



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 12:48 PM UTC

PDB ID : 5TGM / pdb_00005tgm
Title : Crystal structure of the S.cerevisiae 80S ribosome in complex with the A-site bound aminoacyl-tRNA analog ACCA-Pro
Authors : Melnikov, S.; Mailliot, J.; Yusupov, M.
Deposited on : 2016-09-28
Resolution : 3.50 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	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.48.1

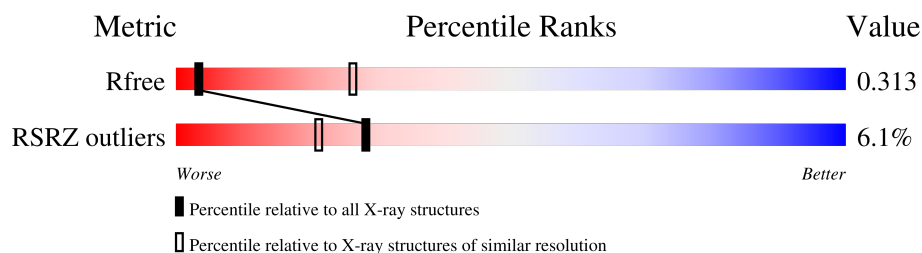
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	164625	1094 (3.56-3.44)
RSRZ outliers	164620	1093 (3.56-3.44)

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
93	MG	1	3735	-	-	-	X
93	MG	1	3785	-	-	-	X
93	MG	1	3788	-	-	-	X
93	MG	1	3827	-	-	-	X
93	MG	1	3837	-	-	-	X
93	MG	1	3839	-	-	-	X
93	MG	1	3852	-	-	-	X
93	MG	1	3854	-	-	-	X
93	MG	1	3874	-	-	-	X
93	MG	1	3883	-	-	-	X
93	MG	1	3896	-	-	-	X
93	MG	1	3908	-	-	-	X
93	MG	1	3911	-	-	-	X
93	MG	1	3914	-	-	-	X
93	MG	1	3980	-	-	-	X
93	MG	1	4015	-	-	-	X
93	MG	1	4026	-	-	-	X
93	MG	2	2055	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
93	MG	2	2057	-	-	-	X
93	MG	2	2060	-	-	-	X
93	MG	2	2067	-	-	-	X
93	MG	2	2070	-	-	-	X
93	MG	2	2071	-	-	-	X
93	MG	2	2074	-	-	-	X
93	MG	2	2082	-	-	-	X
93	MG	2	2084	-	-	-	X
93	MG	2	2099	-	-	-	X
93	MG	2	2101	-	-	-	X
93	MG	2	2112	-	-	-	X
93	MG	2	2115	-	-	-	X
93	MG	2	2117	-	-	-	X
93	MG	2	2127	-	-	-	X
93	MG	2	2132	-	-	-	X
93	MG	3	213	-	-	-	X
93	MG	4	225	-	-	-	X
93	MG	5	3758	-	-	-	X
93	MG	5	3765	-	-	-	X
93	MG	5	3837	-	-	-	X
93	MG	5	3845	-	-	-	X
93	MG	5	3866	-	-	-	X
93	MG	5	3869	-	-	-	X
93	MG	5	3889	-	-	-	X
93	MG	5	3901	-	-	-	X
93	MG	5	3902	-	-	-	X
93	MG	5	3909	-	-	-	X
93	MG	5	3916	-	-	-	X
93	MG	5	3920	-	-	-	X
93	MG	5	3924	-	-	-	X
93	MG	5	3929	-	-	-	X
93	MG	5	3931	-	-	-	X
93	MG	5	3936	-	-	-	X
93	MG	5	3937	-	-	-	X
93	MG	5	3969	-	-	-	X
93	MG	5	3988	-	-	-	X
93	MG	5	4015	-	-	-	X
93	MG	5	4019	-	-	-	X
93	MG	5	4098	-	-	-	X
93	MG	5	4108	-	-	-	X
93	MG	6	2074	-	-	-	X
93	MG	6	2075	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
93	MG	6	2079	-	-	-	X
93	MG	6	2080	-	-	-	X
93	MG	6	2083	-	-	-	X
93	MG	6	2098	-	-	-	X
93	MG	6	2102	-	-	-	X
93	MG	6	2105	-	-	-	X
93	MG	6	2109	-	-	-	X
93	MG	6	2111	-	-	-	X
93	MG	6	2114	-	-	-	X
93	MG	6	2117	-	-	-	X
93	MG	6	2170	-	-	-	X
93	MG	6	2180	-	-	-	X
93	MG	7	213	-	-	-	X
93	MG	7	226	-	-	-	X
93	MG	C9	201	-	-	-	X
93	MG	M7	202	-	-	-	X
93	MG	c8	202	-	-	-	X
93	MG	d3	201	-	-	-	X

