



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 25, 2026 – 02:00 AM UTC

PDB ID : 6HHQ / pdb_00006hhq
Title : Crystal structure of compound C45 bound to the yeast 80S ribosome
Authors : Pellegrino, S.; Vanderwal, C.D.; Yusupov, M.
Deposited on : 2018-08-28
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

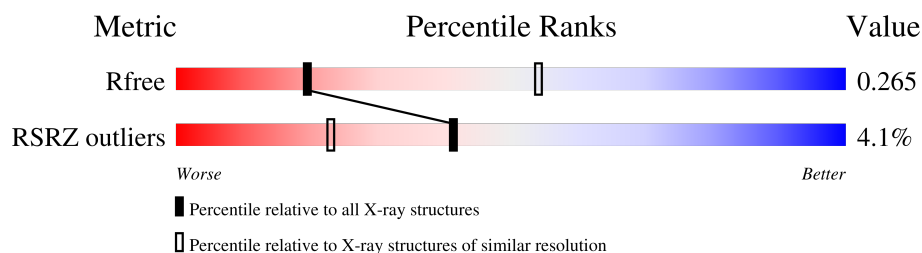
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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
83	MG	1	3730	-	-	-	X
83	MG	1	3860	-	-	-	X
83	MG	1	3931	-	-	-	X
83	MG	1	3973	-	-	-	X
83	MG	1	4094	-	-	-	X
83	MG	1	4158	-	-	-	X
83	MG	1	4180	-	-	-	X
83	MG	1	4210	-	-	-	X
83	MG	3	221	-	-	-	X
83	MG	A	1946	-	-	-	X
83	MG	A	1949	-	-	-	X
83	MG	A	1955	-	-	-	X
83	MG	A	1956	-	-	-	X
83	MG	A	1957	-	-	-	X
83	MG	A	1964	-	-	-	X
83	MG	A	1966	-	-	-	X
83	MG	A	1970	-	-	-	X
83	MG	A	1976	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
83	MG	A	1980	-	-	-	X
83	MG	A	1996	-	-	-	X
83	MG	A	2001	-	-	-	X
83	MG	A	2002	-	-	-	X
83	MG	A	2010	-	-	-	X
83	MG	A	2015	-	-	-	X
83	MG	A	2018	-	-	-	X
83	MG	A	2021	-	-	-	X
83	MG	A	2033	-	-	-	X
83	MG	A	2051	-	-	-	X
83	MG	A	2059	-	-	-	X
83	MG	A	2061	-	-	-	X
83	MG	A	2063	-	-	-	X
83	MG	AR	3768	-	-	-	X
83	MG	AR	3804	-	-	-	X
83	MG	AR	4112	-	-	-	X
83	MG	AR	4229	-	-	-	X
83	MG	CR	203	-	-	-	X
83	MG	d9	103	-	-	-	X
83	MG	e	103	-	-	-	X
83	MG	sR	2073	-	-	-	X
83	MG	sR	2081	-	-	-	X
83	MG	sR	2087	-	-	-	X
83	MG	sR	2088	-	-	-	X
83	MG	sR	2109	-	-	-	X
83	MG	sR	2159	-	-	-	X
83	MG	sR	2174	-	-	-	X
83	MG	sR	2188	-	-	-	X
83	MG	sR	2194	-	-	-	X
83	MG	sR	2199	-	-	-	X
83	MG	t	202	-	-	-	X

2 Entry composition [i](#)

There are 86 unique types of molecules in this entry. The entry contains 409486 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 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			
1	AR	3147	Total	C	N	O	P	0	0	0
			67313	30067	12134	21965	3147			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
2	AS	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			
3	AT	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	j	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
4	CD	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	k	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
5	CE	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	l	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
6	CF	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	m	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
7	CG	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	n	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
8	CH	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	o	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
9	CI	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	p	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	q	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
11	CK	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	r	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			
12	CL	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			

- Molecule 13 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	s	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			
13	CM	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	t	193	Total	C	N	O	0	0	0
			1543	962	315	266			
14	CN	193	Total	C	N	O	0	0	0
			1543	962	315	266			

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	u	136	Total	C	N	O	0	0	0
			1053	675	199	177			
15	CO	136	Total	C	N	O	0	0	0
			1053	675	199	177			

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	v	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			
16	CP	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	w	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			
17	CQ	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	x	183	Total	C	N	O		0	0	0
			1420	882	281	257				
18	CR	183	Total	C	N	O		0	0	0
			1420	882	281	257				

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	y	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			
19	CS	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	z	188	Total	C	N	O		0	0	0
			1521	935	326	260				
20	CT	188	Total	C	N	O		0	0	0
			1521	935	326	260				

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
21	CU	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	2	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			
22	CV	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	5	100	Total	C	N	O		0	0	0
			796	516	131	149				
23	CW	100	Total	C	N	O		0	0	0
			796	516	131	149				

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	6	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
24	CX	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	7	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			
25	CY	124	Total	C	N	O	S	0	0	0
			836	525	166	144	1			

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	8	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	CZ	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			

- Molecule 27 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	9	126	Total	C	N	O		0	0	0
			993	625	192	176				
27	DA	124	Total	C	N	O		0	0	0
			976	614	190	172				

- Molecule 28 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	AA	135	Total	C	N	O		0	0	0
			1092	710	202	180				
28	DB	135	Total	C	N	O		0	0	0
			1092	710	202	180				

- Molecule 29 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	AB	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			
29	DC	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	AC	58	Total	C	N	O		0	0	0
			462	289	100	73				
30	DD	58	Total	C	N	O		0	0	0
			462	289	100	73				

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	AD	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			
31	DE	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AE	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			
32	DF	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	AF	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			
33	DG	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	AG	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			
34	DH	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			

- Molecule 35 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	AH	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			
35	DI	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			

- Molecule 36 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	AI	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			
36	DJ	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			

- Molecule 37 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	AJ	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			
37	DK	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			

- Molecule 38 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	AK	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			
38	DL	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			

- Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	AL	77	Total	C	N	O	0	0	0
			612	391	115	106			
39	DM	77	Total	C	N	O	0	0	0
			612	391	115	106			

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	AM	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			
40	DN	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	AN	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			
41	DO	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			

- Molecule 42 is a protein called 60S ribosomal protein L41-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	AO	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	DP	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

- Molecule 43 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	AP	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			
43	DQ	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	AQ	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			
44	DR	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			

- Molecule 45 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	i	159	Total	C	N	O	S	0	0	0
			1104	652	221	231				
45	sM	63	Total	C	N	O	S	0	0	0
			475	280	99	96				

- Molecule 46 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	p0	143	Total	C	N	O	S	0	0	0
			1076	686	192	195	3			

- Molecule 47 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	A	1781	Total	C	N	O	P	0	0	0
			37948	16965	6715	12487	1781			

- Molecule 48 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B	206	Total	C	N	O	S	0	0	0
			1577	1014	278	283	2			
48	s0	206	Total	C	N	O	S	0	0	0
			1583	1017	281	283	2			

- Molecule 49 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	C	214	Total	C	N	O	S	0	0	0
			1709	1084	310	311	4			
49	s1	216	Total	C	N	O	S	0	0	0
			1722	1091	312	315	4			

- Molecule 50 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	D	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			
50	s2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			

- Molecule 51 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	E	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			
51	s3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			

- Molecule 52 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	F	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			
52	s4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			

- Molecule 53 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	G	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	s5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			

- Molecule 54 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	H	226	Total	C	N	O	S	0	0	0
			1799	1129	346	321	3			
54	s6	218	Total	C	N	O	S	0	0	0
			1755	1102	337	313	3			

- Molecule 55 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	I	184	Total	C	N	O	S	0	0	0
			1481	951	265	265				
55	s7	186	Total	C	N	O	S	0	0	0
			1491	957	267	267				

- Molecule 56 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	J	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			
56	s8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

- Molecule 57 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	K	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			
57	s9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

- Molecule 58 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	L	96	Total	C	N	O	S	0	0	0
			772	499	126	145	2			
58	c0	96	Total	C	N	O	S	0	0	0
			761	490	125	144	2			

- Molecule 59 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	M	155	Total	C	N	O	S	0	0	0
			1213	774	230	206	3			
59	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

- Molecule 60 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	N	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			
60	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

- Molecule 61 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	O	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			
61	c3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			

- Molecule 62 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
62	P	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			
62	c4	128	Total	C	N	O	S	0	0	0
			949	582	188	176	3			

- Molecule 63 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
63	Q	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			
63	c5	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	7			

- Molecule 64 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
64	R	141	Total	C	N	O	0	0	0
			1105	708	203	194			
64	c6	142	Total	C	N	O	0	0	0
			1111	711	204	196			

- Molecule 65 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
65	S	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			
65	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

- Molecule 66 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	T	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			
66	c8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			

- Molecule 67 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	U	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			
67	c9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			

- Molecule 68 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	V	107	Total	C	N	O	S	0	0	0
			855	539	156	159	1			
68	d0	110	Total	C	N	O	S	0	0	0
			882	554	161	166	1			

- Molecule 69 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	W	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	d1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			

- Molecule 70 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
70	X	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			
70	d2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			

- Molecule 71 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
71	Y	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			
71	d3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			

- Molecule 72 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	Z	134	Total	C	N	O		0	0	0
			1073	676	208	189				
72	d4	134	Total	C	N	O		0	0	0
			1073	676	208	189				

- Molecule 73 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
73	a	70	Total	C	N	O		0	0	0
			563	360	104	99				
73	d5	69	Total	C	N	O		0	0	0
			558	357	103	98				

- Molecule 74 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
74	b	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			
74	d6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

- Molecule 75 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	c	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			
75	d7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			

- Molecule 76 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	d	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			
76	d8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			

- Molecule 77 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	e	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			
77	d9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			

- Molecule 78 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	f	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			
78	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

- Molecule 79 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	g	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			
79	e1	51	Total	C	N	O	S	0	0	0
			397	249	73	71	4			

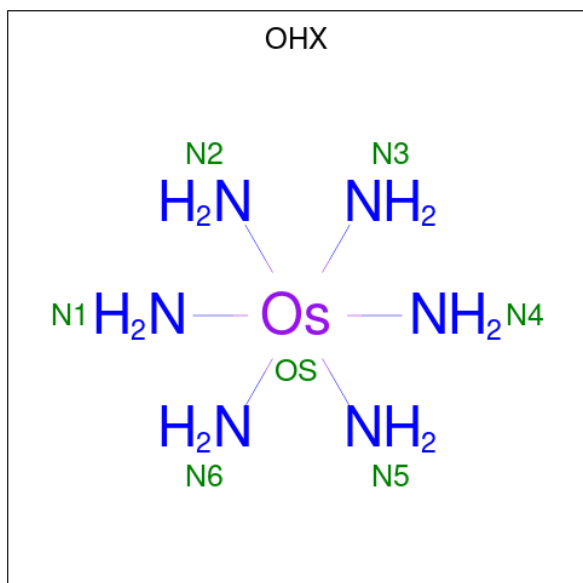
- Molecule 80 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	h	318	Total	C	N	O	S	0	0	0
			2437	1541	418	470	8			
80	Rb	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 81 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	sR	1783	Total	C	N	O	P	0	0	0
			37990	16984	6723	12500	1783			

- Molecule 82 is osmium (III) hexammine (CCD ID: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	Os		0	0
			1	1			
82	3	1	Total	N	Os	0	0
			7	6	1		
82	3	1	Total	N	Os	0	0
			7	6	1		
82	3	1	Total	N	Os	0	0
			7	6	1		
82	3	1	Total	N	Os	0	0
			7	6	1		
82	3	1	Total	N	Os	0	0
			7	6	1		
82	3	1	Total	N	Os	0	0
			7	6	1		
82	3	1	Total	N	Os	0	0
			7	6	1		
82	3	1	Total	N	Os	0	0
			7	6	1		
82	4	1	Total	N	Os	0	0
			7	6	1		
82	4	1	Total	N	Os	0	0
			7	6	1		
82	4	1	Total	N	Os	0	0
			7	6	1		
82	4	1	Total	N	Os	0	0
			7	6	1		
82	4	1	Total	N	Os	0	0
			7	6	1		
82	4	1	Total	N	Os	0	0
			7	6	1		
82	4	1	Total	N	Os	0	0
			7	6	1		
82	4	1	Total	N	Os	0	0
			7	6	1		
82	4	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	4	1	Total 7	N 6	Os 1	0	0
82	4	1	Total 7	N 6	Os 1	0	0
82	4	1	Total 7	N 6	Os 1	0	0
82	4	1	Total 7	N 6	Os 1	0	0
82	k	1	Total 7	N 6	Os 1	0	0
82	l	1	Total 7	N 6	Os 1	0	0
82	n	1	Total 7	N 6	Os 1	0	0
82	r	1	Total 7	N 6	Os 1	0	0
82	v	1	Total 7	N 6	Os 1	0	0
82	v	1	Total 7	N 6	Os 1	0	0
82	w	1	Total 7	N 6	Os 1	0	0
82	x	1	Total 7	N 6	Os 1	0	0
82	y	1	Total 7	N 6	Os 1	0	0
82	z	1	Total 7	N 6	Os 1	0	0
82	2	1	Total 7	N 6	Os 1	0	0
82	AC	1	Total 7	N 6	Os 1	0	0
82	AE	1	Total 7	N 6	Os 1	0	0
82	AG	1	Total 7	N 6	Os 1	0	0
82	AK	1	Total 7	N 6	Os 1	0	0
82	AK	1	Total 7	N 6	Os 1	0	0
82	AP	1	Total 7	N 6	Os 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AS	1	Total	N	Os	0	0
			7	6	1		
82	AS	1	Total	N	Os	0	0
			7	6	1		
82	AS	1	Total	N	Os	0	0
			7	6	1		
82	AS	1	Total	N	Os	0	0
			7	6	1		
82	AS	1	Total	N	Os	0	0
			7	6	1		
82	AS	1	Total	N	Os	0	0
			7	6	1		
82	AS	1	Total	N	Os	0	0
			7	6	1		
82	AS	1	Total	N	Os	0	0
			7	6	1		
82	AT	1	Total	N	Os	0	0
			7	6	1		
82	AT	1	Total	N	Os	0	0
			7	6	1		
82	AT	1	Total	N	Os	0	0
			7	6	1		
82	AT	1	Total	N	Os	0	0
			7	6	1		
82	AT	1	Total	N	Os	0	0
			7	6	1		
82	AT	1	Total	N	Os	0	0
			7	6	1		
82	AT	1	Total	N	Os	0	0
			7	6	1		
82	AT	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AT	1	Total 7	N 6	Os 1	0	0
82	AT	1	Total 7	N 6	Os 1	0	0
82	AT	1	Total 7	N 6	Os 1	0	0
82	AT	1	Total 7	N 6	Os 1	0	0
82	AT	1	Total 7	N 6	Os 1	0	0
82	AT	1	Total 7	N 6	Os 1	0	0
82	AT	1	Total 7	N 6	Os 1	0	0
82	CE	1	Total 7	N 6	Os 1	0	0
82	CE	1	Total 7	N 6	Os 1	0	0
82	CF	1	Total 7	N 6	Os 1	0	0
82	CG	1	Total 7	N 6	Os 1	0	0
82	CG	1	Total 7	N 6	Os 1	0	0
82	CG	1	Total 7	N 6	Os 1	0	0
82	CH	1	Total 7	N 6	Os 1	0	0
82	CK	1	Total 7	N 6	Os 1	0	0
82	CL	1	Total 7	N 6	Os 1	0	0
82	CL	1	Total 7	N 6	Os 1	0	0
82	CM	1	Total 7	N 6	Os 1	0	0
82	CO	1	Total 7	N 6	Os 1	0	0
82	CP	1	Total 7	N 6	Os 1	0	0
82	CQ	1	Total 7	N 6	Os 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	CS	1	Total	Os		0	0
			1	1			
82	CX	1	Total	N	Os	0	0
			7	6	1		
82	CX	1	Total	N	Os	0	0
			7	6	1		
82	DD	1	Total	N	Os	0	0
			7	6	1		
82	DG	1	Total	N	Os	0	0
			7	6	1		
82	DH	1	Total	N	Os	0	0
			7	6	1		
82	DQ	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	J	1	Total	N	Os	0	0
			7	6	1		
82	J	1	Total	N	Os	0	0
			7	6	1		
82	O	1	Total	N	Os	0	0
			7	6	1		
82	Q	1	Total	N	Os	0	0
			7	6	1		
82	T	1	Total	N	Os	0	0
			7	6	1		
82	e	1	Total	N	Os	0	0
			7	6	1		
82	h	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	Rb	1	Total	N	Os	0	0
			7	6	1		
82	s1	1	Total	N	Os	0	0
			7	6	1		
82	s4	1	Total	N	Os	0	0
			7	6	1		
82	s8	1	Total	N	Os	0	0
			7	6	1		
82	c1	1	Total	N	Os	0	0
			7	6	1		
82	c3	1	Total	N	Os	0	0
			7	6	1		
82	c5	1	Total	N	Os	0	0
			7	6	1		
82	c8	1	Total	N	Os	0	0
			7	6	1		
82	d4	1	Total	N	Os	0	0
			7	6	1		
82	d9	1	Total	N	Os	0	0
			7	6	1		

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	1	499	Total 499	Mg 499	0	0
83	3	13	Total 13	Mg 13	0	0
83	4	23	Total 23	Mg 23	0	0
83	j	2	Total 2	Mg 2	0	0
83	k	1	Total 1	Mg 1	0	0
83	l	3	Total 3	Mg 3	0	0
83	o	1	Total 1	Mg 1	0	0
83	r	2	Total 2	Mg 2	0	0
83	s	1	Total 1	Mg 1	0	0
83	t	3	Total 3	Mg 3	0	0
83	v	5	Total 5	Mg 5	0	0
83	w	1	Total 1	Mg 1	0	0
83	x	5	Total 5	Mg 5	0	0
83	z	1	Total 1	Mg 1	0	0
83	6	3	Total 3	Mg 3	0	0
83	9	1	Total 1	Mg 1	0	0
83	AB	8	Total 8	Mg 8	0	0
83	AF	2	Total 2	Mg 2	0	0
83	AG	1	Total 1	Mg 1	0	0
83	AH	1	Total 1	Mg 1	0	0
83	AK	2	Total 2	Mg 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	AM	1	Total 1	Mg 1	0	0
83	AP	1	Total 1	Mg 1	0	0
83	AR	523	Total 523	Mg 523	0	0
83	AS	19	Total 19	Mg 19	0	0
83	AT	15	Total 15	Mg 15	0	0
83	CD	3	Total 3	Mg 3	0	0
83	CE	3	Total 3	Mg 3	0	0
83	CF	2	Total 2	Mg 2	0	0
83	CG	3	Total 3	Mg 3	0	0
83	CI	2	Total 2	Mg 2	0	0
83	CJ	1	Total 1	Mg 1	0	0
83	CK	3	Total 3	Mg 3	0	0
83	CL	1	Total 1	Mg 1	0	0
83	CM	1	Total 1	Mg 1	0	0
83	CO	1	Total 1	Mg 1	0	0
83	CP	4	Total 4	Mg 4	0	0
83	CQ	2	Total 2	Mg 2	0	0
83	CR	8	Total 8	Mg 8	0	0
83	CU	2	Total 2	Mg 2	0	0
83	CX	3	Total 3	Mg 3	0	0
83	CY	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

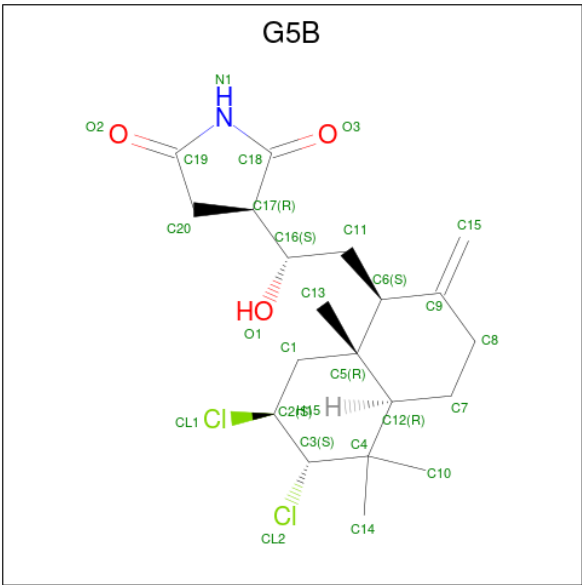
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	DA	2	Total 2	Mg 2	0	0
83	DC	4	Total 4	Mg 4	0	0
83	DD	1	Total 1	Mg 1	0	0
83	DE	1	Total 1	Mg 1	0	0
83	DH	1	Total 1	Mg 1	0	0
83	DI	1	Total 1	Mg 1	0	0
83	DL	1	Total 1	Mg 1	0	0
83	DN	1	Total 1	Mg 1	0	0
83	DO	1	Total 1	Mg 1	0	0
83	DP	1	Total 1	Mg 1	0	0
83	DQ	3	Total 3	Mg 3	0	0
83	DR	2	Total 2	Mg 2	0	0
83	sM	2	Total 2	Mg 2	0	0
83	A	129	Total 129	Mg 129	0	0
83	D	1	Total 1	Mg 1	0	0
83	F	1	Total 1	Mg 1	0	0
83	H	1	Total 1	Mg 1	0	0
83	J	1	Total 1	Mg 1	0	0
83	O	1	Total 1	Mg 1	0	0
83	Y	1	Total 1	Mg 1	0	0
83	b	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	e	1	Total 1	Mg 1	0	0
83	sR	154	Total 154	Mg 154	0	0
83	s1	1	Total 1	Mg 1	0	0
83	s2	1	Total 1	Mg 1	0	0
83	s4	1	Total 1	Mg 1	0	0
83	s8	2	Total 2	Mg 2	0	0
83	c1	2	Total 2	Mg 2	0	0
83	c4	1	Total 1	Mg 1	0	0
83	c6	1	Total 1	Mg 1	0	0
83	c8	1	Total 1	Mg 1	0	0
83	c9	1	Total 1	Mg 1	0	0
83	d3	3	Total 3	Mg 3	0	0
83	d4	3	Total 3	Mg 3	0	0
83	d5	1	Total 1	Mg 1	0	0
83	d6	1	Total 1	Mg 1	0	0
83	d9	1	Total 1	Mg 1	0	0

- Molecule 84 is (3 {R})-3-[(1 {S})-2-[(1 {S},4 {a} {R},6 {S},7 {S},8 {a} {R})-6,7-bis(chloranyl)-5,5,8 {a}-trimethyl-2-methylidene-3,4,4 {a},6,7,8-hexahydro-1 {H}-naphthalen-1-yl]-1-oxidanyl-ethyl]pyrrolidine-2,5-dione (CCD ID: G5B) (formula: C₂₀H₂₉Cl₂NO₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
84	1	1	Total 26	C 20	Cl 2	N 1	O 3	0	0
84	AR	1	Total 26	C 20	Cl 2	N 1	O 3	0	0

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

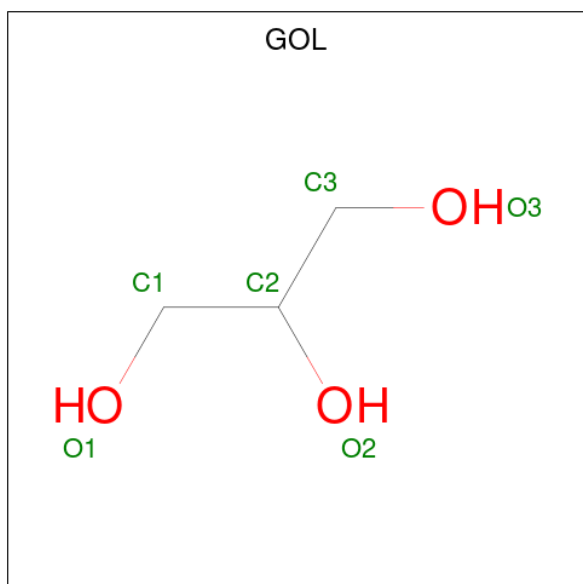
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	AK	1	Total	Zn	0	0
			1	1		
85	AN	1	Total	Zn	0	0
			1	1		
85	AP	1	Total	Zn	0	0
			1	1		
85	AQ	1	Total	Zn	0	0
			1	1		
85	DL	1	Total	Zn	0	0
			1	1		
85	DO	1	Total	Zn	0	0
			1	1		
85	DQ	1	Total	Zn	0	0
			1	1		
85	DR	1	Total	Zn	0	0
			1	1		
85	b	1	Total	Zn	0	0
			1	1		
85	c	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	e	1	Total	Zn	0	0
			1	1		
85	g	1	Total	Zn	0	0
			1	1		
85	d6	1	Total	Zn	0	0
			1	1		
85	d7	1	Total	Zn	0	0
			1	1		
85	d9	1	Total	Zn	0	0
			1	1		
85	e1	1	Total	Zn	0	0
			1	1		

- Molecule 86 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	AR	1	Total	C	O	0	0
			6	3	3		
86	AR	1	Total	C	O	0	0
			6	3	3		