2 Entry composition

There are 98 unique types of molecules in this entry. The entry contains 411589 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	1781	Total	C	N	O	P	0	1	0
			37970	16975	6720	12493	1782			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S0	206	Total	C	N	O	S	0	0	0
			1577	1014	278	283	2			
2	s0	206	Total	C	N	O	S	0	0	0
			1583	1017	281	283	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S1	214	Total	C	N	O	S	0	0	0
			1709	1084	310	311	4			
3	s1	216	Total	C	N	O	S	0	0	0
			1722	1091	312	315	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	S2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			
4	s2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	S3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	S4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			
6	s4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	S5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			
7	s5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	S6	226	Total	C	N	O	S	0	0	0
			1799	1129	346	321	3			
8	s6	218	Total	C	N	O	S	0	0	0
			1755	1102	337	313	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	S7	184	Total	C	N	O	0	0	0
			1481	951	265	265			
9	s7	186	Total	C	N	O	0	0	0
			1491	957	267	267			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	S8	188	Total	C	N	O	0	0	0
			1489	925	298	264			
10	s8	188	Total	C	N	O	0	0	0
			1489	925	298	264			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	S9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			
11	s9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	C0	96	Total	C	N	O	S	0	0	0
			773	500	126	145	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	155	Total	C	N	O	S	0	0	0
			1214	775	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C1	147	ALA	GLY	conflict	UNP P0CX47
c1	147	ALA	GLY	conflict	UNP P0CX47

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	C2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			
14	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	C3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			
15	c3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	C4	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			
16	c4	128	Total	C	N	O	S	0	0	0
			949	582	188	176	3			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C4	127	ARG	-	expression tag	UNP P06367
C4	128	LYS	-	expression tag	UNP P06367
C4	129	LYS	-	expression tag	UNP P06367
C4	130	GLY	-	expression tag	UNP P06367
C4	131	GLY	-	expression tag	UNP P06367
C4	132	ARG	-	expression tag	UNP P06367
C4	133	ARG	-	expression tag	UNP P06367
C4	134	GLY	-	expression tag	UNP P06367
C4	135	ARG	-	expression tag	UNP P06367
C4	136	ARG	-	expression tag	UNP P06367
C4	137	LEU	-	expression tag	UNP P06367
c4	127	ARG	-	expression tag	UNP P06367
c4	128	LYS	-	expression tag	UNP P06367
c4	129	LYS	-	expression tag	UNP P06367
c4	130	GLY	-	expression tag	UNP P06367
c4	131	GLY	-	expression tag	UNP P06367
c4	132	ARG	-	expression tag	UNP P06367
c4	133	ARG	-	expression tag	UNP P06367
c4	134	GLY	-	expression tag	UNP P06367
c4	135	ARG	-	expression tag	UNP P06367
c4	136	ARG	-	expression tag	UNP P06367
c4	137	LEU	-	expression tag	UNP P06367

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	C5	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			
17	c5	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	7			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	C6	141	Total	C	N	O	0	0	0
			1105	708	203	194			
18	c6	142	Total	C	N	O	0	0	0
			1111	711	204	196			

- Molecule 19 is a protein called ES17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	C7	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	C8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			
20	c8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	C9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			
21	c9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	D0	107	Total	C	N	O	S	0	0	0
			855	539	156	159	1			
22	d0	110	Total	C	N	O	S	0	0	0
			882	554	161	166	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	D1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			
23	d1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	D2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			
24	d2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	D3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			
25	d3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	D4	134	Total	C	N	O	0	0	0
			1073	676	208	189			
26	d4	134	Total	C	N	O	0	0	0
			1073	676	208	189			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	D5	70	Total	C	N	O	0	0	0
			563	360	104	99			
27	d5	69	Total	C	N	O	0	0	0
			558	357	103	98			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	D6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			
28	d6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	D7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			
29	d7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	D8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			
30	d8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			
31	d9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	E0	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			
32	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	E1	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			
33	e1	76	Total	C	N	O	S	0	0	0
			608	388	117	99	4			

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	SR	318	Total	C	N	O	S	0	0	0
			2437	1541	418	470	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SR	161	ALA	LYS	conflict	UNP P38011

- Molecule 35 is a protein called Ribosome-bound protein Stm1,Suppressor protein STM1,Ribosome-bound protein Stm1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O	0	0	0
			1105	655	221	229			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SM	134	LEU	ASP	conflict	UNP P39015

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
37	7	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	4	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			
38	8	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	l2	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	L3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
40	l3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	L4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
41	l4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	L5	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
42	l5	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	L6	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
43	l6	157	Total	C	N	O	S	0	0	0
			1248	806	224	217	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	L7	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
44	l7	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	L9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
46	19	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	M0	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			
47	m0	213	Total	C	N	O	S	0	0	0
			1722	1094	325	297	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	M1	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			
48	m1	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	M3	193	Total	C	N	O		0	0	0
			1543	962	315	266				
49	m3	194	Total	C	N	O		0	0	0
			1548	965	316	267				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	M4	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	m4	137	Total	C	N	O	S	0	0	0
			1059	678	200	179	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	M5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			
51	m5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			
52	m6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	M7	183	Total	C	N	O		0	0	0
			1420	882	281	257				
53	m7	155	Total	C	N	O		0	0	0
			1227	764	238	225				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	M8	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			
54	m8	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	M9	188	Total	C	N	O		0	0	0
			1521	935	326	260				
55	m9	188	Total	C	N	O		0	0	0
			1521	935	326	260				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	N0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
56	n0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	N1	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			
57	n1	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	N2	100	Total	C	N	O		0	0	0
			796	516	131	149				
58	n2	98	Total	C	N	O		0	0	0
			778	505	127	146				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	N3	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
59	n3	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	N4	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	N5	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	n5	120	Total	C	N	O	S	0	0	0
			959	617	168	172	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
62	N6	126	Total	C	N	O		0	0	0
			993	625	192	176				
62	n6	126	Total	C	N	O		0	0	0
			993	625	192	176				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
63	N7	135	Total	C	N	O		0	0	0
			1092	710	202	180				
63	n7	135	Total	C	N	O		0	0	0
			1092	710	202	180				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	N8	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			
64	n8	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
65	N9	58	Total	C	N	O		0	0	0
			462	289	100	73				
65	n9	58	Total	C	N	O		0	0	0
			462	289	100	73				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	O0	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			
66	o0	100	Total	C	N	O	S	0	0	0
			767	492	128	146	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	O1	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			
67	o1	109	Total	C	N	O	S	0	0	0
			883	559	167	156	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	O2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			
68	o2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	O3	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			
69	o3	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
70	O4	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			
70	o4	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
71	O5	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			
71	o5	119	Total	C	N	O	S	0	0	0
			965	612	185	167	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	O6	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			
72	o6	99	Total	C	N	O	S	0	0	0
			770	481	156	131	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
73	O7	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			
73	o7	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
74	O8	77	Total	C	N	O		0	0	0
			612	391	115	106				
74	o8	77	Total	C	N	O		0	0	0
			608	388	114	106				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	O9	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			
75	o9	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	Q0	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			
76	q0	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	Q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	Q2	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			
78	q2	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	Q3	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			
79	q3	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	6	1795	Total	C	N	O	P	0	1	0
			38260	17105	6763	12596	1796			

- Molecule 81 is a protein called 40S ribosomal protein S10-A,40S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	c0	96	Total	C	N	O	S	0	0	0
			762	491	125	144	2			

- Molecule 82 is a protein called ES17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c7	90	ALA	-	insertion	UNP A0A0J9X224

- Molecule 83 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
83	sR	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 84 is a protein called Suppressor protein STM1,Ribosome-bound protein Stm1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
84	sM	104	Total	C	N	O		0	0	0
			681	404	140	137				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
sM	59	ALA	GLY	conflict	UNP P39015

- Molecule 85 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
85	5	3150	Total	C	N	O	P	0	0	0
			67376	30095	12145	21987	3149			