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	303.77Å 287.95Å 435.45Å 90.00° 98.96° 90.00°	Depositor
Resolution (Å)	54.71 – 3.10 54.71 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.71-3.10) 99.9 (54.71-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.13Å)	Xtriage
Refinement program	PHENIX dev_2450, PHENIX dev_2450	Depositor
R, R_{free}	0.217 , 0.264 0.218 , 0.265	Depositor DCC
R_{free} test set	26494 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å ²)	67.0	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	409486	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 2586 ligands modelled in this entry, 2 are modelled with single atom and 1525 are monoatomic - leaving 1059 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	$\# Z > 2$
82	OHX	A	1851	-	0,6,6	-	-	-		
82	OHX	AR	3542	-	0,6,6	-	-	-		
82	OHX	1	3674	-	0,6,6	-	-	-		
82	OHX	1	3477	-	0,6,6	-	-	-		
82	OHX	AR	3682	-	0,6,6	-	-	-		
82	OHX	AR	3674	-	0,6,6	-	-	-		
82	OHX	1	3470	-	0,6,6	-	-	-		
82	OHX	1	3656	-	0,6,6	-	-	-		
82	OHX	sR	1925	-	0,6,6	-	-	-		
82	OHX	sR	2035	-	0,6,6	-	-	-		
82	OHX	CL	302	-	0,6,6	-	-	-		
82	OHX	1	3529	-	0,6,6	-	-	-		
82	OHX	1	3510	-	0,6,6	-	-	-		
82	OHX	1	3535	-	0,6,6	-	-	-		
82	OHX	AR	3448	-	0,6,6	-	-	-		
82	OHX	sR	2005	-	0,6,6	-	-	-		
82	OHX	1	3518	-	0,6,6	-	-	-		
82	OHX	AR	3535	-	0,6,6	-	-	-		
82	OHX	sR	1999	-	0,6,6	-	-	-		
82	OHX	1	3442	-	0,6,6	-	-	-		
82	OHX	A	1872	-	0,6,6	-	-	-		
82	OHX	sR	1961	-	0,6,6	-	-	-		
82	OHX	AT	202	-	0,6,6	-	-	-		
82	OHX	sR	1983	-	0,6,6	-	-	-		
82	OHX	1	3669	-	0,6,6	-	-	-		
82	OHX	AR	3501	-	0,6,6	-	-	-		
82	OHX	2	201	-	0,6,6	-	-	-		
82	OHX	sR	1962	-	0,6,6	-	-	-		
82	OHX	sR	2040	-	0,6,6	-	-	-		
82	OHX	x	201	-	0,6,6	-	-	-		
82	OHX	e	102	-	0,6,6	-	-	-		
82	OHX	1	3626	-	0,6,6	-	-	-		
82	OHX	1	3432	-	0,6,6	-	-	-		
82	OHX	1	3719	-	0,6,6	-	-	-		
82	OHX	AR	3432	-	0,6,6	-	-	-		
82	OHX	sR	2013	-	0,6,6	-	-	-		
82	OHX	AR	3411	-	0,6,6	-	-	-		
82	OHX	AR	3719	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	AT	216	-	0,6,6	-	-	-		
82	OHX	AR	3639	-	0,6,6	-	-	-		
82	OHX	A	1835	-	0,6,6	-	-	-		
82	OHX	4	205	-	0,6,6	-	-	-		
82	OHX	1	3610	-	0,6,6	-	-	-		
82	OHX	1	3706	-	0,6,6	-	-	-		
82	OHX	1	3551	-	0,6,6	-	-	-		
82	OHX	AR	3663	-	0,6,6	-	-	-		
82	OHX	1	3544	-	0,6,6	-	-	-		
82	OHX	AS	208	-	0,6,6	-	-	-		
82	OHX	AR	3706	-	0,6,6	-	-	-		
82	OHX	1	3465	-	0,6,6	-	-	-		
82	OHX	sR	2037	-	0,6,6	-	-	-		
82	OHX	AR	3465	-	0,6,6	-	-	-		
82	OHX	sR	2012	-	0,6,6	-	-	-		
82	OHX	AR	3670	-	0,6,6	-	-	-		
82	OHX	1	3522	-	0,6,6	-	-	-		
82	OHX	sR	1968	-	0,6,6	-	-	-		
82	OHX	sR	1969	-	0,6,6	-	-	-		
82	OHX	AR	3522	-	0,6,6	-	-	-		
82	OHX	1	3688	-	0,6,6	-	-	-		
82	OHX	A	1910	-	0,6,6	-	-	-		
82	OHX	sR	1958	-	0,6,6	-	-	-		
82	OHX	1	3621	-	0,6,6	-	-	-		
82	OHX	sR	1980	-	0,6,6	-	-	-		
82	OHX	AS	202	-	0,6,6	-	-	-		
82	OHX	A	1942	-	0,6,6	-	-	-		
82	OHX	1	3416	-	0,6,6	-	-	-		
82	OHX	AR	3621	-	0,6,6	-	-	-		
82	OHX	1	3434	-	0,6,6	-	-	-		
82	OHX	AR	3725	-	0,6,6	-	-	-		
82	OHX	A	1908	-	0,6,6	-	-	-		
82	OHX	3	203	-	0,6,6	-	-	-		
82	OHX	1	3604	-	0,6,6	-	-	-		
82	OHX	1	3620	-	0,6,6	-	-	-		
82	OHX	AR	3434	-	0,6,6	-	-	-		
82	OHX	AR	3518	-	0,6,6	-	-	-		
82	OHX	sR	1973	-	0,6,6	-	-	-		
82	OHX	AR	3604	-	0,6,6	-	-	-		
82	OHX	AR	3620	-	0,6,6	-	-	-		
82	OHX	AR	3534	-	0,6,6	-	-	-		
82	OHX	sR	1982	-	0,6,6	-	-	-		
82	OHX	1	3624	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	CH	201	-	0,6,6	-	-	-		
82	OHX	AR	3510	-	0,6,6	-	-	-		
82	OHX	1	3661	-	0,6,6	-	-	-		
82	OHX	AR	3454	-	0,6,6	-	-	-		
82	OHX	1	3499	-	0,6,6	-	-	-		
82	OHX	AR	3515	-	0,6,6	-	-	-		
82	OHX	AR	3499	-	0,6,6	-	-	-		
82	OHX	A	1934	-	0,6,6	-	-	-		
82	OHX	1	3468	-	0,6,6	-	-	-		
82	OHX	sR	1907	-	0,6,6	-	-	-		
82	OHX	1	3652	-	0,6,6	-	-	-		
82	OHX	AR	3468	-	0,6,6	-	-	-		
82	OHX	AR	3652	-	0,6,6	-	-	-		
82	OHX	sR	2016	-	0,6,6	-	-	-		
82	OHX	AR	3452	-	0,6,6	-	-	-		
82	OHX	4	201	-	0,6,6	-	-	-		
82	OHX	1	3447	-	0,6,6	-	-	-		
82	OHX	1	3601	-	0,6,6	-	-	-		
82	OHX	1	3577	-	0,6,6	-	-	-		
82	OHX	4	213	-	0,6,6	-	-	-		
82	OHX	AR	3577	-	0,6,6	-	-	-		
82	OHX	A	1941	47	0,6,6	-	-	-		
82	OHX	1	3683	-	0,6,6	-	-	-		
82	OHX	sR	1903	-	0,6,6	-	-	-		
82	OHX	AR	3525	-	0,6,6	-	-	-		
82	OHX	1	3550	-	0,6,6	-	-	-		
82	OHX	AR	3591	-	0,6,6	-	-	-		
82	OHX	1	3435	-	0,6,6	-	-	-		
82	OHX	1	3568	-	0,6,6	-	-	-		
82	OHX	sR	1992	-	0,6,6	-	-	-		
82	OHX	AR	3409	-	0,6,6	-	-	-		
82	OHX	1	3453	-	0,6,6	-	-	-		
82	OHX	AG	201	-	0,6,6	-	-	-		
82	OHX	1	3491	-	0,6,6	-	-	-		
82	OHX	AR	3453	-	0,6,6	-	-	-		
82	OHX	1	3638	-	0,6,6	-	-	-		
82	OHX	AR	3657	-	0,6,6	-	-	-		
82	OHX	1	3711	-	0,6,6	-	-	-		
82	OHX	1	3658	-	0,6,6	-	-	-		
82	OHX	sR	1977	-	0,6,6	-	-	-		
82	OHX	AR	3444	-	0,6,6	-	-	-		
82	OHX	1	3540	-	0,6,6	-	-	-		
82	OHX	AR	3658	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3689	-	0,6,6	-	-	-		
82	OHX	1	3545	-	0,6,6	-	-	-		
82	OHX	AR	3629	-	0,6,6	-	-	-		
82	OHX	1	3538	-	0,6,6	-	-	-		
82	OHX	1	3664	-	0,6,6	-	-	-		
82	OHX	AR	3517	-	0,6,6	-	-	-		
82	OHX	AS	210	-	0,6,6	-	-	-		
82	OHX	sR	1939	-	0,6,6	-	-	-		
82	OHX	AR	3664	-	0,6,6	-	-	-		
82	OHX	sR	1913	-	0,6,6	-	-	-		
82	OHX	1	3488	-	0,6,6	-	-	-		
82	OHX	AS	204	-	0,6,6	-	-	-		
82	OHX	1	3569	-	0,6,6	-	-	-		
82	OHX	AT	208	-	0,6,6	-	-	-		
82	OHX	A	1832	-	0,6,6	-	-	-		
82	OHX	1	3495	-	0,6,6	-	-	-		
82	OHX	AR	3495	-	0,6,6	-	-	-		
82	OHX	1	3599	-	0,6,6	-	-	-		
82	OHX	1	3526	-	0,6,6	-	-	-		
82	OHX	1	3589	-	0,6,6	-	-	-		
82	OHX	1	3642	-	0,6,6	-	-	-		
82	OHX	AT	201	-	0,6,6	-	-	-		
82	OHX	AR	3589	-	0,6,6	-	-	-		
82	OHX	1	3692	-	0,6,6	-	-	-		
82	OHX	AR	3474	-	0,6,6	-	-	-		
82	OHX	A	1939	-	0,6,6	-	-	-		
82	OHX	A	1919	-	0,6,6	-	-	-		
82	OHX	1	3717	-	0,6,6	-	-	-		
82	OHX	1	3497	-	0,6,6	-	-	-		
82	OHX	AR	3497	-	0,6,6	-	-	-		
82	OHX	A	1898	-	0,6,6	-	-	-		
82	OHX	1	3655	-	0,6,6	-	-	-		
82	OHX	3	206	-	0,6,6	-	-	-		
82	OHX	sR	1931	-	0,6,6	-	-	-		
82	OHX	1	3478	-	0,6,6	-	-	-		
82	OHX	AR	3445	-	0,6,6	-	-	-		
82	OHX	AR	3478	-	0,6,6	-	-	-		
82	OHX	AR	3646	-	0,6,6	-	-	-		
82	OHX	sR	1956	-	0,6,6	-	-	-		
82	OHX	A	1827	-	0,6,6	-	-	-		
82	OHX	AR	3735	-	0,6,6	-	-	-		
82	OHX	1	3413	-	0,6,6	-	-	-		
82	OHX	AR	3653	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	AR	3651	-	0,6,6	-	-	-		
82	OHX	AR	3416	-	0,6,6	-	-	-		
82	OHX	AR	3738	-	0,6,6	-	-	-		
82	OHX	1	3695	-	0,6,6	-	-	-		
82	OHX	1	3402	-	0,6,6	-	-	-		
82	OHX	AR	3695	-	0,6,6	-	-	-		
82	OHX	AR	3402	-	0,6,6	-	-	-		
82	OHX	A	1922	-	0,6,6	-	-	-		
82	OHX	AR	3433	-	0,6,6	-	-	-		
82	OHX	sR	2042	-	0,6,6	-	-	-		
82	OHX	A	1855	-	0,6,6	-	-	-		
82	OHX	1	3501	-	0,6,6	-	-	-		
82	OHX	AR	3668	-	0,6,6	-	-	-		
82	OHX	A	1826	-	0,6,6	-	-	-		
82	OHX	1	3444	-	0,6,6	-	-	-		
82	OHX	AR	3539	-	0,6,6	-	-	-		
82	OHX	AR	3546	-	0,6,6	-	-	-		
82	OHX	AR	3673	-	0,6,6	-	-	-		
82	OHX	AR	3572	-	0,6,6	-	-	-		
82	OHX	sR	2032	-	0,6,6	-	-	-		
82	OHX	1	3618	-	0,6,6	-	-	-		
82	OHX	1	3533	-	0,6,6	-	-	-		
82	OHX	1	3622	-	0,6,6	-	-	-		
82	OHX	A	1906	47	0,6,6	-	-	-		
82	OHX	A	1918	-	0,6,6	-	-	-		
82	OHX	sR	2020	-	0,6,6	-	-	-		
82	OHX	AR	3622	-	0,6,6	-	-	-		
82	OHX	sR	1979	-	0,6,6	-	-	-		
82	OHX	AR	3613	-	0,6,6	-	-	-		
82	OHX	1	3436	-	0,6,6	-	-	-		
82	OHX	1	3666	-	0,6,6	-	-	-		
82	OHX	sR	1970	-	0,6,6	-	-	-		
82	OHX	1	3707	-	0,6,6	-	-	-		
82	OHX	sR	1975	-	0,6,6	-	-	-		
82	OHX	AR	3414	-	0,6,6	-	-	-		
82	OHX	AR	3484	-	0,6,6	-	-	-		
82	OHX	1	3512	-	0,6,6	-	-	-		
82	OHX	sR	2038	-	0,6,6	-	-	-		
82	OHX	AR	3512	-	0,6,6	-	-	-		
82	OHX	A	1803	-	0,6,6	-	-	-		
82	OHX	1	3410	-	0,6,6	-	-	-		
82	OHX	1	3575	-	0,6,6	-	-	-		
82	OHX	A	1866	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	sR	1946	-	0,6,6	-	-	-		
82	OHX	1	3528	-	0,6,6	-	-	-		
82	OHX	1	3709	-	0,6,6	-	-	-		
82	OHX	A	1932	-	0,6,6	-	-	-		
82	OHX	AR	3528	-	0,6,6	-	-	-		
82	OHX	AR	3677	-	0,6,6	-	-	-		
82	OHX	1	3520	-	0,6,6	-	-	-		
82	OHX	1	3710	-	0,6,6	-	-	-		
82	OHX	AR	3713	-	0,6,6	-	-	-		
82	OHX	1	3584	-	0,6,6	-	-	-		
82	OHX	A	1927	-	0,6,6	-	-	-		
82	OHX	1	3561	-	0,6,6	-	-	-		
82	OHX	AR	3679	-	0,6,6	-	-	-		
82	OHX	A	1821	-	0,6,6	-	-	-		
82	OHX	A	1875	-	0,6,6	-	-	-		
82	OHX	A	1843	-	0,6,6	-	-	-		
82	OHX	AR	3626	-	0,6,6	-	-	-		
82	OHX	A	1842	-	0,6,6	-	-	-		
82	OHX	AR	3590	-	0,6,6	-	-	-		
82	OHX	AR	3511	-	0,6,6	-	-	-		
82	OHX	sR	1981	-	0,6,6	-	-	-		
82	OHX	AR	3594	-	0,6,6	-	-	-		
82	OHX	A	1856	-	0,6,6	-	-	-		
82	OHX	AR	3685	-	0,6,6	-	-	-		
82	OHX	AR	3614	-	0,6,6	-	-	-		
82	OHX	1	3452	-	0,6,6	-	-	-		
82	OHX	1	3429	-	0,6,6	-	-	-		
82	OHX	v	302	-	0,6,6	-	-	-		
82	OHX	AR	3595	-	0,6,6	-	-	-		
82	OHX	sR	2049	81	0,6,6	-	-	-		
82	OHX	AR	3429	-	0,6,6	-	-	-		
82	OHX	CF	401	-	0,6,6	-	-	-		
82	OHX	AR	3506	-	0,6,6	-	-	-		
82	OHX	AR	3461	-	0,6,6	-	-	-		
82	OHX	DH	201	-	0,6,6	-	-	-		
82	OHX	sR	2021	-	0,6,6	-	-	-		
82	OHX	1	3723	-	0,6,6	-	-	-		
82	OHX	AR	3582	-	0,6,6	-	-	-		
82	OHX	A	1883	-	0,6,6	-	-	-		
82	OHX	1	3481	-	0,6,6	-	-	-		
82	OHX	r	301	-	0,6,6	-	-	-		
82	OHX	AR	3420	-	0,6,6	-	-	-		
82	OHX	4	210	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3609	-	0,6,6	-	-	-		
82	OHX	AR	3446	-	0,6,6	-	-	-		
82	OHX	1	3697	82	0,6,6	-	-	-		
82	OHX	1	3566	-	0,6,6	-	-	-		
82	OHX	A	1811	-	0,6,6	-	-	-		
82	OHX	AR	3566	-	0,6,6	-	-	-		
82	OHX	AR	3483	-	0,6,6	-	-	-		
82	OHX	AR	3656	-	0,6,6	-	-	-		
82	OHX	AR	3694	-	0,6,6	-	-	-		
82	OHX	AR	3728	-	0,6,6	-	-	-		
82	OHX	1	3593	-	0,6,6	-	-	-		
82	OHX	AR	3413	-	0,6,6	-	-	-		
82	OHX	AT	209	-	0,6,6	-	-	-		
82	OHX	1	3700	-	0,6,6	-	-	-		
82	OHX	AR	3593	-	0,6,6	-	-	-		
82	OHX	d4	201	-	0,6,6	-	-	-		
82	OHX	AR	3700	-	0,6,6	-	-	-		
82	OHX	1	3504	-	0,6,6	-	-	-		
82	OHX	AR	3686	-	0,6,6	-	-	-		
82	OHX	sR	1993	-	0,6,6	-	-	-		
82	OHX	AR	3441	-	0,6,6	-	-	-		
82	OHX	J	302	-	0,6,6	-	-	-		
82	OHX	sR	1909	-	0,6,6	-	-	-		
82	OHX	sR	1986	-	0,6,6	-	-	-		
82	OHX	sR	1953	-	0,6,6	-	-	-		
82	OHX	1	3708	-	0,6,6	-	-	-		
82	OHX	1	3433	-	0,6,6	-	-	-		
82	OHX	1	3480	-	0,6,6	-	-	-		
82	OHX	AR	3553	-	0,6,6	-	-	-		
82	OHX	AR	3708	-	0,6,6	-	-	-		
82	OHX	y	201	-	0,6,6	-	-	-		
82	OHX	1	3684	-	0,6,6	-	-	-		
82	OHX	sR	1957	-	0,6,6	-	-	-		
82	OHX	1	3715	-	0,6,6	-	-	-		
82	OHX	AS	209	-	0,6,6	-	-	-		
82	OHX	AR	3715	-	0,6,6	-	-	-		
82	OHX	1	3405	-	0,6,6	-	-	-		
82	OHX	A	1813	-	0,6,6	-	-	-		
82	OHX	AR	3430	-	0,6,6	-	-	-		
82	OHX	A	1920	82	0,6,6	-	-	-		
82	OHX	1	3557	-	0,6,6	-	-	-		
82	OHX	DG	201	-	0,6,6	-	-	-		
82	OHX	1	3628	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	AR	3557	-	0,6,6	-	-	-		
84	G5B	1	4224	-	27,28,28	0.38	0	36,45,45	1.00	2 (5%)
82	OHX	AR	3587	-	0,6,6	-	-	-		
82	OHX	1	3428	-	0,6,6	-	-	-		
82	OHX	AR	3628	-	0,6,6	-	-	-		
82	OHX	1	3464	-	0,6,6	-	-	-		
82	OHX	sR	2014	-	0,6,6	-	-	-		
82	OHX	A	1834	-	0,6,6	-	-	-		
82	OHX	AR	3464	-	0,6,6	-	-	-		
82	OHX	1	3635	-	0,6,6	-	-	-		
82	OHX	A	1925	-	0,6,6	-	-	-		
82	OHX	sR	2046	-	0,6,6	-	-	-		
82	OHX	1	3590	-	0,6,6	-	-	-		
82	OHX	AT	207	-	0,6,6	-	-	-		
82	OHX	1	3691	-	0,6,6	-	-	-		
82	OHX	A	1844	-	0,6,6	-	-	-		
82	OHX	3	204	-	0,6,6	-	-	-		
82	OHX	sR	2025	-	0,6,6	-	-	-		
82	OHX	1	3685	-	0,6,6	-	-	-		
82	OHX	1	3698	-	0,6,6	-	-	-		
82	OHX	A	1802	-	0,6,6	-	-	-		
82	OHX	AR	3680	-	0,6,6	-	-	-		
82	OHX	sR	1971	-	0,6,6	-	-	-		
82	OHX	1	3503	-	0,6,6	-	-	-		
82	OHX	AR	3698	-	0,6,6	-	-	-		
82	OHX	sR	1917	-	0,6,6	-	-	-		
82	OHX	1	3718	-	0,6,6	-	-	-		
82	OHX	s8	301	-	0,6,6	-	-	-		
82	OHX	A	1806	-	0,6,6	-	-	-		
82	OHX	AR	3718	-	0,6,6	-	-	-		
82	OHX	AR	3407	-	0,6,6	-	-	-		
82	OHX	sR	2000	-	0,6,6	-	-	-		
82	OHX	AR	3717	-	0,6,6	-	-	-		
82	OHX	AS	207	-	0,6,6	-	-	-		
82	OHX	AR	3529	-	0,6,6	-	-	-		
82	OHX	A	1839	-	0,6,6	-	-	-		
82	OHX	AR	3734	-	0,6,6	-	-	-		
82	OHX	1	3445	-	0,6,6	-	-	-		
82	OHX	1	3492	-	0,6,6	-	-	-		
82	OHX	A	1888	-	0,6,6	-	-	-		
82	OHX	sR	2029	-	0,6,6	-	-	-		
82	OHX	1	3679	-	0,6,6	-	-	-		
82	OHX	1	3493	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3485	-	0,6,6	-	-	-		
82	OHX	1	3654	-	0,6,6	-	-	-		
82	OHX	c5	201	-	0,6,6	-	-	-		
82	OHX	A	1871	-	0,6,6	-	-	-		
82	OHX	1	3680	-	0,6,6	-	-	-		
82	OHX	AR	3654	-	0,6,6	-	-	-		
82	OHX	AR	3615	-	0,6,6	-	-	-		
82	OHX	sR	1930	-	0,6,6	-	-	-		
82	OHX	1	3583	-	0,6,6	-	-	-		
82	OHX	1	3463	-	0,6,6	-	-	-		
82	OHX	1	3665	-	0,6,6	-	-	-		
82	OHX	1	3631	-	0,6,6	-	-	-		
82	OHX	sR	1943	-	0,6,6	-	-	-		
82	OHX	AR	3583	-	0,6,6	-	-	-		
82	OHX	sR	1949	-	0,6,6	-	-	-		
82	OHX	s4	301	-	0,6,6	-	-	-		
82	OHX	1	3673	-	0,6,6	-	-	-		
82	OHX	1	3572	-	0,6,6	-	-	-		
82	OHX	sR	2027	-	0,6,6	-	-	-		
82	OHX	CL	301	-	0,6,6	-	-	-		
82	OHX	A	1884	-	0,6,6	-	-	-		
82	OHX	1	3617	-	0,6,6	-	-	-		
82	OHX	AR	3617	-	0,6,6	-	-	-		
82	OHX	A	1876	82	0,6,6	-	-	-		
82	OHX	1	3579	-	0,6,6	-	-	-		
82	OHX	AR	3451	-	0,6,6	-	-	-		
82	OHX	1	3406	-	0,6,6	-	-	-		
82	OHX	AR	3564	-	0,6,6	-	-	-		
82	OHX	1	3430	-	0,6,6	-	-	-		
82	OHX	AR	3548	-	0,6,6	-	-	-		
82	OHX	AR	3406	-	0,6,6	-	-	-		
82	OHX	sR	1987	-	0,6,6	-	-	-		
82	OHX	A	1860	-	0,6,6	-	-	-		
82	OHX	sR	2004	-	0,6,6	-	-	-		
82	OHX	sR	1972	-	0,6,6	-	-	-		
82	OHX	A	1853	-	0,6,6	-	-	-		
82	OHX	A	1859	-	0,6,6	-	-	-		
82	OHX	sR	1988	-	0,6,6	-	-	-		
82	OHX	1	3678	-	0,6,6	-	-	-		
82	OHX	1	3640	-	0,6,6	-	-	-		
82	OHX	AR	3640	-	0,6,6	-	-	-		
82	OHX	CG	301	-	0,6,6	-	-	-		
82	OHX	1	3494	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	4	214	-	0,6,6	-	-	-		
82	OHX	AR	3494	-	0,6,6	-	-	-		
82	OHX	1	3438	-	0,6,6	-	-	-		
82	OHX	1	3614	-	0,6,6	-	-	-		
82	OHX	1	3427	-	0,6,6	-	-	-		
82	OHX	A	1810	-	0,6,6	-	-	-		
82	OHX	A	1823	-	0,6,6	-	-	-		
82	OHX	sR	1974	-	0,6,6	-	-	-		
82	OHX	sR	2022	-	0,6,6	-	-	-		
82	OHX	A	1849	-	0,6,6	-	-	-		
82	OHX	1	3713	-	0,6,6	-	-	-		
82	OHX	AT	205	-	0,6,6	-	-	-		
82	OHX	AR	3688	-	0,6,6	-	-	-		
82	OHX	A	1833	-	0,6,6	-	-	-		
82	OHX	1	401	-	0,6,6	-	-	-		
82	OHX	3	207	-	0,6,6	-	-	-		
82	OHX	1	3633	-	0,6,6	-	-	-		
82	OHX	1	3525	-	0,6,6	-	-	-		
82	OHX	1	3543	-	0,6,6	-	-	-		
82	OHX	AR	3633	-	0,6,6	-	-	-		
82	OHX	T	201	-	0,6,6	-	-	-		
82	OHX	1	3541	-	0,6,6	-	-	-		
82	OHX	1	3585	-	0,6,6	-	-	-		
82	OHX	AR	3543	-	0,6,6	-	-	-		
82	OHX	1	3676	-	0,6,6	-	-	-		
82	OHX	AR	3599	-	0,6,6	-	-	-		
82	OHX	AR	3585	-	0,6,6	-	-	-		
82	OHX	sR	1910	-	0,6,6	-	-	-		
82	OHX	sR	1911	-	0,6,6	-	-	-		
82	OHX	1	3459	-	0,6,6	-	-	-		
82	OHX	1	3667	-	0,6,6	-	-	-		
82	OHX	AR	3661	-	0,6,6	-	-	-		
82	OHX	1	3403	-	0,6,6	-	-	-		
82	OHX	AR	3463	-	0,6,6	-	-	-		
82	OHX	1	3602	-	0,6,6	-	-	-		
82	OHX	AR	3523	-	0,6,6	-	-	-		
82	OHX	1	3608	-	0,6,6	-	-	-		
82	OHX	AR	3602	-	0,6,6	-	-	-		
82	OHX	1	3440	-	0,6,6	-	-	-		
82	OHX	A	1816	-	0,6,6	-	-	-		
82	OHX	sR	1924	-	0,6,6	-	-	-		
82	OHX	AR	3424	-	0,6,6	-	-	-		
82	OHX	AR	3440	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	A	1912	-	0,6,6	-	-	-		
82	OHX	sR	1935	-	0,6,6	-	-	-		
82	OHX	AR	3500	-	0,6,6	-	-	-		
82	OHX	1	3560	-	0,6,6	-	-	-		
82	OHX	AS	203	-	0,6,6	-	-	-		
82	OHX	sR	1990	-	0,6,6	-	-	-		
82	OHX	1	3670	-	0,6,6	-	-	-		
82	OHX	sR	2024	-	0,6,6	-	-	-		
82	OHX	1	3696	-	0,6,6	-	-	-		
82	OHX	A	1824	-	0,6,6	-	-	-		
82	OHX	1	3411	-	0,6,6	-	-	-		
82	OHX	AR	3696	-	0,6,6	-	-	-		
82	OHX	sR	1959	-	0,6,6	-	-	-		
82	OHX	A	1897	47	0,6,6	-	-	-		
82	OHX	sR	1984	-	0,6,6	-	-	-		
82	OHX	1	3722	-	0,6,6	-	-	-		
82	OHX	1	3441	-	0,6,6	-	-	-		
82	OHX	A	1812	-	0,6,6	-	-	-		
82	OHX	sR	1919	-	0,6,6	-	-	-		
82	OHX	1	3422	-	0,6,6	-	-	-		
82	OHX	A	1889	-	0,6,6	-	-	-		
82	OHX	AR	3485	-	0,6,6	-	-	-		
82	OHX	sR	1960	-	0,6,6	-	-	-		
82	OHX	d9	102	-	0,6,6	-	-	-		
82	OHX	A	1854	-	0,6,6	-	-	-		
82	OHX	1	3448	-	0,6,6	-	-	-		
82	OHX	AR	3726	-	0,6,6	-	-	-		
82	OHX	1	3649	-	0,6,6	-	-	-		
82	OHX	AR	3643	-	0,6,6	-	-	-		
82	OHX	A	1818	-	0,6,6	-	-	-		
82	OHX	1	3600	-	0,6,6	-	-	-		
82	OHX	sR	2008	-	0,6,6	-	-	-		
82	OHX	3	202	-	0,6,6	-	-	-		
82	OHX	AR	3600	-	0,6,6	-	-	-		
82	OHX	sR	2045	-	0,6,6	-	-	-		
82	OHX	1	3454	-	0,6,6	-	-	-		
82	OHX	AE	201	-	0,6,6	-	-	-		
82	OHX	A	1862	-	0,6,6	-	-	-		
82	OHX	sR	2028	-	0,6,6	-	-	-		
82	OHX	AR	3729	-	0,6,6	-	-	-		
82	OHX	1	3675	-	0,6,6	-	-	-		
82	OHX	A	1882	-	0,6,6	-	-	-		
82	OHX	A	1847	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	A	1870	-	0,6,6	-	-	-		
82	OHX	sR	1955	-	0,6,6	-	-	-		
82	OHX	1	3487	-	0,6,6	-	-	-		
82	OHX	1	3431	-	0,6,6	-	-	-		
82	OHX	1	3556	-	0,6,6	-	-	-		
82	OHX	AR	3526	82	0,6,6	-	-	-		
82	OHX	A	1881	-	0,6,6	-	-	-		
82	OHX	1	3592	-	0,6,6	-	-	-		
82	OHX	AR	3431	-	0,6,6	-	-	-		
82	OHX	AR	3443	82	0,6,6	-	-	-		
82	OHX	1	3597	-	0,6,6	-	-	-		
82	OHX	1	3462	-	0,6,6	-	-	-		
82	OHX	AR	3487	-	0,6,6	-	-	-		
82	OHX	AR	3556	-	0,6,6	-	-	-		
82	OHX	AR	3467	-	0,6,6	-	-	-		
82	OHX	AR	3592	-	0,6,6	-	-	-		
82	OHX	AR	3462	-	0,6,6	-	-	-		
82	OHX	AR	3597	-	0,6,6	-	-	-		
82	OHX	sR	1922	-	0,6,6	-	-	-		
82	OHX	sR	1942	-	0,6,6	-	-	-		
82	OHX	AC	101	-	0,6,6	-	-	-		
82	OHX	1	3460	-	0,6,6	-	-	-		
82	OHX	AR	3460	-	0,6,6	-	-	-		
82	OHX	1	3514	-	0,6,6	-	-	-		
82	OHX	J	301	-	0,6,6	-	-	-		
82	OHX	1	3475	-	0,6,6	-	-	-		
82	OHX	1	3660	-	0,6,6	-	-	-		
82	OHX	AR	3514	-	0,6,6	-	-	-		
82	OHX	AR	3721	-	0,6,6	-	-	-		
82	OHX	AR	3475	-	0,6,6	-	-	-		
82	OHX	AR	3660	-	0,6,6	-	-	-		
82	OHX	A	1921	-	0,6,6	-	-	-		
82	OHX	AR	3649	-	0,6,6	-	-	-		
82	OHX	AR	3437	-	0,6,6	-	-	-		
82	OHX	AR	3584	-	0,6,6	-	-	-		
82	OHX	sR	1934	-	0,6,6	-	-	-		
82	OHX	sR	1965	-	0,6,6	-	-	-		
82	OHX	1	3616	-	0,6,6	-	-	-		
82	OHX	sR	2023	-	0,6,6	-	-	-		
82	OHX	AR	3405	-	0,6,6	-	-	-		
82	OHX	AR	3574	-	0,6,6	-	-	-		
82	OHX	sR	1940	-	0,6,6	-	-	-		
82	OHX	1	3507	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	A	1929	-	0,6,6	-	-	-		
82	OHX	AR	3507	-	0,6,6	-	-	-		
82	OHX	1	3439	-	0,6,6	-	-	-		
82	OHX	1	3657	-	0,6,6	-	-	-		
82	OHX	A	1838	-	0,6,6	-	-	-		
82	OHX	1	3547	-	0,6,6	-	-	-		
82	OHX	AR	3669	-	0,6,6	-	-	-		
82	OHX	A	1878	-	0,6,6	-	-	-		
82	OHX	1	3629	-	0,6,6	-	-	-		
82	OHX	1	3682	-	0,6,6	-	-	-		
82	OHX	AR	3714	-	0,6,6	-	-	-		
82	OHX	AR	3675	-	0,6,6	-	-	-		
82	OHX	1	3472	-	0,6,6	-	-	-		
82	OHX	1	3564	-	0,6,6	-	-	-		
82	OHX	A	1857	-	0,6,6	-	-	-		
86	GOL	AR	4262	-	5,5,5	0.30	0	5,5,5	0.40	0
82	OHX	AR	3618	-	0,6,6	-	-	-		
82	OHX	AR	3472	-	0,6,6	-	-	-		
82	OHX	AR	3481	-	0,6,6	-	-	-		
82	OHX	A	1879	-	0,6,6	-	-	-		
82	OHX	1	3576	-	0,6,6	-	-	-		
82	OHX	AR	3609	-	0,6,6	-	-	-		
82	OHX	AR	3576	-	0,6,6	-	-	-		
82	OHX	AS	201	-	0,6,6	-	-	-		
82	OHX	1	3554	-	0,6,6	-	-	-		
82	OHX	A	1885	-	0,6,6	-	-	-		
82	OHX	A	1831	-	0,6,6	-	-	-		
82	OHX	AR	3676	-	0,6,6	-	-	-		
82	OHX	A	1819	-	0,6,6	-	-	-		
82	OHX	Rb	401	-	0,6,6	-	-	-		
82	OHX	k	401	-	0,6,6	-	-	-		
82	OHX	A	1825	-	0,6,6	-	-	-		
82	OHX	AR	3509	-	0,6,6	-	-	-		
82	OHX	A	1900	-	0,6,6	-	-	-		
82	OHX	A	1850	-	0,6,6	-	-	-		
82	OHX	sR	1952	-	0,6,6	-	-	-		
82	OHX	sR	2034	-	0,6,6	-	-	-		
82	OHX	sR	2044	-	0,6,6	-	-	-		
82	OHX	AR	3650	-	0,6,6	-	-	-		
82	OHX	1	3471	-	0,6,6	-	-	-		
82	OHX	1	3490	-	0,6,6	-	-	-		
82	OHX	AR	3724	-	0,6,6	-	-	-		
82	OHX	AR	3436	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3632	-	0,6,6	-	-	-		
82	OHX	AR	3490	-	0,6,6	-	-	-		
82	OHX	AR	3632	-	0,6,6	-	-	-		
82	OHX	A	1861	-	0,6,6	-	-	-		
82	OHX	A	1804	-	0,6,6	-	-	-		
82	OHX	1	3496	-	0,6,6	-	-	-		
82	OHX	1	3549	-	0,6,6	-	-	-		
82	OHX	1	3555	-	0,6,6	-	-	-		
82	OHX	AR	3496	-	0,6,6	-	-	-		
82	OHX	AR	3536	-	0,6,6	-	-	-		
82	OHX	A	1928	-	0,6,6	-	-	-		
82	OHX	AR	3502	-	0,6,6	-	-	-		
82	OHX	AR	3575	-	0,6,6	-	-	-		
82	OHX	AR	3616	-	0,6,6	-	-	-		
82	OHX	AP	502	-	0,6,6	-	-	-		
82	OHX	A	1805	-	0,6,6	-	-	-		
82	OHX	1	3671	-	0,6,6	-	-	-		
82	OHX	CO	201	-	0,6,6	-	-	-		
82	OHX	AR	3601	-	0,6,6	-	-	-		
82	OHX	AR	3612	-	0,6,6	-	-	-		
82	OHX	c8	201	-	0,6,6	-	-	-		
82	OHX	4	209	-	0,6,6	-	-	-		
82	OHX	1	3515	-	0,6,6	-	-	-		
82	OHX	AR	3544	-	0,6,6	-	-	-		
82	OHX	AR	3421	-	0,6,6	-	-	-		
82	OHX	A	1822	82	0,6,6	-	-	-		
82	OHX	A	1828	-	0,6,6	-	-	-		
82	OHX	A	1837	-	0,6,6	-	-	-		
82	OHX	sR	1978	-	0,6,6	-	-	-		
82	OHX	sR	1941	-	0,6,6	-	-	-		
82	OHX	AT	215	-	0,6,6	-	-	-		
82	OHX	A	1923	-	0,6,6	-	-	-		
82	OHX	1	3424	-	0,6,6	-	-	-		
82	OHX	1	3530	-	0,6,6	-	-	-		
82	OHX	O	201	-	0,6,6	-	-	-		
82	OHX	AR	3530	-	0,6,6	-	-	-		
82	OHX	A	1907	-	0,6,6	-	-	-		
82	OHX	AR	3731	-	0,6,6	-	-	-		
82	OHX	sR	2048	-	0,6,6	-	-	-		
82	OHX	CG	302	-	0,6,6	-	-	-		
82	OHX	AR	3723	82	0,6,6	-	-	-		
82	OHX	sR	1904	-	0,6,6	-	-	-		
82	OHX	AR	3435	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3627	-	0,6,6	-	-	-		
82	OHX	1	3588	82	0,6,6	-	-	-		
82	OHX	AR	3569	-	0,6,6	-	-	-		
82	OHX	AR	3588	-	0,6,6	-	-	-		
82	OHX	sR	1947	-	0,6,6	-	-	-		
82	OHX	AR	3697	-	0,6,6	-	-	-		
82	OHX	1	3574	-	0,6,6	-	-	-		
82	OHX	A	1914	-	0,6,6	-	-	-		
82	OHX	AR	3541	-	0,6,6	-	-	-		
82	OHX	A	1903	-	0,6,6	-	-	-		
82	OHX	1	3418	-	0,6,6	-	-	-		
82	OHX	A	1845	-	0,6,6	-	-	-		
82	OHX	AR	3418	-	0,6,6	-	-	-		
82	OHX	sR	1963	-	0,6,6	-	-	-		
82	OHX	1	3643	-	0,6,6	-	-	-		
82	OHX	1	3659	-	0,6,6	-	-	-		
82	OHX	AR	3480	-	0,6,6	-	-	-		
82	OHX	A	1830	-	0,6,6	-	-	-		
82	OHX	1	3645	-	0,6,6	-	-	-		
82	OHX	CQ	201	-	0,6,6	-	-	-		
82	OHX	AR	3645	-	0,6,6	-	-	-		
82	OHX	1	3408	-	0,6,6	-	-	-		
82	OHX	AR	3560	-	0,6,6	-	-	-		
82	OHX	1	3607	-	0,6,6	-	-	-		
82	OHX	AR	3449	-	0,6,6	-	-	-		
82	OHX	z	201	-	0,6,6	-	-	-		
82	OHX	1	3701	-	0,6,6	-	-	-		
82	OHX	A	1913	-	0,6,6	-	-	-		
82	OHX	sR	1989	-	0,6,6	-	-	-		
82	OHX	sR	1912	-	0,6,6	-	-	-		
82	OHX	1	3419	-	0,6,6	-	-	-		
82	OHX	A	1874	-	0,6,6	-	-	-		
82	OHX	AR	3419	-	0,6,6	-	-	-		
82	OHX	AS	205	-	0,6,6	-	-	-		
82	OHX	1	3421	-	0,6,6	-	-	-		
82	OHX	CX	201	-	0,6,6	-	-	-		
82	OHX	1	3613	-	0,6,6	-	-	-		
82	OHX	AR	3552	-	0,6,6	-	-	-		
82	OHX	sR	1926	-	0,6,6	-	-	-		
82	OHX	AR	3635	-	0,6,6	-	-	-		
82	OHX	sR	2017	-	0,6,6	-	-	-		
82	OHX	A	1840	-	0,6,6	-	-	-		
82	OHX	1	3625	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	A	1894	-	0,6,6	-	-	-		
82	OHX	1	3443	-	0,6,6	-	-	-		
82	OHX	sR	1976	-	0,6,6	-	-	-		
82	OHX	AR	3625	-	0,6,6	-	-	-		
82	OHX	A	1905	-	0,6,6	-	-	-		
82	OHX	DQ	502	-	0,6,6	-	-	-		
82	OHX	1	3404	-	0,6,6	-	-	-		
82	OHX	A	1848	-	0,6,6	-	-	-		
82	OHX	AR	3503	-	0,6,6	-	-	-		
82	OHX	1	3517	-	0,6,6	-	-	-		
82	OHX	sR	2009	-	0,6,6	-	-	-		
82	OHX	A	1909	-	0,6,6	-	-	-		
82	OHX	sR	1902	-	0,6,6	-	-	-		
82	OHX	1	3694	-	0,6,6	-	-	-		
82	OHX	AR	3683	-	0,6,6	-	-	-		
82	OHX	AT	203	82	0,6,6	-	-	-		
82	OHX	A	1926	-	0,6,6	-	-	-		
82	OHX	sR	1951	-	0,6,6	-	-	-		
82	OHX	1	3580	-	0,6,6	-	-	-		
82	OHX	AT	211	-	0,6,6	-	-	-		
82	OHX	AR	3641	-	0,6,6	-	-	-		
82	OHX	AR	3580	-	0,6,6	-	-	-		
82	OHX	AR	3459	-	0,6,6	-	-	-		
82	OHX	sR	2031	-	0,6,6	-	-	-		
82	OHX	1	3586	-	0,6,6	-	-	-		
82	OHX	AR	3493	-	0,6,6	-	-	-		
82	OHX	AR	3586	-	0,6,6	-	-	-		
82	OHX	AR	3624	-	0,6,6	-	-	-		
82	OHX	A	1863	-	0,6,6	-	-	-		
82	OHX	sR	1906	-	0,6,6	-	-	-		
82	OHX	1	3461	-	0,6,6	-	-	-		
82	OHX	1	3702	-	0,6,6	-	-	-		
82	OHX	1	3603	-	0,6,6	-	-	-		
82	OHX	AR	3665	-	0,6,6	-	-	-		
82	OHX	1	3509	-	0,6,6	-	-	-		
82	OHX	sR	1944	-	0,6,6	-	-	-		
82	OHX	1	3720	-	0,6,6	-	-	-		
82	OHX	AR	3631	-	0,6,6	-	-	-		
82	OHX	AR	3563	-	0,6,6	-	-	-		
82	OHX	1	3531	-	0,6,6	-	-	-		
82	OHX	sR	1928	-	0,6,6	-	-	-		
82	OHX	sR	1929	-	0,6,6	-	-	-		
82	OHX	A	1858	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	sR	1932	-	0,6,6	-	-	-		
82	OHX	1	3414	-	0,6,6	-	-	-		
82	OHX	A	1865	-	0,6,6	-	-	-		
82	OHX	1	3516	-	0,6,6	-	-	-		
82	OHX	A	1877	-	0,6,6	-	-	-		
82	OHX	AR	3516	-	0,6,6	-	-	-		
82	OHX	1	3606	-	0,6,6	-	-	-		
82	OHX	sR	1998	-	0,6,6	-	-	-		
82	OHX	AR	3489	-	0,6,6	-	-	-		
82	OHX	1	3644	-	0,6,6	-	-	-		
82	OHX	AR	3606	-	0,6,6	-	-	-		
82	OHX	1	3536	-	0,6,6	-	-	-		
82	OHX	sR	2047	-	0,6,6	-	-	-		
82	OHX	1	3407	-	0,6,6	-	-	-		
82	OHX	1	3502	-	0,6,6	-	-	-		
82	OHX	sR	1923	-	0,6,6	-	-	-		
86	GOL	AR	4263	-	5,5,5	0.08	0	5,5,5	0.25	0
82	OHX	AR	3627	-	0,6,6	-	-	-		
82	OHX	AR	3412	-	0,6,6	-	-	-		
82	OHX	AR	3427	-	0,6,6	-	-	-		
82	OHX	DD	101	-	0,6,6	-	-	-		
82	OHX	4	206	-	0,6,6	-	-	-		
82	OHX	sR	1901	-	0,6,6	-	-	-		
82	OHX	4	207	-	0,6,6	-	-	-		
82	OHX	AR	3425	-	0,6,6	-	-	-		
82	OHX	A	1931	-	0,6,6	-	-	-		
82	OHX	AR	3704	-	0,6,6	-	-	-		
82	OHX	A	1899	-	0,6,6	-	-	-		
82	OHX	1	3714	-	0,6,6	-	-	-		
82	OHX	sR	2026	-	0,6,6	-	-	-		
82	OHX	AR	3486	-	0,6,6	-	-	-		
84	G5B	AR	4264	-	27,28,28	0.33	0	36,45,45	0.59	0
82	OHX	AR	3667	-	0,6,6	-	-	-		
82	OHX	AR	3477	-	0,6,6	-	-	-		
82	OHX	AR	3531	-	0,6,6	-	-	-		
82	OHX	A	1938	-	0,6,6	-	-	-		
82	OHX	1	3505	-	0,6,6	-	-	-		
82	OHX	AR	3687	-	0,6,6	-	-	-		
82	OHX	1	3619	-	0,6,6	-	-	-		
82	OHX	A	1901	-	0,6,6	-	-	-		
82	OHX	sR	1936	-	0,6,6	-	-	-		
82	OHX	c1	201	-	0,6,6	-	-	-		
82	OHX	AR	3608	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3521	-	0,6,6	-	-	-		
82	OHX	AR	3408	-	0,6,6	-	-	-		
82	OHX	sR	1918	-	0,6,6	-	-	-		
82	OHX	A	1896	-	0,6,6	-	-	-		
82	OHX	AR	3732	-	0,6,6	-	-	-		
82	OHX	1	3559	-	0,6,6	-	-	-		
82	OHX	1	3668	-	0,6,6	-	-	-		
82	OHX	1	3595	-	0,6,6	-	-	-		
82	OHX	AR	3533	-	0,6,6	-	-	-		
82	OHX	1	3663	-	0,6,6	-	-	-		
82	OHX	1	3532	-	0,6,6	-	-	-		
82	OHX	AR	3450	-	0,6,6	-	-	-		
82	OHX	AR	3532	-	0,6,6	-	-	-		
82	OHX	1	3571	-	0,6,6	-	-	-		
82	OHX	AR	3571	-	0,6,6	-	-	-		
82	OHX	3	201	-	0,6,6	-	-	-		
82	OHX	sR	1920	-	0,6,6	-	-	-		
82	OHX	sR	2030	-	0,6,6	-	-	-		
82	OHX	1	3473	-	0,6,6	-	-	-		
82	OHX	1	3636	-	0,6,6	-	-	-		
82	OHX	AR	3491	-	0,6,6	-	-	-		
82	OHX	1	3466	-	0,6,6	-	-	-		
82	OHX	AR	3422	-	0,6,6	-	-	-		
82	OHX	AT	212	82	0,6,6	-	-	-		
82	OHX	1	3721	1	0,6,6	-	-	-		
82	OHX	AR	3702	-	0,6,6	-	-	-		
82	OHX	AR	3466	-	0,6,6	-	-	-		
82	OHX	AR	3730	-	0,6,6	-	-	-		
82	OHX	1	3704	-	0,6,6	-	-	-		
82	OHX	sR	1905	-	0,6,6	-	-	-		
82	OHX	sR	2002	-	0,6,6	-	-	-		
82	OHX	1	3534	-	0,6,6	-	-	-		
82	OHX	1	3449	-	0,6,6	-	-	-		
82	OHX	AR	3469	-	0,6,6	-	-	-		
82	OHX	1	3634	-	0,6,6	-	-	-		
82	OHX	A	1846	-	0,6,6	-	-	-		
82	OHX	1	3582	-	0,6,6	-	-	-		
82	OHX	1	3686	-	0,6,6	-	-	-		
82	OHX	sR	1945	-	0,6,6	-	-	-		
82	OHX	AR	3634	-	0,6,6	-	-	-		
82	OHX	AT	214	-	0,6,6	-	-	-		
82	OHX	A	1868	-	0,6,6	-	-	-		
82	OHX	1	3415	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	sR	1964	-	0,6,6	-	-	-		
82	OHX	AR	3415	-	0,6,6	-	-	-		
82	OHX	1	3623	-	0,6,6	-	-	-		
82	OHX	1	3690	82	0,6,6	-	-	-		
82	OHX	1	3662	-	0,6,6	-	-	-		
82	OHX	AR	3638	-	0,6,6	-	-	-		
82	OHX	1	3552	-	0,6,6	-	-	-		
82	OHX	AR	3623	-	0,6,6	-	-	-		
82	OHX	AR	3690	-	0,6,6	-	-	-		
82	OHX	AR	3662	-	0,6,6	-	-	-		
82	OHX	A	1817	-	0,6,6	-	-	-		
82	OHX	1	3548	-	0,6,6	-	-	-		
82	OHX	AR	3559	-	0,6,6	-	-	-		
82	OHX	A	1933	-	0,6,6	-	-	-		
82	OHX	1	3508	-	0,6,6	-	-	-		
82	OHX	sR	1966	-	0,6,6	-	-	-		
82	OHX	AR	3705	-	0,6,6	-	-	-		
82	OHX	AR	3508	-	0,6,6	-	-	-		
82	OHX	CK	201	-	0,6,6	-	-	-		
82	OHX	4	211	-	0,6,6	-	-	-		
82	OHX	sR	1916	-	0,6,6	-	-	-		
82	OHX	s1	301	-	0,6,6	-	-	-		
82	OHX	AR	3549	-	0,6,6	-	-	-		
82	OHX	1	3596	-	0,6,6	-	-	-		
82	OHX	1	3677	-	0,6,6	-	-	-		
82	OHX	1	3681	-	0,6,6	-	-	-		
82	OHX	sR	1954	-	0,6,6	-	-	-		
82	OHX	AR	3596	-	0,6,6	-	-	-		
82	OHX	1	3591	-	0,6,6	-	-	-		
82	OHX	1	3641	-	0,6,6	-	-	-		
82	OHX	1	3409	-	0,6,6	-	-	-		
82	OHX	4	202	-	0,6,6	-	-	-		
82	OHX	A	1916	-	0,6,6	-	-	-		
82	OHX	sR	2041	-	0,6,6	-	-	-		
82	OHX	sR	2015	-	0,6,6	-	-	-		
82	OHX	1	3573	-	0,6,6	-	-	-		
82	OHX	AR	3573	-	0,6,6	-	-	-		
82	OHX	AR	3439	-	0,6,6	-	-	-		
82	OHX	A	1815	-	0,6,6	-	-	-		
82	OHX	sR	2001	-	0,6,6	-	-	-		
82	OHX	Q	201	-	0,6,6	-	-	-		
82	OHX	3	208	-	0,6,6	-	-	-		
82	OHX	AR	3505	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	sR	2006	-	0,6,6	-	-	-		
82	OHX	A	1895	-	0,6,6	-	-	-		
82	OHX	AR	3684	-	0,6,6	-	-	-		
82	OHX	1	3565	-	0,6,6	-	-	-		
82	OHX	1	3630	-	0,6,6	-	-	-		
82	OHX	sR	2036	-	0,6,6	-	-	-		
82	OHX	AR	3709	82	0,6,6	-	-	-		
82	OHX	AR	3565	-	0,6,6	-	-	-		
82	OHX	1	3567	-	0,6,6	-	-	-		
82	OHX	1	3570	-	0,6,6	-	-	-		
82	OHX	AR	3630	-	0,6,6	-	-	-		
82	OHX	A	1937	-	0,6,6	-	-	-		
82	OHX	1	3699	-	0,6,6	-	-	-		
82	OHX	1	3467	-	0,6,6	-	-	-		
82	OHX	AR	3567	-	0,6,6	-	-	-		
82	OHX	AR	3570	-	0,6,6	-	-	-		
82	OHX	AR	3699	-	0,6,6	-	-	-		
82	OHX	A	1841	-	0,6,6	-	-	-		
82	OHX	AR	3727	-	0,6,6	-	-	-		
82	OHX	AR	3689	-	0,6,6	-	-	-		
82	OHX	1	3412	-	0,6,6	-	-	-		
82	OHX	1	3474	-	0,6,6	-	-	-		
82	OHX	AR	3554	-	0,6,6	-	-	-		
82	OHX	4	212	-	0,6,6	-	-	-		
82	OHX	AR	3498	-	0,6,6	-	-	-		
82	OHX	AR	3681	-	0,6,6	-	-	-		
82	OHX	A	1886	-	0,6,6	-	-	-		
82	OHX	sR	2010	-	0,6,6	-	-	-		
82	OHX	A	1808	-	0,6,6	-	-	-		
82	OHX	sR	1937	-	0,6,6	-	-	-		
82	OHX	CE	401	-	0,6,6	-	-	-		
82	OHX	1	3646	-	0,6,6	-	-	-		
82	OHX	1	3455	-	0,6,6	-	-	-		
82	OHX	AR	3707	-	0,6,6	-	-	-		
82	OHX	sR	1994	-	0,6,6	-	-	-		
82	OHX	AR	3471	-	0,6,6	-	-	-		
82	OHX	AR	3455	-	0,6,6	-	-	-		
82	OHX	1	3451	-	0,6,6	-	-	-		
82	OHX	1	3581	-	0,6,6	-	-	-		
82	OHX	1	3479	-	0,6,6	-	-	-		
82	OHX	AR	3581	-	0,6,6	-	-	-		
82	OHX	A	1869	-	0,6,6	-	-	-		
82	OHX	1	3423	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3578	-	0,6,6	-	-	-		
82	OHX	3	205	-	0,6,6	-	-	-		
82	OHX	AR	3479	-	0,6,6	-	-	-		
82	OHX	1	3651	-	0,6,6	-	-	-		
82	OHX	AR	3423	-	0,6,6	-	-	-		
82	OHX	AR	3578	-	0,6,6	-	-	-		
82	OHX	AR	3603	-	0,6,6	-	-	-		
82	OHX	A	1820	-	0,6,6	-	-	-		
82	OHX	1	3653	-	0,6,6	-	-	-		
82	OHX	AR	3555	-	0,6,6	-	-	-		
82	OHX	1	3639	-	0,6,6	-	-	-		
82	OHX	1	3425	-	0,6,6	-	-	-		
82	OHX	AR	3482	-	0,6,6	-	-	-		
82	OHX	sR	1996	-	0,6,6	-	-	-		
82	OHX	1	3450	-	0,6,6	-	-	-		
82	OHX	4	204	-	0,6,6	-	-	-		
82	OHX	AR	3666	-	0,6,6	-	-	-		
82	OHX	sR	1915	-	0,6,6	-	-	-		
82	OHX	AR	3520	-	0,6,6	-	-	-		
82	OHX	AR	3547	-	0,6,6	-	-	-		
82	OHX	AR	3403	-	0,6,6	-	-	-		
82	OHX	1	3637	-	0,6,6	-	-	-		
82	OHX	1	3672	-	0,6,6	-	-	-		
82	OHX	AK	102	-	0,6,6	-	-	-		
82	OHX	AR	3671	-	0,6,6	-	-	-		
82	OHX	1	3527	-	0,6,6	-	-	-		
82	OHX	AR	3637	-	0,6,6	-	-	-		
82	OHX	AR	3672	-	0,6,6	-	-	-		
82	OHX	CX	202	-	0,6,6	-	-	-		
82	OHX	A	1852	-	0,6,6	-	-	-		
82	OHX	1	3486	-	0,6,6	-	-	-		
82	OHX	AR	3470	-	0,6,6	-	-	-		
82	OHX	AR	3527	-	0,6,6	-	-	-		
82	OHX	A	1930	-	0,6,6	-	-	-		
82	OHX	sR	1908	-	0,6,6	-	-	-		
82	OHX	sR	2007	-	0,6,6	-	-	-		
82	OHX	1	3524	-	0,6,6	-	-	-		
82	OHX	AR	3524	-	0,6,6	-	-	-		
82	OHX	1	3523	-	0,6,6	-	-	-		
82	OHX	1	3648	-	0,6,6	-	-	-		
82	OHX	1	3687	-	0,6,6	-	-	-		
82	OHX	A	1911	-	0,6,6	-	-	-		
82	OHX	AR	3648	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	A	1890	-	0,6,6	-	-	-		
82	OHX	A	1915	-	0,6,6	-	-	-		
82	OHX	AR	3447	-	0,6,6	-	-	-		
82	OHX	1	3500	-	0,6,6	-	-	-		
82	OHX	1	3546	-	0,6,6	-	-	-		
82	OHX	AR	3442	-	0,6,6	-	-	-		
82	OHX	1	3482	-	0,6,6	-	-	-		
82	OHX	1	3457	-	0,6,6	-	-	-		
82	OHX	A	1892	-	0,6,6	-	-	-		
82	OHX	AR	3457	-	0,6,6	-	-	-		
82	OHX	AR	3644	-	0,6,6	-	-	-		
82	OHX	4	208	-	0,6,6	-	-	-		
82	OHX	1	3417	-	0,6,6	-	-	-		
82	OHX	AR	3417	-	0,6,6	-	-	-		
82	OHX	AK	103	-	0,6,6	-	-	-		
82	OHX	AR	3579	-	0,6,6	-	-	-		
82	OHX	AR	3733	-	0,6,6	-	-	-		
82	OHX	1	3437	-	0,6,6	-	-	-		
82	OHX	1	3484	-	0,6,6	-	-	-		
82	OHX	AR	3401	-	0,6,6	-	-	-		
82	OHX	AT	210	-	0,6,6	-	-	-		
82	OHX	A	1867	-	0,6,6	-	-	-		
82	OHX	sR	1995	-	0,6,6	-	-	-		
82	OHX	AT	204	-	0,6,6	-	-	-		
82	OHX	sR	2019	-	0,6,6	-	-	-		
82	OHX	AR	3736	-	0,6,6	-	-	-		
82	OHX	A	1891	-	0,6,6	-	-	-		
82	OHX	sR	2018	-	0,6,6	-	-	-		
82	OHX	AR	3678	-	0,6,6	-	-	-		
82	OHX	sR	1927	-	0,6,6	-	-	-		
82	OHX	1	3605	-	0,6,6	-	-	-		
82	OHX	A	1904	-	0,6,6	-	-	-		
82	OHX	AR	3521	-	0,6,6	-	-	-		
82	OHX	1	3558	-	0,6,6	-	-	-		
82	OHX	AR	3605	-	0,6,6	-	-	-		
82	OHX	AR	3438	-	0,6,6	-	-	-		
82	OHX	1	3469	-	0,6,6	-	-	-		
82	OHX	AR	3659	-	0,6,6	-	-	-		
82	OHX	1	3401	-	0,6,6	-	-	-		
82	OHX	1	3612	-	0,6,6	-	-	-		
82	OHX	AR	3737	1	0,6,6	-	-	-		
82	OHX	A	1809	82	0,6,6	-	-	-		
82	OHX	1	3458	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3511	-	0,6,6	-	-	-		
82	OHX	A	1887	-	0,6,6	-	-	-		
82	OHX	1	3594	-	0,6,6	-	-	-		
82	OHX	1	3703	-	0,6,6	-	-	-		
82	OHX	AR	3458	-	0,6,6	-	-	-		
82	OHX	AR	3607	-	0,6,6	-	-	-		
82	OHX	CP	501	-	0,6,6	-	-	-		
82	OHX	sR	2043	-	0,6,6	-	-	-		
82	OHX	AR	3703	-	0,6,6	-	-	-		
82	OHX	AR	3504	-	0,6,6	-	-	-		
82	OHX	AR	3701	-	0,6,6	-	-	-		
82	OHX	sR	1950	-	0,6,6	-	-	-		
82	OHX	1	3426	-	0,6,6	-	-	-		
82	OHX	sR	2011	-	0,6,6	-	-	-		
82	OHX	1	3519	-	0,6,6	-	-	-		
82	OHX	AR	3426	-	0,6,6	-	-	-		
82	OHX	AR	3428	-	0,6,6	-	-	-		
82	OHX	1	3598	-	0,6,6	-	-	-		
82	OHX	1	3705	-	0,6,6	-	-	-		
82	OHX	AR	3519	-	0,6,6	-	-	-		
82	OHX	CM	201	-	0,6,6	-	-	-		
82	OHX	A	1836	-	0,6,6	-	-	-		
82	OHX	1	3506	-	0,6,6	-	-	-		
82	OHX	AR	3598	-	0,6,6	-	-	-		
82	OHX	4	203	-	0,6,6	-	-	-		
82	OHX	A	1893	-	0,6,6	-	-	-		
82	OHX	A	1880	-	0,6,6	-	-	-		
82	OHX	sR	1914	-	0,6,6	-	-	-		
82	OHX	1	3615	-	0,6,6	-	-	-		
82	OHX	A	1936	-	0,6,6	-	-	-		
82	OHX	1	3716	-	0,6,6	-	-	-		
82	OHX	1	3537	82	0,6,6	-	-	-		
82	OHX	AR	3691	-	0,6,6	-	-	-		
82	OHX	1	3420	-	0,6,6	-	-	-		
82	OHX	AR	3716	-	0,6,6	-	-	-		
82	OHX	AR	3722	-	0,6,6	-	-	-		
82	OHX	AR	3537	-	0,6,6	-	-	-		
82	OHX	A	1814	-	0,6,6	-	-	-		
82	OHX	h	401	-	0,6,6	-	-	-		
82	OHX	1	3446	-	0,6,6	-	-	-		
82	OHX	AR	3561	-	0,6,6	-	-	-		
82	OHX	AR	3636	-	0,6,6	-	-	-		
82	OHX	A	1801	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3483	-	0,6,6	-	-	-		
82	OHX	1	3539	-	0,6,6	-	-	-		
82	OHX	1	3650	-	0,6,6	-	-	-		
82	OHX	3	209	-	0,6,6	-	-	-		
82	OHX	AR	3404	-	0,6,6	-	-	-		
82	OHX	1	3563	-	0,6,6	-	-	-		
82	OHX	1	3456	-	0,6,6	-	-	-		
82	OHX	1	3611	-	0,6,6	-	-	-		
82	OHX	AR	3610	-	0,6,6	-	-	-		
82	OHX	AR	3456	-	0,6,6	-	-	-		
82	OHX	A	1924	-	0,6,6	-	-	-		
82	OHX	AR	3611	-	0,6,6	-	-	-		
82	OHX	A	1935	-	0,6,6	-	-	-		
82	OHX	AR	3550	-	0,6,6	-	-	-		
82	OHX	AT	206	-	0,6,6	-	-	-		
82	OHX	1	3712	-	0,6,6	-	-	-		
82	OHX	AR	3558	-	0,6,6	-	-	-		
82	OHX	1	3647	-	0,6,6	-	-	-		
82	OHX	AR	3568	-	0,6,6	-	-	-		
82	OHX	A	1940	-	0,6,6	-	-	-		
82	OHX	AR	3712	-	0,6,6	-	-	-		
82	OHX	sR	1985	-	0,6,6	-	-	-		
82	OHX	AR	3647	-	0,6,6	-	-	-		
82	OHX	1	3553	-	0,6,6	-	-	-		
82	OHX	AR	3551	-	0,6,6	-	-	-		
82	OHX	CE	402	-	0,6,6	-	-	-		
82	OHX	AR	3492	-	0,6,6	-	-	-		
82	OHX	AR	3720	-	0,6,6	-	-	-		
82	OHX	A	1864	-	0,6,6	-	-	-		
82	OHX	A	1902	-	0,6,6	-	-	-		
82	OHX	c3	201	-	0,6,6	-	-	-		
82	OHX	w	201	-	0,6,6	-	-	-		
82	OHX	1	3693	-	0,6,6	-	-	-		
82	OHX	AR	3619	-	0,6,6	-	-	-		
82	OHX	CG	303	-	0,6,6	-	-	-		
82	OHX	1	3562	-	0,6,6	-	-	-		
82	OHX	AR	3540	-	0,6,6	-	-	-		
82	OHX	AR	3693	-	0,6,6	-	-	-		
82	OHX	sR	1933	-	0,6,6	-	-	-		
82	OHX	AR	3562	-	0,6,6	-	-	-		
82	OHX	sR	2033	-	0,6,6	-	-	-		
82	OHX	AR	3538	-	0,6,6	-	-	-		
82	OHX	sR	1967	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	AS	206	-	0,6,6	-	-	-		
82	OHX	1	3587	-	0,6,6	-	-	-		
82	OHX	AR	3488	-	0,6,6	-	-	-		
82	OHX	v	301	-	0,6,6	-	-	-		
82	OHX	1	3498	-	0,6,6	-	-	-		
82	OHX	1	3489	-	0,6,6	-	-	-		
82	OHX	A	1829	-	0,6,6	-	-	-		
82	OHX	sR	2039	-	0,6,6	-	-	-		
82	OHX	A	1917	-	0,6,6	-	-	-		
82	OHX	sR	1948	-	0,6,6	-	-	-		
82	OHX	AR	3642	-	0,6,6	-	-	-		
82	OHX	AT	213	-	0,6,6	-	-	-		
82	OHX	n	201	-	0,6,6	-	-	-		
82	OHX	A	1873	-	0,6,6	-	-	-		
82	OHX	AR	3410	-	0,6,6	-	-	-		
82	OHX	AR	3692	-	0,6,6	-	-	-		
82	OHX	AR	3473	-	0,6,6	-	-	-		
82	OHX	sR	1938	-	0,6,6	-	-	-		
82	OHX	sR	1921	-	0,6,6	-	-	-		
82	OHX	sR	2003	-	0,6,6	-	-	-		
82	OHX	AR	3711	-	0,6,6	-	-	-		
82	OHX	1	3476	-	0,6,6	-	-	-		
82	OHX	sR	1997	-	0,6,6	-	-	-		
82	OHX	1	3513	-	0,6,6	-	-	-		
82	OHX	A	1807	-	0,6,6	-	-	-		
82	OHX	AR	3476	-	0,6,6	-	-	-		
82	OHX	AR	3655	-	0,6,6	-	-	-		
82	OHX	sR	1991	-	0,6,6	-	-	-		
82	OHX	AR	3513	-	0,6,6	-	-	-		
82	OHX	AR	3545	-	0,6,6	-	-	-		
82	OHX	AR	3710	-	0,6,6	-	-	-		
82	OHX	1	3542	-	0,6,6	-	-	-		

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
84	G5B	1	4224	-	-	1/8/62/62	0/3/3/3
86	GOL	AR	4262	-	-	2/4/4/4	-
86	GOL	AR	4263	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	G5B	AR	4264	-	-	1/8/62/62	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	1	4224	G5B	C11-C6-C5	-4.13	109.39	114.23
84	1	4224	G5B	C11-C6-C9	2.82	117.03	113.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

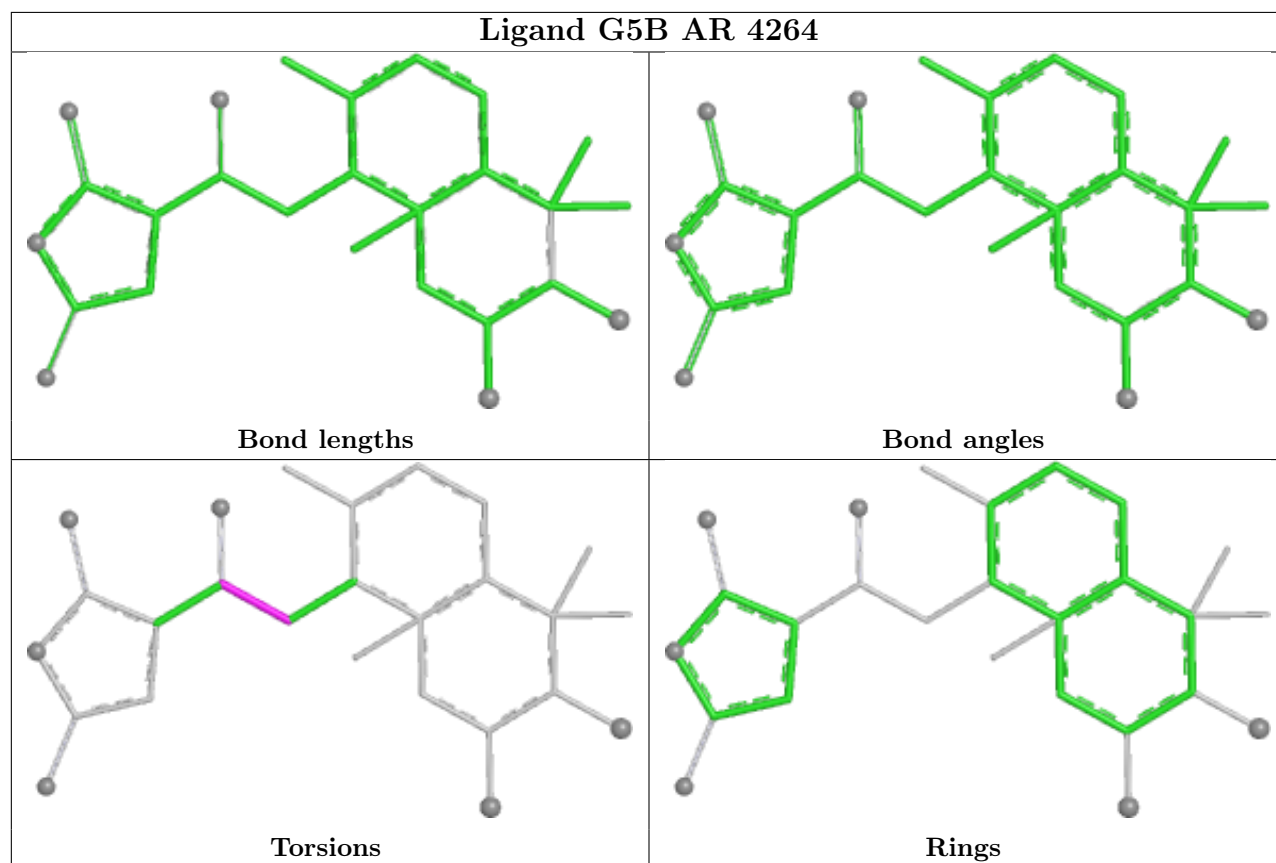
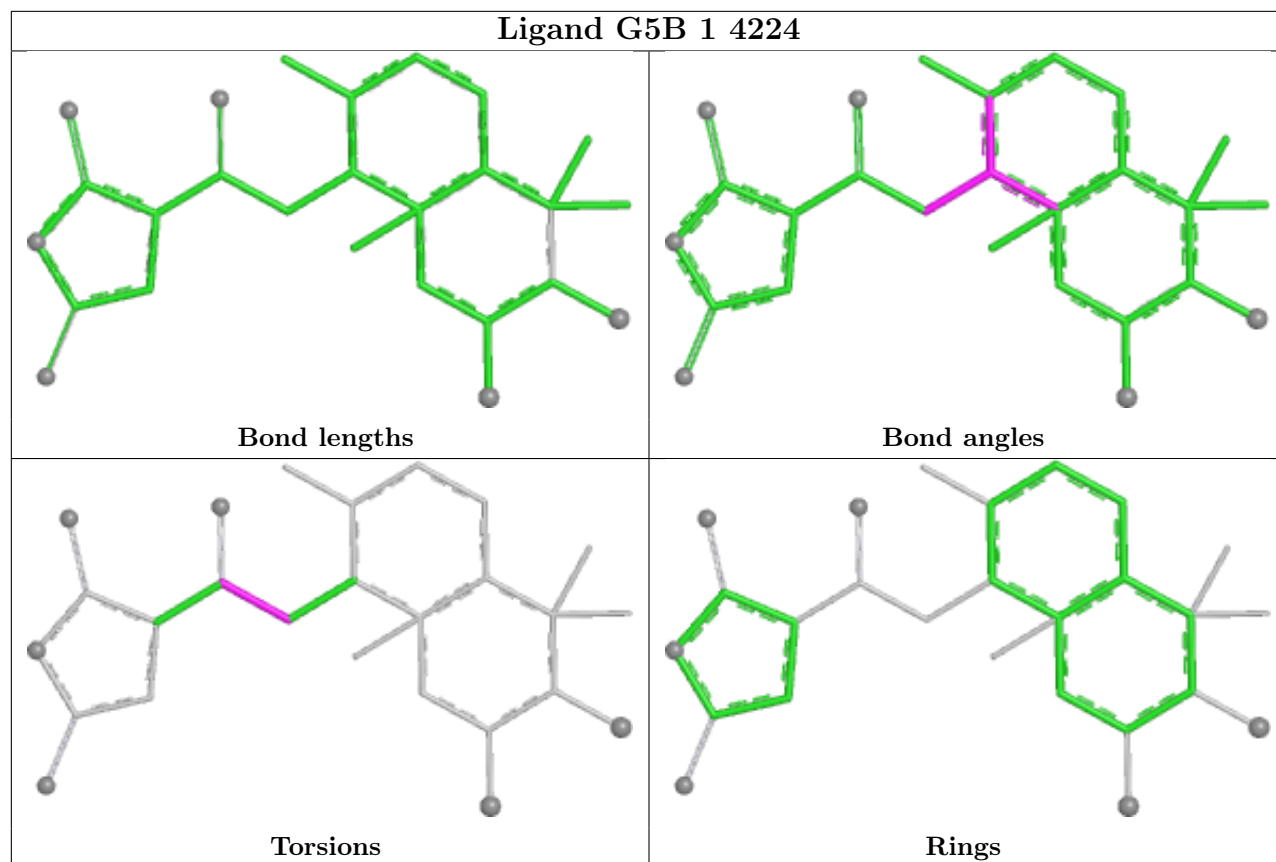
Mol	Chain	Res	Type	Atoms
86	AR	4262	GOL	C1-C2-C3-O3
86	AR	4262	GOL	O2-C2-C3-O3
84	1	4224	G5B	C6-C11-C16-O1
84	AR	4264	G5B	C6-C11-C16-O1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	AR	3441	OHX	0	1

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.



4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
58	c0	1
47	A	1
14	t	1
52	F	1
48	s0	1
7	CG	1
52	s4	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	c0	84:GLU	C	87:HIS	N	9.26
1	A	1716:C	O3'	1717:G	P	4.20
1	t	132:ALA	C	133:PRO	N	1.75
1	F	82:TYR	C	83:PRO	N	1.18
1	s0	160:ILE	C	161:PRO	N	1.16

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	1	3149/3396 (92%)	-0.13	95 (3%)	52	31	20, 42, 104, 200	0
1	AR	3147/3396 (92%)	-0.15	122 (3%)	43	24	21, 40, 100, 196	0
2	3	121/121 (100%)	-0.27	0	100	100	34, 58, 70, 71	0
2	AS	121/121 (100%)	-0.43	1 (0%)	82	65	27, 43, 53, 56	0
3	4	158/158 (100%)	-0.25	5 (3%)	50	30	24, 40, 73, 107	0
3	AT	158/158 (100%)	-0.17	5 (3%)	50	30	29, 48, 78, 95	0
4	CD	252/254 (99%)	0.11	9 (3%)	46	26	25, 40, 57, 64	0
4	j	252/254 (99%)	0.00	4 (1%)	70	49	25, 39, 53, 62	0
5	CE	386/387 (99%)	-0.10	5 (1%)	75	56	22, 33, 43, 76	0
5	k	386/387 (99%)	0.00	3 (0%)	82	65	28, 44, 54, 64	0
6	CF	361/362 (99%)	-0.03	2 (0%)	85	70	25, 39, 53, 67	0
6	l	361/362 (99%)	-0.15	1 (0%)	90	80	21, 34, 49, 56	0
7	CG	296/297 (99%)	0.14	7 (2%)	59	38	34, 44, 64, 79	0
7	m	296/297 (99%)	0.26	4 (1%)	73	53	41, 61, 74, 95	0
8	CH	156/176 (88%)	0.02	1 (0%)	85	70	33, 41, 58, 70	0
8	n	156/176 (88%)	-0.10	0	100	100	33, 37, 49, 62	0
9	CI	222/244 (90%)	-0.03	3 (1%)	73	53	26, 31, 61, 93	0
9	o	222/244 (90%)	-0.08	2 (0%)	81	63	27, 33, 52, 79	0
10	CJ	233/256 (91%)	0.49	12 (5%)	33	17	54, 64, 94, 103	0
10	p	233/256 (91%)	0.38	4 (1%)	69	48	45, 57, 85, 93	0
11	CK	191/191 (100%)	-0.09	4 (2%)	63	42	33, 39, 53, 62	0
11	q	191/191 (100%)	0.14	0	100	100	42, 52, 62, 72	0
12	CL	211/221 (95%)	0.05	6 (2%)	55	34	26, 39, 62, 90	0
12	r	211/221 (95%)	0.12	3 (1%)	73	53	29, 42, 73, 81	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	CM	169/174 (97%)	0.16	2 (1%) 76 58	36, 51, 65, 76	0
13	s	169/174 (97%)	0.29	0 100 100	51, 67, 76, 82	0
14	CN	193/199 (96%)	0.06	4 (2%) 63 42	26, 49, 80, 95	0
14	t	193/199 (96%)	0.03	3 (1%) 70 49	23, 41, 73, 94	0
15	CO	136/138 (98%)	-0.05	4 (2%) 53 32	31, 36, 53, 68	0
15	u	136/138 (98%)	-0.02	1 (0%) 84 68	34, 42, 53, 60	0
16	CP	203/204 (99%)	0.23	2 (0%) 79 61	28, 44, 53, 57	0
16	v	203/204 (99%)	0.12	1 (0%) 87 73	24, 37, 46, 51	0
17	CQ	197/199 (98%)	-0.09	4 (2%) 65 44	23, 26, 51, 56	0
17	w	197/199 (98%)	-0.13	3 (1%) 72 52	27, 33, 48, 50	0
18	CR	183/184 (99%)	0.59	26 (14%) 6 3	25, 31, 109, 140	0
18	x	183/184 (99%)	0.13	8 (4%) 39 21	28, 35, 76, 106	0
19	CS	185/186 (99%)	0.02	2 (1%) 78 59	28, 39, 47, 53	0
19	y	185/186 (99%)	0.08	5 (2%) 56 35	27, 36, 48, 65	0
20	CT	188/189 (99%)	0.47	12 (6%) 25 14	38, 49, 119, 134	0
20	z	188/189 (99%)	0.40	6 (3%) 50 30	43, 55, 125, 139	0
21	0	172/172 (100%)	-0.03	2 (1%) 76 58	33, 40, 50, 54	0
21	CU	172/172 (100%)	-0.13	2 (1%) 76 58	28, 32, 40, 48	0
22	2	159/160 (99%)	0.01	1 (0%) 85 70	27, 40, 73, 80	0
22	CV	159/160 (99%)	-0.01	1 (0%) 85 70	24, 34, 67, 73	0
23	5	100/121 (82%)	0.66	4 (4%) 42 23	71, 82, 89, 95	0
23	CW	100/121 (82%)	0.42	3 (3%) 52 31	60, 70, 76, 90	0
24	6	136/137 (99%)	-0.03	2 (1%) 72 52	31, 40, 48, 52	0
24	CX	136/137 (99%)	-0.12	4 (2%) 53 32	24, 32, 42, 45	0
25	7	98/155 (63%)	1.06	25 (25%) 1 1	40, 52, 124, 127	0
25	CY	124/155 (80%)	0.69	15 (12%) 8 5	32, 64, 109, 125	0
26	8	121/142 (85%)	0.10	1 (0%) 82 65	36, 46, 59, 90	0
26	CZ	121/142 (85%)	0.25	3 (2%) 58 37	38, 49, 68, 78	0
27	9	126/127 (99%)	-0.05	1 (0%) 82 65	27, 42, 51, 54	0
27	DA	124/127 (97%)	0.29	2 (1%) 70 49	32, 49, 60, 64	0
28	AA	135/136 (99%)	0.26	1 (0%) 84 68	55, 65, 79, 87	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DB	135/136 (99%)	0.53	1 (0%) 84 68	61, 72, 92, 99	0
29	AB	148/149 (99%)	-0.03	1 (0%) 84 68	20, 36, 52, 60	0
29	DC	148/149 (99%)	0.03	0 100 100	22, 41, 54, 56	0
30	AC	58/59 (98%)	0.28	5 (8%) 16 9	24, 43, 85, 97	0
30	DD	58/59 (98%)	0.18	1 (1%) 69 48	23, 42, 64, 70	0
31	AD	97/105 (92%)	0.05	1 (1%) 79 61	53, 60, 77, 81	0
31	DE	97/105 (92%)	0.36	1 (1%) 79 61	53, 63, 79, 82	0
32	AE	109/113 (96%)	0.22	4 (3%) 45 25	40, 51, 74, 86	0
32	DF	109/113 (96%)	0.16	3 (2%) 55 34	33, 42, 69, 85	0
33	AF	127/130 (97%)	0.04	4 (3%) 51 30	22, 34, 41, 51	0
33	DG	127/130 (97%)	0.06	2 (1%) 70 49	22, 39, 47, 56	0
34	AG	106/107 (99%)	-0.01	0 100 100	28, 32, 49, 54	0
34	DH	106/107 (99%)	-0.01	3 (2%) 55 34	26, 32, 57, 70	0
35	AH	112/121 (92%)	0.58	4 (3%) 46 26	38, 52, 86, 95	0
35	DI	112/121 (92%)	0.53	3 (2%) 56 35	39, 55, 86, 95	0
36	AI	119/120 (99%)	0.12	2 (1%) 69 48	34, 48, 55, 59	0
36	DJ	119/120 (99%)	0.32	3 (2%) 58 37	44, 54, 65, 72	0
37	AJ	99/100 (99%)	0.20	1 (1%) 79 61	39, 48, 71, 84	0
37	DK	99/100 (99%)	0.26	3 (3%) 52 31	46, 56, 72, 85	0
38	AK	87/88 (98%)	0.08	3 (3%) 48 28	25, 30, 47, 66	0
38	DL	87/88 (98%)	0.15	2 (2%) 61 39	26, 33, 58, 86	0
39	AL	77/78 (98%)	0.33	0 100 100	59, 70, 85, 88	0
39	DM	77/78 (98%)	0.38	2 (2%) 57 36	60, 70, 81, 86	0
40	AM	50/51 (98%)	0.24	2 (4%) 42 23	33, 36, 43, 46	0
40	DN	50/51 (98%)	0.09	0 100 100	35, 39, 48, 52	0
41	AN	52/128 (40%)	0.24	1 (1%) 66 45	39, 44, 53, 56	0
41	DO	52/128 (40%)	0.02	2 (3%) 44 25	28, 30, 41, 48	0
42	AO	25/25 (100%)	0.87	2 (8%) 18 10	48, 50, 54, 55	0
42	DP	25/25 (100%)	0.55	0 100 100	34, 39, 46, 49	0
43	AP	105/106 (99%)	0.07	0 100 100	26, 41, 62, 77	0
43	DQ	105/106 (99%)	-0.06	0 100 100	27, 38, 52, 70	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	AQ	91/92 (98%)	-0.12	0 100 100	32, 40, 50, 55	0
44	DR	91/92 (98%)	0.01	0 100 100	30, 40, 51, 60	0
45	i	159/273 (58%)	0.96	22 (13%) 6 4	47, 77, 123, 128	0
45	sM	63/273 (23%)	0.75	3 (4%) 35 19	48, 76, 88, 91	0
46	p0	143/312 (45%)	1.01	19 (13%) 7 4	73, 90, 152, 161	0
47	A	1781/1797 (99%)	0.46	92 (5%) 33 17	47, 77, 163, 229	0
48	B	206/252 (81%)	0.81	15 (7%) 21 11	82, 94, 103, 116	0
48	s0	206/252 (81%)	0.38	8 (3%) 43 24	60, 73, 85, 89	0
49	C	214/255 (83%)	1.17	27 (12%) 8 4	84, 110, 135, 144	0
49	s1	216/255 (84%)	0.39	9 (4%) 40 22	53, 65, 92, 107	0
50	D	217/254 (85%)	0.46	5 (2%) 61 39	61, 74, 88, 95	0
50	s2	217/254 (85%)	0.25	8 (3%) 45 25	46, 57, 68, 77	0
51	E	223/240 (92%)	0.40	5 (2%) 62 41	67, 79, 105, 113	0
51	s3	223/240 (92%)	0.61	8 (3%) 46 26	62, 85, 103, 108	0
52	F	260/261 (99%)	0.46	5 (1%) 66 45	58, 74, 83, 101	0
52	s4	260/261 (99%)	0.24	2 (0%) 82 65	42, 60, 73, 100	0
53	G	206/225 (91%)	0.98	18 (8%) 16 9	85, 101, 112, 120	0
53	s5	206/225 (91%)	0.65	10 (4%) 35 18	64, 82, 97, 101	0
54	H	226/236 (95%)	0.79	20 (8%) 15 9	57, 86, 105, 114	0
54	s6	218/236 (92%)	0.37	6 (2%) 55 34	43, 68, 84, 99	0
55	I	184/190 (96%)	0.78	12 (6%) 25 13	73, 99, 127, 132	0
55	s7	186/190 (97%)	0.65	9 (4%) 35 19	54, 85, 117, 126	0
56	J	188/200 (94%)	0.56	9 (4%) 35 19	50, 61, 94, 105	0
56	s8	188/200 (94%)	0.48	6 (3%) 50 30	39, 57, 96, 108	0
57	K	185/197 (93%)	0.92	16 (8%) 16 9	68, 83, 118, 149	0
57	s9	185/197 (93%)	0.46	12 (6%) 25 13	54, 65, 89, 113	0
58	L	96/105 (91%)	0.89	8 (8%) 17 9	72, 91, 115, 130	0
58	c0	96/105 (91%)	1.29	17 (17%) 4 2	82, 110, 128, 145	0
59	M	155/156 (99%)	0.71	16 (10%) 12 6	51, 59, 92, 101	0
59	c1	146/156 (93%)	0.43	8 (5%) 30 16	39, 52, 76, 97	0
60	N	124/143 (86%)	1.30	19 (15%) 5 3	114, 126, 146, 155	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	c2	124/143 (86%)	1.82	43 (34%) 1 0	148, 162, 179, 183	0
61	O	150/151 (99%)	0.53	2 (1%) 75 56	58, 73, 84, 88	0
61	c3	150/151 (99%)	0.23	0 100 100	45, 57, 70, 83	0
62	P	127/138 (92%)	1.19	18 (14%) 6 3	59, 112, 126, 127	0
62	c4	128/138 (92%)	0.38	3 (2%) 61 39	38, 69, 76, 78	0
63	Q	124/142 (87%)	0.78	12 (9%) 13 7	67, 80, 105, 127	0
63	c5	135/142 (95%)	0.93	16 (11%) 9 5	68, 80, 99, 109	0
64	R	141/143 (98%)	1.10	20 (14%) 6 3	72, 94, 99, 101	0
64	c6	142/143 (99%)	0.92	16 (11%) 10 5	58, 76, 88, 102	0
65	S	120/136 (88%)	1.11	18 (15%) 5 3	81, 94, 112, 114	0
65	c7	117/136 (86%)	0.60	3 (2%) 57 36	66, 77, 95, 101	0
66	T	145/146 (99%)	0.76	7 (4%) 35 19	66, 89, 111, 118	0
66	c8	145/146 (99%)	0.54	4 (2%) 55 34	60, 74, 95, 104	0
67	U	143/144 (99%)	1.02	12 (8%) 17 9	76, 90, 103, 110	0
67	c9	143/144 (99%)	0.42	1 (0%) 84 68	60, 70, 86, 94	0
68	V	107/121 (88%)	1.06	16 (14%) 5 3	64, 96, 118, 123	0
68	d0	110/121 (90%)	0.89	8 (7%) 21 11	61, 89, 122, 132	0
69	W	87/87 (100%)	0.40	2 (2%) 61 39	77, 82, 95, 102	0
69	d1	87/87 (100%)	0.09	0 100 100	55, 62, 79, 85	0
70	X	129/130 (99%)	0.52	3 (2%) 61 39	59, 69, 76, 86	0
70	d2	129/130 (99%)	0.28	0 100 100	43, 52, 58, 66	0
71	Y	144/145 (99%)	0.48	4 (2%) 55 34	50, 55, 63, 70	0
71	d3	144/145 (99%)	0.15	2 (1%) 73 53	38, 42, 53, 59	0
72	Z	134/135 (99%)	0.60	4 (2%) 52 31	64, 85, 97, 104	0
72	d4	134/135 (99%)	0.39	4 (2%) 52 31	49, 67, 78, 96	0
73	a	70/108 (64%)	1.18	14 (20%) 3 1	97, 109, 116, 118	0
73	d5	69/108 (63%)	0.88	7 (10%) 12 6	75, 92, 101, 103	0
74	b	97/119 (81%)	0.97	9 (9%) 14 8	61, 75, 126, 131	0
74	d6	97/119 (81%)	0.45	3 (3%) 51 30	43, 52, 78, 85	0
75	c	81/82 (98%)	0.85	5 (6%) 26 14	72, 84, 112, 115	0
75	d7	81/82 (98%)	0.55	2 (2%) 58 37	53, 67, 97, 99	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
76	d	63/67 (94%)	1.00	7 (11%) 10 5	95, 110, 118, 122	0
76	d8	63/67 (94%)	0.73	2 (3%) 50 30	79, 91, 100, 107	0
77	d9	53/56 (94%)	1.02	9 (16%) 4 2	61, 69, 100, 105	0
77	e	53/56 (94%)	0.83	9 (16%) 4 2	66, 70, 85, 89	0
78	e0	62/63 (98%)	0.54	3 (4%) 35 19	44, 66, 84, 91	0
78	f	60/63 (95%)	0.72	7 (11%) 9 5	53, 83, 111, 113	0
79	e1	51/152 (33%)	1.58	13 (25%) 1 1	128, 142, 157, 160	0
79	g	71/152 (46%)	1.64	25 (35%) 1 0	87, 107, 119, 121	0
80	Rb	318/319 (99%)	0.93	14 (4%) 39 21	83, 95, 103, 111	0
80	h	318/319 (99%)	0.68	13 (4%) 41 23	88, 100, 113, 125	0
81	sR	1783/1800 (99%)	0.29	80 (4%) 38 20	33, 64, 134, 203	0
All	All	33026/35567 (92%)	0.27	1358 (4%) 41 23	20, 55, 110, 229	0

The worst 5 of 1358 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	CR	179	GLN	8.1
18	CR	176	ILE	8.0
18	CR	182	ILE	7.7
79	g	87	THR	6.6
38	DL	88	ALA	6.6