- Molecule 86 is a protein called 60S ribosomal protein L8-A,60S Ribosomal Protein L8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
86	l8	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

- Molecule 87 is a protein called 60S Ribosomal Protein L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
87	m2	150	Total	C	N	O		0	0	0
			750	450	150	150				

- Molecule 88 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
88	n4	135	Total	C	N	O	S	0	0	0
			1038	651	206	180	1			

- Molecule 89 is a protein called 60S Ribosomal Protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
89	p0	143	Total	C	N	O	S	0	0	0
			1077	687	192	195	3			

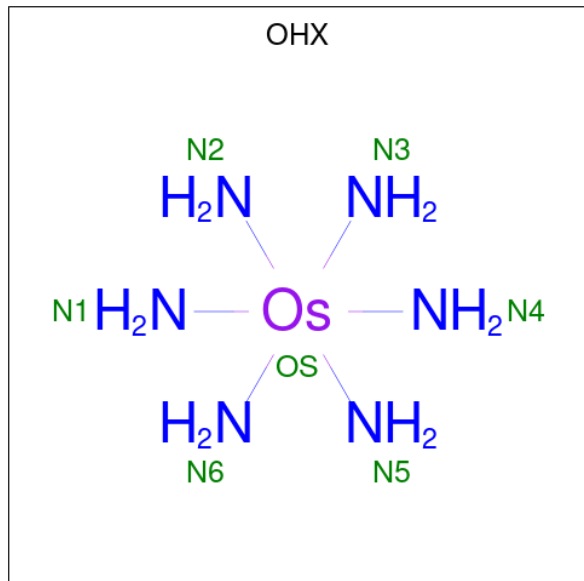
- Molecule 90 is a protein called 60S Ribosomal Protein P1/2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
90	p1	47	Total	C	N	O	0	0	0
			235	141	47	47			
90	p2	46	Total	C	N	O	0	0	0
			230	138	46	46			

- Molecule 91 is a RNA chain called Peptidyl-tRNA analog ACCA-Leu-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
91	P	2	Total	C	N	O	P	0	0	0
			37	18	6	12	1			
91	p	2	Total	C	N	O	P	0	0	0
			40	18	6	14	2			