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

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

5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	sR	2188	1/1	-0.48	0.61	120,120,120,120	0
83	MG	1	4146	1/1	-0.33	0.39	174,174,174,174	0
83	MG	sR	2073	1/1	-0.05	0.42	96,96,96,96	0
83	MG	A	1996	1/1	0.05	0.48	101,101,101,101	0
83	MG	A	2057	1/1	0.07	0.38	109,109,109,109	0
83	MG	1	4094	1/1	0.16	0.42	104,104,104,104	0
83	MG	1	4180	1/1	0.34	0.45	52,52,52,52	0
83	MG	A	2061	1/1	0.35	0.49	77,77,77,77	0
83	MG	AR	3804	1/1	0.41	0.47	88,88,88,88	0
83	MG	A	2010	1/1	0.42	0.59	102,102,102,102	0
83	MG	A	2018	1/1	0.42	0.51	80,80,80,80	0
83	MG	A	2002	1/1	0.43	0.46	94,94,94,94	0
83	MG	A	2021	1/1	0.43	0.45	86,86,86,86	0
83	MG	AR	4139	1/1	0.46	0.25	127,127,127,127	0
83	MG	AR	4112	1/1	0.49	0.40	73,73,73,73	0
83	MG	A	2046	1/1	0.50	0.34	96,96,96,96	0
83	MG	sR	2111	1/1	0.51	0.33	78,78,78,78	0
83	MG	1	4158	1/1	0.53	0.51	91,91,91,91	0
83	MG	sR	2058	1/1	0.54	0.39	90,90,90,90	0
83	MG	e	103	1/1	0.54	0.42	81,81,81,81	0
83	MG	t	202	1/1	0.57	0.41	76,76,76,76	0
83	MG	A	2037	1/1	0.59	0.28	64,64,64,64	0
83	MG	AR	4051	1/1	0.59	0.27	46,46,46,46	0
83	MG	sR	2148	1/1	0.59	0.22	62,62,62,62	0
83	MG	1	3828	1/1	0.59	0.31	39,39,39,39	0
83	MG	sR	2194	1/1	0.59	0.45	83,83,83,83	0
83	MG	sR	2191	1/1	0.60	0.37	75,75,75,75	0
83	MG	A	2009	1/1	0.61	0.27	79,79,79,79	0
83	MG	A	1988	1/1	0.61	0.29	77,77,77,77	0
83	MG	AR	4141	1/1	0.61	0.37	82,82,82,82	0
83	MG	DN	101	1/1	0.61	0.19	49,49,49,49	0
83	MG	d5	201	1/1	0.61	0.17	74,74,74,74	0
83	MG	A	2032	1/1	0.62	0.28	81,81,81,81	0
83	MG	sR	2131	1/1	0.62	0.32	73,73,73,73	0
83	MG	sR	2133	1/1	0.62	0.19	65,65,65,65	0
83	MG	A	1957	1/1	0.62	0.48	63,63,63,63	0
83	MG	3	221	1/1	0.63	0.44	74,74,74,74	0
83	MG	sR	2159	1/1	0.63	0.41	95,95,95,95	0
83	MG	CR	203	1/1	0.63	0.48	93,93,93,93	0
83	MG	AR	3768	1/1	0.64	0.41	76,76,76,76	0
83	MG	A	2012	1/1	0.64	0.36	83,83,83,83	0
83	MG	A	2001	1/1	0.64	0.49	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	A	1970	1/1	0.65	0.51	77,77,77,77	0
83	MG	d9	103	1/1	0.65	0.51	94,94,94,94	0
83	MG	A	1956	1/1	0.66	0.40	59,59,59,59	0
83	MG	AR	4222	1/1	0.66	0.26	30,30,30,30	0
83	MG	sR	2116	1/1	0.67	0.39	66,66,66,66	0
83	MG	A	1968	1/1	0.67	0.36	82,82,82,82	0
83	MG	CG	306	1/1	0.67	0.18	52,52,52,52	0
83	MG	A	2058	1/1	0.67	0.35	76,76,76,76	0
83	MG	AR	4113	1/1	0.67	0.32	61,61,61,61	0
83	MG	A	1994	1/1	0.67	0.39	86,86,86,86	0
83	MG	1	4100	1/1	0.67	0.33	56,56,56,56	0
83	MG	sR	2063	1/1	0.67	0.37	64,64,64,64	0
83	MG	AR	4060	1/1	0.67	0.27	66,66,66,66	0
83	MG	AR	3830	1/1	0.67	0.33	48,48,48,48	0
83	MG	1	3931	1/1	0.68	0.41	68,68,68,68	0
83	MG	A	2007	1/1	0.68	0.32	87,87,87,87	0
83	MG	A	2030	1/1	0.68	0.38	90,90,90,90	0
83	MG	AR	4124	1/1	0.68	0.31	70,70,70,70	0
83	MG	sR	2174	1/1	0.68	0.45	81,81,81,81	0
83	MG	1	4080	1/1	0.68	0.14	38,38,38,38	0
83	MG	AR	4039	1/1	0.68	0.36	73,73,73,73	0
83	MG	sR	2087	1/1	0.68	0.48	62,62,62,62	0
83	MG	d4	203	1/1	0.68	0.23	66,66,66,66	0
83	MG	A	2052	1/1	0.68	0.32	66,66,66,66	0
83	MG	A	2015	1/1	0.68	0.40	75,75,75,75	0
83	MG	A	1986	1/1	0.69	0.23	58,58,58,58	0
83	MG	AR	3807	1/1	0.69	0.24	95,95,95,95	0
83	MG	c9	201	1/1	0.69	0.29	65,65,65,65	0
83	MG	c6	201	1/1	0.70	0.26	76,76,76,76	0
83	MG	sR	2056	1/1	0.70	0.36	61,61,61,61	0
83	MG	A	2023	1/1	0.70	0.40	62,62,62,62	0
83	MG	sR	2060	1/1	0.70	0.34	69,69,69,69	0
83	MG	1	3916	1/1	0.70	0.38	59,59,59,59	0
83	MG	1	3730	1/1	0.71	0.44	78,78,78,78	0
83	MG	sR	2112	1/1	0.71	0.30	50,50,50,50	0
83	MG	1	3974	1/1	0.71	0.30	62,62,62,62	0
83	MG	AR	4135	1/1	0.71	0.12	25,25,25,25	0
83	MG	A	2004	1/1	0.72	0.38	51,51,51,51	0
83	MG	1	3819	1/1	0.72	0.30	69,69,69,69	0
83	MG	AR	4109	1/1	0.72	0.11	74,74,74,74	0
83	MG	A	1972	1/1	0.72	0.27	59,59,59,59	0
83	MG	sR	2106	1/1	0.73	0.40	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	1	3709	7/7	0.73	0.24	127,127,127,127	0
83	MG	1	3959	1/1	0.73	0.28	61,61,61,61	0
83	MG	A	1976	1/1	0.73	0.41	67,67,67,67	0
83	MG	1	3973	1/1	0.73	0.41	78,78,78,78	0
83	MG	A	2006	1/1	0.73	0.11	108,108,108,108	0
83	MG	sR	2145	1/1	0.73	0.36	89,89,89,89	0
83	MG	AM	101	1/1	0.73	0.16	49,49,49,49	0
83	MG	1	4177	1/1	0.73	0.32	66,66,66,66	0
83	MG	1	4088	1/1	0.74	0.31	86,86,86,86	0
83	MG	sR	2051	1/1	0.74	0.31	46,46,46,46	0
83	MG	1	3833	1/1	0.74	0.32	28,28,28,28	0
83	MG	1	3860	1/1	0.74	0.40	46,46,46,46	0
83	MG	sR	2166	1/1	0.74	0.14	56,56,56,56	0
83	MG	1	4105	1/1	0.74	0.22	48,48,48,48	0
82	OHX	AR	3662	7/7	0.74	0.25	137,137,137,137	0
83	MG	AR	3757	1/1	0.74	0.24	58,58,58,58	0
83	MG	AR	4247	1/1	0.74	0.22	39,39,39,39	0
83	MG	sR	2196	1/1	0.74	0.36	62,62,62,62	0
83	MG	AT	227	1/1	0.74	0.26	51,51,51,51	0
83	MG	A	2011	1/1	0.74	0.33	72,72,72,72	0
83	MG	AR	3758	1/1	0.74	0.36	76,76,76,76	0
83	MG	1	3767	1/1	0.74	0.24	62,62,62,62	0
83	MG	D	301	1/1	0.74	0.39	66,66,66,66	0
83	MG	A	2014	1/1	0.75	0.34	67,67,67,67	0
83	MG	A	1949	1/1	0.75	0.42	53,53,53,53	0
83	MG	sR	2127	1/1	0.75	0.26	50,50,50,50	0
83	MG	AR	4229	1/1	0.75	0.46	44,44,44,44	0
83	MG	AR	3946	1/1	0.75	0.17	44,44,44,44	0
83	MG	sR	2100	1/1	0.75	0.34	61,61,61,61	0
83	MG	1	3978	1/1	0.75	0.28	28,28,28,28	0
83	MG	sR	2109	1/1	0.75	0.45	71,71,71,71	0
83	MG	sR	2165	1/1	0.75	0.22	85,85,85,85	0
83	MG	A	1946	1/1	0.75	0.45	70,70,70,70	0
83	MG	AR	4202	1/1	0.76	0.33	72,72,72,72	0
83	MG	1	4116	1/1	0.76	0.27	40,40,40,40	0
83	MG	A	2029	1/1	0.76	0.26	59,59,59,59	0
83	MG	1	4040	1/1	0.76	0.34	79,79,79,79	0
83	MG	AR	4006	1/1	0.76	0.21	76,76,76,76	0
83	MG	sR	2114	1/1	0.76	0.31	71,71,71,71	0
83	MG	AR	4016	1/1	0.76	0.33	51,51,51,51	0
83	MG	A	2043	1/1	0.76	0.38	63,63,63,63	0
83	MG	1	3744	1/1	0.76	0.34	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
83	MG	A	2048	1/1	0.76	0.29	60,60,60,60	0
82	OHX	1	3691	7/7	0.76	0.17	154,154,154,154	0
83	MG	AR	3742	1/1	0.76	0.11	34,34,34,34	0
83	MG	sR	2155	1/1	0.76	0.13	44,44,44,44	0
83	MG	sR	2115	1/1	0.77	0.25	67,67,67,67	0
83	MG	1	3728	1/1	0.77	0.34	57,57,57,57	0
83	MG	A	1980	1/1	0.77	0.42	55,55,55,55	0
83	MG	A	2063	1/1	0.77	0.55	76,76,76,76	0
82	OHX	AR	3731	7/7	0.77	0.24	135,135,135,135	0
83	MG	AR	4025	1/1	0.77	0.12	37,37,37,37	0
83	MG	A	1991	1/1	0.77	0.36	80,80,80,80	0
83	MG	1	4210	1/1	0.77	0.42	58,58,58,58	0
83	MG	A	2025	1/1	0.77	0.40	75,75,75,75	0
83	MG	1	3887	1/1	0.77	0.33	42,42,42,42	0
83	MG	AR	4148	1/1	0.77	0.23	54,54,54,54	0
83	MG	A	1950	1/1	0.77	0.32	65,65,65,65	0
83	MG	sR	2081	1/1	0.77	0.41	63,63,63,63	0
83	MG	A	2033	1/1	0.77	0.47	53,53,53,53	0
83	MG	AR	4168	1/1	0.77	0.17	56,56,56,56	0
83	MG	AR	4057	1/1	0.77	0.21	25,25,25,25	0
83	MG	sR	2108	1/1	0.77	0.36	40,40,40,40	0
83	MG	A	1966	1/1	0.77	0.52	75,75,75,75	0
83	MG	AR	3905	1/1	0.77	0.36	25,25,25,25	0
83	MG	4	230	1/1	0.77	0.09	37,37,37,37	0
83	MG	AR	3981	1/1	0.77	0.23	80,80,80,80	0
83	MG	AR	4149	1/1	0.78	0.09	37,37,37,37	0
83	MG	1	3852	1/1	0.78	0.29	43,43,43,43	0
83	MG	AR	3888	1/1	0.78	0.34	25,25,25,25	0
83	MG	AR	3893	1/1	0.78	0.23	30,30,30,30	0
83	MG	sR	2069	1/1	0.78	0.36	55,55,55,55	0
82	OHX	z	201	7/7	0.78	0.19	123,123,123,123	0
83	MG	AR	3927	1/1	0.78	0.32	35,35,35,35	0
83	MG	AS	225	1/1	0.78	0.11	45,45,45,45	0
82	OHX	CM	201	7/7	0.78	0.20	120,120,120,120	0
83	MG	sR	2176	1/1	0.78	0.27	63,63,63,63	0
83	MG	sR	2179	1/1	0.78	0.33	51,51,51,51	0
82	OHX	CO	201	7/7	0.78	0.18	148,148,148,148	0
83	MG	A	1984	1/1	0.78	0.34	66,66,66,66	0
83	MG	A	1985	1/1	0.78	0.28	63,63,63,63	0
83	MG	A	2059	1/1	0.78	0.43	69,69,69,69	0
82	OHX	A	1919	7/7	0.78	0.22	117,117,117,117	0
83	MG	1	3939	1/1	0.78	0.14	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	s1	301	7/7	0.78	0.25	126,126,126,126	0
83	MG	A	1992	1/1	0.78	0.20	52,52,52,52	0
82	OHX	AR	3682	7/7	0.78	0.24	121,121,121,121	0
83	MG	A	2066	1/1	0.79	0.36	58,58,58,58	0
83	MG	sR	2119	1/1	0.79	0.25	63,63,63,63	0
83	MG	1	4098	1/1	0.79	0.09	39,39,39,39	0
82	OHX	A	1937	7/7	0.79	0.20	130,130,130,130	0
83	MG	1	4021	1/1	0.79	0.36	62,62,62,62	0
83	MG	AR	3951	1/1	0.79	0.21	70,70,70,70	0
83	MG	1	3888	1/1	0.79	0.20	39,39,39,39	0
83	MG	AR	3987	1/1	0.79	0.12	35,35,35,35	0
83	MG	A	1955	1/1	0.79	0.51	71,71,71,71	0
83	MG	1	4044	1/1	0.79	0.15	62,62,62,62	0
83	MG	1	4062	1/1	0.79	0.16	71,71,71,71	0
83	MG	A	1961	1/1	0.79	0.35	61,61,61,61	0
83	MG	sR	2082	1/1	0.79	0.25	70,70,70,70	0
83	MG	A	1964	1/1	0.79	0.44	60,60,60,60	0
83	MG	sR	2180	1/1	0.79	0.31	59,59,59,59	0
83	MG	sR	2088	1/1	0.79	0.47	82,82,82,82	0
83	MG	1	4065	1/1	0.79	0.29	53,53,53,53	0
83	MG	A	2051	1/1	0.79	0.44	50,50,50,50	0
83	MG	1	3972	1/1	0.79	0.25	56,56,56,56	0
83	MG	sR	2199	1/1	0.79	0.45	65,65,65,65	0
82	OHX	A	1939	7/7	0.79	0.17	138,138,138,138	0
83	MG	3	210	1/1	0.79	0.31	60,60,60,60	0
82	OHX	AR	3713	7/7	0.79	0.23	121,121,121,121	0
83	MG	AR	4105	1/1	0.79	0.31	62,62,62,62	0
83	MG	4	218	1/1	0.79	0.36	55,55,55,55	0
85	ZN	c	101	1/1	0.79	0.13	119,119,119,119	0
83	MG	sR	2130	1/1	0.80	0.16	68,68,68,68	0
83	MG	sR	2053	1/1	0.80	0.32	66,66,66,66	0
83	MG	sR	2132	1/1	0.80	0.12	38,38,38,38	0
83	MG	1	4081	1/1	0.80	0.32	49,49,49,49	0
83	MG	AR	3743	1/1	0.80	0.23	29,29,29,29	0
83	MG	A	1952	1/1	0.80	0.48	53,53,53,53	0
83	MG	1	3905	1/1	0.80	0.24	39,39,39,39	0
82	OHX	AR	3721	7/7	0.80	0.25	118,118,118,118	0
83	MG	AR	4095	1/1	0.80	0.20	37,37,37,37	0
83	MG	A	1958	1/1	0.80	0.37	47,47,47,47	0
83	MG	A	1959	1/1	0.80	0.39	55,55,55,55	0
82	OHX	sR	2045	7/7	0.80	0.18	139,139,139,139	0
83	MG	AR	3953	1/1	0.80	0.15	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	sR	2099	1/1	0.80	0.40	63,63,63,63	0
83	MG	AR	4250	1/1	0.80	0.29	49,49,49,49	0
83	MG	AR	3794	1/1	0.80	0.26	25,25,25,25	0
83	MG	AR	3982	1/1	0.80	0.37	61,61,61,61	0
83	MG	CE	403	1/1	0.80	0.34	21,21,21,21	0
83	MG	A	2060	1/1	0.80	0.43	49,49,49,49	0
83	MG	s8	302	1/1	0.80	0.23	45,45,45,45	0
83	MG	1	4079	1/1	0.80	0.10	47,47,47,47	0
83	MG	CP	504	1/1	0.80	0.25	48,48,48,48	0
83	MG	z	202	1/1	0.80	0.10	50,50,50,50	0
83	MG	6	202	1/1	0.80	0.23	58,58,58,58	0
83	MG	A	2022	1/1	0.80	0.39	53,53,53,53	0
83	MG	1	3934	1/1	0.80	0.13	32,32,32,32	0
83	MG	1	4135	1/1	0.81	0.16	46,46,46,46	0
83	MG	1	4142	1/1	0.81	0.20	55,55,55,55	0
83	MG	1	3927	1/1	0.81	0.30	31,31,31,31	0
83	MG	A	2040	1/1	0.81	0.29	84,84,84,84	0
83	MG	AS	214	1/1	0.81	0.39	55,55,55,55	0
83	MG	AS	218	1/1	0.81	0.16	50,50,50,50	0
83	MG	1	3841	1/1	0.81	0.39	33,33,33,33	0
83	MG	AT	221	1/1	0.81	0.15	32,32,32,32	0
83	MG	A	1990	1/1	0.81	0.36	56,56,56,56	0
83	MG	1	3756	1/1	0.81	0.37	38,38,38,38	0
83	MG	AT	230	1/1	0.81	0.44	61,61,61,61	0
83	MG	AR	4075	1/1	0.81	0.28	50,50,50,50	0
83	MG	AR	4078	1/1	0.81	0.36	34,34,34,34	0
83	MG	A	1997	1/1	0.81	0.26	88,88,88,88	0
83	MG	1	3854	1/1	0.81	0.36	54,54,54,54	0
83	MG	1	3940	1/1	0.81	0.23	52,52,52,52	0
83	MG	A	2069	1/1	0.81	0.40	58,58,58,58	0
83	MG	1	3957	1/1	0.81	0.17	54,54,54,54	0
83	MG	sM	301	1/1	0.81	0.19	37,37,37,37	0
82	OHX	AR	3711	7/7	0.81	0.18	133,133,133,133	0
83	MG	1	3878	1/1	0.81	0.28	27,27,27,27	0
83	MG	1	4089	1/1	0.81	0.17	38,38,38,38	0
82	OHX	A	1938	7/7	0.81	0.40	106,106,106,106	0
83	MG	1	3823	1/1	0.81	0.27	36,36,36,36	0
82	OHX	AR	3732	7/7	0.81	0.15	181,181,181,181	0
83	MG	sR	2067	1/1	0.81	0.39	61,61,61,61	0
82	OHX	AS	210	7/7	0.81	0.21	112,112,112,112	0
83	MG	1	4106	1/1	0.81	0.16	33,33,33,33	0
83	MG	A	2020	1/1	0.81	0.32	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	4111	1/1	0.81	0.26	58,58,58,58	0
83	MG	AR	4178	1/1	0.81	0.12	46,46,46,46	0
83	MG	AR	4200	1/1	0.81	0.30	70,70,70,70	0
83	MG	1	4022	1/1	0.81	0.34	37,37,37,37	0
83	MG	AR	4217	1/1	0.81	0.28	42,42,42,42	0
83	MG	AR	4020	1/1	0.81	0.24	40,40,40,40	0
83	MG	sR	2146	1/1	0.82	0.23	71,71,71,71	0
83	MG	4	231	1/1	0.82	0.19	35,35,35,35	0
83	MG	A	2062	1/1	0.82	0.51	82,82,82,82	0
83	MG	AR	3939	1/1	0.82	0.30	26,26,26,26	0
83	MG	A	1974	1/1	0.82	0.46	54,54,54,54	0
83	MG	A	2068	1/1	0.82	0.43	67,67,67,67	0
83	MG	AR	4253	1/1	0.82	0.21	38,38,38,38	0
83	MG	A	1979	1/1	0.82	0.41	53,53,53,53	0
83	MG	J	303	1/1	0.82	0.29	51,51,51,51	0
82	OHX	sR	2047	7/7	0.82	0.18	127,127,127,127	0
83	MG	AR	4056	1/1	0.82	0.15	82,82,82,82	0
83	MG	1	3966	1/1	0.82	0.24	36,36,36,36	0
83	MG	sR	2055	1/1	0.82	0.32	42,42,42,42	0
83	MG	1	4066	1/1	0.82	0.20	26,26,26,26	0
83	MG	sR	2198	1/1	0.82	0.38	60,60,60,60	0
82	OHX	AR	3724	7/7	0.82	0.25	115,115,115,115	0
83	MG	AP	503	1/1	0.82	0.19	52,52,52,52	0
83	MG	AR	3842	1/1	0.82	0.29	35,35,35,35	0
83	MG	1	4008	1/1	0.82	0.29	72,72,72,72	0
83	MG	4	226	1/1	0.82	0.23	42,42,42,42	0
83	MG	AR	4017	1/1	0.82	0.24	61,61,61,61	0
83	MG	sR	2141	1/1	0.82	0.12	37,37,37,37	0
83	MG	1	4179	1/1	0.82	0.31	34,34,34,34	0
86	GOL	AR	4263	6/6	0.82	0.28	40,40,40,40	0
82	OHX	1	3720	7/7	0.83	0.24	112,112,112,112	0
83	MG	1	3735	1/1	0.83	0.30	39,39,39,39	0
83	MG	AR	3809	1/1	0.83	0.22	37,37,37,37	0
83	MG	1	3742	1/1	0.83	0.29	37,37,37,37	0
82	OHX	1	3700	7/7	0.83	0.22	111,111,111,111	0
83	MG	AR	3859	1/1	0.83	0.28	34,34,34,34	0
83	MG	AR	4071	1/1	0.83	0.28	28,28,28,28	0
83	MG	A	1973	1/1	0.83	0.46	67,67,67,67	0
83	MG	1	3958	1/1	0.83	0.28	51,51,51,51	0
83	MG	1	4119	1/1	0.83	0.14	44,44,44,44	0
83	MG	4	233	1/1	0.83	0.24	52,52,52,52	0
83	MG	1	3745	1/1	0.83	0.34	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3752	1/1	0.83	0.22	31,31,31,31	0
82	OHX	sR	2021	7/7	0.83	0.18	137,137,137,137	0
83	MG	A	2036	1/1	0.83	0.23	48,48,48,48	0
83	MG	AR	3949	1/1	0.83	0.22	40,40,40,40	0
82	OHX	1	3698	7/7	0.83	0.17	131,131,131,131	0
83	MG	1	3789	1/1	0.83	0.22	40,40,40,40	0
83	MG	DI	201	1/1	0.83	0.31	53,53,53,53	0
83	MG	sR	2094	1/1	0.83	0.43	59,59,59,59	0
83	MG	AR	3969	1/1	0.83	0.22	50,50,50,50	0
82	OHX	1	3716	7/7	0.83	0.21	112,112,112,112	0
83	MG	A	1943	1/1	0.83	0.51	72,72,72,72	0
83	MG	AR	4146	1/1	0.83	0.14	69,69,69,69	0
82	OHX	A	1930	7/7	0.83	0.13	193,193,193,193	0
83	MG	AR	3752	1/1	0.83	0.26	50,50,50,50	0
83	MG	1	4202	1/1	0.83	0.24	43,43,43,43	0
83	MG	1	4204	1/1	0.83	0.25	54,54,54,54	0
83	MG	AR	4189	1/1	0.83	0.28	53,53,53,53	0
82	OHX	1	3717	7/7	0.83	0.22	117,117,117,117	0
83	MG	1	4217	1/1	0.83	0.22	50,50,50,50	0
83	MG	1	4047	1/1	0.84	0.23	46,46,46,46	0
83	MG	DE	201	1/1	0.84	0.14	55,55,55,55	0
83	MG	sR	2079	1/1	0.84	0.43	63,63,63,63	0
82	OHX	A	1935	7/7	0.84	0.19	122,122,122,122	0
83	MG	1	3932	1/1	0.84	0.43	52,52,52,52	0
83	MG	AR	3836	1/1	0.84	0.19	38,38,38,38	0
83	MG	1	3826	1/1	0.84	0.31	64,64,64,64	0
83	MG	1	3936	1/1	0.84	0.30	45,45,45,45	0
82	OHX	sR	2032	7/7	0.84	0.19	118,118,118,118	0
82	OHX	sR	2034	7/7	0.84	0.28	110,110,110,110	0
83	MG	A	1951	1/1	0.84	0.30	65,65,65,65	0
83	MG	1	3944	1/1	0.84	0.30	52,52,52,52	0
83	MG	A	1954	1/1	0.84	0.32	62,62,62,62	0
83	MG	AR	3923	1/1	0.84	0.31	31,31,31,31	0
83	MG	AR	4140	1/1	0.84	0.08	27,27,27,27	0
83	MG	1	3741	1/1	0.84	0.19	25,25,25,25	0
82	OHX	sR	2036	7/7	0.84	0.24	118,118,118,118	0
82	OHX	sR	2039	7/7	0.84	0.23	118,118,118,118	0
83	MG	1	3960	1/1	0.84	0.14	38,38,38,38	0
83	MG	AR	4151	1/1	0.84	0.11	60,60,60,60	0
83	MG	sR	2128	1/1	0.84	0.35	58,58,58,58	0
83	MG	4	236	1/1	0.84	0.28	42,42,42,42	0
83	MG	A	2041	1/1	0.84	0.20	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	sR	2040	7/7	0.84	0.22	111,111,111,111	0
83	MG	AR	3964	1/1	0.84	0.43	79,79,79,79	0
83	MG	A	1971	1/1	0.84	0.44	61,61,61,61	0
82	OHX	sR	2044	7/7	0.84	0.19	126,126,126,126	0
83	MG	1	3881	1/1	0.84	0.06	41,41,41,41	0
83	MG	AH	201	1/1	0.84	0.30	49,49,49,49	0
82	OHX	1	3708	7/7	0.84	0.23	110,110,110,110	0
83	MG	AR	3988	1/1	0.84	0.22	37,37,37,37	0
83	MG	AR	4002	1/1	0.84	0.13	61,61,61,61	0
83	MG	A	1982	1/1	0.84	0.28	57,57,57,57	0
83	MG	A	1983	1/1	0.84	0.32	57,57,57,57	0
82	OHX	AR	3700	7/7	0.84	0.33	106,106,106,106	0
83	MG	1	3991	1/1	0.84	0.18	65,65,65,65	0
82	OHX	sR	2048	7/7	0.84	0.24	112,112,112,112	0
83	MG	1	4143	1/1	0.84	0.22	23,23,23,23	0
83	MG	A	2070	1/1	0.84	0.21	76,76,76,76	0
83	MG	1	3908	1/1	0.84	0.23	35,35,35,35	0
83	MG	H	301	1/1	0.84	0.30	82,82,82,82	0
83	MG	1	3911	1/1	0.84	0.37	29,29,29,29	0
83	MG	AR	3761	1/1	0.84	0.24	47,47,47,47	0
83	MG	sR	2201	1/1	0.84	0.13	62,62,62,62	0
83	MG	1	4175	1/1	0.84	0.12	22,22,22,22	0
83	MG	1	3816	1/1	0.84	0.30	53,53,53,53	0
83	MG	CF	403	1/1	0.84	0.14	38,38,38,38	0
83	MG	AR	3802	1/1	0.84	0.19	31,31,31,31	0
83	MG	CJ	301	1/1	0.84	0.32	68,68,68,68	0
82	OHX	AR	3720	7/7	0.84	0.16	137,137,137,137	0
83	MG	A	2005	1/1	0.84	0.44	65,65,65,65	0
83	MG	CQ	203	1/1	0.84	0.17	27,27,27,27	0
83	MG	AR	3952	1/1	0.85	0.19	40,40,40,40	0
83	MG	AB	201	1/1	0.85	0.12	20,20,20,20	0
83	MG	1	3737	1/1	0.85	0.29	35,35,35,35	0
83	MG	sR	2089	1/1	0.85	0.28	41,41,41,41	0
82	OHX	A	1871	7/7	0.85	0.19	116,116,116,116	0
83	MG	sR	2098	1/1	0.85	0.31	38,38,38,38	0
82	OHX	sR	2038	7/7	0.85	0.20	125,125,125,125	0
83	MG	1	4023	1/1	0.85	0.22	82,82,82,82	0
82	OHX	4	212	7/7	0.85	0.19	112,112,112,112	0
83	MG	1	4163	1/1	0.85	0.12	44,44,44,44	0
83	MG	1	4171	1/1	0.85	0.18	23,23,23,23	0
83	MG	1	4173	1/1	0.85	0.12	27,27,27,27	0
82	OHX	A	1921	7/7	0.85	0.16	140,140,140,140	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3751	1/1	0.85	0.12	50,50,50,50	0
83	MG	1	3945	1/1	0.85	0.19	55,55,55,55	0
83	MG	AR	3797	1/1	0.85	0.32	23,23,23,23	0
83	MG	sR	2117	1/1	0.85	0.15	49,49,49,49	0
83	MG	AR	4028	1/1	0.85	0.09	29,29,29,29	0
83	MG	A	1981	1/1	0.85	0.35	61,61,61,61	0
83	MG	1	3949	1/1	0.85	0.39	63,63,63,63	0
83	MG	AT	225	1/1	0.85	0.12	50,50,50,50	0
83	MG	A	2053	1/1	0.85	0.49	46,46,46,46	0
83	MG	1	3950	1/1	0.85	0.23	31,31,31,31	0
83	MG	1	3952	1/1	0.85	0.19	65,65,65,65	0
83	MG	sR	2135	1/1	0.85	0.27	70,70,70,70	0
83	MG	sR	2137	1/1	0.85	0.34	66,66,66,66	0
82	OHX	sR	2042	7/7	0.85	0.23	118,118,118,118	0
83	MG	AR	4059	1/1	0.85	0.13	33,33,33,33	0
83	MG	AR	3810	1/1	0.85	0.10	28,28,28,28	0
83	MG	1	3884	1/1	0.85	0.32	33,33,33,33	0
82	OHX	1	3695	7/7	0.85	0.20	120,120,120,120	0
83	MG	AR	4076	1/1	0.85	0.19	51,51,51,51	0
83	MG	A	1995	1/1	0.85	0.19	81,81,81,81	0
83	MG	3	217	1/1	0.85	0.31	53,53,53,53	0
83	MG	AR	3848	1/1	0.85	0.30	36,36,36,36	0
83	MG	A	1998	1/1	0.85	0.23	58,58,58,58	0
82	OHX	1	3696	7/7	0.85	0.22	138,138,138,138	0
83	MG	DL	102	1/1	0.85	0.31	27,27,27,27	0
83	MG	sR	2183	1/1	0.85	0.35	34,34,34,34	0
82	OHX	AR	3730	7/7	0.85	0.23	109,109,109,109	0
83	MG	1	4095	1/1	0.85	0.14	38,38,38,38	0
83	MG	sR	2193	1/1	0.85	0.33	37,37,37,37	0
82	OHX	AR	3678	7/7	0.85	0.21	111,111,111,111	0
83	MG	AR	3912	1/1	0.85	0.45	38,38,38,38	0
83	MG	A	2008	1/1	0.85	0.31	54,54,54,54	0
83	MG	AR	3916	1/1	0.85	0.35	37,37,37,37	0
82	OHX	1	3714	7/7	0.85	0.18	112,112,112,112	0
82	OHX	1	3671	7/7	0.85	0.22	115,115,115,115	0
83	MG	sR	2065	1/1	0.85	0.48	64,64,64,64	0
82	OHX	1	3656	7/7	0.85	0.19	114,114,114,114	0
83	MG	1	3988	1/1	0.85	0.45	63,63,63,63	0
83	MG	sR	2070	1/1	0.85	0.33	38,38,38,38	0
82	OHX	1	3702	7/7	0.85	0.13	162,162,162,162	0
83	MG	1	4004	1/1	0.85	0.09	33,33,33,33	0
83	MG	A	2019	1/1	0.85	0.29	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	sR	2072	1/1	0.86	0.31	61,61,61,61	0
83	MG	AR	4029	1/1	0.86	0.15	52,52,52,52	0
83	MG	sR	2078	1/1	0.86	0.28	48,48,48,48	0
83	MG	CP	502	1/1	0.86	0.25	40,40,40,40	0
83	MG	1	4169	1/1	0.86	0.10	34,34,34,34	0
83	MG	AR	4046	1/1	0.86	0.12	43,43,43,43	0
82	OHX	A	1932	7/7	0.86	0.10	215,215,215,215	0
83	MG	1	4032	1/1	0.86	0.29	63,63,63,63	0
83	MG	1	3731	1/1	0.86	0.21	33,33,33,33	0
82	OHX	A	1933	7/7	0.86	0.22	117,117,117,117	0
82	OHX	1	3687	7/7	0.86	0.19	116,116,116,116	0
83	MG	1	4060	1/1	0.86	0.26	30,30,30,30	0
83	MG	1	4195	1/1	0.86	0.32	42,42,42,42	0
83	MG	AR	3817	1/1	0.86	0.31	51,51,51,51	0
82	OHX	1	3660	7/7	0.86	0.19	117,117,117,117	0
82	OHX	AR	3716	7/7	0.86	0.19	120,120,120,120	0
82	OHX	sR	2041	7/7	0.86	0.38	92,92,92,92	0
82	OHX	1	3686	7/7	0.86	0.18	121,121,121,121	0
83	MG	A	1953	1/1	0.86	0.44	53,53,53,53	0
83	MG	1	3864	1/1	0.86	0.25	50,50,50,50	0
83	MG	AR	3865	1/1	0.86	0.23	43,43,43,43	0
83	MG	AR	3879	1/1	0.86	0.34	33,33,33,33	0
83	MG	AR	4127	1/1	0.86	0.13	37,37,37,37	0
83	MG	AR	3881	1/1	0.86	0.35	57,57,57,57	0
83	MG	1	3953	1/1	0.86	0.10	39,39,39,39	0
83	MG	AR	3889	1/1	0.86	0.19	38,38,38,38	0
83	MG	A	1962	1/1	0.86	0.18	58,58,58,58	0
83	MG	1	3871	1/1	0.86	0.16	37,37,37,37	0
83	MG	1	3876	1/1	0.86	0.38	29,29,29,29	0
83	MG	1	4092	1/1	0.86	0.11	30,30,30,30	0
83	MG	sR	2136	1/1	0.86	0.34	63,63,63,63	0
82	OHX	sR	2018	7/7	0.86	0.15	136,136,136,136	0
82	OHX	AS	208	7/7	0.86	0.20	115,115,115,115	0
83	MG	1	3755	1/1	0.86	0.25	37,37,37,37	0
83	MG	AR	3938	1/1	0.86	0.20	39,39,39,39	0
83	MG	AR	4180	1/1	0.86	0.16	36,36,36,36	0
83	MG	4	234	1/1	0.86	0.14	31,31,31,31	0
83	MG	A	1978	1/1	0.86	0.45	51,51,51,51	0
83	MG	AR	4194	1/1	0.86	0.40	52,52,52,52	0
83	MG	1	3967	1/1	0.86	0.34	54,54,54,54	0
83	MG	A	2064	1/1	0.86	0.44	68,68,68,68	0
83	MG	1	4101	1/1	0.86	0.17	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	sR	2024	7/7	0.86	0.19	121,121,121,121	0
83	MG	1	3760	1/1	0.86	0.21	38,38,38,38	0
83	MG	1	3763	1/1	0.86	0.28	26,26,26,26	0
83	MG	A	2071	1/1	0.86	0.28	56,56,56,56	0
83	MG	1	3976	1/1	0.86	0.17	24,24,24,24	0
83	MG	AK	104	1/1	0.86	0.22	47,47,47,47	0
82	OHX	sR	2025	7/7	0.86	0.20	110,110,110,110	0
83	MG	1	3768	1/1	0.86	0.31	55,55,55,55	0
83	MG	AS	217	1/1	0.86	0.17	52,52,52,52	0
83	MG	AR	3739	1/1	0.86	0.20	45,45,45,45	0
83	MG	AS	223	1/1	0.86	0.12	60,60,60,60	0
83	MG	1	4136	1/1	0.86	0.18	41,41,41,41	0
83	MG	1	3915	1/1	0.86	0.41	45,45,45,45	0
83	MG	AR	3744	1/1	0.86	0.17	32,32,32,32	0
83	MG	1	3780	1/1	0.86	0.39	50,50,50,50	0
82	OHX	sR	2027	7/7	0.86	0.21	114,114,114,114	0
82	OHX	AR	3607	7/7	0.86	0.16	124,124,124,124	0
83	MG	AR	3759	1/1	0.86	0.25	29,29,29,29	0
83	MG	1	3729	1/1	0.86	0.40	59,59,59,59	0
82	OHX	AR	3718	7/7	0.87	0.17	134,134,134,134	0
83	MG	4	215	1/1	0.87	0.33	41,41,41,41	0
83	MG	1	3762	1/1	0.87	0.20	39,39,39,39	0
83	MG	AR	4133	1/1	0.87	0.13	59,59,59,59	0
82	OHX	AR	3674	7/7	0.87	0.20	110,110,110,110	0
83	MG	Y	201	1/1	0.87	0.18	50,50,50,50	0
83	MG	AR	4137	1/1	0.87	0.26	51,51,51,51	0
82	OHX	AR	3710	7/7	0.87	0.20	112,112,112,112	0
82	OHX	sR	2002	7/7	0.87	0.30	97,97,97,97	0
83	MG	AR	3891	1/1	0.87	0.27	25,25,25,25	0
82	OHX	sR	2006	7/7	0.87	0.20	121,121,121,121	0
82	OHX	AR	3677	7/7	0.87	0.18	117,117,117,117	0
83	MG	1	3814	1/1	0.87	0.21	42,42,42,42	0
83	MG	1	3992	1/1	0.87	0.13	41,41,41,41	0
83	MG	x	203	1/1	0.87	0.12	27,27,27,27	0
82	OHX	sR	2019	7/7	0.87	0.20	113,113,113,113	0
83	MG	AR	3933	1/1	0.87	0.11	57,57,57,57	0
83	MG	1	4132	1/1	0.87	0.21	27,27,27,27	0
83	MG	AR	4191	1/1	0.87	0.24	44,44,44,44	0
82	OHX	A	1877	7/7	0.87	0.22	118,118,118,118	0
83	MG	A	1987	1/1	0.87	0.28	60,60,60,60	0
83	MG	1	3820	1/1	0.87	0.20	33,33,33,33	0
83	MG	A	1989	1/1	0.87	0.20	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	A	1901	7/7	0.87	0.20	115,115,115,115	0
83	MG	sR	2083	1/1	0.87	0.35	56,56,56,56	0
83	MG	AR	4214	1/1	0.87	0.15	26,26,26,26	0
83	MG	AR	4215	1/1	0.87	0.14	35,35,35,35	0
82	OHX	A	1909	7/7	0.87	0.16	117,117,117,117	0
83	MG	AR	4221	1/1	0.87	0.34	44,44,44,44	0
83	MG	sR	2095	1/1	0.87	0.34	48,48,48,48	0
82	OHX	sR	2026	7/7	0.87	0.23	116,116,116,116	0
82	OHX	A	1912	7/7	0.87	0.18	125,125,125,125	0
83	MG	AR	4233	1/1	0.87	0.26	57,57,57,57	0
83	MG	sR	2105	1/1	0.87	0.50	56,56,56,56	0
83	MG	AR	3954	1/1	0.87	0.18	28,28,28,28	0
83	MG	AR	3961	1/1	0.87	0.27	51,51,51,51	0
83	MG	AR	3741	1/1	0.87	0.39	50,50,50,50	0
82	OHX	AR	3725	7/7	0.87	0.20	111,111,111,111	0
83	MG	AR	3977	1/1	0.87	0.31	32,32,32,32	0
83	MG	1	4167	1/1	0.87	0.24	55,55,55,55	0
83	MG	AS	219	1/1	0.87	0.16	48,48,48,48	0
82	OHX	AR	3729	7/7	0.87	0.17	114,114,114,114	0
83	MG	1	4052	1/1	0.87	0.11	38,38,38,38	0
83	MG	sR	2118	1/1	0.87	0.15	52,52,52,52	0
82	OHX	A	1927	7/7	0.87	0.17	132,132,132,132	0
83	MG	sR	2120	1/1	0.87	0.24	50,50,50,50	0
83	MG	1	3859	1/1	0.87	0.28	35,35,35,35	0
83	MG	A	2013	1/1	0.87	0.37	68,68,68,68	0
82	OHX	sR	2037	7/7	0.87	0.21	114,114,114,114	0
83	MG	AR	4014	1/1	0.87	0.10	27,27,27,27	0
83	MG	1	4178	1/1	0.87	0.28	42,42,42,42	0
83	MG	CE	405	1/1	0.87	0.17	28,28,28,28	0
83	MG	1	3862	1/1	0.87	0.27	32,32,32,32	0
83	MG	AR	3792	1/1	0.87	0.18	29,29,29,29	0
83	MG	1	4067	1/1	0.87	0.33	59,59,59,59	0
83	MG	sR	2138	1/1	0.87	0.12	45,45,45,45	0
83	MG	AR	4027	1/1	0.87	0.19	57,57,57,57	0
82	OHX	AR	3712	7/7	0.87	0.31	104,104,104,104	0
83	MG	A	2027	1/1	0.87	0.23	55,55,55,55	0
83	MG	1	3870	1/1	0.87	0.35	55,55,55,55	0
83	MG	sR	2149	1/1	0.87	0.15	64,64,64,64	0
83	MG	sR	2150	1/1	0.87	0.18	75,75,75,75	0
82	OHX	1	3633	7/7	0.87	0.17	128,128,128,128	0
83	MG	CR	205	1/1	0.87	0.14	28,28,28,28	0
83	MG	sR	2161	1/1	0.87	0.23	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	CR	207	1/1	0.87	0.20	37,37,37,37	0
83	MG	A	2034	1/1	0.87	0.44	73,73,73,73	0
83	MG	sR	2167	1/1	0.87	0.30	63,63,63,63	0
83	MG	DA	201	1/1	0.87	0.21	52,52,52,52	0
83	MG	DC	203	1/1	0.87	0.10	28,28,28,28	0
83	MG	1	4209	1/1	0.87	0.31	34,34,34,34	0
83	MG	1	4082	1/1	0.87	0.19	29,29,29,29	0
83	MG	1	3874	1/1	0.87	0.29	35,35,35,35	0
83	MG	AR	3813	1/1	0.87	0.19	64,64,64,64	0
83	MG	1	4223	1/1	0.87	0.13	34,34,34,34	0
83	MG	AR	3819	1/1	0.87	0.26	34,34,34,34	0
83	MG	AR	4062	1/1	0.87	0.31	55,55,55,55	0
83	MG	AR	4065	1/1	0.87	0.20	32,32,32,32	0
82	OHX	AR	3715	7/7	0.87	0.24	111,111,111,111	0
83	MG	AR	3834	1/1	0.87	0.09	21,21,21,21	0
83	MG	3	215	1/1	0.87	0.29	59,59,59,59	0
83	MG	s2	301	1/1	0.87	0.17	48,48,48,48	0
82	OHX	1	3710	7/7	0.87	0.28	106,106,106,106	0
83	MG	AR	4093	1/1	0.87	0.09	39,39,39,39	0
83	MG	AR	4094	1/1	0.87	0.19	68,68,68,68	0
83	MG	AR	3844	1/1	0.87	0.32	44,44,44,44	0
83	MG	AR	4104	1/1	0.87	0.18	86,86,86,86	0
83	MG	d6	202	1/1	0.87	0.20	43,43,43,43	0
83	MG	3	219	1/1	0.87	0.10	63,63,63,63	0
83	MG	AR	3854	1/1	0.87	0.28	30,30,30,30	0
83	MG	AR	3857	1/1	0.87	0.32	21,21,21,21	0
83	MG	A	1977	1/1	0.88	0.42	57,57,57,57	0
83	MG	1	4018	1/1	0.88	0.22	36,36,36,36	0
82	OHX	AR	3706	7/7	0.88	0.20	112,112,112,112	0
83	MG	AK	105	1/1	0.88	0.20	33,33,33,33	0
83	MG	1	3929	1/1	0.88	0.14	47,47,47,47	0
83	MG	1	3829	1/1	0.88	0.24	22,22,22,22	0
83	MG	sR	2066	1/1	0.88	0.31	48,48,48,48	0
82	OHX	A	1940	7/7	0.88	0.16	128,128,128,128	0
83	MG	1	3839	1/1	0.88	0.30	18,18,18,18	0
82	OHX	J	302	7/7	0.88	0.16	125,125,125,125	0
83	MG	1	4045	1/1	0.88	0.11	33,33,33,33	0
83	MG	1	4174	1/1	0.88	0.35	27,27,27,27	0
83	MG	sR	2076	1/1	0.88	0.38	55,55,55,55	0
83	MG	AR	3749	1/1	0.88	0.30	32,32,32,32	0
82	OHX	AR	3726	7/7	0.88	0.34	105,105,105,105	0
82	OHX	1	3674	7/7	0.88	0.20	113,113,113,113	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	AR	4236	1/1	0.88	0.17	34,34,34,34	0
82	OHX	AR	3630	7/7	0.88	0.17	120,120,120,120	0
83	MG	sR	2086	1/1	0.88	0.27	35,35,35,35	0
83	MG	A	1993	1/1	0.88	0.47	74,74,74,74	0
83	MG	AR	4248	1/1	0.88	0.20	31,31,31,31	0
82	OHX	sR	2046	7/7	0.88	0.18	112,112,112,112	0
82	OHX	1	3616	7/7	0.88	0.18	114,114,114,114	0
83	MG	AR	4255	1/1	0.88	0.37	48,48,48,48	0
83	MG	sR	2097	1/1	0.88	0.32	44,44,44,44	0
83	MG	AR	4257	1/1	0.88	0.42	32,32,32,32	0
83	MG	AR	3990	1/1	0.88	0.17	26,26,26,26	0
83	MG	AR	3763	1/1	0.88	0.23	36,36,36,36	0
83	MG	sR	2103	1/1	0.88	0.37	38,38,38,38	0
83	MG	A	2003	1/1	0.88	0.31	55,55,55,55	0
82	OHX	A	1924	7/7	0.88	0.17	126,126,126,126	0
83	MG	AR	3769	1/1	0.88	0.11	33,33,33,33	0
83	MG	AR	3782	1/1	0.88	0.11	35,35,35,35	0
83	MG	1	3764	1/1	0.88	0.23	28,28,28,28	0
82	OHX	A	1925	7/7	0.88	0.14	149,149,149,149	0
83	MG	AR	4021	1/1	0.88	0.26	35,35,35,35	0
83	MG	AT	226	1/1	0.88	0.10	38,38,38,38	0
83	MG	1	4205	1/1	0.88	0.34	44,44,44,44	0
83	MG	1	3956	1/1	0.88	0.07	24,24,24,24	0
82	OHX	1	3628	7/7	0.88	0.16	111,111,111,111	0
83	MG	1	4211	1/1	0.88	0.18	29,29,29,29	0
83	MG	1	4216	1/1	0.88	0.40	44,44,44,44	0
83	MG	sR	2125	1/1	0.88	0.30	42,42,42,42	0
82	OHX	AR	3676	7/7	0.88	0.23	109,109,109,109	0
83	MG	AR	4047	1/1	0.88	0.26	52,52,52,52	0
83	MG	AR	4050	1/1	0.88	0.11	38,38,38,38	0
82	OHX	1	3712	7/7	0.88	0.42	99,99,99,99	0
83	MG	1	3793	1/1	0.88	0.30	51,51,51,51	0
83	MG	AR	3818	1/1	0.88	0.29	50,50,50,50	0
83	MG	3	214	1/1	0.88	0.35	31,31,31,31	0
83	MG	AR	3829	1/1	0.88	0.10	44,44,44,44	0
82	OHX	4	213	7/7	0.88	0.20	109,109,109,109	0
83	MG	1	3886	1/1	0.88	0.33	22,22,22,22	0
83	MG	sR	2139	1/1	0.88	0.43	59,59,59,59	0
82	OHX	A	1934	7/7	0.88	0.41	103,103,103,103	0
83	MG	DH	202	1/1	0.88	0.19	29,29,29,29	0
83	MG	AR	3841	1/1	0.88	0.10	31,31,31,31	0
83	MG	1	3818	1/1	0.88	0.17	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	1	3707	7/7	0.88	0.20	111,111,111,111	0
83	MG	DP	101	1/1	0.88	0.29	38,38,38,38	0
83	MG	sR	2151	1/1	0.88	0.23	48,48,48,48	0
83	MG	4	216	1/1	0.88	0.36	48,48,48,48	0
83	MG	1	3738	1/1	0.88	0.46	51,51,51,51	0
83	MG	1	3909	1/1	0.88	0.41	41,41,41,41	0
83	MG	sR	2164	1/1	0.88	0.11	43,43,43,43	0
83	MG	1	3979	1/1	0.88	0.26	31,31,31,31	0
83	MG	AR	3860	1/1	0.88	0.29	29,29,29,29	0
83	MG	1	4107	1/1	0.88	0.21	47,47,47,47	0
83	MG	1	3821	1/1	0.88	0.26	39,39,39,39	0
82	OHX	AR	3687	7/7	0.88	0.15	136,136,136,136	0
83	MG	AR	4121	1/1	0.88	0.20	26,26,26,26	0
83	MG	AR	3886	1/1	0.88	0.38	35,35,35,35	0
83	MG	AR	3887	1/1	0.88	0.41	43,43,43,43	0
83	MG	AR	4128	1/1	0.88	0.12	36,36,36,36	0
83	MG	1	4117	1/1	0.88	0.26	54,54,54,54	0
83	MG	s	300	1/1	0.88	0.24	64,64,64,64	0
82	OHX	AR	3600	7/7	0.88	0.17	110,110,110,110	0
83	MG	sR	2195	1/1	0.88	0.22	58,58,58,58	0
83	MG	v	304	1/1	0.88	0.17	37,37,37,37	0
83	MG	A	2067	1/1	0.88	0.34	56,56,56,56	0
83	MG	w	202	1/1	0.88	0.10	40,40,40,40	0
83	MG	AR	3906	1/1	0.88	0.32	31,31,31,31	0
83	MG	AR	3910	1/1	0.88	0.23	36,36,36,36	0
83	MG	A	1969	1/1	0.88	0.36	51,51,51,51	0
83	MG	1	3993	1/1	0.88	0.42	57,57,57,57	0
83	MG	1	3917	1/1	0.88	0.28	22,22,22,22	0
83	MG	1	4006	1/1	0.88	0.18	38,38,38,38	0
83	MG	1	3918	1/1	0.88	0.29	19,19,19,19	0
83	MG	b	202	1/1	0.88	0.17	63,63,63,63	0
83	MG	AR	4171	1/1	0.88	0.15	34,34,34,34	0
83	MG	A	1975	1/1	0.88	0.39	55,55,55,55	0
83	MG	AB	208	1/1	0.88	0.34	45,45,45,45	0
83	MG	A	2065	1/1	0.89	0.35	51,51,51,51	0
83	MG	AR	3822	1/1	0.89	0.17	38,38,38,38	0
83	MG	AR	4055	1/1	0.89	0.17	29,29,29,29	0
83	MG	AR	3823	1/1	0.89	0.14	38,38,38,38	0
83	MG	3	211	1/1	0.89	0.12	39,39,39,39	0
83	MG	1	4070	1/1	0.89	0.25	54,54,54,54	0
83	MG	1	3851	1/1	0.89	0.25	24,24,24,24	0
83	MG	AR	4061	1/1	0.89	0.15	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	F	301	1/1	0.89	0.30	62,62,62,62	0
82	OHX	A	1917	7/7	0.89	0.20	115,115,115,115	0
83	MG	AR	3839	1/1	0.89	0.29	24,24,24,24	0
83	MG	AR	4067	1/1	0.89	0.25	31,31,31,31	0
82	OHX	A	1918	7/7	0.89	0.15	124,124,124,124	0
82	OHX	1	3644	7/7	0.89	0.15	134,134,134,134	0
83	MG	1	4083	1/1	0.89	0.10	32,32,32,32	0
82	OHX	AR	3727	7/7	0.89	0.29	107,107,107,107	0
83	MG	AR	4088	1/1	0.89	0.06	39,39,39,39	0
83	MG	AR	4091	1/1	0.89	0.21	48,48,48,48	0
82	OHX	sR	2023	7/7	0.89	0.18	122,122,122,122	0
83	MG	1	3766	1/1	0.89	0.29	21,21,21,21	0
83	MG	1	4093	1/1	0.89	0.13	41,41,41,41	0
83	MG	1	3866	1/1	0.89	0.31	32,32,32,32	0
82	OHX	s8	301	7/7	0.89	0.16	127,127,127,127	0
83	MG	AR	3867	1/1	0.89	0.46	46,46,46,46	0
82	OHX	c3	201	7/7	0.89	0.17	113,113,113,113	0
83	MG	1	3961	1/1	0.89	0.33	47,47,47,47	0
83	MG	AR	4114	1/1	0.89	0.12	64,64,64,64	0
83	MG	AR	4120	1/1	0.89	0.23	40,40,40,40	0
83	MG	AR	3883	1/1	0.89	0.42	43,43,43,43	0
83	MG	AR	3884	1/1	0.89	0.22	38,38,38,38	0
83	MG	AR	3885	1/1	0.89	0.30	40,40,40,40	0
83	MG	o	301	1/1	0.89	0.15	34,34,34,34	0
83	MG	1	3962	1/1	0.89	0.28	49,49,49,49	0
83	MG	1	3774	1/1	0.89	0.18	35,35,35,35	0
83	MG	1	3775	1/1	0.89	0.32	37,37,37,37	0
83	MG	1	3877	1/1	0.89	0.29	45,45,45,45	0
82	OHX	d9	102	7/7	0.89	0.18	125,125,125,125	0
83	MG	AR	3895	1/1	0.89	0.27	39,39,39,39	0
83	MG	AR	3902	1/1	0.89	0.29	21,21,21,21	0
83	MG	AR	4147	1/1	0.89	0.09	46,46,46,46	0
83	MG	1	3782	1/1	0.89	0.24	32,32,32,32	0
83	MG	1	3786	1/1	0.89	0.26	22,22,22,22	0
83	MG	AR	3908	1/1	0.89	0.43	33,33,33,33	0
82	OHX	1	3655	7/7	0.89	0.19	111,111,111,111	0
83	MG	sR	2101	1/1	0.89	0.42	57,57,57,57	0
83	MG	1	3791	1/1	0.89	0.14	43,43,43,43	0
83	MG	AR	3914	1/1	0.89	0.34	32,32,32,32	0
83	MG	1	3792	1/1	0.89	0.23	35,35,35,35	0
83	MG	1	3890	1/1	0.89	0.36	27,27,27,27	0
83	MG	1	3902	1/1	0.89	0.34	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	AR	3930	1/1	0.89	0.19	37,37,37,37	0
82	OHX	1	3701	7/7	0.89	0.32	103,103,103,103	0
83	MG	1	3995	1/1	0.89	0.32	40,40,40,40	0
83	MG	AR	4203	1/1	0.89	0.11	50,50,50,50	0
83	MG	1	3807	1/1	0.89	0.23	28,28,28,28	0
83	MG	1	4160	1/1	0.89	0.24	54,54,54,54	0
83	MG	A	2000	1/1	0.89	0.45	69,69,69,69	0
83	MG	1	3808	1/1	0.89	0.28	42,42,42,42	0
82	OHX	1	3675	7/7	0.89	0.18	111,111,111,111	0
83	MG	sR	2122	1/1	0.89	0.26	48,48,48,48	0
82	OHX	1	3676	7/7	0.89	0.17	113,113,113,113	0
83	MG	sR	2126	1/1	0.89	0.18	62,62,62,62	0
83	MG	AR	4227	1/1	0.89	0.23	36,36,36,36	0
83	MG	1	3732	1/1	0.89	0.32	33,33,33,33	0
82	OHX	1	3614	7/7	0.89	0.18	111,111,111,111	0
83	MG	AR	4235	1/1	0.89	0.34	38,38,38,38	0
82	OHX	1	3659	7/7	0.89	0.21	118,118,118,118	0
83	MG	AR	4238	1/1	0.89	0.11	30,30,30,30	0
83	MG	AR	4245	1/1	0.89	0.33	43,43,43,43	0
82	OHX	1	3690	7/7	0.89	0.17	123,123,123,123	0
83	MG	AR	3967	1/1	0.89	0.14	42,42,42,42	0
83	MG	AR	3968	1/1	0.89	0.29	40,40,40,40	0
83	MG	1	4176	1/1	0.89	0.43	43,43,43,43	0
83	MG	AR	3971	1/1	0.89	0.27	30,30,30,30	0
83	MG	AR	3973	1/1	0.89	0.10	26,26,26,26	0
83	MG	1	4036	1/1	0.89	0.23	43,43,43,43	0
83	MG	AR	3978	1/1	0.89	0.22	41,41,41,41	0
82	OHX	AR	3667	7/7	0.89	0.20	116,116,116,116	0
83	MG	AR	3764	1/1	0.89	0.20	31,31,31,31	0
82	OHX	1	3550	7/7	0.89	0.13	125,125,125,125	0
82	OHX	1	3692	7/7	0.89	0.37	83,83,83,83	0
83	MG	sR	2157	1/1	0.89	0.22	42,42,42,42	0
83	MG	AS	228	1/1	0.89	0.26	44,44,44,44	0
83	MG	A	2028	1/1	0.89	0.25	60,60,60,60	0
83	MG	sR	2163	1/1	0.89	0.30	49,49,49,49	0
83	MG	AR	3771	1/1	0.89	0.30	68,68,68,68	0
83	MG	AR	3992	1/1	0.89	0.22	23,23,23,23	0
83	MG	AR	3994	1/1	0.89	0.10	48,48,48,48	0
83	MG	AR	3996	1/1	0.89	0.17	21,21,21,21	0
83	MG	sR	2168	1/1	0.89	0.23	48,48,48,48	0
83	MG	sR	2172	1/1	0.89	0.24	70,70,70,70	0
83	MG	sR	2173	1/1	0.89	0.38	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	AR	3776	1/1	0.89	0.31	52,52,52,52	0
83	MG	1	4190	1/1	0.89	0.26	21,21,21,21	0
83	MG	1	4192	1/1	0.89	0.22	29,29,29,29	0
83	MG	A	2038	1/1	0.89	0.39	65,65,65,65	0
82	OHX	1	3665	7/7	0.89	0.33	107,107,107,107	0
83	MG	sR	2185	1/1	0.89	0.47	46,46,46,46	0
83	MG	1	4048	1/1	0.89	0.22	43,43,43,43	0
83	MG	A	2042	1/1	0.89	0.14	81,81,81,81	0
83	MG	1	4049	1/1	0.89	0.27	37,37,37,37	0
83	MG	A	2045	1/1	0.89	0.37	49,49,49,49	0
83	MG	CL	303	1/1	0.89	0.34	26,26,26,26	0
83	MG	CM	202	1/1	0.89	0.24	52,52,52,52	0
83	MG	A	2049	1/1	0.89	0.19	54,54,54,54	0
83	MG	A	2050	1/1	0.89	0.48	39,39,39,39	0
82	OHX	1	3669	7/7	0.89	0.16	112,112,112,112	0
83	MG	sR	2203	1/1	0.89	0.28	42,42,42,42	0
83	MG	1	4059	1/1	0.89	0.14	42,42,42,42	0
83	MG	1	3938	1/1	0.89	0.14	36,36,36,36	0
83	MG	c1	202	1/1	0.89	0.22	42,42,42,42	0
82	OHX	1	3718	7/7	0.89	0.33	94,94,94,94	0
83	MG	1	4063	1/1	0.89	0.23	52,52,52,52	0
83	MG	AR	4031	1/1	0.89	0.11	26,26,26,26	0
82	OHX	A	1915	7/7	0.89	0.17	125,125,125,125	0
83	MG	DC	201	1/1	0.89	0.14	20,20,20,20	0
83	MG	1	3941	1/1	0.89	0.15	45,45,45,45	0
83	MG	1	3843	1/1	0.89	0.32	27,27,27,27	0
83	MG	AR	3820	1/1	0.89	0.21	53,53,53,53	0
82	OHX	AR	3655	7/7	0.90	0.18	110,110,110,110	0
83	MG	1	4051	1/1	0.90	0.07	44,44,44,44	0
83	MG	1	3809	1/1	0.90	0.09	31,31,31,31	0
83	MG	AT	219	1/1	0.90	0.20	46,46,46,46	0
83	MG	1	4056	1/1	0.90	0.10	27,27,27,27	0
83	MG	AR	4066	1/1	0.90	0.36	58,58,58,58	0
83	MG	1	4057	1/1	0.90	0.10	38,38,38,38	0
83	MG	1	3879	1/1	0.90	0.36	24,24,24,24	0
83	MG	AT	228	1/1	0.90	0.24	46,46,46,46	0
82	OHX	AR	3658	7/7	0.90	0.33	98,98,98,98	0
83	MG	CD	303	1/1	0.90	0.11	31,31,31,31	0
83	MG	1	3815	1/1	0.90	0.21	28,28,28,28	0
82	OHX	1	3672	7/7	0.90	0.19	114,114,114,114	0
82	OHX	1	3666	7/7	0.90	0.37	86,86,86,86	0
83	MG	AR	4089	1/1	0.90	0.17	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	AR	3530	7/7	0.90	0.25	69,69,69,69	0
82	OHX	AR	3633	7/7	0.90	0.14	142,142,142,142	0
83	MG	1	4194	1/1	0.90	0.35	38,38,38,38	0
83	MG	1	4068	1/1	0.90	0.23	43,43,43,43	0
83	MG	1	3895	1/1	0.90	0.38	38,38,38,38	0
83	MG	1	3898	1/1	0.90	0.36	33,33,33,33	0
82	OHX	AR	3642	7/7	0.90	0.25	101,101,101,101	0
83	MG	A	2026	1/1	0.90	0.24	59,59,59,59	0
83	MG	1	4208	1/1	0.90	0.19	39,39,39,39	0
83	MG	AR	3775	1/1	0.90	0.21	42,42,42,42	0
82	OHX	A	1923	7/7	0.90	0.17	123,123,123,123	0
82	OHX	AR	3649	7/7	0.90	0.28	101,101,101,101	0
83	MG	AR	3787	1/1	0.90	0.30	53,53,53,53	0
82	OHX	AR	3650	7/7	0.90	0.33	103,103,103,103	0
83	MG	1	4084	1/1	0.90	0.11	33,33,33,33	0
82	OHX	CE	402	7/7	0.90	0.17	112,112,112,112	0
83	MG	1	3914	1/1	0.90	0.27	28,28,28,28	0
83	MG	1	3981	1/1	0.90	0.29	35,35,35,35	0
83	MG	A	2039	1/1	0.90	0.41	59,59,59,59	0
83	MG	1	3986	1/1	0.90	0.20	42,42,42,42	0
83	MG	1	3773	1/1	0.90	0.18	29,29,29,29	0
82	OHX	CF	401	7/7	0.90	0.24	107,107,107,107	0
82	OHX	AR	3719	7/7	0.90	0.38	83,83,83,83	0
83	MG	AR	4143	1/1	0.90	0.23	33,33,33,33	0
83	MG	1	4099	1/1	0.90	0.22	45,45,45,45	0
83	MG	3	220	1/1	0.90	0.06	42,42,42,42	0
83	MG	1	3776	1/1	0.90	0.20	29,29,29,29	0
83	MG	1	3994	1/1	0.90	0.09	28,28,28,28	0
83	MG	1	3777	1/1	0.90	0.23	38,38,38,38	0
83	MG	1	4002	1/1	0.90	0.10	48,48,48,48	0
83	MG	1	3928	1/1	0.90	0.16	33,33,33,33	0
83	MG	A	2055	1/1	0.90	0.41	40,40,40,40	0
83	MG	4	227	1/1	0.90	0.26	52,52,52,52	0
82	OHX	AR	3652	7/7	0.90	0.19	110,110,110,110	0
82	OHX	A	1853	7/7	0.90	0.18	112,112,112,112	0
83	MG	AR	3838	1/1	0.90	0.31	31,31,31,31	0
83	MG	1	3858	1/1	0.90	0.33	26,26,26,26	0
83	MG	AR	4004	1/1	0.90	0.18	35,35,35,35	0
82	OHX	AR	3689	7/7	0.90	0.23	105,105,105,105	0
83	MG	AR	4010	1/1	0.90	0.35	66,66,66,66	0
83	MG	AR	4207	1/1	0.90	0.28	43,43,43,43	0
83	MG	AR	4212	1/1	0.90	0.38	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	AR	4011	1/1	0.90	0.10	27,27,27,27	0
83	MG	1	4128	1/1	0.90	0.15	75,75,75,75	0
83	MG	AR	3843	1/1	0.90	0.26	24,24,24,24	0
83	MG	AR	4218	1/1	0.90	0.25	21,21,21,21	0
83	MG	4	237	1/1	0.90	0.31	39,39,39,39	0
83	MG	1	3787	1/1	0.90	0.27	21,21,21,21	0
82	OHX	AR	3722	7/7	0.90	0.17	120,120,120,120	0
83	MG	AR	3856	1/1	0.90	0.22	33,33,33,33	0
83	MG	sR	2182	1/1	0.90	0.37	37,37,37,37	0
83	MG	AR	4232	1/1	0.90	0.33	49,49,49,49	0
83	MG	1	4029	1/1	0.90	0.45	59,59,59,59	0
83	MG	1	4140	1/1	0.90	0.16	43,43,43,43	0
83	MG	sR	2189	1/1	0.90	0.48	64,64,64,64	0
82	OHX	AR	3697	7/7	0.90	0.31	106,106,106,106	0
83	MG	sR	2192	1/1	0.90	0.31	41,41,41,41	0
82	OHX	A	1905	7/7	0.90	0.20	118,118,118,118	0
83	MG	AR	4038	1/1	0.90	0.23	41,41,41,41	0
83	MG	AR	4246	1/1	0.90	0.42	49,49,49,49	0
83	MG	x	204	1/1	0.90	0.15	33,33,33,33	0
83	MG	sR	2057	1/1	0.90	0.27	43,43,43,43	0
83	MG	AR	3875	1/1	0.90	0.30	29,29,29,29	0
83	MG	1	3867	1/1	0.90	0.32	31,31,31,31	0
83	MG	1	4156	1/1	0.90	0.07	46,46,46,46	0
82	OHX	A	1908	7/7	0.90	0.17	122,122,122,122	0
83	MG	s4	302	1/1	0.90	0.24	47,47,47,47	0
83	MG	1	3795	1/1	0.90	0.08	33,33,33,33	0
83	MG	AR	4260	1/1	0.90	0.22	33,33,33,33	0
83	MG	c4	201	1/1	0.90	0.23	46,46,46,46	0
83	MG	sR	2068	1/1	0.90	0.37	35,35,35,35	0
83	MG	AS	211	1/1	0.90	0.34	36,36,36,36	0
83	MG	d3	201	1/1	0.90	0.28	48,48,48,48	0
83	MG	1	3804	1/1	0.90	0.22	59,59,59,59	0
83	MG	AS	215	1/1	0.90	0.38	26,26,26,26	0
83	MG	1	4164	1/1	0.90	0.10	47,47,47,47	0
83	MG	AR	4058	1/1	0.90	0.16	45,45,45,45	0
82	OHX	sR	2043	7/7	0.90	0.18	120,120,120,120	0
83	MG	AS	220	1/1	0.90	0.16	41,41,41,41	0
83	MG	1	4191	1/1	0.91	0.39	37,37,37,37	0
83	MG	1	3921	1/1	0.91	0.30	31,31,31,31	0
83	MG	1	3923	1/1	0.91	0.28	33,33,33,33	0
83	MG	1	3926	1/1	0.91	0.20	31,31,31,31	0
82	OHX	AR	3626	7/7	0.91	0.15	119,119,119,119	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	1	3668	7/7	0.91	0.35	79,79,79,79	0
83	MG	AR	4034	1/1	0.91	0.24	55,55,55,55	0
82	OHX	1	3625	7/7	0.91	0.17	110,110,110,110	0
83	MG	1	4207	1/1	0.91	0.30	38,38,38,38	0
83	MG	AR	4043	1/1	0.91	0.14	51,51,51,51	0
82	OHX	A	1913	7/7	0.91	0.17	111,111,111,111	0
83	MG	CK	203	1/1	0.91	0.20	38,38,38,38	0
83	MG	AR	3824	1/1	0.91	0.27	37,37,37,37	0
83	MG	AR	4048	1/1	0.91	0.13	44,44,44,44	0
83	MG	AR	4049	1/1	0.91	0.21	45,45,45,45	0
83	MG	AR	3825	1/1	0.91	0.21	43,43,43,43	0
83	MG	CQ	202	1/1	0.91	0.07	33,33,33,33	0
83	MG	AR	3827	1/1	0.91	0.08	22,22,22,22	0
83	MG	CR	201	1/1	0.91	0.32	26,26,26,26	0
83	MG	AR	4052	1/1	0.91	0.24	39,39,39,39	0
83	MG	1	3825	1/1	0.91	0.35	59,59,59,59	0
83	MG	O	202	1/1	0.91	0.41	59,59,59,59	0
82	OHX	A	1914	7/7	0.91	0.21	125,125,125,125	0
83	MG	CR	208	1/1	0.91	0.21	31,31,31,31	0
83	MG	CX	205	1/1	0.91	0.09	31,31,31,31	0
83	MG	1	3935	1/1	0.91	0.12	36,36,36,36	0
82	OHX	AR	3695	7/7	0.91	0.31	107,107,107,107	0
83	MG	1	3754	1/1	0.91	0.32	39,39,39,39	0
83	MG	DC	204	1/1	0.91	0.12	33,33,33,33	0
83	MG	DD	102	1/1	0.91	0.11	29,29,29,29	0
82	OHX	1	3706	7/7	0.91	0.35	106,106,106,106	0
82	OHX	sR	2031	7/7	0.91	0.20	110,110,110,110	0
83	MG	1	3840	1/1	0.91	0.29	31,31,31,31	0
83	MG	sR	2064	1/1	0.91	0.33	47,47,47,47	0
83	MG	1	3759	1/1	0.91	0.20	32,32,32,32	0
83	MG	1	3842	1/1	0.91	0.31	32,32,32,32	0
83	MG	1	3948	1/1	0.91	0.31	40,40,40,40	0
82	OHX	1	3597	7/7	0.91	0.33	100,100,100,100	0
83	MG	1	3848	1/1	0.91	0.27	22,22,22,22	0
82	OHX	AR	3701	7/7	0.91	0.16	114,114,114,114	0
82	OHX	AR	3703	7/7	0.91	0.29	99,99,99,99	0
82	OHX	3	208	7/7	0.91	0.16	112,112,112,112	0
82	OHX	AR	3707	7/7	0.91	0.12	149,149,149,149	0
83	MG	AR	4090	1/1	0.91	0.26	46,46,46,46	0
83	MG	4	221	1/1	0.91	0.30	27,27,27,27	0
83	MG	AR	3873	1/1	0.91	0.24	41,41,41,41	0
83	MG	4	224	1/1	0.91	0.24	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	3	209	7/7	0.91	0.19	118,118,118,118	0
83	MG	sR	2084	1/1	0.91	0.28	61,61,61,61	0
82	OHX	A	1926	7/7	0.91	0.17	115,115,115,115	0
83	MG	4	228	1/1	0.91	0.14	28,28,28,28	0
83	MG	1	3769	1/1	0.91	0.22	37,37,37,37	0
83	MG	A	1960	1/1	0.91	0.48	53,53,53,53	0
83	MG	AR	4111	1/1	0.91	0.13	38,38,38,38	0
83	MG	1	3771	1/1	0.91	0.23	39,39,39,39	0
83	MG	A	1963	1/1	0.91	0.37	48,48,48,48	0
82	OHX	1	3658	7/7	0.91	0.21	114,114,114,114	0
82	OHX	A	1928	7/7	0.91	0.16	118,118,118,118	0
83	MG	A	1967	1/1	0.91	0.46	64,64,64,64	0
83	MG	AR	4117	1/1	0.91	0.11	29,29,29,29	0
83	MG	1	3868	1/1	0.91	0.25	34,34,34,34	0
83	MG	1	3968	1/1	0.91	0.18	28,28,28,28	0
82	OHX	A	1929	7/7	0.91	0.18	116,116,116,116	0
82	OHX	1	3645	7/7	0.91	0.28	99,99,99,99	0
83	MG	t	201	1/1	0.91	0.10	39,39,39,39	0
83	MG	AR	4129	1/1	0.91	0.17	38,38,38,38	0
83	MG	AR	4131	1/1	0.91	0.22	54,54,54,54	0
83	MG	sR	2113	1/1	0.91	0.14	57,57,57,57	0
83	MG	AR	3899	1/1	0.91	0.35	26,26,26,26	0
83	MG	1	3872	1/1	0.91	0.25	37,37,37,37	0
82	OHX	CG	303	7/7	0.91	0.38	105,105,105,105	0
82	OHX	AR	3659	7/7	0.91	0.30	95,95,95,95	0
83	MG	AR	3907	1/1	0.91	0.30	27,27,27,27	0
83	MG	1	3781	1/1	0.91	0.25	20,20,20,20	0
82	OHX	1	3648	7/7	0.91	0.31	98,98,98,98	0
83	MG	1	3784	1/1	0.91	0.33	28,28,28,28	0
83	MG	sR	2123	1/1	0.91	0.29	55,55,55,55	0
83	MG	1	4122	1/1	0.91	0.11	38,38,38,38	0
82	OHX	AR	3519	7/7	0.91	0.16	122,122,122,122	0
83	MG	AR	3920	1/1	0.91	0.22	24,24,24,24	0
83	MG	AR	4150	1/1	0.91	0.09	36,36,36,36	0
83	MG	AB	207	1/1	0.91	0.13	29,29,29,29	0
83	MG	AR	3924	1/1	0.91	0.26	35,35,35,35	0
83	MG	1	4130	1/1	0.91	0.15	48,48,48,48	0
83	MG	AR	4176	1/1	0.91	0.20	28,28,28,28	0
83	MG	1	3989	1/1	0.91	0.13	41,41,41,41	0
83	MG	1	4133	1/1	0.91	0.19	41,41,41,41	0
83	MG	1	4134	1/1	0.91	0.19	24,24,24,24	0
83	MG	1	3882	1/1	0.91	0.32	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	A	1936	7/7	0.91	0.17	123,123,123,123	0
83	MG	AR	4197	1/1	0.91	0.14	48,48,48,48	0
83	MG	AR	3948	1/1	0.91	0.28	35,35,35,35	0
83	MG	A	1999	1/1	0.91	0.32	55,55,55,55	0
83	MG	1	4137	1/1	0.91	0.16	70,70,70,70	0
82	OHX	1	3711	7/7	0.91	0.35	95,95,95,95	0
83	MG	AR	4205	1/1	0.91	0.10	30,30,30,30	0
82	OHX	A	1875	7/7	0.91	0.14	123,123,123,123	0
83	MG	AR	4208	1/1	0.91	0.32	52,52,52,52	0
82	OHX	c5	201	7/7	0.91	0.13	130,130,130,130	0
83	MG	1	4145	1/1	0.91	0.10	32,32,32,32	0
83	MG	AR	3956	1/1	0.91	0.32	36,36,36,36	0
83	MG	AR	3745	1/1	0.91	0.23	36,36,36,36	0
83	MG	1	3996	1/1	0.91	0.21	21,21,21,21	0
83	MG	AR	4219	1/1	0.91	0.28	39,39,39,39	0
83	MG	1	4151	1/1	0.91	0.19	28,28,28,28	0
82	OHX	1	3652	7/7	0.91	0.29	76,76,76,76	0
83	MG	AR	4224	1/1	0.91	0.24	28,28,28,28	0
83	MG	sR	2170	1/1	0.91	0.23	54,54,54,54	0
83	MG	1	3794	1/1	0.91	0.18	45,45,45,45	0
82	OHX	A	1885	7/7	0.91	0.27	96,96,96,96	0
83	MG	A	2017	1/1	0.91	0.20	60,60,60,60	0
83	MG	AR	4230	1/1	0.91	0.31	35,35,35,35	0
83	MG	1	3803	1/1	0.91	0.37	35,35,35,35	0
83	MG	1	4014	1/1	0.91	0.34	33,33,33,33	0
82	OHX	A	1893	7/7	0.91	0.19	111,111,111,111	0
83	MG	AR	3980	1/1	0.91	0.17	40,40,40,40	0
83	MG	sR	2184	1/1	0.91	0.31	33,33,33,33	0
83	MG	1	4019	1/1	0.91	0.11	40,40,40,40	0
83	MG	AR	4242	1/1	0.91	0.30	41,41,41,41	0
83	MG	1	4020	1/1	0.91	0.22	48,48,48,48	0
83	MG	AR	3984	1/1	0.91	0.09	32,32,32,32	0
83	MG	AR	3985	1/1	0.91	0.18	61,61,61,61	0
83	MG	AR	3770	1/1	0.91	0.29	40,40,40,40	0
82	OHX	sR	1990	7/7	0.91	0.32	103,103,103,103	0
82	OHX	sR	1997	7/7	0.91	0.16	117,117,117,117	0
82	OHX	A	1898	7/7	0.91	0.17	115,115,115,115	0
83	MG	AR	3781	1/1	0.91	0.20	22,22,22,22	0
83	MG	A	2035	1/1	0.91	0.17	87,87,87,87	0
83	MG	1	4027	1/1	0.91	0.27	39,39,39,39	0
83	MG	AR	3998	1/1	0.91	0.17	36,36,36,36	0
83	MG	AR	3783	1/1	0.91	0.21	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3812	1/1	0.91	0.29	32,32,32,32	0
83	MG	1	3733	1/1	0.91	0.33	28,28,28,28	0
82	OHX	1	3653	7/7	0.91	0.21	105,105,105,105	0
82	OHX	sR	2011	7/7	0.91	0.24	110,110,110,110	0
83	MG	AR	4012	1/1	0.91	0.22	29,29,29,29	0
83	MG	1	4184	1/1	0.91	0.25	28,28,28,28	0
83	MG	AR	3803	1/1	0.91	0.27	50,50,50,50	0
83	MG	A	2047	1/1	0.91	0.25	60,60,60,60	0
83	MG	1	4189	1/1	0.91	0.29	18,18,18,18	0
83	MG	AS	229	1/1	0.91	0.27	43,43,43,43	0
83	MG	AT	218	1/1	0.91	0.28	31,31,31,31	0
83	MG	AR	4018	1/1	0.91	0.14	36,36,36,36	0
86	GOL	AR	4262	6/6	0.91	0.17	27,27,27,27	0
82	OHX	AR	3622	7/7	0.91	0.16	114,114,114,114	0
83	MG	AR	4068	1/1	0.92	0.24	28,28,28,28	0
83	MG	AR	4070	1/1	0.92	0.26	27,27,27,27	0
83	MG	CK	202	1/1	0.92	0.08	36,36,36,36	0
82	OHX	1	3699	7/7	0.92	0.28	107,107,107,107	0
83	MG	AR	3896	1/1	0.92	0.28	23,23,23,23	0
83	MG	AR	3897	1/1	0.92	0.33	25,25,25,25	0
82	OHX	1	3601	7/7	0.92	0.28	94,94,94,94	0
83	MG	1	4054	1/1	0.92	0.18	51,51,51,51	0
83	MG	CP	505	1/1	0.92	0.16	40,40,40,40	0
83	MG	1	3799	1/1	0.92	0.32	64,64,64,64	0
82	OHX	AR	3529	7/7	0.92	0.26	80,80,80,80	0
82	OHX	AR	3699	7/7	0.92	0.36	109,109,109,109	0
82	OHX	A	1880	7/7	0.92	0.17	119,119,119,119	0
82	OHX	1	3603	7/7	0.92	0.31	85,85,85,85	0
82	OHX	sR	2030	7/7	0.92	0.38	95,95,95,95	0