- Molecule 92 is osmium (III) hexammine (CCD ID: OHX) (formula: H₁₂N₆Os).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	2	1	Total	N	Os	0	0
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92	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	SR	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	3	1	Total	N	Os	0	0
			7	6	1		
92	3	1	Total	N	Os	0	0
			7	6	1		
92	3	1	Total	N	Os	0	0
			7	6	1		
92	3	1	Total	N	Os	0	0
			7	6	1		
92	3	1	Total	N	Os	0	0
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92	3	1	Total	N	Os	0	0
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92	3	1	Total	N	Os	0	0
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92	3	1	Total	N	Os	0	0
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92	3	1	Total	N	Os	0	0
			7	6	1		
92	4	1	Total	N	Os	0	0
			7	6	1		
92	4	1	Total	N	Os	0	0
			7	6	1		
92	4	1	Total	N	Os	0	0
			7	6	1		
92	4	1	Total	N	Os	0	0
			7	6	1		
92	4	1	Total	N	Os	0	0
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92	4	1	Total	N	Os	0	0
			7	6	1		
92	4	1	Total	N	Os	0	0
			7	6	1		
92	4	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	4	1	Total 7	N 6	Os 1	0	0
92	L3	1	Total 7	N 6	Os 1	0	0
92	L3	1	Total 7	N 6	Os 1	0	0
92	L4	1	Total 7	N 6	Os 1	0	0
92	L6	1	Total 7	N 6	Os 1	0	0
92	L6	1	Total 7	N 6	Os 1	0	0
92	M0	1	Total 7	N 6	Os 1	0	0
92	M5	1	Total 7	N 6	Os 1	0	0
92	M5	1	Total 7	N 6	Os 1	0	0
92	M6	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	M7	1	Total	N	Os	0	0
			7	6	1		
92	M8	1	Total	N	Os	0	0
			7	6	1		
92	M9	1	Total	N	Os	0	0
			7	6	1		
92	N9	1	Total	N	Os	0	0
			7	6	1		
92	O3	1	Total	N	Os	0	0
			7	6	1		
92	O4	1	Total	N	Os	0	0
			7	6	1		
92	O7	1	Total	N	Os	0	0
			7	6	1		
92	O9	1	Total	N	Os	0	0
			7	6	1		
92	Q2	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	s1	1	Total	N	Os	0	0
			7	6	1		
92	s4	1	Total	N	Os	0	0
			7	6	1		
92	s8	1	Total	N	Os	0	0
			7	6	1		
92	s9	1	Total	N	Os	0	0
			7	6	1		
92	c3	1	Total	N	Os	0	0
			7	6	1		
92	c5	1	Total	N	Os	0	0
			7	6	1		
92	c8	1	Total	N	Os	0	0
			7	6	1		
92	d4	1	Total	N	Os	0	0
			7	6	1		
92	sR	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
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92	5	1	Total	N	Os	0	0
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92	5	1	Total	N	Os	0	0
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92	5	1	Total	N	Os	0	0
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			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	5	1	Total	N	Os	0	0
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92	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	7	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	l3	1	Total	N	Os	0	0
			7	6	1		
92	l3	1	Total	N	Os	0	0
			7	6	1		
92	l5	1	Total	N	Os	0	0
			7	6	1		
92	l5	1	Total	N	Os	0	0
			7	6	1		
92	l9	1	Total	N	Os	0	0
			7	6	1		
92	m0	1	Total	N	Os	0	0
			7	6	1		
92	m0	1	Total	N	Os	0	0
			7	6	1		
92	m0	1	Total	N	Os	0	0
			7	6	1		
92	m5	1	Total	N	Os	0	0
			7	6	1		
92	m5	1	Total	N	Os	0	0
			7	6	1		
92	m6	1	Total	N	Os	0	0
			7	6	1		
92	m8	1	Total	N	Os	0	0
			7	6	1		
92	m9	1	Total	N	Os	0	0
			7	6	1		
92	n9	1	Total	N	Os	0	0
			7	6	1		
92	o3	1	Total	N	Os	0	0
			7	6	1		
92	o7	1	Total	N	Os	0	0
			7	6	1		
92	o7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 93 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
93	2	91	Total	Mg	0	0
			91	91		
93	S4	1	Total	Mg	0	0
			1	1		
93	C1	1	Total	Mg	0	0
			1	1		
93	C9	1	Total	Mg	0	0
			1	1		
93	D9	2	Total	Mg	0	0
			2	2		
93	1	400	Total	Mg	0	0
			400	400		
93	3	8	Total	Mg	0	0
			8	8		
93	4	18	Total	Mg	0	0
			18	18		
93	L2	2	Total	Mg	0	0
			2	2		
93	L3	2	Total	Mg	0	0
			2	2		
93	L4	4	Total	Mg	0	0
			4	4		
93	L7	1	Total	Mg	0	0
			1	1		
93	M0	1	Total	Mg	0	0
			1	1		
93	M3	1	Total	Mg	0	0
			1	1		
93	M5	1	Total	Mg	0	0
			1	1		
93	M7	5	Total	Mg	0	0
			5	5		
93	N0	1	Total	Mg	0	0
			1	1		
93	N3	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
93	N6	2	Total 2	Mg 2	0	0
93	N8	6	Total 6	Mg 6	0	0
93	O4	1	Total 1	Mg 1	0	0
93	O7	2	Total 2	Mg 2	0	0
93	Q2	1	Total 1	Mg 1	0	0
93	6	130	Total 130	Mg 130	0	0
93	s6	1	Total 1	Mg 1	0	0
93	c8	1	Total 1	Mg 1	0	0
93	d3	1	Total 1	Mg 1	0	0
93	d4	1	Total 1	Mg 1	0	0
93	d6	1	Total 1	Mg 1	0	0
93	d7	1	Total 1	Mg 1	0	0
93	sM	2	Total 2	Mg 2	0	0
93	5	430	Total 430	Mg 430	0	0
93	7	16	Total 16	Mg 16	0	0
93	8	12	Total 12	Mg 12	0	0
93	l2	3	Total 3	Mg 3	0	0
93	l3	4	Total 4	Mg 4	0	0
93	l5	1	Total 1	Mg 1	0	0
93	l6	1	Total 1	Mg 1	0	0
93	l7	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
93	l9	1	Total 1	Mg 1	0	0
93	m4	1	Total 1	Mg 1	0	0
93	m5	2	Total 2	Mg 2	0	0
93	m6	4	Total 4	Mg 4	0	0
93	m7	3	Total 3	Mg 3	0	0
93	n0	2	Total 2	Mg 2	0	0
93	n3	1	Total 1	Mg 1	0	0
93	n6	2	Total 2	Mg 2	0	0
93	n8	3	Total 3	Mg 3	0	0
93	n9	2	Total 2	Mg 2	0	0
93	o2	2	Total 2	Mg 2	0	0
93	o3	2	Total 2	Mg 2	0	0
93	o9	1	Total 1	Mg 1	0	0
93	q1	1	Total 1	Mg 1	0	0
93	P	1	Total 1	Mg 1	0	0
93	p	2	Total 2	Mg 2	0	0