83	MG	AR	4098	1/1	0.92	0.19	33,33,33,33	0
83	MG	1	3965	1/1	0.92	0.16	36,36,36,36	0
83	MG	AR	3751	1/1	0.92	0.31	27,27,27,27	0
83	MG	1	4181	1/1	0.92	0.34	44,44,44,44	0
83	MG	AR	4110	1/1	0.92	0.11	55,55,55,55	0
83	MG	sR	2052	1/1	0.92	0.34	38,38,38,38	0
83	MG	AR	3921	1/1	0.92	0.41	43,43,43,43	0
83	MG	AR	3922	1/1	0.92	0.29	22,22,22,22	0
83	MG	AR	3755	1/1	0.92	0.28	17,17,17,17	0
83	MG	1	3810	1/1	0.92	0.36	41,41,41,41	0
83	MG	AR	4116	1/1	0.92	0.24	23,23,23,23	0
83	MG	AR	3925	1/1	0.92	0.31	22,22,22,22	0
83	MG	sR	2062	1/1	0.92	0.37	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	4187	1/1	0.92	0.12	34,34,34,34	0
82	OHX	A	1889	7/7	0.92	0.15	130,130,130,130	0
83	MG	DR	502	1/1	0.92	0.09	56,56,56,56	0
83	MG	AR	3931	1/1	0.92	0.19	38,38,38,38	0
82	OHX	AR	3566	7/7	0.92	0.17	100,100,100,100	0
83	MG	AR	3937	1/1	0.92	0.16	33,33,33,33	0
83	MG	A	1947	1/1	0.92	0.47	53,53,53,53	0
83	MG	A	1948	1/1	0.92	0.27	49,49,49,49	0
83	MG	1	4069	1/1	0.92	0.15	40,40,40,40	0
83	MG	1	3969	1/1	0.92	0.14	35,35,35,35	0
83	MG	AR	3942	1/1	0.92	0.17	25,25,25,25	0
83	MG	sR	2077	1/1	0.92	0.30	50,50,50,50	0
83	MG	AR	3945	1/1	0.92	0.10	27,27,27,27	0
83	MG	1	4074	1/1	0.92	0.20	46,46,46,46	0
83	MG	AR	3947	1/1	0.92	0.12	34,34,34,34	0
82	OHX	A	1895	7/7	0.92	0.16	110,110,110,110	0
83	MG	1	4196	1/1	0.92	0.31	29,29,29,29	0
83	MG	1	4200	1/1	0.92	0.27	29,29,29,29	0
83	MG	AR	4144	1/1	0.92	0.10	39,39,39,39	0
83	MG	AR	4145	1/1	0.92	0.08	34,34,34,34	0
82	OHX	sR	2035	7/7	0.92	0.29	107,107,107,107	0
82	OHX	A	1896	7/7	0.92	0.27	101,101,101,101	0
83	MG	AR	3778	1/1	0.92	0.24	32,32,32,32	0
83	MG	1	3975	1/1	0.92	0.13	38,38,38,38	0
83	MG	AR	3958	1/1	0.92	0.22	23,23,23,23	0
83	MG	AR	3959	1/1	0.92	0.23	55,55,55,55	0
83	MG	AR	4152	1/1	0.92	0.16	25,25,25,25	0
83	MG	AR	4155	1/1	0.92	0.07	27,27,27,27	0
83	MG	AR	4162	1/1	0.92	0.24	23,23,23,23	0
83	MG	1	4206	1/1	0.92	0.35	36,36,36,36	0
82	OHX	1	3689	7/7	0.92	0.16	115,115,115,115	0
83	MG	AR	4172	1/1	0.92	0.43	31,31,31,31	0
83	MG	AR	3966	1/1	0.92	0.43	70,70,70,70	0
83	MG	1	3977	1/1	0.92	0.33	42,42,42,42	0
83	MG	1	4085	1/1	0.92	0.19	45,45,45,45	0
83	MG	AR	4184	1/1	0.92	0.22	44,44,44,44	0
83	MG	AR	4188	1/1	0.92	0.22	31,31,31,31	0
83	MG	AR	3793	1/1	0.92	0.14	36,36,36,36	0
83	MG	1	3896	1/1	0.92	0.29	25,25,25,25	0
83	MG	AR	4193	1/1	0.92	0.14	65,65,65,65	0
82	OHX	AR	3605	7/7	0.92	0.14	118,118,118,118	0
83	MG	AR	3974	1/1	0.92	0.26	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	AR	4199	1/1	0.92	0.10	41,41,41,41	0
83	MG	AR	3976	1/1	0.92	0.31	49,49,49,49	0
83	MG	sR	2121	1/1	0.92	0.21	45,45,45,45	0
83	MG	1	4213	1/1	0.92	0.21	30,30,30,30	0
83	MG	1	3761	1/1	0.92	0.23	24,24,24,24	0
82	OHX	AR	3665	7/7	0.92	0.15	117,117,117,117	0
83	MG	1	3987	1/1	0.92	0.14	30,30,30,30	0
83	MG	1	3824	1/1	0.92	0.33	25,25,25,25	0
83	MG	AR	4210	1/1	0.92	0.11	33,33,33,33	0
82	OHX	A	1906	7/7	0.92	0.12	160,160,160,160	0
83	MG	1	3990	1/1	0.92	0.18	36,36,36,36	0
83	MG	AR	3986	1/1	0.92	0.24	46,46,46,46	0
82	OHX	AR	3708	7/7	0.92	0.29	103,103,103,103	0
83	MG	sR	2134	1/1	0.92	0.09	40,40,40,40	0
82	OHX	AR	3666	7/7	0.92	0.11	143,143,143,143	0
83	MG	3	218	1/1	0.92	0.30	56,56,56,56	0
83	MG	1	4102	1/1	0.92	0.13	31,31,31,31	0
82	OHX	A	1911	7/7	0.92	0.34	99,99,99,99	0
82	OHX	J	301	7/7	0.92	0.25	106,106,106,106	0
83	MG	AR	4226	1/1	0.92	0.27	22,22,22,22	0
83	MG	sR	2143	1/1	0.92	0.06	48,48,48,48	0
83	MG	3	222	1/1	0.92	0.24	27,27,27,27	0
82	OHX	1	3629	7/7	0.92	0.15	113,113,113,113	0
82	OHX	Q	201	7/7	0.92	0.13	131,131,131,131	0
82	OHX	e	102	7/7	0.92	0.18	110,110,110,110	0
82	OHX	sR	1960	7/7	0.92	0.20	92,92,92,92	0
83	MG	AR	4234	1/1	0.92	0.20	20,20,20,20	0
83	MG	AR	3833	1/1	0.92	0.24	23,23,23,23	0
82	OHX	Rb	401	7/7	0.92	0.14	127,127,127,127	0
83	MG	4	225	1/1	0.92	0.09	40,40,40,40	0
83	MG	AR	4241	1/1	0.92	0.32	25,25,25,25	0
83	MG	1	3847	1/1	0.92	0.34	30,30,30,30	0
83	MG	1	4123	1/1	0.92	0.12	30,30,30,30	0
83	MG	1	4126	1/1	0.92	0.31	21,21,21,21	0
82	OHX	sR	1972	7/7	0.92	0.17	110,110,110,110	0
83	MG	1	3849	1/1	0.92	0.14	26,26,26,26	0
82	OHX	sR	1980	7/7	0.92	0.38	76,76,76,76	0
82	OHX	sR	1985	7/7	0.92	0.15	116,116,116,116	0
83	MG	4	235	1/1	0.92	0.10	30,30,30,30	0
82	OHX	sR	1987	7/7	0.92	0.18	117,117,117,117	0
83	MG	1	3855	1/1	0.92	0.23	21,21,21,21	0
83	MG	1	3857	1/1	0.92	0.11	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	AS	213	1/1	0.92	0.28	47,47,47,47	0
82	OHX	d4	201	7/7	0.92	0.14	116,116,116,116	0
83	MG	AR	3861	1/1	0.92	0.34	23,23,23,23	0
83	MG	AR	4041	1/1	0.92	0.21	69,69,69,69	0
82	OHX	AR	3618	7/7	0.92	0.14	114,114,114,114	0
82	OHX	1	3609	7/7	0.92	0.20	105,105,105,105	0
83	MG	sR	2187	1/1	0.92	0.27	43,43,43,43	0
83	MG	AR	3868	1/1	0.92	0.18	24,24,24,24	0
83	MG	AR	3871	1/1	0.92	0.29	39,39,39,39	0
83	MG	AS	224	1/1	0.92	0.15	36,36,36,36	0
83	MG	1	4035	1/1	0.92	0.13	42,42,42,42	0
83	MG	AS	226	1/1	0.92	0.22	46,46,46,46	0
83	MG	AS	227	1/1	0.92	0.35	38,38,38,38	0
82	OHX	1	3595	7/7	0.92	0.16	110,110,110,110	0
83	MG	AR	3876	1/1	0.92	0.31	31,31,31,31	0
83	MG	AT	217	1/1	0.92	0.19	29,29,29,29	0
83	MG	AR	3878	1/1	0.92	0.26	24,24,24,24	0
83	MG	1	4039	1/1	0.92	0.21	33,33,33,33	0
82	OHX	CG	301	7/7	0.92	0.16	109,109,109,109	0
83	MG	AT	222	1/1	0.92	0.26	39,39,39,39	0
83	MG	AT	223	1/1	0.92	0.19	55,55,55,55	0
83	MG	1	4043	1/1	0.92	0.12	35,35,35,35	0
83	MG	6	201	1/1	0.92	0.32	25,25,25,25	0
83	MG	1	3790	1/1	0.92	0.25	48,48,48,48	0
82	OHX	1	3486	7/7	0.92	0.22	73,73,73,73	0
82	OHX	1	3619	7/7	0.92	0.24	102,102,102,102	0
83	MG	AT	231	1/1	0.92	0.27	30,30,30,30	0
83	MG	CD	301	1/1	0.92	0.32	40,40,40,40	0
83	MG	1	3869	1/1	0.92	0.21	42,42,42,42	0
83	MG	AF	201	1/1	0.92	0.12	23,23,23,23	0
83	MG	CE	404	1/1	0.92	0.12	22,22,22,22	0
82	OHX	1	3650	7/7	0.92	0.22	98,98,98,98	0
83	MG	1	4168	1/1	0.92	0.22	36,36,36,36	0
83	MG	CG	305	1/1	0.92	0.06	49,49,49,49	0
82	OHX	A	1894	7/7	0.93	0.16	118,118,118,118	0
83	MG	AR	3814	1/1	0.93	0.42	30,30,30,30	0
83	MG	AR	3816	1/1	0.93	0.21	47,47,47,47	0
82	OHX	1	3594	7/7	0.93	0.14	120,120,120,120	0
83	MG	1	4033	1/1	0.93	0.10	30,30,30,30	0
83	MG	1	4193	1/1	0.93	0.24	35,35,35,35	0
83	MG	1	4034	1/1	0.93	0.08	46,46,46,46	0
83	MG	AR	3821	1/1	0.93	0.29	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	1	3626	7/7	0.93	0.14	109,109,109,109	0
82	OHX	AR	3702	7/7	0.93	0.32	82,82,82,82	0
83	MG	AR	4035	1/1	0.93	0.06	41,41,41,41	0
83	MG	1	4197	1/1	0.93	0.12	26,26,26,26	0
83	MG	A	2054	1/1	0.93	0.42	44,44,44,44	0
83	MG	AT	220	1/1	0.93	0.33	37,37,37,37	0
83	MG	A	2056	1/1	0.93	0.38	36,36,36,36	0
83	MG	1	4198	1/1	0.93	0.19	29,29,29,29	0
83	MG	1	3783	1/1	0.93	0.31	59,59,59,59	0
83	MG	1	4201	1/1	0.93	0.31	33,33,33,33	0
83	MG	AT	224	1/1	0.93	0.12	37,37,37,37	0
83	MG	1	3900	1/1	0.93	0.28	21,21,21,21	0
83	MG	AR	3831	1/1	0.93	0.12	38,38,38,38	0
83	MG	1	4041	1/1	0.93	0.10	27,27,27,27	0
82	OHX	A	1899	7/7	0.93	0.28	100,100,100,100	0
83	MG	AT	229	1/1	0.93	0.28	31,31,31,31	0
83	MG	AR	3835	1/1	0.93	0.30	28,28,28,28	0
82	OHX	1	3627	7/7	0.93	0.28	97,97,97,97	0
83	MG	1	3907	1/1	0.93	0.29	28,28,28,28	0
82	OHX	sR	2029	7/7	0.93	0.31	86,86,86,86	0
82	OHX	A	1903	7/7	0.93	0.16	113,113,113,113	0
82	OHX	AR	3705	7/7	0.93	0.26	97,97,97,97	0
82	OHX	AR	3624	7/7	0.93	0.15	109,109,109,109	0
82	OHX	1	3713	7/7	0.93	0.20	105,105,105,105	0
83	MG	1	4214	1/1	0.93	0.26	33,33,33,33	0
83	MG	AR	3849	1/1	0.93	0.34	24,24,24,24	0
83	MG	AR	3853	1/1	0.93	0.34	21,21,21,21	0
83	MG	1	4215	1/1	0.93	0.30	38,38,38,38	0
83	MG	AR	3855	1/1	0.93	0.26	23,23,23,23	0
82	OHX	1	3604	7/7	0.93	0.26	101,101,101,101	0
82	OHX	1	3605	7/7	0.93	0.26	105,105,105,105	0
83	MG	1	4221	1/1	0.93	0.43	41,41,41,41	0
82	OHX	AR	3637	7/7	0.93	0.20	103,103,103,103	0
83	MG	1	3797	1/1	0.93	0.32	24,24,24,24	0
83	MG	AR	3864	1/1	0.93	0.25	25,25,25,25	0
83	MG	1	3798	1/1	0.93	0.31	22,22,22,22	0
83	MG	3	212	1/1	0.93	0.41	59,59,59,59	0
83	MG	sR	2059	1/1	0.93	0.32	46,46,46,46	0
83	MG	CR	202	1/1	0.93	0.23	28,28,28,28	0
83	MG	3	213	1/1	0.93	0.22	32,32,32,32	0
83	MG	1	3925	1/1	0.93	0.26	26,26,26,26	0
83	MG	CR	206	1/1	0.93	0.22	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	AR	3638	7/7	0.93	0.35	100,100,100,100	0
83	MG	AR	3874	1/1	0.93	0.28	30,30,30,30	0
83	MG	CX	203	1/1	0.93	0.27	21,21,21,21	0
83	MG	1	4064	1/1	0.93	0.14	30,30,30,30	0
83	MG	1	3802	1/1	0.93	0.10	39,39,39,39	0
83	MG	DA	202	1/1	0.93	0.20	39,39,39,39	0
83	MG	sR	2071	1/1	0.93	0.36	47,47,47,47	0
82	OHX	AR	3640	7/7	0.93	0.37	90,90,90,90	0
82	OHX	AR	3641	7/7	0.93	0.18	104,104,104,104	0
83	MG	sR	2075	1/1	0.93	0.31	42,42,42,42	0
83	MG	1	3805	1/1	0.93	0.10	33,33,33,33	0
83	MG	AR	4108	1/1	0.93	0.11	24,24,24,24	0
82	OHX	1	3630	7/7	0.93	0.17	114,114,114,114	0
83	MG	1	3933	1/1	0.93	0.18	35,35,35,35	0
83	MG	sR	2080	1/1	0.93	0.23	42,42,42,42	0
82	OHX	AR	3643	7/7	0.93	0.34	94,94,94,94	0
83	MG	4	217	1/1	0.93	0.35	41,41,41,41	0
82	OHX	1	3664	7/7	0.93	0.29	94,94,94,94	0
83	MG	DO	202	1/1	0.93	0.09	37,37,37,37	0
83	MG	sR	2085	1/1	0.93	0.36	37,37,37,37	0
82	OHX	1	3608	7/7	0.93	0.24	96,96,96,96	0
83	MG	DQ	505	1/1	0.93	0.17	34,34,34,34	0
83	MG	4	222	1/1	0.93	0.24	22,22,22,22	0
83	MG	DR	503	1/1	0.93	0.16	54,54,54,54	0
83	MG	sR	2091	1/1	0.93	0.32	38,38,38,38	0
82	OHX	A	1922	7/7	0.93	0.32	85,85,85,85	0
82	OHX	1	3635	7/7	0.93	0.19	107,107,107,107	0
82	OHX	1	3643	7/7	0.93	0.28	100,100,100,100	0
83	MG	AR	4122	1/1	0.93	0.13	41,41,41,41	0
82	OHX	AR	3657	7/7	0.93	0.26	82,82,82,82	0
82	OHX	4	209	7/7	0.93	0.14	116,116,116,116	0
82	OHX	1	3530	7/7	0.93	0.14	128,128,128,128	0
83	MG	AR	3901	1/1	0.93	0.36	42,42,42,42	0
82	OHX	s4	301	7/7	0.93	0.17	118,118,118,118	0
83	MG	AR	3903	1/1	0.93	0.28	25,25,25,25	0
83	MG	sR	2107	1/1	0.93	0.37	51,51,51,51	0
83	MG	1	4090	1/1	0.93	0.06	27,27,27,27	0
83	MG	1	4091	1/1	0.93	0.09	42,42,42,42	0
82	OHX	AR	3661	7/7	0.93	0.22	109,109,109,109	0
82	OHX	AR	3728	7/7	0.93	0.24	100,100,100,100	0
82	OHX	1	3596	7/7	0.93	0.30	99,99,99,99	0
83	MG	AR	4142	1/1	0.93	0.07	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	j	301	1/1	0.93	0.23	25,25,25,25	0
82	OHX	A	1931	7/7	0.93	0.35	87,87,87,87	0
82	OHX	AR	3663	7/7	0.93	0.30	102,102,102,102	0
83	MG	AR	3917	1/1	0.93	0.37	35,35,35,35	0
83	MG	1	3727	1/1	0.93	0.22	31,31,31,31	0
83	MG	A	1965	1/1	0.93	0.43	54,54,54,54	0
82	OHX	4	214	7/7	0.93	0.21	106,106,106,106	0
83	MG	1	3830	1/1	0.93	0.32	37,37,37,37	0
82	OHX	l	401	7/7	0.93	0.24	106,106,106,106	0
83	MG	1	4104	1/1	0.93	0.11	39,39,39,39	0
82	OHX	1	3499	7/7	0.93	0.15	89,89,89,89	0
82	OHX	AR	3672	7/7	0.93	0.25	102,102,102,102	0
83	MG	AR	3928	1/1	0.93	0.41	34,34,34,34	0
82	OHX	AT	214	7/7	0.93	0.26	98,98,98,98	0
83	MG	AR	4170	1/1	0.93	0.17	31,31,31,31	0
83	MG	1	4108	1/1	0.93	0.20	60,60,60,60	0
83	MG	AR	3932	1/1	0.93	0.07	37,37,37,37	0
82	OHX	AR	3500	7/7	0.93	0.15	90,90,90,90	0
83	MG	1	4113	1/1	0.93	0.11	43,43,43,43	0
82	OHX	AR	3508	7/7	0.93	0.17	91,91,91,91	0
83	MG	AR	4183	1/1	0.93	0.26	36,36,36,36	0
83	MG	1	3846	1/1	0.93	0.24	61,61,61,61	0
83	MG	AR	4185	1/1	0.93	0.07	29,29,29,29	0
83	MG	AG	202	1/1	0.93	0.17	48,48,48,48	0
83	MG	AR	3943	1/1	0.93	0.23	43,43,43,43	0
82	OHX	1	3703	7/7	0.93	0.33	98,98,98,98	0
82	OHX	CG	302	7/7	0.93	0.23	107,107,107,107	0
83	MG	1	3739	1/1	0.93	0.25	29,29,29,29	0
82	OHX	1	3704	7/7	0.93	0.36	99,99,99,99	0
82	OHX	CL	302	7/7	0.93	0.21	88,88,88,88	0
82	OHX	1	3618	7/7	0.93	0.11	170,170,170,170	0
83	MG	sR	2152	1/1	0.93	0.12	48,48,48,48	0
82	OHX	h	401	7/7	0.93	0.13	134,134,134,134	0
83	MG	1	3749	1/1	0.93	0.20	37,37,37,37	0
82	OHX	sR	1950	7/7	0.93	0.18	104,104,104,104	0
82	OHX	AR	3686	7/7	0.93	0.32	86,86,86,86	0
83	MG	1	3982	1/1	0.93	0.10	26,26,26,26	0
83	MG	1	3984	1/1	0.93	0.14	36,36,36,36	0
83	MG	AR	3960	1/1	0.93	0.15	41,41,41,41	0
82	OHX	sR	1962	7/7	0.93	0.26	102,102,102,102	0
83	MG	1	4141	1/1	0.93	0.12	36,36,36,36	0
82	OHX	sR	1966	7/7	0.93	0.18	101,101,101,101	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	sR	1969	7/7	0.93	0.17	91,91,91,91	0
83	MG	1	3758	1/1	0.93	0.17	40,40,40,40	0
83	MG	AR	4220	1/1	0.93	0.32	38,38,38,38	0
82	OHX	A	1846	7/7	0.93	0.13	126,126,126,126	0
82	OHX	1	3651	7/7	0.93	0.18	109,109,109,109	0
82	OHX	A	1858	7/7	0.93	0.12	127,127,127,127	0
82	OHX	AR	3688	7/7	0.93	0.36	97,97,97,97	0
83	MG	sR	2181	1/1	0.93	0.22	44,44,44,44	0
82	OHX	AR	3580	7/7	0.93	0.13	135,135,135,135	0
83	MG	AR	4228	1/1	0.93	0.24	26,26,26,26	0
82	OHX	sR	1995	7/7	0.93	0.12	128,128,128,128	0
83	MG	1	3873	1/1	0.93	0.15	28,28,28,28	0
83	MG	1	4165	1/1	0.93	0.10	33,33,33,33	0
83	MG	1	3765	1/1	0.93	0.20	36,36,36,36	0
83	MG	1	3875	1/1	0.93	0.38	29,29,29,29	0
83	MG	sR	2190	1/1	0.93	0.34	53,53,53,53	0
82	OHX	1	3561	7/7	0.93	0.27	84,84,84,84	0
83	MG	A	2016	1/1	0.93	0.22	61,61,61,61	0
82	OHX	AR	3696	7/7	0.93	0.33	91,91,91,91	0
83	MG	AR	4237	1/1	0.93	0.17	34,34,34,34	0
83	MG	1	4010	1/1	0.93	0.16	31,31,31,31	0
83	MG	1	4011	1/1	0.93	0.31	45,45,45,45	0
83	MG	AR	3784	1/1	0.93	0.14	29,29,29,29	0
83	MG	1	4012	1/1	0.93	0.13	30,30,30,30	0
83	MG	AR	3791	1/1	0.93	0.31	32,32,32,32	0
82	OHX	A	1881	7/7	0.93	0.09	173,173,173,173	0
82	OHX	sR	2007	7/7	0.93	0.16	111,111,111,111	0
83	MG	AR	3997	1/1	0.93	0.07	22,22,22,22	0
83	MG	1	3880	1/1	0.93	0.36	30,30,30,30	0
83	MG	AR	4254	1/1	0.93	0.26	34,34,34,34	0
82	OHX	sR	2010	7/7	0.93	0.27	107,107,107,107	0
83	MG	A	2031	1/1	0.93	0.26	64,64,64,64	0
83	MG	AR	4256	1/1	0.93	0.09	26,26,26,26	0
82	OHX	AR	3602	7/7	0.93	0.19	104,104,104,104	0
82	OHX	AR	3698	7/7	0.93	0.31	103,103,103,103	0
83	MG	AR	4009	1/1	0.93	0.13	29,29,29,29	0
82	OHX	1	3684	7/7	0.93	0.17	110,110,110,110	0
83	MG	AR	3806	1/1	0.93	0.14	30,30,30,30	0
83	MG	1	4185	1/1	0.93	0.22	24,24,24,24	0
82	OHX	sR	2020	7/7	0.93	0.15	111,111,111,111	0
83	MG	1	4028	1/1	0.93	0.10	38,38,38,38	0
83	MG	1	3740	1/1	0.94	0.09	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	AR	3815	1/1	0.94	0.22	21,21,21,21	0
83	MG	1	3831	1/1	0.94	0.25	31,31,31,31	0
82	OHX	AR	3664	7/7	0.94	0.23	96,96,96,96	0
83	MG	1	3942	1/1	0.94	0.27	41,41,41,41	0
83	MG	AR	4251	1/1	0.94	0.29	39,39,39,39	0
83	MG	AR	4008	1/1	0.94	0.21	37,37,37,37	0
83	MG	1	3836	1/1	0.94	0.30	27,27,27,27	0
83	MG	1	3837	1/1	0.94	0.21	24,24,24,24	0
83	MG	1	3946	1/1	0.94	0.06	30,30,30,30	0
83	MG	1	3947	1/1	0.94	0.19	36,36,36,36	0
83	MG	AR	4259	1/1	0.94	0.36	44,44,44,44	0
83	MG	1	4075	1/1	0.94	0.20	25,25,25,25	0
83	MG	1	4077	1/1	0.94	0.11	42,42,42,42	0
82	OHX	sR	1981	7/7	0.94	0.26	88,88,88,88	0
83	MG	1	3743	1/1	0.94	0.24	41,41,41,41	0
82	OHX	AR	3603	7/7	0.94	0.28	85,85,85,85	0
83	MG	AS	216	1/1	0.94	0.09	37,37,37,37	0
82	OHX	1	3705	7/7	0.94	0.27	74,74,74,74	0
83	MG	AR	4023	1/1	0.94	0.10	38,38,38,38	0
82	OHX	sR	1989	7/7	0.94	0.16	100,100,100,100	0
83	MG	AR	4026	1/1	0.94	0.14	34,34,34,34	0
83	MG	AS	221	1/1	0.94	0.28	37,37,37,37	0
83	MG	1	3954	1/1	0.94	0.15	34,34,34,34	0
83	MG	1	3844	1/1	0.94	0.26	35,35,35,35	0
82	OHX	1	3622	7/7	0.94	0.17	100,100,100,100	0
83	MG	3	216	1/1	0.94	0.13	38,38,38,38	0
83	MG	AR	4032	1/1	0.94	0.16	47,47,47,47	0
83	MG	AR	3837	1/1	0.94	0.16	24,24,24,24	0
82	OHX	sR	1992	7/7	0.94	0.20	94,94,94,94	0
83	MG	1	3753	1/1	0.94	0.21	40,40,40,40	0
82	OHX	A	1900	7/7	0.94	0.20	110,110,110,110	0
82	OHX	AR	3668	7/7	0.94	0.34	71,71,71,71	0
82	OHX	sR	1998	7/7	0.94	0.24	107,107,107,107	0
82	OHX	AR	3671	7/7	0.94	0.33	97,97,97,97	0
82	OHX	A	1904	7/7	0.94	0.28	94,94,94,94	0
82	OHX	4	211	7/7	0.94	0.25	87,87,87,87	0
83	MG	AR	3851	1/1	0.94	0.21	25,25,25,25	0
83	MG	AR	3852	1/1	0.94	0.31	46,46,46,46	0
82	OHX	AR	3673	7/7	0.94	0.25	103,103,103,103	0
82	OHX	AR	3619	7/7	0.94	0.29	76,76,76,76	0
83	MG	AR	4054	1/1	0.94	0.19	44,44,44,44	0
83	MG	4	219	1/1	0.94	0.26	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
83	MG	4	220	1/1	0.94	0.27	29,29,29,29	0
82	OHX	sR	2015	7/7	0.94	0.27	90,90,90,90	0
83	MG	1	3861	1/1	0.94	0.42	26,26,26,26	0
83	MG	CD	302	1/1	0.94	0.37	27,27,27,27	0
82	OHX	1	3592	7/7	0.94	0.12	129,129,129,129	0
83	MG	sR	2054	1/1	0.94	0.34	47,47,47,47	0
83	MG	1	3863	1/1	0.94	0.29	22,22,22,22	0
83	MG	AR	3863	1/1	0.94	0.33	30,30,30,30	0
82	OHX	1	3654	7/7	0.94	0.14	114,114,114,114	0
83	MG	AR	4063	1/1	0.94	0.11	29,29,29,29	0
82	OHX	1	3615	7/7	0.94	0.27	98,98,98,98	0
82	OHX	AR	3680	7/7	0.94	0.30	93,93,93,93	0
83	MG	sR	2061	1/1	0.94	0.34	47,47,47,47	0
83	MG	1	4110	1/1	0.94	0.21	26,26,26,26	0
82	OHX	sR	2022	7/7	0.94	0.34	91,91,91,91	0
83	MG	AR	3872	1/1	0.94	0.25	29,29,29,29	0
83	MG	1	3980	1/1	0.94	0.23	36,36,36,36	0
83	MG	AR	4073	1/1	0.94	0.16	52,52,52,52	0
82	OHX	1	3693	7/7	0.94	0.25	90,90,90,90	0
82	OHX	1	3593	7/7	0.94	0.19	99,99,99,99	0
82	OHX	AR	3735	7/7	0.94	0.29	85,85,85,85	0
83	MG	AR	4080	1/1	0.94	0.14	43,43,43,43	0
83	MG	AR	4084	1/1	0.94	0.23	38,38,38,38	0
83	MG	AR	4085	1/1	0.94	0.11	40,40,40,40	0
83	MG	AR	3877	1/1	0.94	0.24	21,21,21,21	0
83	MG	sR	2074	1/1	0.94	0.38	41,41,41,41	0
83	MG	1	4121	1/1	0.94	0.18	39,39,39,39	0
82	OHX	AS	207	7/7	0.94	0.15	101,101,101,101	0
82	OHX	1	3673	7/7	0.94	0.25	101,101,101,101	0
83	MG	AR	3882	1/1	0.94	0.21	25,25,25,25	0
82	OHX	sR	2028	7/7	0.94	0.32	73,73,73,73	0
83	MG	CU	201	1/1	0.94	0.09	31,31,31,31	0
83	MG	1	4127	1/1	0.94	0.19	51,51,51,51	0
83	MG	CX	204	1/1	0.94	0.07	33,33,33,33	0
82	OHX	1	3554	7/7	0.94	0.26	91,91,91,91	0
83	MG	AR	4099	1/1	0.94	0.17	45,45,45,45	0
83	MG	AR	4101	1/1	0.94	0.07	27,27,27,27	0
83	MG	AR	4102	1/1	0.94	0.10	32,32,32,32	0
83	MG	t	203	1/1	0.94	0.17	22,22,22,22	0
82	OHX	AT	213	7/7	0.94	0.23	106,106,106,106	0
83	MG	AR	4107	1/1	0.94	0.12	27,27,27,27	0
83	MG	sR	2090	1/1	0.94	0.20	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	v	305	1/1	0.94	0.24	39,39,39,39	0
83	MG	sR	2092	1/1	0.94	0.43	58,58,58,58	0
83	MG	sR	2093	1/1	0.94	0.42	40,40,40,40	0
83	MG	v	306	1/1	0.94	0.21	43,43,43,43	0
83	MG	AR	3890	1/1	0.94	0.35	31,31,31,31	0
83	MG	sR	2096	1/1	0.94	0.30	37,37,37,37	0
83	MG	v	307	1/1	0.94	0.22	34,34,34,34	0
83	MG	AR	3892	1/1	0.94	0.35	40,40,40,40	0
82	OHX	1	3646	7/7	0.94	0.20	103,103,103,103	0
82	OHX	AT	216	7/7	0.94	0.29	95,95,95,95	0
83	MG	AR	4115	1/1	0.94	0.11	47,47,47,47	0
83	MG	sR	2102	1/1	0.94	0.34	42,42,42,42	0
82	OHX	sR	2033	7/7	0.94	0.29	97,97,97,97	0
82	OHX	1	3715	7/7	0.94	0.11	140,140,140,140	0
83	MG	AR	4118	1/1	0.94	0.44	70,70,70,70	0
82	OHX	1	3610	7/7	0.94	0.33	91,91,91,91	0
83	MG	A	1944	1/1	0.94	0.31	36,36,36,36	0
82	OHX	AR	3540	7/7	0.94	0.20	88,88,88,88	0
83	MG	1	3998	1/1	0.94	0.20	31,31,31,31	0
83	MG	1	4000	1/1	0.94	0.21	43,43,43,43	0
83	MG	AR	4126	1/1	0.94	0.20	32,32,32,32	0
83	MG	AR	3904	1/1	0.94	0.27	26,26,26,26	0
83	MG	1	4001	1/1	0.94	0.13	29,29,29,29	0
82	OHX	AR	3644	7/7	0.94	0.25	103,103,103,103	0
83	MG	AR	4130	1/1	0.94	0.10	26,26,26,26	0
83	MG	AF	202	1/1	0.94	0.09	24,24,24,24	0
82	OHX	AR	3646	7/7	0.94	0.28	98,98,98,98	0
82	OHX	AR	3647	7/7	0.94	0.34	92,92,92,92	0
83	MG	AR	3911	1/1	0.94	0.23	26,26,26,26	0
83	MG	1	4150	1/1	0.94	0.07	41,41,41,41	0
82	OHX	AR	3648	7/7	0.94	0.24	81,81,81,81	0
83	MG	1	4152	1/1	0.94	0.14	40,40,40,40	0
83	MG	1	4154	1/1	0.94	0.22	38,38,38,38	0
83	MG	1	3889	1/1	0.94	0.21	25,25,25,25	0
83	MG	AR	3740	1/1	0.94	0.20	24,24,24,24	0
82	OHX	AR	3544	7/7	0.94	0.13	127,127,127,127	0
82	OHX	CS	201	1/7	0.94	0.09	137,137,137,137	0
82	OHX	A	1818	7/7	0.94	0.15	80,80,80,80	0
82	OHX	1	3679	7/7	0.94	0.27	106,106,106,106	0
83	MG	AR	3926	1/1	0.94	0.26	25,25,25,25	0
82	OHX	AR	3704	7/7	0.94	0.31	77,77,77,77	0
83	MG	AR	3748	1/1	0.94	0.28	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	AR	3929	1/1	0.94	0.42	30,30,30,30	0
83	MG	1	4166	1/1	0.94	0.10	34,34,34,34	0
82	OHX	A	1854	7/7	0.94	0.25	97,97,97,97	0
83	MG	sR	2140	1/1	0.94	0.17	45,45,45,45	0
83	MG	AR	4165	1/1	0.94	0.22	38,38,38,38	0
83	MG	sR	2142	1/1	0.94	0.17	65,65,65,65	0
83	MG	AR	4167	1/1	0.94	0.14	49,49,49,49	0
83	MG	1	3801	1/1	0.94	0.09	31,31,31,31	0
83	MG	1	3906	1/1	0.94	0.25	33,33,33,33	0
83	MG	sR	2147	1/1	0.94	0.15	45,45,45,45	0
83	MG	AR	3756	1/1	0.94	0.16	27,27,27,27	0
82	OHX	AR	3574	7/7	0.94	0.20	103,103,103,103	0
83	MG	1	4172	1/1	0.94	0.16	42,42,42,42	0
83	MG	1	4024	1/1	0.94	0.19	33,33,33,33	0
82	OHX	A	1869	7/7	0.94	0.25	108,108,108,108	0
83	MG	sR	2154	1/1	0.94	0.11	43,43,43,43	0
83	MG	AR	4182	1/1	0.94	0.10	41,41,41,41	0
82	OHX	AR	3653	7/7	0.94	0.31	82,82,82,82	0
83	MG	sR	2158	1/1	0.94	0.12	57,57,57,57	0
82	OHX	A	1874	7/7	0.94	0.10	136,136,136,136	0
83	MG	1	3912	1/1	0.94	0.29	20,20,20,20	0
83	MG	AR	4186	1/1	0.94	0.34	23,23,23,23	0
83	MG	1	3913	1/1	0.94	0.27	26,26,26,26	0
83	MG	1	3806	1/1	0.94	0.39	36,36,36,36	0
83	MG	AR	4190	1/1	0.94	0.07	32,32,32,32	0
83	MG	AR	3950	1/1	0.94	0.15	32,32,32,32	0
82	OHX	1	3661	7/7	0.94	0.26	83,83,83,83	0
83	MG	sR	2169	1/1	0.94	0.24	40,40,40,40	0
83	MG	AR	3774	1/1	0.94	0.20	32,32,32,32	0
82	OHX	O	201	7/7	0.94	0.14	125,125,125,125	0
83	MG	AR	4198	1/1	0.94	0.13	40,40,40,40	0
83	MG	1	4037	1/1	0.94	0.24	30,30,30,30	0
83	MG	sR	2175	1/1	0.94	0.14	82,82,82,82	0
83	MG	AR	3777	1/1	0.94	0.23	28,28,28,28	0
83	MG	sR	2177	1/1	0.94	0.20	50,50,50,50	0
83	MG	AR	3957	1/1	0.94	0.31	36,36,36,36	0
82	OHX	AR	3582	7/7	0.94	0.27	95,95,95,95	0
83	MG	AR	3779	1/1	0.94	0.28	21,21,21,21	0
83	MG	AR	4206	1/1	0.94	0.09	33,33,33,33	0
83	MG	AR	3780	1/1	0.94	0.16	27,27,27,27	0
82	OHX	A	1879	7/7	0.94	0.15	114,114,114,114	0
83	MG	1	3920	1/1	0.94	0.29	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	c8	201	7/7	0.94	0.14	115,115,115,115	0
82	OHX	AR	3587	7/7	0.94	0.15	107,107,107,107	0
83	MG	AR	3786	1/1	0.94	0.22	43,43,43,43	0
83	MG	AR	4216	1/1	0.94	0.04	38,38,38,38	0
83	MG	1	3924	1/1	0.94	0.24	22,22,22,22	0
83	MG	AR	3790	1/1	0.94	0.14	27,27,27,27	0
82	OHX	sR	1932	7/7	0.94	0.16	88,88,88,88	0
82	OHX	AR	3593	7/7	0.94	0.31	74,74,74,74	0
82	OHX	sR	1955	7/7	0.94	0.14	133,133,133,133	0
82	OHX	AR	3595	7/7	0.94	0.29	79,79,79,79	0
83	MG	sR	2197	1/1	0.94	0.37	38,38,38,38	0
83	MG	AR	4223	1/1	0.94	0.20	29,29,29,29	0
82	OHX	1	3620	7/7	0.94	0.27	93,93,93,93	0
83	MG	sR	2200	1/1	0.94	0.21	36,36,36,36	0
83	MG	AR	3798	1/1	0.94	0.10	25,25,25,25	0
83	MG	AR	3799	1/1	0.94	0.24	35,35,35,35	0
83	MG	AR	3801	1/1	0.94	0.24	44,44,44,44	0
82	OHX	A	1891	7/7	0.94	0.15	122,122,122,122	0
83	MG	1	4199	1/1	0.94	0.19	37,37,37,37	0
82	OHX	AR	3714	7/7	0.94	0.21	109,109,109,109	0
82	OHX	sR	1971	7/7	0.94	0.25	102,102,102,102	0
83	MG	A	2024	1/1	0.94	0.30	53,53,53,53	0
82	OHX	1	3632	7/7	0.94	0.26	90,90,90,90	0
83	MG	AR	3808	1/1	0.94	0.22	29,29,29,29	0
83	MG	AR	3991	1/1	0.94	0.15	35,35,35,35	0
82	OHX	sR	1976	7/7	0.94	0.14	115,115,115,115	0
82	OHX	sR	1977	7/7	0.94	0.17	104,104,104,104	0
83	MG	AR	4239	1/1	0.94	0.20	30,30,30,30	0
83	MG	AR	3995	1/1	0.94	0.25	40,40,40,40	0
85	ZN	d7	101	1/1	0.94	0.10	108,108,108,108	0
82	OHX	sR	1979	7/7	0.94	0.28	101,101,101,101	0
83	MG	AR	4243	1/1	0.94	0.14	20,20,20,20	0
82	OHX	1	3667	7/7	0.95	0.22	103,103,103,103	0
82	OHX	AR	3684	7/7	0.95	0.21	108,108,108,108	0
83	MG	AR	4225	1/1	0.95	0.34	45,45,45,45	0
83	MG	AR	3773	1/1	0.95	0.17	30,30,30,30	0
83	MG	1	4148	1/1	0.95	0.16	31,31,31,31	0
83	MG	1	3827	1/1	0.95	0.31	21,21,21,21	0
82	OHX	1	3444	7/7	0.95	0.17	66,66,66,66	0
82	OHX	1	3638	7/7	0.95	0.11	116,116,116,116	0
83	MG	1	4153	1/1	0.95	0.17	42,42,42,42	0
83	MG	AR	3983	1/1	0.95	0.20	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	AR	3589	7/7	0.95	0.21	96,96,96,96	0
82	OHX	AR	3592	7/7	0.95	0.33	78,78,78,78	0
82	OHX	AR	3690	7/7	0.95	0.26	81,81,81,81	0
83	MG	1	4159	1/1	0.95	0.06	33,33,33,33	0
83	MG	A	2044	1/1	0.95	0.18	70,70,70,70	0
83	MG	1	3834	1/1	0.95	0.32	18,18,18,18	0
83	MG	AR	3989	1/1	0.95	0.13	36,36,36,36	0
83	MG	AR	4240	1/1	0.95	0.07	33,33,33,33	0
83	MG	1	4162	1/1	0.95	0.09	35,35,35,35	0
82	OHX	AR	3694	7/7	0.95	0.33	86,86,86,86	0
83	MG	1	3983	1/1	0.95	0.14	27,27,27,27	0
83	MG	AR	3788	1/1	0.95	0.20	24,24,24,24	0
83	MG	AR	3789	1/1	0.95	0.18	29,29,29,29	0
82	OHX	1	3670	7/7	0.95	0.26	83,83,83,83	0
83	MG	1	3985	1/1	0.95	0.07	39,39,39,39	0
82	OHX	A	1902	7/7	0.95	0.27	91,91,91,91	0
83	MG	AR	4000	1/1	0.95	0.25	47,47,47,47	0
83	MG	AR	4252	1/1	0.95	0.28	26,26,26,26	0
82	OHX	AR	3594	7/7	0.95	0.28	88,88,88,88	0
83	MG	AR	4003	1/1	0.95	0.29	38,38,38,38	0
82	OHX	1	3640	7/7	0.95	0.24	95,95,95,95	0
82	OHX	AR	3598	7/7	0.95	0.24	98,98,98,98	0
82	OHX	1	3642	7/7	0.95	0.23	107,107,107,107	0
83	MG	AR	4258	1/1	0.95	0.35	26,26,26,26	0
82	OHX	1	3556	7/7	0.95	0.14	111,111,111,111	0
83	MG	AR	3800	1/1	0.95	0.30	22,22,22,22	0
82	OHX	1	3557	7/7	0.95	0.12	109,109,109,109	0
82	OHX	A	1910	7/7	0.95	0.26	97,97,97,97	0
82	OHX	1	3613	7/7	0.95	0.31	87,87,87,87	0
82	OHX	AR	3606	7/7	0.95	0.26	73,73,73,73	0
83	MG	AR	3805	1/1	0.95	0.19	27,27,27,27	0
83	MG	1	3850	1/1	0.95	0.21	25,25,25,25	0
83	MG	AR	4019	1/1	0.95	0.17	31,31,31,31	0
82	OHX	1	3495	7/7	0.95	0.11	97,97,97,97	0
82	OHX	AR	3611	7/7	0.95	0.27	90,90,90,90	0
83	MG	AR	4022	1/1	0.95	0.19	41,41,41,41	0
82	OHX	AR	3613	7/7	0.95	0.22	106,106,106,106	0
83	MG	1	4183	1/1	0.95	0.29	20,20,20,20	0
83	MG	AR	3812	1/1	0.95	0.24	41,41,41,41	0
82	OHX	1	3563	7/7	0.95	0.17	99,99,99,99	0
83	MG	1	4003	1/1	0.95	0.28	54,54,54,54	0
83	MG	1	4186	1/1	0.95	0.14	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3856	1/1	0.95	0.30	31,31,31,31	0
82	OHX	c1	201	7/7	0.95	0.28	101,101,101,101	0
82	OHX	1	3680	7/7	0.95	0.29	98,98,98,98	0
82	OHX	AR	3620	7/7	0.95	0.23	86,86,86,86	0
82	OHX	AR	3621	7/7	0.95	0.26	95,95,95,95	0
82	OHX	1	3681	7/7	0.95	0.28	96,96,96,96	0
82	OHX	AR	3623	7/7	0.95	0.25	98,98,98,98	0
82	OHX	1	3649	7/7	0.95	0.30	83,83,83,83	0
83	MG	AR	4045	1/1	0.95	0.13	38,38,38,38	0
82	OHX	AR	3625	7/7	0.95	0.20	106,106,106,106	0
83	MG	1	3865	1/1	0.95	0.19	21,21,21,21	0
82	OHX	1	3685	7/7	0.95	0.26	101,101,101,101	0
82	OHX	AR	3717	7/7	0.95	0.24	95,95,95,95	0
82	OHX	AR	3627	7/7	0.95	0.23	107,107,107,107	0
82	OHX	AR	3628	7/7	0.95	0.21	100,100,100,100	0
83	MG	AR	3832	1/1	0.95	0.14	30,30,30,30	0
82	OHX	1	3722	7/7	0.95	0.32	58,58,58,58	0
83	MG	1	4203	1/1	0.95	0.27	35,35,35,35	0
82	OHX	AR	3631	7/7	0.95	0.16	108,108,108,108	0
83	MG	1	3736	1/1	0.95	0.21	30,30,30,30	0
83	MG	1	4030	1/1	0.95	0.16	54,54,54,54	0
82	OHX	1	3724	1/7	0.95	0.18	143,143,143,143	0
82	OHX	AR	3634	7/7	0.95	0.31	91,91,91,91	0
82	OHX	AR	3636	7/7	0.95	0.29	88,88,88,88	0
82	OHX	3	207	7/7	0.95	0.16	97,97,97,97	0
82	OHX	1	3565	7/7	0.95	0.18	103,103,103,103	0
82	OHX	AR	3639	7/7	0.95	0.24	92,92,92,92	0
83	MG	1	4038	1/1	0.95	0.11	33,33,33,33	0
83	MG	CK	204	1/1	0.95	0.20	32,32,32,32	0
82	OHX	1	3454	7/7	0.95	0.15	91,91,91,91	0
82	OHX	4	208	7/7	0.95	0.31	79,79,79,79	0
83	MG	CO	202	1/1	0.95	0.07	34,34,34,34	0
82	OHX	1	3688	7/7	0.95	0.23	100,100,100,100	0
83	MG	1	4219	1/1	0.95	0.21	31,31,31,31	0
83	MG	1	4220	1/1	0.95	0.13	45,45,45,45	0
83	MG	AR	4074	1/1	0.95	0.27	36,36,36,36	0
83	MG	1	3747	1/1	0.95	0.15	29,29,29,29	0
83	MG	1	3748	1/1	0.95	0.23	32,32,32,32	0
83	MG	AR	4077	1/1	0.95	0.12	47,47,47,47	0
82	OHX	A	1941	7/7	0.95	0.32	78,78,78,78	0
83	MG	AR	4079	1/1	0.95	0.25	46,46,46,46	0
83	MG	AR	3858	1/1	0.95	0.26	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	AR	4083	1/1	0.95	0.21	47,47,47,47	0
82	OHX	A	1942	7/7	0.95	0.14	111,111,111,111	0
82	OHX	1	3501	7/7	0.95	0.12	105,105,105,105	0
83	MG	CU	202	1/1	0.95	0.16	32,32,32,32	0
82	OHX	AR	3734	7/7	0.95	0.34	64,64,64,64	0
83	MG	1	4050	1/1	0.95	0.20	25,25,25,25	0
82	OHX	1	3479	7/7	0.95	0.15	88,88,88,88	0
82	OHX	1	3532	7/7	0.95	0.27	79,79,79,79	0
83	MG	1	4053	1/1	0.95	0.11	34,34,34,34	0
82	OHX	1	3623	7/7	0.95	0.12	120,120,120,120	0
83	MG	DC	202	1/1	0.95	0.19	41,41,41,41	0
83	MG	AR	3869	1/1	0.95	0.20	26,26,26,26	0
82	OHX	1	3534	7/7	0.95	0.24	82,82,82,82	0
82	OHX	sR	1919	7/7	0.95	0.16	73,73,73,73	0
83	MG	1	3901	1/1	0.95	0.16	22,22,22,22	0
82	OHX	r	301	7/7	0.95	0.16	74,74,74,74	0
83	MG	1	3904	1/1	0.95	0.35	33,33,33,33	0
82	OHX	sR	1940	7/7	0.95	0.12	105,105,105,105	0
83	MG	AR	4106	1/1	0.95	0.09	27,27,27,27	0
82	OHX	x	201	7/7	0.95	0.29	101,101,101,101	0
82	OHX	AR	3651	7/7	0.95	0.29	90,90,90,90	0
83	MG	DQ	503	1/1	0.95	0.06	34,34,34,34	0
82	OHX	1	3694	7/7	0.95	0.29	81,81,81,81	0
82	OHX	AP	502	7/7	0.95	0.27	63,63,63,63	0
82	OHX	AR	3496	7/7	0.95	0.16	86,86,86,86	0
82	OHX	AR	3656	7/7	0.95	0.27	104,104,104,104	0
82	OHX	1	3538	7/7	0.95	0.18	90,90,90,90	0
83	MG	sR	2124	1/1	0.95	0.17	42,42,42,42	0
83	MG	1	4071	1/1	0.95	0.14	39,39,39,39	0
82	OHX	CK	201	7/7	0.95	0.20	97,97,97,97	0
82	OHX	sR	1973	7/7	0.95	0.16	105,105,105,105	0
82	OHX	1	3599	7/7	0.95	0.12	117,117,117,117	0
83	MG	1	4078	1/1	0.95	0.19	36,36,36,36	0
82	OHX	1	3542	7/7	0.95	0.20	96,96,96,96	0
83	MG	4	232	1/1	0.95	0.18	60,60,60,60	0
82	OHX	1	3602	7/7	0.95	0.19	94,94,94,94	0
82	OHX	1	3662	7/7	0.95	0.26	88,88,88,88	0
83	MG	AR	3894	1/1	0.95	0.26	22,22,22,22	0
82	OHX	AR	3539	7/7	0.95	0.12	106,106,106,106	0
83	MG	1	3922	1/1	0.95	0.31	22,22,22,22	0
83	MG	1	3778	1/1	0.95	0.24	31,31,31,31	0
83	MG	1	3779	1/1	0.95	0.39	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	AR	3900	1/1	0.95	0.18	21,21,21,21	0
83	MG	k	402	1/1	0.95	0.28	30,30,30,30	0
83	MG	AR	4134	1/1	0.95	0.15	27,27,27,27	0
83	MG	l	404	1/1	0.95	0.14	83,83,83,83	0
83	MG	sR	2144	1/1	0.95	0.28	51,51,51,51	0
82	OHX	sR	1983	7/7	0.95	0.12	112,112,112,112	0
82	OHX	sR	1984	7/7	0.95	0.20	90,90,90,90	0
82	OHX	A	1831	7/7	0.95	0.11	105,105,105,105	0
82	OHX	1	3663	7/7	0.95	0.15	84,84,84,84	0
82	OHX	A	1851	7/7	0.95	0.11	111,111,111,111	0
82	OHX	1	3545	7/7	0.95	0.14	93,93,93,93	0
83	MG	AR	3909	1/1	0.95	0.26	22,22,22,22	0
82	OHX	AR	3546	7/7	0.95	0.17	83,83,83,83	0
83	MG	1	3788	1/1	0.95	0.12	30,30,30,30	0
83	MG	1	4096	1/1	0.95	0.28	47,47,47,47	0
83	MG	sR	2156	1/1	0.95	0.35	51,51,51,51	0
83	MG	1	4097	1/1	0.95	0.22	39,39,39,39	0
83	MG	x	202	1/1	0.95	0.26	29,29,29,29	0
82	OHX	sR	1994	7/7	0.95	0.22	104,104,104,104	0
83	MG	sR	2160	1/1	0.95	0.17	42,42,42,42	0
82	OHX	A	1855	7/7	0.95	0.15	97,97,97,97	0
83	MG	x	205	1/1	0.95	0.19	36,36,36,36	0
83	MG	AR	4154	1/1	0.95	0.14	34,34,34,34	0
83	MG	x	206	1/1	0.95	0.18	30,30,30,30	0
83	MG	AR	4158	1/1	0.95	0.18	37,37,37,37	0
83	MG	AR	4159	1/1	0.95	0.08	30,30,30,30	0
83	MG	AR	4161	1/1	0.95	0.09	32,32,32,32	0
82	OHX	A	1857	7/7	0.95	0.26	93,93,93,93	0
83	MG	AR	4163	1/1	0.95	0.09	38,38,38,38	0
82	OHX	AR	3554	7/7	0.95	0.28	89,89,89,89	0
83	MG	AR	4166	1/1	0.95	0.16	60,60,60,60	0
82	OHX	sR	2000	7/7	0.95	0.18	107,107,107,107	0
82	OHX	A	1859	7/7	0.95	0.17	107,107,107,107	0
82	OHX	sR	2004	7/7	0.95	0.24	105,105,105,105	0
82	OHX	sR	2005	7/7	0.95	0.28	83,83,83,83	0
82	OHX	A	1863	7/7	0.95	0.13	114,114,114,114	0
83	MG	AR	4173	1/1	0.95	0.22	30,30,30,30	0
82	OHX	A	1864	7/7	0.95	0.23	92,92,92,92	0
82	OHX	sR	2009	7/7	0.95	0.18	85,85,85,85	0
82	OHX	A	1865	7/7	0.95	0.20	103,103,103,103	0
82	OHX	AR	3557	7/7	0.95	0.22	77,77,77,77	0
83	MG	AR	3935	1/1	0.95	0.16	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	4114	1/1	0.95	0.14	58,58,58,58	0
82	OHX	sR	2013	7/7	0.95	0.26	83,83,83,83	0
82	OHX	sR	2014	7/7	0.95	0.29	93,93,93,93	0
83	MG	AR	3941	1/1	0.95	0.24	23,23,23,23	0
82	OHX	AR	3561	7/7	0.95	0.14	106,106,106,106	0
83	MG	1	4120	1/1	0.95	0.18	31,31,31,31	0
82	OHX	sR	2016	7/7	0.95	0.26	89,89,89,89	0
82	OHX	sR	2017	7/7	0.95	0.21	100,100,100,100	0
82	OHX	A	1873	7/7	0.95	0.11	121,121,121,121	0
83	MG	1	4124	1/1	0.95	0.13	29,29,29,29	0
82	OHX	AR	3565	7/7	0.95	0.26	89,89,89,89	0
82	OHX	1	3480	7/7	0.95	0.15	69,69,69,69	0
82	OHX	AR	3567	7/7	0.95	0.10	122,122,122,122	0
83	MG	AR	4201	1/1	0.95	0.14	37,37,37,37	0
82	OHX	A	1878	7/7	0.95	0.13	120,120,120,120	0
82	OHX	AR	3570	7/7	0.95	0.14	96,96,96,96	0
83	MG	AR	3754	1/1	0.95	0.23	23,23,23,23	0
83	MG	AR	3955	1/1	0.95	0.14	53,53,53,53	0
82	OHX	AR	3571	7/7	0.95	0.24	76,76,76,76	0
83	MG	1	3964	1/1	0.95	0.16	30,30,30,30	0
83	MG	c1	203	1/1	0.95	0.26	51,51,51,51	0
82	OHX	AR	3573	7/7	0.95	0.22	90,90,90,90	0
82	OHX	A	1883	7/7	0.95	0.23	101,101,101,101	0
83	MG	AR	4213	1/1	0.95	0.22	25,25,25,25	0
82	OHX	A	1884	7/7	0.95	0.18	86,86,86,86	0
83	MG	d3	203	1/1	0.95	0.30	40,40,40,40	0
83	MG	AR	3760	1/1	0.95	0.17	36,36,36,36	0
83	MG	d4	204	1/1	0.95	0.36	57,57,57,57	0
83	MG	1	3822	1/1	0.95	0.24	28,28,28,28	0
82	OHX	1	3552	7/7	0.95	0.17	103,103,103,103	0
83	MG	1	3971	1/1	0.95	0.14	39,39,39,39	0
84	G5B	1	4224	26/26	0.95	0.11	27,27,27,27	0
83	MG	AR	3767	1/1	0.95	0.11	22,22,22,22	0
82	OHX	AR	3681	7/7	0.95	0.26	94,94,94,94	0
85	ZN	e1	501	1/1	0.95	0.06	136,136,136,136	0
83	MG	AR	3970	1/1	0.95	0.24	33,33,33,33	0
83	MG	1	4144	1/1	0.95	0.12	27,27,27,27	0
82	OHX	AR	3505	7/7	0.96	0.13	82,82,82,82	0
83	MG	1	4182	1/1	0.96	0.24	31,31,31,31	0
83	MG	1	4007	1/1	0.96	0.08	28,28,28,28	0
83	MG	AR	4005	1/1	0.96	0.05	27,27,27,27	0
82	OHX	A	1920	7/7	0.96	0.20	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	AR	3632	7/7	0.96	0.16	83,83,83,83	0
82	OHX	1	3483	7/7	0.96	0.12	95,95,95,95	0
82	OHX	AR	3515	7/7	0.96	0.11	123,123,123,123	0
83	MG	1	4188	1/1	0.96	0.34	41,41,41,41	0
82	OHX	1	3564	7/7	0.96	0.27	82,82,82,82	0
83	MG	AR	4013	1/1	0.96	0.14	42,42,42,42	0
83	MG	AR	4244	1/1	0.96	0.23	28,28,28,28	0
83	MG	AR	3811	1/1	0.96	0.21	44,44,44,44	0
83	MG	1	4016	1/1	0.96	0.21	29,29,29,29	0
82	OHX	1	3485	7/7	0.96	0.15	82,82,82,82	0
82	OHX	1	3570	7/7	0.96	0.23	92,92,92,92	0
83	MG	AR	4249	1/1	0.96	0.28	42,42,42,42	0
82	OHX	AR	3532	7/7	0.96	0.21	69,69,69,69	0
83	MG	1	3725	1/1	0.96	0.33	32,32,32,32	0
83	MG	1	3726	1/1	0.96	0.32	40,40,40,40	0
82	OHX	AR	3538	7/7	0.96	0.24	89,89,89,89	0
82	OHX	1	3571	7/7	0.96	0.16	103,103,103,103	0
82	OHX	1	3572	7/7	0.96	0.23	91,91,91,91	0
82	OHX	AR	3541	7/7	0.96	0.10	99,99,99,99	0
82	OHX	1	3575	7/7	0.96	0.23	85,85,85,85	0
82	OHX	AR	3545	7/7	0.96	0.22	98,98,98,98	0
82	OHX	AR	3737	7/7	0.96	0.26	58,58,58,58	0
82	OHX	1	3579	7/7	0.96	0.23	82,82,82,82	0
82	OHX	AR	3551	7/7	0.96	0.20	83,83,83,83	0
82	OHX	1	3582	7/7	0.96	0.24	86,86,86,86	0
82	OHX	AT	210	7/7	0.96	0.22	85,85,85,85	0
83	MG	AR	4037	1/1	0.96	0.18	29,29,29,29	0
82	OHX	AT	211	7/7	0.96	0.10	108,108,108,108	0
82	OHX	AR	3555	7/7	0.96	0.24	80,80,80,80	0
83	MG	AR	4040	1/1	0.96	0.20	30,30,30,30	0
82	OHX	1	3586	7/7	0.96	0.16	104,104,104,104	0
83	MG	AR	4042	1/1	0.96	0.13	33,33,33,33	0
82	OHX	AT	215	7/7	0.96	0.15	108,108,108,108	0
83	MG	AS	222	1/1	0.96	0.16	45,45,45,45	0
83	MG	AR	4044	1/1	0.96	0.13	42,42,42,42	0
82	OHX	1	3590	7/7	0.96	0.32	84,84,84,84	0
83	MG	1	4212	1/1	0.96	0.20	42,42,42,42	0
83	MG	1	4042	1/1	0.96	0.09	37,37,37,37	0
82	OHX	AR	3563	7/7	0.96	0.12	110,110,110,110	0
83	MG	sR	2050	1/1	0.96	0.34	40,40,40,40	0
83	MG	1	3883	1/1	0.96	0.26	22,22,22,22	0
82	OHX	AR	3564	7/7	0.96	0.25	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	4046	1/1	0.96	0.09	27,27,27,27	0
83	MG	1	3885	1/1	0.96	0.39	32,32,32,32	0
83	MG	AR	4053	1/1	0.96	0.15	33,33,33,33	0
82	OHX	1	3471	7/7	0.96	0.14	69,69,69,69	0
83	MG	AR	3846	1/1	0.96	0.40	30,30,30,30	0
82	OHX	1	3535	7/7	0.96	0.24	74,74,74,74	0
82	OHX	1	3536	7/7	0.96	0.14	95,95,95,95	0
83	MG	1	3750	1/1	0.96	0.21	23,23,23,23	0
82	OHX	1	3473	7/7	0.96	0.12	86,86,86,86	0
83	MG	1	3892	1/1	0.96	0.23	23,23,23,23	0
83	MG	1	3894	1/1	0.96	0.27	19,19,19,19	0
83	MG	1	4055	1/1	0.96	0.35	31,31,31,31	0
82	OHX	CL	301	7/7	0.96	0.15	97,97,97,97	0
83	MG	AR	4064	1/1	0.96	0.12	36,36,36,36	0
82	OHX	AR	3660	7/7	0.96	0.28	81,81,81,81	0
83	MG	1	4058	1/1	0.96	0.10	28,28,28,28	0
82	OHX	sR	1946	7/7	0.96	0.20	85,85,85,85	0
82	OHX	sR	1949	7/7	0.96	0.12	104,104,104,104	0
83	MG	AR	4069	1/1	0.96	0.06	43,43,43,43	0
83	MG	1	4061	1/1	0.96	0.12	40,40,40,40	0
82	OHX	1	3634	7/7	0.96	0.26	93,93,93,93	0
83	MG	AR	4072	1/1	0.96	0.07	29,29,29,29	0
82	OHX	sR	1951	7/7	0.96	0.12	102,102,102,102	0
82	OHX	sR	1952	7/7	0.96	0.09	121,121,121,121	0
83	MG	AR	3866	1/1	0.96	0.30	27,27,27,27	0
82	OHX	AR	3572	7/7	0.96	0.16	105,105,105,105	0
82	OHX	sR	1956	7/7	0.96	0.10	135,135,135,135	0
82	OHX	sR	1958	7/7	0.96	0.20	84,84,84,84	0
82	OHX	1	3540	7/7	0.96	0.21	78,78,78,78	0
82	OHX	1	3636	7/7	0.96	0.21	93,93,93,93	0
83	MG	AR	4081	1/1	0.96	0.21	35,35,35,35	0
82	OHX	A	1821	7/7	0.96	0.13	95,95,95,95	0
83	MG	CP	503	1/1	0.96	0.06	35,35,35,35	0
82	OHX	AR	3578	7/7	0.96	0.27	87,87,87,87	0
83	MG	1	4073	1/1	0.96	0.09	41,41,41,41	0
82	OHX	A	1835	7/7	0.96	0.18	107,107,107,107	0
82	OHX	A	1840	7/7	0.96	0.21	99,99,99,99	0
83	MG	1	4076	1/1	0.96	0.11	32,32,32,32	0
82	OHX	A	1843	7/7	0.96	0.23	83,83,83,83	0
83	MG	AR	3880	1/1	0.96	0.34	26,26,26,26	0
83	MG	4	229	1/1	0.96	0.15	45,45,45,45	0
82	OHX	sR	1975	7/7	0.96	0.22	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	AR	4096	1/1	0.96	0.07	31,31,31,31	0
83	MG	1	3772	1/1	0.96	0.11	23,23,23,23	0
82	OHX	A	1844	7/7	0.96	0.11	109,109,109,109	0
83	MG	AR	4100	1/1	0.96	0.15	23,23,23,23	0
83	MG	1	3919	1/1	0.96	0.36	22,22,22,22	0
82	OHX	A	1845	7/7	0.96	0.14	110,110,110,110	0
83	MG	AR	4103	1/1	0.96	0.13	36,36,36,36	0
82	OHX	AR	3579	7/7	0.96	0.27	94,94,94,94	0
82	OHX	A	1849	7/7	0.96	0.19	103,103,103,103	0
82	OHX	1	3637	7/7	0.96	0.24	91,91,91,91	0
83	MG	1	4087	1/1	0.96	0.18	24,24,24,24	0
83	MG	j	302	1/1	0.96	0.10	28,28,28,28	0
82	OHX	sR	1982	7/7	0.96	0.14	114,114,114,114	0
83	MG	l	402	1/1	0.96	0.11	46,46,46,46	0
83	MG	sR	2110	1/1	0.96	0.23	39,39,39,39	0
82	OHX	1	3677	7/7	0.96	0.23	82,82,82,82	0
82	OHX	AR	3670	7/7	0.96	0.21	99,99,99,99	0
83	MG	r	302	1/1	0.96	0.18	35,35,35,35	0
82	OHX	AR	3583	7/7	0.96	0.16	86,86,86,86	0
82	OHX	sR	1986	7/7	0.96	0.28	87,87,87,87	0
82	OHX	1	3496	7/7	0.96	0.16	74,74,74,74	0
83	MG	1	3930	1/1	0.96	0.39	44,44,44,44	0
83	MG	v	303	1/1	0.96	0.14	27,27,27,27	0
83	MG	DQ	504	1/1	0.96	0.11	31,31,31,31	0
83	MG	AR	4119	1/1	0.96	0.08	36,36,36,36	0
82	OHX	sR	1988	7/7	0.96	0.22	104,104,104,104	0
83	MG	1	3785	1/1	0.96	0.27	18,18,18,18	0
82	OHX	1	3639	7/7	0.96	0.23	88,88,88,88	0
83	MG	sM	302	1/1	0.96	0.09	38,38,38,38	0
82	OHX	AR	3590	7/7	0.96	0.18	94,94,94,94	0
82	OHX	sR	1991	7/7	0.96	0.25	95,95,95,95	0
83	MG	A	1945	1/1	0.96	0.37	47,47,47,47	0
82	OHX	A	1860	7/7	0.96	0.10	122,122,122,122	0
83	MG	1	3937	1/1	0.96	0.24	30,30,30,30	0
82	OHX	sR	1993	7/7	0.96	0.21	93,93,93,93	0
82	OHX	AR	3675	7/7	0.96	0.11	121,121,121,121	0
82	OHX	3	203	7/7	0.96	0.14	75,75,75,75	0
82	OHX	3	205	7/7	0.96	0.16	94,94,94,94	0
82	OHX	A	1866	7/7	0.96	0.17	100,100,100,100	0
82	OHX	sR	1999	7/7	0.96	0.24	98,98,98,98	0
83	MG	AR	3918	1/1	0.96	0.30	25,25,25,25	0
83	MG	AR	4138	1/1	0.96	0.12	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	4109	1/1	0.96	0.16	45,45,45,45	0
83	MG	AB	202	1/1	0.96	0.21	22,22,22,22	0
83	MG	AB	203	1/1	0.96	0.12	40,40,40,40	0
83	MG	1	3796	1/1	0.96	0.12	28,28,28,28	0
82	OHX	3	206	7/7	0.96	0.19	98,98,98,98	0
82	OHX	sR	2001	7/7	0.96	0.25	83,83,83,83	0
82	OHX	A	1870	7/7	0.96	0.25	92,92,92,92	0
83	MG	1	4115	1/1	0.96	0.10	32,32,32,32	0
82	OHX	AR	3679	7/7	0.96	0.29	88,88,88,88	0
82	OHX	1	3543	7/7	0.96	0.18	98,98,98,98	0
83	MG	1	4118	1/1	0.96	0.15	38,38,38,38	0
82	OHX	AR	3596	7/7	0.96	0.27	81,81,81,81	0
82	OHX	AR	3597	7/7	0.96	0.26	86,86,86,86	0
82	OHX	sR	2008	7/7	0.96	0.14	106,106,106,106	0
83	MG	AR	3934	1/1	0.96	0.16	33,33,33,33	0
83	MG	1	3955	1/1	0.96	0.15	23,23,23,23	0
83	MG	AR	3936	1/1	0.96	0.08	23,23,23,23	0
82	OHX	1	3641	7/7	0.96	0.19	92,92,92,92	0
82	OHX	AR	3685	7/7	0.96	0.23	89,89,89,89	0
82	OHX	AR	3599	7/7	0.96	0.22	93,93,93,93	0
83	MG	AR	3940	1/1	0.96	0.18	25,25,25,25	0
83	MG	AR	4164	1/1	0.96	0.09	36,36,36,36	0
83	MG	sR	2162	1/1	0.96	0.08	25,25,25,25	0
82	OHX	1	3600	7/7	0.96	0.32	78,78,78,78	0
82	OHX	AR	3601	7/7	0.96	0.23	89,89,89,89	0
83	MG	AR	3747	1/1	0.96	0.21	37,37,37,37	0
83	MG	1	3811	1/1	0.96	0.30	32,32,32,32	0
83	MG	1	4131	1/1	0.96	0.13	22,22,22,22	0
82	OHX	A	1882	7/7	0.96	0.23	88,88,88,88	0
83	MG	1	3963	1/1	0.96	0.18	30,30,30,30	0
83	MG	AR	3753	1/1	0.96	0.09	26,26,26,26	0
82	OHX	4	207	7/7	0.96	0.19	92,92,92,92	0
83	MG	AR	4177	1/1	0.96	0.12	33,33,33,33	0
82	OHX	1	3544	7/7	0.96	0.18	97,97,97,97	0
82	OHX	AR	3693	7/7	0.96	0.27	90,90,90,90	0
83	MG	1	3817	1/1	0.96	0.19	25,25,25,25	0
83	MG	1	4138	1/1	0.96	0.07	44,44,44,44	0
83	MG	sR	2178	1/1	0.96	0.13	45,45,45,45	0
82	OHX	A	1887	7/7	0.96	0.12	114,114,114,114	0
82	OHX	A	1888	7/7	0.96	0.21	90,90,90,90	0
82	OHX	AR	3604	7/7	0.96	0.23	97,97,97,97	0
83	MG	AR	4187	1/1	0.96	0.10	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	A	1890	7/7	0.96	0.24	100,100,100,100	0
82	OHX	1	3462	7/7	0.96	0.14	80,80,80,80	0
82	OHX	A	1892	7/7	0.96	0.22	100,100,100,100	0
82	OHX	1	3469	7/7	0.96	0.12	80,80,80,80	0
82	OHX	1	3551	7/7	0.96	0.19	91,91,91,91	0
82	OHX	AR	3608	7/7	0.96	0.18	96,96,96,96	0
82	OHX	AR	3609	7/7	0.96	0.28	76,76,76,76	0
83	MG	AR	3772	1/1	0.96	0.23	23,23,23,23	0
82	OHX	A	1897	7/7	0.96	0.15	119,119,119,119	0
82	OHX	AR	3610	7/7	0.96	0.24	78,78,78,78	0
82	OHX	1	3513	7/7	0.96	0.17	80,80,80,80	0
83	MG	AR	3972	1/1	0.96	0.17	44,44,44,44	0
82	OHX	1	3606	7/7	0.96	0.14	95,95,95,95	0
83	MG	1	4157	1/1	0.96	0.10	41,41,41,41	0
83	MG	AR	3975	1/1	0.96	0.11	31,31,31,31	0
83	MG	1	3832	1/1	0.96	0.35	31,31,31,31	0
82	OHX	AR	3614	7/7	0.96	0.18	96,96,96,96	0
82	OHX	AR	3616	7/7	0.96	0.24	83,83,83,83	0
83	MG	AR	4211	1/1	0.96	0.10	29,29,29,29	0
82	OHX	AR	3617	7/7	0.96	0.24	87,87,87,87	0
82	OHX	1	3607	7/7	0.96	0.21	94,94,94,94	0
83	MG	1	3838	1/1	0.96	0.35	20,20,20,20	0
83	MG	s8	303	1/1	0.96	0.16	42,42,42,42	0
82	OHX	1	3516	7/7	0.96	0.20	81,81,81,81	0
82	OHX	1	3524	7/7	0.96	0.23	78,78,78,78	0
82	OHX	1	3525	7/7	0.96	0.28	86,86,86,86	0
82	OHX	1	3612	7/7	0.96	0.25	87,87,87,87	0
83	MG	c8	202	1/1	0.96	0.36	68,68,68,68	0
82	OHX	AR	3428	7/7	0.96	0.16	57,57,57,57	0
82	OHX	AR	3475	7/7	0.96	0.11	84,84,84,84	0
83	MG	d3	202	1/1	0.96	0.16	41,41,41,41	0
82	OHX	AR	3476	7/7	0.96	0.14	71,71,71,71	0
83	MG	d4	202	1/1	0.96	0.15	43,43,43,43	0
82	OHX	AR	3495	7/7	0.96	0.14	97,97,97,97	0
82	OHX	1	3529	7/7	0.96	0.23	74,74,74,74	0
82	OHX	1	3562	7/7	0.96	0.20	99,99,99,99	0
83	MG	AR	3795	1/1	0.96	0.24	22,22,22,22	0
82	OHX	A	1916	7/7	0.96	0.11	130,130,130,130	0
82	OHX	AR	3629	7/7	0.96	0.29	98,98,98,98	0
84	G5B	AR	4264	26/26	0.96	0.09	29,29,29,29	0
82	OHX	sR	2049	7/7	0.96	0.26	72,72,72,72	0
82	OHX	AR	3502	7/7	0.96	0.12	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	4005	1/1	0.96	0.21	40,40,40,40	0
83	MG	AR	4231	1/1	0.96	0.22	36,36,36,36	0
83	MG	AR	4001	1/1	0.96	0.09	24,24,24,24	0
82	OHX	1	3585	7/7	0.97	0.15	103,103,103,103	0
82	OHX	AR	3509	7/7	0.97	0.09	101,101,101,101	0
82	OHX	1	3624	7/7	0.97	0.23	82,82,82,82	0
83	MG	AR	3826	1/1	0.97	0.32	24,24,24,24	0
82	OHX	1	3549	7/7	0.97	0.25	80,80,80,80	0
82	OHX	AR	3521	7/7	0.97	0.23	74,74,74,74	0
82	OHX	AR	3522	7/7	0.97	0.23	85,85,85,85	0
83	MG	AR	4030	1/1	0.97	0.20	36,36,36,36	0
82	OHX	AR	3525	7/7	0.97	0.19	76,76,76,76	0
82	OHX	AR	3526	7/7	0.97	0.22	82,82,82,82	0
83	MG	AR	4033	1/1	0.97	0.09	25,25,25,25	0
82	OHX	AR	3528	7/7	0.97	0.15	81,81,81,81	0
82	OHX	1	3587	7/7	0.97	0.24	76,76,76,76	0
82	OHX	1	3589	7/7	0.97	0.24	69,69,69,69	0
83	MG	1	4218	1/1	0.97	0.09	23,23,23,23	0
82	OHX	1	3505	7/7	0.97	0.21	74,74,74,74	0
82	OHX	AR	3635	7/7	0.97	0.18	96,96,96,96	0
82	OHX	AR	3533	7/7	0.97	0.17	81,81,81,81	0
83	MG	AR	3840	1/1	0.97	0.12	33,33,33,33	0
82	OHX	AR	3534	7/7	0.97	0.11	106,106,106,106	0
83	MG	AS	212	1/1	0.97	0.19	25,25,25,25	0
82	OHX	AR	3736	7/7	0.97	0.29	53,53,53,53	0
82	OHX	AR	3535	7/7	0.97	0.23	81,81,81,81	0
82	OHX	AR	3738	7/7	0.97	0.29	71,71,71,71	0
83	MG	AR	3845	1/1	0.97	0.23	23,23,23,23	0
82	OHX	AS	206	7/7	0.97	0.13	84,84,84,84	0
83	MG	AR	3847	1/1	0.97	0.34	22,22,22,22	0
82	OHX	AR	3536	7/7	0.97	0.20	76,76,76,76	0
82	OHX	1	3591	7/7	0.97	0.27	88,88,88,88	0
83	MG	AR	3850	1/1	0.97	0.39	22,22,22,22	0
83	MG	1	3734	1/1	0.97	0.23	24,24,24,24	0
82	OHX	AS	209	7/7	0.97	0.24	74,74,74,74	0
82	OHX	1	3507	7/7	0.97	0.10	98,98,98,98	0
82	OHX	AT	205	7/7	0.97	0.16	80,80,80,80	0
83	MG	1	3891	1/1	0.97	0.32	26,26,26,26	0
82	OHX	AT	206	7/7	0.97	0.12	96,96,96,96	0
83	MG	1	3893	1/1	0.97	0.27	22,22,22,22	0
82	OHX	AT	207	7/7	0.97	0.13	91,91,91,91	0
82	OHX	AT	208	7/7	0.97	0.24	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
82	OHX	1	3631	7/7	0.97	0.28	82,82,82,82	0
82	OHX	1	3531	7/7	0.97	0.10	115,115,115,115	0
83	MG	AR	3862	1/1	0.97	0.39	38,38,38,38	0
82	OHX	AT	212	7/7	0.97	0.21	93,93,93,93	0
82	OHX	AR	3543	7/7	0.97	0.20	99,99,99,99	0
82	OHX	AR	3645	7/7	0.97	0.21	90,90,90,90	0
83	MG	1	3903	1/1	0.97	0.33	29,29,29,29	0
83	MG	1	3746	1/1	0.97	0.28	26,26,26,26	0
82	OHX	1	3508	7/7	0.97	0.13	81,81,81,81	0
82	OHX	1	3555	7/7	0.97	0.23	87,87,87,87	0
83	MG	AR	3870	1/1	0.97	0.33	21,21,21,21	0
82	OHX	1	3512	7/7	0.97	0.17	78,78,78,78	0
82	OHX	AR	3547	7/7	0.97	0.26	64,64,64,64	0
82	OHX	AR	3548	7/7	0.97	0.17	85,85,85,85	0
83	MG	1	3910	1/1	0.97	0.32	40,40,40,40	0
82	OHX	T	201	7/7	0.97	0.11	91,91,91,91	0
82	OHX	AR	3549	7/7	0.97	0.23	73,73,73,73	0
82	OHX	1	3719	7/7	0.97	0.15	93,93,93,93	0
82	OHX	AR	3553	7/7	0.97	0.11	104,104,104,104	0
82	OHX	sR	1928	7/7	0.97	0.11	101,101,101,101	0
83	MG	CF	402	1/1	0.97	0.10	27,27,27,27	0
83	MG	AR	4082	1/1	0.97	0.09	25,25,25,25	0
82	OHX	AR	3654	7/7	0.97	0.25	83,83,83,83	0
82	OHX	sR	1939	7/7	0.97	0.11	91,91,91,91	0
83	MG	CI	301	1/1	0.97	0.08	29,29,29,29	0
83	MG	CI	302	1/1	0.97	0.21	35,35,35,35	0
82	OHX	1	3430	7/7	0.97	0.15	62,62,62,62	0
83	MG	AR	4086	1/1	0.97	0.14	38,38,38,38	0
83	MG	AR	4087	1/1	0.97	0.23	49,49,49,49	0
82	OHX	sR	1941	7/7	0.97	0.13	81,81,81,81	0
82	OHX	sR	1944	7/7	0.97	0.09	103,103,103,103	0
82	OHX	sR	1945	7/7	0.97	0.17	81,81,81,81	0
83	MG	l	403	1/1	0.97	0.11	25,25,25,25	0
82	OHX	1	3598	7/7	0.97	0.25	73,73,73,73	0
82	OHX	AR	3556	7/7	0.97	0.20	72,72,72,72	0
82	OHX	CP	501	7/7	0.97	0.19	94,94,94,94	0
83	MG	r	303	1/1	0.97	0.07	37,37,37,37	0
83	MG	AR	4097	1/1	0.97	0.15	32,32,32,32	0
82	OHX	1	3723	7/7	0.97	0.27	72,72,72,72	0
82	OHX	DQ	502	7/7	0.97	0.23	64,64,64,64	0
82	OHX	sR	1953	7/7	0.97	0.14	91,91,91,91	0
83	MG	1	3770	1/1	0.97	0.12	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	sR	1954	7/7	0.97	0.09	127,127,127,127	0
82	OHX	A	1809	7/7	0.97	0.19	94,94,94,94	0
82	OHX	A	1811	7/7	0.97	0.15	89,89,89,89	0
82	OHX	A	1815	7/7	0.97	0.13	101,101,101,101	0
82	OHX	sR	1959	7/7	0.97	0.16	92,92,92,92	0
82	OHX	AR	3559	7/7	0.97	0.23	78,78,78,78	0
82	OHX	sR	1961	7/7	0.97	0.17	86,86,86,86	0
82	OHX	AR	3560	7/7	0.97	0.12	100,100,100,100	0
82	OHX	sR	1963	7/7	0.97	0.22	83,83,83,83	0
82	OHX	sR	1964	7/7	0.97	0.16	97,97,97,97	0
83	MG	sR	2104	1/1	0.97	0.38	37,37,37,37	0
82	OHX	sR	1965	7/7	0.97	0.21	82,82,82,82	0