- Molecule 94 is ZINC ION (CCD ID: ZN) (formula: Zn).

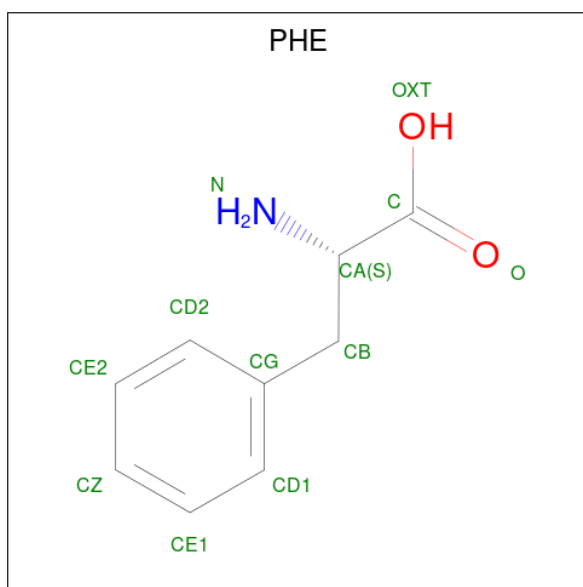
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
94	D6	1	Total 1	Zn 1	0	0
94	D7	1	Total 1	Zn 1	0	0
94	D9	1	Total 1	Zn 1	0	0

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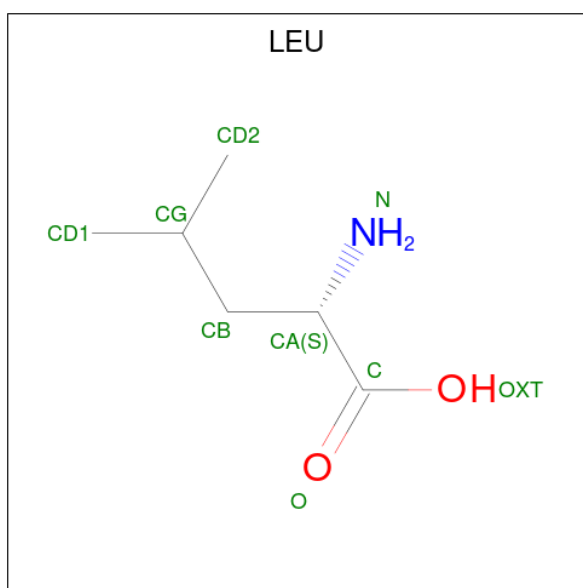
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
94	E1	1	Total 1	Zn 1	0	0
94	O7	1	Total 1	Zn 1	0	0
94	Q0	1	Total 1	Zn 1	0	0
94	Q2	1	Total 1	Zn 1	0	0
94	Q3	1	Total 1	Zn 1	0	0
94	d6	1	Total 1	Zn 1	0	0
94	d7	1	Total 1	Zn 1	0	0
94	d9	1	Total 1	Zn 1	0	0
94	e1	1	Total 1	Zn 1	0	0
94	o7	1	Total 1	Zn 1	0	0
94	q0	1	Total 1	Zn 1	0	0
94	q2	1	Total 1	Zn 1	0	0
94	q3	1	Total 1	Zn 1	0	0