82	OHX	A	1830	7/7	0.97	0.14	87,87,87,87	0
82	OHX	sR	1967	7/7	0.97	0.20	98,98,98,98	0
82	OHX	1	3678	7/7	0.97	0.20	94,94,94,94	0
83	MG	6	203	1/1	0.97	0.28	40,40,40,40	0
83	MG	9	201	1/1	0.97	0.18	34,34,34,34	0
83	MG	1	4112	1/1	0.97	0.09	36,36,36,36	0
82	OHX	sR	1970	7/7	0.97	0.20	90,90,90,90	0
83	MG	AR	3915	1/1	0.97	0.30	32,32,32,32	0
82	OHX	A	1832	7/7	0.97	0.18	98,98,98,98	0
83	MG	AB	204	1/1	0.97	0.08	25,25,25,25	0
83	MG	AB	205	1/1	0.97	0.18	26,26,26,26	0
83	MG	AR	4125	1/1	0.97	0.31	26,26,26,26	0
83	MG	AB	206	1/1	0.97	0.20	22,22,22,22	0
82	OHX	A	1833	7/7	0.97	0.16	90,90,90,90	0
82	OHX	A	1834	7/7	0.97	0.11	111,111,111,111	0
82	OHX	3	201	7/7	0.97	0.11	76,76,76,76	0
82	OHX	A	1836	7/7	0.97	0.13	84,84,84,84	0
82	OHX	A	1839	7/7	0.97	0.10	105,105,105,105	0
83	MG	AR	4132	1/1	0.97	0.07	29,29,29,29	0
83	MG	1	3951	1/1	0.97	0.18	28,28,28,28	0
82	OHX	sR	1978	7/7	0.97	0.23	81,81,81,81	0
82	OHX	1	3559	7/7	0.97	0.16	98,98,98,98	0
82	OHX	A	1841	7/7	0.97	0.15	106,106,106,106	0
83	MG	sR	2129	1/1	0.97	0.22	39,39,39,39	0
82	OHX	A	1842	7/7	0.97	0.24	88,88,88,88	0
82	OHX	3	204	7/7	0.97	0.17	75,75,75,75	0
82	OHX	1	3560	7/7	0.97	0.12	102,102,102,102	0
82	OHX	1	3482	7/7	0.97	0.11	105,105,105,105	0
83	MG	1	4129	1/1	0.97	0.09	46,46,46,46	0
82	OHX	1	3683	7/7	0.97	0.24	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	A	1847	7/7	0.97	0.19	90,90,90,90	0
82	OHX	A	1848	7/7	0.97	0.11	106,106,106,106	0
82	OHX	1	3537	7/7	0.97	0.23	78,78,78,78	0
82	OHX	A	1850	7/7	0.97	0.17	95,95,95,95	0
82	OHX	AR	3669	7/7	0.97	0.33	65,65,65,65	0
83	MG	AR	3750	1/1	0.97	0.26	25,25,25,25	0
82	OHX	A	1852	7/7	0.97	0.27	92,92,92,92	0
82	OHX	1	3518	7/7	0.97	0.26	72,72,72,72	0
83	MG	AR	3944	1/1	0.97	0.07	26,26,26,26	0
82	OHX	1	3539	7/7	0.97	0.20	87,87,87,87	0
82	OHX	1	3522	7/7	0.97	0.14	79,79,79,79	0
83	MG	AR	4156	1/1	0.97	0.19	50,50,50,50	0
82	OHX	A	1856	7/7	0.97	0.20	103,103,103,103	0
83	MG	1	3970	1/1	0.97	0.09	41,41,41,41	0
83	MG	AR	4160	1/1	0.97	0.07	31,31,31,31	0
82	OHX	sR	1996	7/7	0.97	0.23	102,102,102,102	0
82	OHX	AR	3576	7/7	0.97	0.23	83,83,83,83	0
83	MG	sR	2153	1/1	0.97	0.19	39,39,39,39	0
83	MG	1	3813	1/1	0.97	0.17	30,30,30,30	0
82	OHX	1	3567	7/7	0.97	0.27	80,80,80,80	0
82	OHX	1	3523	7/7	0.97	0.26	82,82,82,82	0
83	MG	AR	3762	1/1	0.97	0.16	33,33,33,33	0
83	MG	1	4149	1/1	0.97	0.06	26,26,26,26	0
82	OHX	1	3647	7/7	0.97	0.20	93,93,93,93	0
83	MG	AR	3765	1/1	0.97	0.34	35,35,35,35	0
82	OHX	A	1861	7/7	0.97	0.10	110,110,110,110	0
82	OHX	A	1862	7/7	0.97	0.22	91,91,91,91	0
82	OHX	1	3472	7/7	0.97	0.12	69,69,69,69	0
83	MG	AR	4174	1/1	0.97	0.07	28,28,28,28	0
82	OHX	1	3503	7/7	0.97	0.15	85,85,85,85	0
83	MG	AR	3962	1/1	0.97	0.15	30,30,30,30	0
83	MG	AR	3963	1/1	0.97	0.07	37,37,37,37	0
82	OHX	AR	3585	7/7	0.97	0.27	78,78,78,78	0
83	MG	AR	3965	1/1	0.97	0.06	30,30,30,30	0
82	OHX	1	3573	7/7	0.97	0.24	81,81,81,81	0
83	MG	sR	2171	1/1	0.97	0.09	71,71,71,71	0
82	OHX	AR	3588	7/7	0.97	0.19	88,88,88,88	0
82	OHX	1	3611	7/7	0.97	0.23	91,91,91,91	0
82	OHX	AR	3683	7/7	0.97	0.27	92,92,92,92	0
83	MG	1	4161	1/1	0.97	0.06	45,45,45,45	0
82	OHX	v	302	7/7	0.97	0.22	85,85,85,85	0
82	OHX	sR	2012	7/7	0.97	0.16	106,106,106,106	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	AR	3591	7/7	0.97	0.24	83,83,83,83	0
82	OHX	1	3526	7/7	0.97	0.11	110,110,110,110	0
83	MG	AR	4192	1/1	0.97	0.21	37,37,37,37	0
82	OHX	A	1876	7/7	0.97	0.22	89,89,89,89	0
82	OHX	y	201	7/7	0.97	0.22	97,97,97,97	0
83	MG	AR	4196	1/1	0.97	0.07	29,29,29,29	0
82	OHX	1	3576	7/7	0.97	0.23	74,74,74,74	0
82	OHX	AE	201	7/7	0.97	0.13	91,91,91,91	0
83	MG	sR	2186	1/1	0.97	0.18	41,41,41,41	0
83	MG	AR	3785	1/1	0.97	0.11	36,36,36,36	0
82	OHX	AG	201	7/7	0.97	0.27	83,83,83,83	0
83	MG	1	3835	1/1	0.97	0.26	38,38,38,38	0
82	OHX	AR	3692	7/7	0.97	0.25	83,83,83,83	0
82	OHX	1	3697	7/7	0.97	0.25	74,74,74,74	0
83	MG	1	3999	1/1	0.97	0.15	36,36,36,36	0
82	OHX	1	3577	7/7	0.97	0.15	81,81,81,81	0
82	OHX	AR	3441	7/7	0.97	0.11	65,65,65,65	0
82	OHX	AR	3445	7/7	0.97	0.11	67,67,67,67	0
83	MG	AR	4209	1/1	0.97	0.12	44,44,44,44	0
82	OHX	A	1886	7/7	0.97	0.10	123,123,123,123	0
82	OHX	AR	3450	7/7	0.97	0.11	83,83,83,83	0
83	MG	AR	3796	1/1	0.97	0.21	24,24,24,24	0
82	OHX	AR	3457	7/7	0.97	0.12	70,70,70,70	0
83	MG	AR	3993	1/1	0.97	0.27	39,39,39,39	0
83	MG	sR	2202	1/1	0.97	0.42	49,49,49,49	0
82	OHX	AR	3460	7/7	0.97	0.12	53,53,53,53	0
83	MG	s1	302	1/1	0.97	0.12	63,63,63,63	0
82	OHX	AR	3467	7/7	0.97	0.12	85,85,85,85	0
82	OHX	AR	3468	7/7	0.97	0.15	64,64,64,64	0
83	MG	1	4009	1/1	0.97	0.27	40,40,40,40	0
82	OHX	AR	3473	7/7	0.97	0.16	62,62,62,62	0
83	MG	AR	3999	1/1	0.97	0.13	27,27,27,27	0
82	OHX	1	3578	7/7	0.97	0.27	79,79,79,79	0
82	OHX	1	3546	7/7	0.97	0.12	107,107,107,107	0
83	MG	1	4013	1/1	0.97	0.06	31,31,31,31	0
82	OHX	AR	3478	7/7	0.97	0.12	70,70,70,70	0
83	MG	1	4015	1/1	0.97	0.14	38,38,38,38	0
82	OHX	AR	3481	7/7	0.97	0.14	78,78,78,78	0
83	MG	1	4017	1/1	0.97	0.16	35,35,35,35	0
83	MG	1	3853	1/1	0.97	0.35	31,31,31,31	0
82	OHX	AR	3484	7/7	0.97	0.20	75,75,75,75	0
82	OHX	AR	3489	7/7	0.97	0.10	94,94,94,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	AR	3709	7/7	0.97	0.21	77,77,77,77	0
82	OHX	AR	3493	7/7	0.97	0.14	77,77,77,77	0
82	OHX	AR	3615	7/7	0.97	0.30	73,73,73,73	0
82	OHX	AR	3494	7/7	0.97	0.23	71,71,71,71	0
83	MG	AR	4015	1/1	0.97	0.20	42,42,42,42	0
82	OHX	1	3617	7/7	0.97	0.19	96,96,96,96	0
82	OHX	1	3581	7/7	0.97	0.14	107,107,107,107	0
85	ZN	g	501	1/1	0.97	0.06	102,102,102,102	0
82	OHX	1	3548	7/7	0.97	0.15	99,99,99,99	0
82	OHX	1	3583	7/7	0.97	0.24	83,83,83,83	0
82	OHX	AR	3504	7/7	0.97	0.23	55,55,55,55	0
82	OHX	1	3584	7/7	0.97	0.14	102,102,102,102	0
83	MG	1	4086	1/1	0.98	0.05	28,28,28,28	0
82	OHX	4	204	7/7	0.98	0.11	90,90,90,90	0
82	OHX	4	205	7/7	0.98	0.15	94,94,94,94	0
82	OHX	4	206	7/7	0.98	0.23	78,78,78,78	0
82	OHX	CQ	201	7/7	0.98	0.14	70,70,70,70	0
82	OHX	AR	3542	7/7	0.98	0.21	64,64,64,64	0
82	OHX	sR	1905	7/7	0.98	0.13	59,59,59,59	0
82	OHX	sR	1908	7/7	0.98	0.13	60,60,60,60	0
82	OHX	CX	202	7/7	0.98	0.19	81,81,81,81	0
82	OHX	sR	1920	7/7	0.98	0.10	80,80,80,80	0
82	OHX	sR	1921	7/7	0.98	0.12	95,95,95,95	0
83	MG	1	3757	1/1	0.98	0.20	26,26,26,26	0
82	OHX	sR	1926	7/7	0.98	0.09	85,85,85,85	0
82	OHX	DH	201	7/7	0.98	0.16	82,82,82,82	0
83	MG	AR	3898	1/1	0.98	0.37	26,26,26,26	0
82	OHX	sR	1929	7/7	0.98	0.08	106,106,106,106	0
82	OHX	sR	1931	7/7	0.98	0.13	79,79,79,79	0
82	OHX	1	3520	7/7	0.98	0.13	81,81,81,81	0
82	OHX	sR	1933	7/7	0.98	0.13	70,70,70,70	0
83	MG	AR	4092	1/1	0.98	0.11	36,36,36,36	0
82	OHX	sR	1934	7/7	0.98	0.12	86,86,86,86	0
82	OHX	sR	1936	7/7	0.98	0.14	75,75,75,75	0
82	OHX	sR	1938	7/7	0.98	0.10	90,90,90,90	0
82	OHX	A	1803	7/7	0.98	0.18	74,74,74,74	0
82	OHX	A	1806	7/7	0.98	0.12	78,78,78,78	0
82	OHX	A	1807	7/7	0.98	0.11	83,83,83,83	0
82	OHX	sR	1942	7/7	0.98	0.14	85,85,85,85	0
82	OHX	sR	1943	7/7	0.98	0.14	87,87,87,87	0
82	OHX	A	1808	7/7	0.98	0.13	81,81,81,81	0
82	OHX	1	3521	7/7	0.98	0.14	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
83	MG	CG	304	1/1	0.98	0.26	35,35,35,35	0
83	MG	AR	3913	1/1	0.98	0.20	26,26,26,26	0
82	OHX	1	3434	7/7	0.98	0.10	65,65,65,65	0
82	OHX	sR	1947	7/7	0.98	0.11	93,93,93,93	0
83	MG	1	3943	1/1	0.98	0.14	39,39,39,39	0
82	OHX	sR	1948	7/7	0.98	0.16	80,80,80,80	0
82	OHX	A	1812	7/7	0.98	0.13	87,87,87,87	0
83	MG	AR	3919	1/1	0.98	0.36	22,22,22,22	0
82	OHX	A	1813	7/7	0.98	0.13	83,83,83,83	0
82	OHX	4	210	7/7	0.98	0.15	103,103,103,103	0
82	OHX	A	1816	7/7	0.98	0.11	83,83,83,83	0
82	OHX	A	1817	7/7	0.98	0.11	76,76,76,76	0
82	OHX	1	3439	7/7	0.98	0.10	64,64,64,64	0
83	MG	1	4125	1/1	0.98	0.23	24,24,24,24	0
82	OHX	1	3682	7/7	0.98	0.18	77,77,77,77	0
82	OHX	A	1822	7/7	0.98	0.11	77,77,77,77	0
82	OHX	sR	1957	7/7	0.98	0.11	89,89,89,89	0
82	OHX	A	1824	7/7	0.98	0.12	91,91,91,91	0
82	OHX	A	1825	7/7	0.98	0.07	104,104,104,104	0
82	OHX	A	1826	7/7	0.98	0.10	93,93,93,93	0
83	MG	AR	3746	1/1	0.98	0.12	24,24,24,24	0
83	MG	CR	204	1/1	0.98	0.14	40,40,40,40	0
83	MG	AR	4123	1/1	0.98	0.11	28,28,28,28	0
82	OHX	A	1827	7/7	0.98	0.10	96,96,96,96	0
82	OHX	A	1828	7/7	0.98	0.14	86,86,86,86	0
82	OHX	A	1829	7/7	0.98	0.16	82,82,82,82	0
82	OHX	1	3441	7/7	0.98	0.10	66,66,66,66	0
82	OHX	AR	3550	7/7	0.98	0.15	91,91,91,91	0
82	OHX	1	3476	7/7	0.98	0.17	68,68,68,68	0
82	OHX	AR	3552	7/7	0.98	0.19	78,78,78,78	0
83	MG	1	4139	1/1	0.98	0.12	44,44,44,44	0
83	MG	CY	201	1/1	0.98	0.04	69,69,69,69	0
82	OHX	sR	1968	7/7	0.98	0.19	82,82,82,82	0
82	OHX	k	401	7/7	0.98	0.18	87,87,87,87	0
82	OHX	1	3442	7/7	0.98	0.12	71,71,71,71	0
82	OHX	1	3527	7/7	0.98	0.13	92,92,92,92	0
83	MG	AR	4136	1/1	0.98	0.11	34,34,34,34	0
83	MG	1	3800	1/1	0.98	0.15	25,25,25,25	0
82	OHX	A	1837	7/7	0.98	0.13	102,102,102,102	0
82	OHX	A	1838	7/7	0.98	0.15	78,78,78,78	0
83	MG	1	4147	1/1	0.98	0.13	56,56,56,56	0
82	OHX	sR	1974	7/7	0.98	0.17	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	1	3580	7/7	0.98	0.15	95,95,95,95	0
82	OHX	1	3528	7/7	0.98	0.09	102,102,102,102	0
82	OHX	1	3425	7/7	0.98	0.10	58,58,58,58	0
82	OHX	1	3481	7/7	0.98	0.14	83,83,83,83	0
82	OHX	1	3445	7/7	0.98	0.08	71,71,71,71	0
82	OHX	AR	3562	7/7	0.98	0.22	90,90,90,90	0
83	MG	1	4155	1/1	0.98	0.08	42,42,42,42	0
82	OHX	1	3447	7/7	0.98	0.10	65,65,65,65	0
82	OHX	AK	103	7/7	0.98	0.13	73,73,73,73	0
82	OHX	1	3448	7/7	0.98	0.10	67,67,67,67	0
82	OHX	1	3449	7/7	0.98	0.10	76,76,76,76	0
82	OHX	AR	3431	7/7	0.98	0.13	58,58,58,58	0
82	OHX	AR	3568	7/7	0.98	0.20	82,82,82,82	0
82	OHX	AR	3569	7/7	0.98	0.15	90,90,90,90	0
83	MG	AR	4157	1/1	0.98	0.06	31,31,31,31	0
82	OHX	AR	3433	7/7	0.98	0.10	53,53,53,53	0
82	OHX	1	3588	7/7	0.98	0.13	110,110,110,110	0
82	OHX	AR	3442	7/7	0.98	0.10	63,63,63,63	0
82	OHX	AR	3444	7/7	0.98	0.09	62,62,62,62	0
82	OHX	1	3487	7/7	0.98	0.17	68,68,68,68	0
82	OHX	AR	3575	7/7	0.98	0.21	88,88,88,88	0
82	OHX	AR	3447	7/7	0.98	0.11	54,54,54,54	0
83	MG	1	4170	1/1	0.98	0.10	49,49,49,49	0
82	OHX	AR	3577	7/7	0.98	0.20	86,86,86,86	0
82	OHX	AR	3448	7/7	0.98	0.09	72,72,72,72	0
82	OHX	1	3489	7/7	0.98	0.12	78,78,78,78	0
83	MG	AR	4169	1/1	0.98	0.11	29,29,29,29	0
82	OHX	AR	3691	7/7	0.98	0.18	62,62,62,62	0
82	OHX	AR	3451	7/7	0.98	0.11	64,64,64,64	0
83	MG	1	3997	1/1	0.98	0.06	56,56,56,56	0
82	OHX	AR	3452	7/7	0.98	0.13	92,92,92,92	0
83	MG	AR	3979	1/1	0.98	0.15	37,37,37,37	0
83	MG	AR	4175	1/1	0.98	0.09	49,49,49,49	0
82	OHX	AR	3453	7/7	0.98	0.10	80,80,80,80	0
82	OHX	AR	3584	7/7	0.98	0.19	77,77,77,77	0
82	OHX	sR	2003	7/7	0.98	0.23	83,83,83,83	0
83	MG	AR	4179	1/1	0.98	0.07	41,41,41,41	0
82	OHX	A	1867	7/7	0.98	0.18	82,82,82,82	0
83	MG	AR	4181	1/1	0.98	0.04	29,29,29,29	0
82	OHX	A	1868	7/7	0.98	0.15	93,93,93,93	0
82	OHX	AR	3455	7/7	0.98	0.09	72,72,72,72	0
82	OHX	AR	3586	7/7	0.98	0.20	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	AR	3456	7/7	0.98	0.12	70,70,70,70	0
82	OHX	A	1872	7/7	0.98	0.08	125,125,125,125	0
82	OHX	1	3490	7/7	0.98	0.17	70,70,70,70	0
82	OHX	AR	3459	7/7	0.98	0.11	69,69,69,69	0
82	OHX	1	3491	7/7	0.98	0.19	56,56,56,56	0
82	OHX	AR	3464	7/7	0.98	0.10	72,72,72,72	0
82	OHX	1	3492	7/7	0.98	0.10	86,86,86,86	0
82	OHX	1	3541	7/7	0.98	0.24	78,78,78,78	0
83	MG	1	3845	1/1	0.98	0.05	26,26,26,26	0
82	OHX	AR	3469	7/7	0.98	0.09	72,72,72,72	0
82	OHX	AR	3470	7/7	0.98	0.10	74,74,74,74	0
82	OHX	1	3493	7/7	0.98	0.12	85,85,85,85	0
82	OHX	AR	3474	7/7	0.98	0.13	56,56,56,56	0
82	OHX	1	3451	7/7	0.98	0.10	75,75,75,75	0
82	OHX	1	3452	7/7	0.98	0.10	77,77,77,77	0
82	OHX	1	3498	7/7	0.98	0.14	76,76,76,76	0
82	OHX	AR	3480	7/7	0.98	0.11	71,71,71,71	0
82	OHX	1	3416	7/7	0.98	0.12	56,56,56,56	0
83	MG	AR	4204	1/1	0.98	0.12	49,49,49,49	0
82	OHX	AR	3482	7/7	0.98	0.13	66,66,66,66	0
83	MG	1	4025	1/1	0.98	0.12	42,42,42,42	0
83	MG	AR	4007	1/1	0.98	0.21	35,35,35,35	0
83	MG	1	4026	1/1	0.98	0.13	32,32,32,32	0
82	OHX	1	3547	7/7	0.98	0.17	90,90,90,90	0
82	OHX	AR	3487	7/7	0.98	0.14	64,64,64,64	0
82	OHX	1	3500	7/7	0.98	0.19	73,73,73,73	0
82	OHX	AR	3491	7/7	0.98	0.12	77,77,77,77	0
83	MG	1	4031	1/1	0.98	0.14	24,24,24,24	0
82	OHX	1	3457	7/7	0.98	0.10	57,57,57,57	0
83	MG	AR	3828	1/1	0.98	0.24	25,25,25,25	0
82	OHX	1	3502	7/7	0.98	0.13	74,74,74,74	0
82	OHX	1	3657	7/7	0.98	0.21	89,89,89,89	0
82	OHX	1	3458	7/7	0.98	0.09	64,64,64,64	0
82	OHX	AR	3723	7/7	0.98	0.17	74,74,74,74	0
82	OHX	AR	3497	7/7	0.98	0.22	69,69,69,69	0
82	OHX	AR	3498	7/7	0.98	0.08	95,95,95,95	0
82	OHX	AR	3499	7/7	0.98	0.10	82,82,82,82	0
82	OHX	1	3504	7/7	0.98	0.17	83,83,83,83	0
83	MG	AR	4024	1/1	0.98	0.09	42,42,42,42	0
82	OHX	1	3553	7/7	0.98	0.21	85,85,85,85	0
82	OHX	AR	3503	7/7	0.98	0.23	73,73,73,73	0
83	MG	1	4222	1/1	0.98	0.27	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	1	3460	7/7	0.98	0.11	88,88,88,88	0
82	OHX	1	3506	7/7	0.98	0.19	73,73,73,73	0
82	OHX	AR	3506	7/7	0.98	0.16	70,70,70,70	0
82	OHX	A	1907	7/7	0.98	0.21	88,88,88,88	0
82	OHX	AR	3733	7/7	0.98	0.25	76,76,76,76	0
82	OHX	1	3431	7/7	0.98	0.12	64,64,64,64	0
82	OHX	1	3463	7/7	0.98	0.09	83,83,83,83	0
82	OHX	AR	3511	7/7	0.98	0.16	69,69,69,69	0
83	MG	AR	4036	1/1	0.98	0.18	44,44,44,44	0
82	OHX	AR	3512	7/7	0.98	0.10	85,85,85,85	0
82	OHX	AR	3513	7/7	0.98	0.18	77,77,77,77	0
82	OHX	AS	202	7/7	0.98	0.14	71,71,71,71	0
82	OHX	AS	203	7/7	0.98	0.16	72,72,72,72	0
82	OHX	AS	204	7/7	0.98	0.19	69,69,69,69	0
82	OHX	AS	205	7/7	0.98	0.10	79,79,79,79	0
82	OHX	AR	3514	7/7	0.98	0.18	81,81,81,81	0
82	OHX	1	3558	7/7	0.98	0.19	74,74,74,74	0
82	OHX	AR	3516	7/7	0.98	0.17	70,70,70,70	0
82	OHX	AR	3517	7/7	0.98	0.18	76,76,76,76	0
82	OHX	AR	3518	7/7	0.98	0.14	80,80,80,80	0
82	OHX	AT	204	7/7	0.98	0.14	78,78,78,78	0
82	OHX	1	3509	7/7	0.98	0.17	77,77,77,77	0
82	OHX	AR	3520	7/7	0.98	0.09	96,96,96,96	0
83	MG	4	223	1/1	0.98	0.18	30,30,30,30	0
82	OHX	1	3721	7/7	0.98	0.26	55,55,55,55	0
82	OHX	1	3510	7/7	0.98	0.19	64,64,64,64	0
82	OHX	AT	209	7/7	0.98	0.12	95,95,95,95	0
82	OHX	AR	3523	7/7	0.98	0.22	74,74,74,74	0
83	MG	1	3897	1/1	0.98	0.34	26,26,26,26	0
82	OHX	AR	3524	7/7	0.98	0.13	84,84,84,84	0
82	OHX	1	3511	7/7	0.98	0.20	67,67,67,67	0
83	MG	1	4072	1/1	0.98	0.04	32,32,32,32	0
82	OHX	1	3466	7/7	0.98	0.10	74,74,74,74	0
82	OHX	AR	3527	7/7	0.98	0.09	88,88,88,88	0
82	OHX	1	3467	7/7	0.98	0.10	84,84,84,84	0
82	OHX	3	202	7/7	0.98	0.19	76,76,76,76	0
82	OHX	CE	401	7/7	0.98	0.13	76,76,76,76	0
82	OHX	1	3433	7/7	0.98	0.13	71,71,71,71	0
82	OHX	1	3517	7/7	0.98	0.19	63,63,63,63	0
82	OHX	1	3566	7/7	0.98	0.22	77,77,77,77	0
82	OHX	1	3470	7/7	0.98	0.11	76,76,76,76	0
82	OHX	1	3568	7/7	0.98	0.08	115,115,115,115	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	1	3569	7/7	0.98	0.20	70,70,70,70	0
82	OHX	AR	3537	7/7	0.98	0.11	67,67,67,67	0
82	OHX	1	3519	7/7	0.98	0.13	94,94,94,94	0
82	OHX	AR	3486	7/7	0.99	0.10	69,69,69,69	0
82	OHX	1	3621	7/7	0.99	0.20	64,64,64,64	0
82	OHX	AR	3488	7/7	0.99	0.10	72,72,72,72	0
82	OHX	1	3465	7/7	0.99	0.09	66,66,66,66	0
82	OHX	A	1819	7/7	0.99	0.08	81,81,81,81	0
82	OHX	A	1820	7/7	0.99	0.09	81,81,81,81	0
82	OHX	1	3437	7/7	0.99	0.10	60,60,60,60	0
82	OHX	AR	3492	7/7	0.99	0.14	66,66,66,66	0
82	OHX	A	1823	7/7	0.99	0.09	83,83,83,83	0
82	OHX	1	3438	7/7	0.99	0.10	54,54,54,54	0
82	OHX	1	3404	7/7	0.99	0.15	45,45,45,45	0
82	OHX	w	201	7/7	0.99	0.14	80,80,80,80	0
82	OHX	1	3440	7/7	0.99	0.09	70,70,70,70	0
82	OHX	1	3417	7/7	0.99	0.11	49,49,49,49	0
82	OHX	1	3419	7/7	0.99	0.10	55,55,55,55	0
82	OHX	2	201	7/7	0.99	0.08	53,53,53,53	0
82	OHX	AC	101	7/7	0.99	0.10	47,47,47,47	0
83	MG	AR	4261	1/1	0.99	0.20	29,29,29,29	0
82	OHX	AR	3501	7/7	0.99	0.16	65,65,65,65	0
82	OHX	1	3443	7/7	0.99	0.11	54,54,54,54	0
82	OHX	sR	1901	7/7	0.99	0.13	47,47,47,47	0
82	OHX	sR	1902	7/7	0.99	0.17	59,59,59,59	0
82	OHX	sR	1904	7/7	0.99	0.09	61,61,61,61	0
82	OHX	1	3474	7/7	0.99	0.08	78,78,78,78	0
82	OHX	sR	1907	7/7	0.99	0.12	59,59,59,59	0
82	OHX	AK	102	7/7	0.99	0.10	71,71,71,71	0
82	OHX	sR	1909	7/7	0.99	0.13	72,72,72,72	0
82	OHX	sR	1910	7/7	0.99	0.10	52,52,52,52	0
82	OHX	sR	1911	7/7	0.99	0.11	65,65,65,65	0
82	OHX	sR	1912	7/7	0.99	0.08	62,62,62,62	0
82	OHX	sR	1913	7/7	0.99	0.08	64,64,64,64	0
82	OHX	sR	1914	7/7	0.99	0.11	80,80,80,80	0
82	OHX	sR	1915	7/7	0.99	0.09	64,64,64,64	0
82	OHX	sR	1916	7/7	0.99	0.08	63,63,63,63	0
82	OHX	sR	1917	7/7	0.99	0.07	67,67,67,67	0
82	OHX	sR	1918	7/7	0.99	0.08	67,67,67,67	0
82	OHX	1	3475	7/7	0.99	0.14	70,70,70,70	0
82	OHX	1	3420	7/7	0.99	0.10	53,53,53,53	0
82	OHX	AR	3507	7/7	0.99	0.15	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	sR	1922	7/7	0.99	0.13	66,66,66,66	0
82	OHX	sR	1923	7/7	0.99	0.12	70,70,70,70	0
82	OHX	sR	1924	7/7	0.99	0.08	78,78,78,78	0
82	OHX	sR	1925	7/7	0.99	0.10	67,67,67,67	0
82	OHX	AR	3401	7/7	0.99	0.13	37,37,37,37	0
82	OHX	sR	1927	7/7	0.99	0.18	67,67,67,67	0
82	OHX	AR	3404	7/7	0.99	0.11	40,40,40,40	0
82	OHX	AR	3510	7/7	0.99	0.09	49,49,49,49	0
82	OHX	sR	1930	7/7	0.99	0.09	64,64,64,64	0
82	OHX	AR	3405	7/7	0.99	0.12	41,41,41,41	0
82	OHX	AR	3406	7/7	0.99	0.09	45,45,45,45	0
82	OHX	AR	3612	7/7	0.99	0.17	63,63,63,63	0
82	OHX	AR	3407	7/7	0.99	0.12	44,44,44,44	0
82	OHX	sR	1935	7/7	0.99	0.14	71,71,71,71	0
83	MG	AR	4153	1/1	0.99	0.04	44,44,44,44	0
82	OHX	AR	3410	7/7	0.99	0.09	35,35,35,35	0
82	OHX	sR	1937	7/7	0.99	0.09	81,81,81,81	0
82	OHX	AR	3411	7/7	0.99	0.15	52,52,52,52	0
82	OHX	AR	3412	7/7	0.99	0.08	47,47,47,47	0
82	OHX	AR	3414	7/7	0.99	0.10	46,46,46,46	0
82	OHX	AR	3415	7/7	0.99	0.11	50,50,50,50	0
82	OHX	AR	3416	7/7	0.99	0.13	49,49,49,49	0
82	OHX	AR	3418	7/7	0.99	0.07	49,49,49,49	0
82	OHX	AR	3420	7/7	0.99	0.08	54,54,54,54	0
82	OHX	AR	3421	7/7	0.99	0.10	52,52,52,52	0
82	OHX	AR	3424	7/7	0.99	0.10	52,52,52,52	0
82	OHX	AR	3425	7/7	0.99	0.12	55,55,55,55	0
82	OHX	AR	3426	7/7	0.99	0.07	50,50,50,50	0
82	OHX	1	3477	7/7	0.99	0.07	82,82,82,82	0
82	OHX	AR	3430	7/7	0.99	0.06	55,55,55,55	0
82	OHX	1	3514	7/7	0.99	0.14	57,57,57,57	0
82	OHX	AR	3432	7/7	0.99	0.07	48,48,48,48	0
82	OHX	1	3515	7/7	0.99	0.10	85,85,85,85	0
82	OHX	AR	3531	7/7	0.99	0.17	61,61,61,61	0
82	OHX	AR	3434	7/7	0.99	0.13	72,72,72,72	0
82	OHX	AR	3435	7/7	0.99	0.05	56,56,56,56	0
82	OHX	AR	3436	7/7	0.99	0.06	57,57,57,57	0
83	MG	1	3899	1/1	0.99	0.28	17,17,17,17	0
82	OHX	AR	3437	7/7	0.99	0.07	56,56,56,56	0
82	OHX	AR	3438	7/7	0.99	0.06	53,53,53,53	0
82	OHX	AR	3439	7/7	0.99	0.11	66,66,66,66	0
82	OHX	AR	3440	7/7	0.99	0.08	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
82	OHX	AS	201	7/7	0.99	0.10	67,67,67,67	0
82	OHX	1	3478	7/7	0.99	0.10	70,70,70,70	0
82	OHX	1	3422	7/7	0.99	0.12	64,64,64,64	0
82	OHX	AR	3443	7/7	0.99	0.15	72,72,72,72	0
82	OHX	1	3446	7/7	0.99	0.08	64,64,64,64	0
82	OHX	1	3424	7/7	0.99	0.14	63,63,63,63	0
82	OHX	AR	3446	7/7	0.99	0.07	59,59,59,59	0
82	OHX	1	3406	7/7	0.99	0.14	45,45,45,45	0
82	OHX	1	3427	7/7	0.99	0.09	59,59,59,59	0
83	MG	AR	3766	1/1	0.99	0.06	27,27,27,27	0
82	OHX	AR	3449	7/7	0.99	0.09	75,75,75,75	0
82	OHX	AT	202	7/7	0.99	0.08	57,57,57,57	0
82	OHX	AT	203	7/7	0.99	0.10	84,84,84,84	0
82	OHX	1	3484	7/7	0.99	0.07	65,65,65,65	0
83	MG	AR	4195	1/1	0.99	0.22	28,28,28,28	0
82	OHX	1	3450	7/7	0.99	0.12	62,62,62,62	0
82	OHX	1	3429	7/7	0.99	0.13	60,60,60,60	0
82	OHX	1	3407	7/7	0.99	0.08	40,40,40,40	0
82	OHX	AR	3454	7/7	0.99	0.12	55,55,55,55	0
82	OHX	1	3488	7/7	0.99	0.16	69,69,69,69	0
82	OHX	1	3409	7/7	0.99	0.10	49,49,49,49	0
82	OHX	1	3455	7/7	0.99	0.10	68,68,68,68	0
82	OHX	AR	3458	7/7	0.99	0.08	61,61,61,61	0
82	OHX	1	3456	7/7	0.99	0.07	70,70,70,70	0
82	OHX	AR	3558	7/7	0.99	0.15	78,78,78,78	0
82	OHX	1	3432	7/7	0.99	0.07	61,61,61,61	0
82	OHX	AR	3461	7/7	0.99	0.09	57,57,57,57	0
82	OHX	AR	3462	7/7	0.99	0.09	63,63,63,63	0
82	OHX	AR	3463	7/7	0.99	0.08	72,72,72,72	0
82	OHX	1	3410	7/7	0.99	0.10	46,46,46,46	0
82	OHX	AR	3465	7/7	0.99	0.17	60,60,60,60	0
82	OHX	AR	3466	7/7	0.99	0.11	74,74,74,74	0
82	OHX	4	201	7/7	0.99	0.12	44,44,44,44	0
82	OHX	CH	201	7/7	0.99	0.13	43,43,43,43	0
82	OHX	4	202	7/7	0.99	0.09	61,61,61,61	0
82	OHX	4	203	7/7	0.99	0.14	71,71,71,71	0
82	OHX	1	3494	7/7	0.99	0.12	73,73,73,73	0
82	OHX	AR	3471	7/7	0.99	0.08	78,78,78,78	0
82	OHX	AR	3472	7/7	0.99	0.14	66,66,66,66	0
82	OHX	1	3533	7/7	0.99	0.14	64,64,64,64	0
82	OHX	1	3459	7/7	0.99	0.11	60,60,60,60	0
82	OHX	1	3574	7/7	0.99	0.10	100,100,100,100	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	CX	201	7/7	0.99	0.08	67,67,67,67	0
82	OHX	1	3414	7/7	0.99	0.11	52,52,52,52	0
82	OHX	DD	101	7/7	0.99	0.12	50,50,50,50	0
82	OHX	DG	201	7/7	0.99	0.19	68,68,68,68	0
82	OHX	AR	3477	7/7	0.99	0.10	79,79,79,79	0
82	OHX	1	3497	7/7	0.99	0.13	45,45,45,45	0
82	OHX	A	1801	7/7	0.99	0.16	64,64,64,64	0
82	OHX	A	1802	7/7	0.99	0.11	68,68,68,68	0
82	OHX	AR	3479	7/7	0.99	0.14	58,58,58,58	0
82	OHX	A	1804	7/7	0.99	0.09	70,70,70,70	0
82	OHX	A	1805	7/7	0.99	0.10	63,63,63,63	0
82	OHX	1	3461	7/7	0.99	0.10	68,68,68,68	0
82	OHX	1	3435	7/7	0.99	0.08	51,51,51,51	0
82	OHX	AR	3581	7/7	0.99	0.17	69,69,69,69	0
82	OHX	1	3436	7/7	0.99	0.07	60,60,60,60	0
85	ZN	b	201	1/1	0.99	0.02	71,71,71,71	0
82	OHX	A	1810	7/7	0.99	0.09	81,81,81,81	0
82	OHX	AR	3483	7/7	0.99	0.12	59,59,59,59	0
82	OHX	1	3464	7/7	0.99	0.10	62,62,62,62	0
85	ZN	d9	101	1/1	0.99	0.05	69,69,69,69	0
82	OHX	AR	3485	7/7	0.99	0.15	69,69,69,69	0
82	OHX	A	1814	7/7	0.99	0.07	76,76,76,76	0
83	MG	1	4103	1/1	0.99	0.10	47,47,47,47	0
82	OHX	1	3412	7/7	1.00	0.05	46,46,46,46	0
82	OHX	AR	3417	7/7	1.00	0.08	55,55,55,55	0
82	OHX	1	3468	7/7	1.00	0.07	46,46,46,46	0
82	OHX	AR	3419	7/7	1.00	0.07	49,49,49,49	0
82	OHX	1	3453	7/7	1.00	0.06	61,61,61,61	0
82	OHX	AT	201	7/7	1.00	0.11	45,45,45,45	0
82	OHX	1	3413	7/7	1.00	0.09	51,51,51,51	0
82	OHX	sR	1903	7/7	1.00	0.09	50,50,50,50	0
82	OHX	AR	3422	7/7	1.00	0.05	49,49,49,49	0
82	OHX	AR	3423	7/7	1.00	0.09	48,48,48,48	0
82	OHX	sR	1906	7/7	1.00	0.11	56,56,56,56	0
82	OHX	1	3426	7/7	1.00	0.06	53,53,53,53	0
82	OHX	1	3402	7/7	1.00	0.11	40,40,40,40	0
82	OHX	1	3428	7/7	1.00	0.06	55,55,55,55	0
82	OHX	AR	3427	7/7	1.00	0.06	47,47,47,47	0
82	OHX	1	3415	7/7	1.00	0.05	47,47,47,47	0
82	OHX	AR	3429	7/7	1.00	0.06	57,57,57,57	0
82	OHX	1	3403	7/7	1.00	0.11	38,38,38,38	0
82	OHX	AR	3402	7/7	1.00	0.12	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	OHX	AR	3490	7/7	1.00	0.07	47,47,47,47	0
82	OHX	AR	3403	7/7	1.00	0.11	34,34,34,34	0
82	OHX	1	3408	7/7	1.00	0.10	49,49,49,49	0
82	OHX	1	3418	7/7	1.00	0.05	45,45,45,45	0
82	OHX	n	201	7/7	1.00	0.10	43,43,43,43	0
82	OHX	1	3401	7/7	1.00	0.11	33,33,33,33	0
85	ZN	AK	101	1/1	1.00	0.02	27,27,27,27	0
85	ZN	AN	500	1/1	1.00	0.01	40,40,40,40	0
85	ZN	AP	501	1/1	1.00	0.05	54,54,54,54	0
85	ZN	AQ	501	1/1	1.00	0.01	43,43,43,43	0
85	ZN	DL	101	1/1	1.00	0.02	35,35,35,35	0
85	ZN	DO	201	1/1	1.00	0.01	29,29,29,29	0
85	ZN	DQ	501	1/1	1.00	0.04	51,51,51,51	0
85	ZN	DR	501	1/1	1.00	0.02	49,49,49,49	0
82	OHX	AR	3408	7/7	1.00	0.11	45,45,45,45	0
82	OHX	AR	3409	7/7	1.00	0.10	44,44,44,44	0
85	ZN	e	101	1/1	1.00	0.01	70,70,70,70	0
82	OHX	v	301	7/7	1.00	0.08	43,43,43,43	0
85	ZN	d6	201	1/1	1.00	0.03	44,44,44,44	0
82	OHX	1	3405	7/7	1.00	0.09	39,39,39,39	0
82	OHX	1	3421	7/7	1.00	0.08	54,54,54,54	0
82	OHX	AR	3413	7/7	1.00	0.06	43,43,43,43	0
82	OHX	1	3411	7/7	1.00	0.09	49,49,49,49	0
82	OHX	1	3423	7/7	1.00	0.07	53,53,53,53	0

5.5 Other polymers [\(i\)](#)

There are no such residues in this entry.