- Molecule 95 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



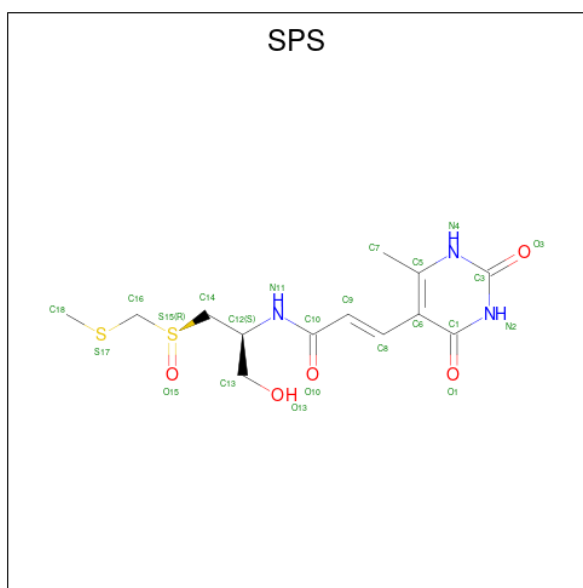
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
95	1	1	Total	C	N	O	0	0
			11	9	1	1		
95	5	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 96 is LEUCINE (CCD ID: LEU) (formula: C₆H₁₃NO₂).



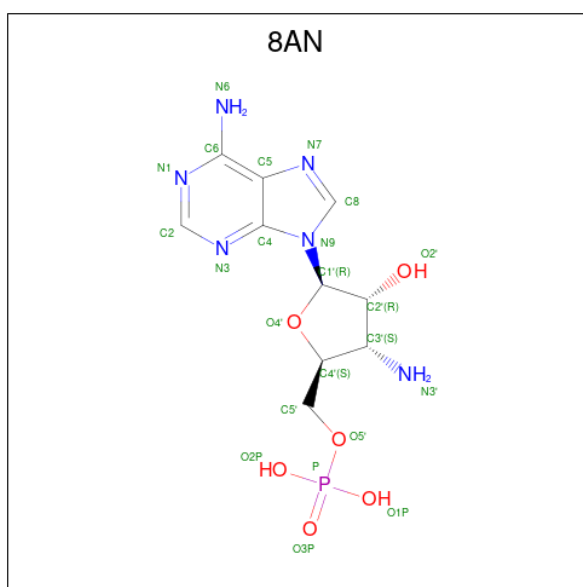
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
96	1	1	Total	C	N	O	0	0
			8	6	1	1		
96	5	1	Total	C	N	O	0	0
			8	6	1	1		

- Molecule 97 is SPARSOMYCIN (CCD ID: SPS) (formula: $C_{13}H_{19}N_3O_5S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
97	P	1	Total	C	N	O	S	0	0
			23	13	3	5	2		
97	p	1	Total	C	N	O	S	0	0
			23	13	3	5	2		

- Molecule 98 is 3'-amino-3'-deoxyadenosine 5'-(dihydrogen phosphate) (CCD ID: 8AN) (formula: $C_{10}H_{15}N_6O_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
98	P	1	Total	C	N	O	P	0	0
			22	10	6	5	1		
98	p	1	Total	C	N	O	P	0	0
			22	10	6	5	1		

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	434.73Å 286.77Å 303.15Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	148.72 – 3.50 148.72 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (148.72-3.50) 99.7 (148.72-3.50)	Depositor EDS
R_{merge}	0.61	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.261 , 0.312 0.263 , 0.313	Depositor DCC
R_{free} test set	18373 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	83.6	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	411589	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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 2310 ligands modelled in this entry, 1207 are monoatomic - leaving 1103 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	$\# Z > 2$
92	OHX	1	3637	36	0,6,6	-	-	-		
92	OHX	4	208	-	0,6,6	-	-	-		
92	OHX	2	1947	-	0,6,6	-	-	-		
92	OHX	L6	201	-	0,6,6	-	-	-		
92	OHX	M7	201	-	0,6,6	-	-	-		
92	OHX	1	3730	36	0,6,6	-	-	-		
92	OHX	1	3599	-	0,6,6	-	-	-		
92	OHX	5	3639	-	0,6,6	-	-	-		
92	OHX	5	3560	-	0,6,6	-	-	-		
92	OHX	5	3697	-	0,6,6	-	-	-		
92	OHX	4	201	-	0,6,6	-	-	-		
92	OHX	1	3658	-	0,6,6	-	-	-		
92	OHX	1	3425	-	0,6,6	-	-	-		
92	OHX	1	3490	-	0,6,6	-	-	-		
92	OHX	1	3533	-	0,6,6	-	-	-		
92	OHX	6	1953	80	0,6,6	-	-	-		
92	OHX	5	3662	-	0,6,6	-	-	-		
92	OHX	2	2023	-	0,6,6	-	-	-		
92	OHX	M9	201	-	0,6,6	-	-	-		
92	OHX	5	3658	85	0,6,6	-	-	-		
92	OHX	5	3664	-	0,6,6	-	-	-		
92	OHX	5	3442	-	0,6,6	-	-	-		
92	OHX	5	3533	85	0,6,6	-	-	-		
92	OHX	5	3550	85	0,6,6	-	-	-		
92	OHX	1	3450	-	0,6,6	-	-	-		
92	OHX	1	3654	-	0,6,6	-	-	-		
92	OHX	s9	201	-	0,6,6	-	-	-		
92	OHX	6	1979	-	0,6,6	-	-	-		
98	8AN	P	102	93,91	17,24,25	0.95	1 (5%)	13,35,38	1.79	4 (30%)
92	OHX	1	3428	-	0,6,6	-	-	-		
92	OHX	1	3530	36	0,6,6	-	-	-		
92	OHX	6	1988	-	0,6,6	-	-	-		
92	OHX	5	3583	-	0,6,6	-	-	-		
92	OHX	1	3523	-	0,6,6	-	-	-		
92	OHX	5	3569	-	0,6,6	-	-	-		
92	OHX	1	3522	-	0,6,6	-	-	-		
92	OHX	3	210	-	0,6,6	-	-	-		
92	OHX	M5	301	-	0,6,6	-	-	-		
92	OHX	1	3480	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	1	3727	36	0,6,6	-	-	-		
92	OHX	m9	201	-	0,6,6	-	-	-		
96	LEU	5	3402	-	5,7,8	0.45	0	6,8,10	0.84	0
92	OHX	5	3480	85	0,6,6	-	-	-		
92	OHX	6	2055	80	0,6,6	-	-	-		
92	OHX	1	3675	-	0,6,6	-	-	-		
92	OHX	8	208	-	0,6,6	-	-	-		
92	OHX	M0	301	-	0,6,6	-	-	-		
92	OHX	6	1948	80	0,6,6	-	-	-		
92	OHX	6	1951	80	0,6,6	-	-	-		
92	OHX	5	3526	-	0,6,6	-	-	-		
92	OHX	6	1934	-	0,6,6	-	-	-		
92	OHX	8	206	38	0,6,6	-	-	-		
92	OHX	5	3514	85	0,6,6	-	-	-		
92	OHX	6	1939	80	0,6,6	-	-	-		
92	OHX	6	1902	80	0,6,6	-	-	-		
92	OHX	5	3728	85	0,6,6	-	-	-		
92	OHX	1	3414	-	0,6,6	-	-	-		
92	OHX	1	3421	-	0,6,6	-	-	-		
92	OHX	5	3449	-	0,6,6	-	-	-		
92	OHX	1	3431	-	0,6,6	-	-	-		
92	OHX	1	3552	-	0,6,6	-	-	-		
92	OHX	1	3605	-	0,6,6	-	-	-		
92	OHX	2	1929	-	0,6,6	-	-	-		
92	OHX	2	1954	-	0,6,6	-	-	-		
92	OHX	6	1996	80	0,6,6	-	-	-		
92	OHX	5	3414	-	0,6,6	-	-	-		
92	OHX	2	2013	-	0,6,6	-	-	-		
92	OHX	5	3421	-	0,6,6	-	-	-		
92	OHX	1	3575	-	0,6,6	-	-	-		
92	OHX	5	3632	-	0,6,6	-	-	-		
92	OHX	6	1929	80	0,6,6	-	-	-		
92	OHX	2	2031	-	0,6,6	-	-	-		
92	OHX	2	1948	-	0,6,6	-	-	-		
92	OHX	1	3609	-	0,6,6	-	-	-		
92	OHX	6	1936	-	0,6,6	-	-	-		
92	OHX	5	3478	-	0,6,6	-	-	-		
92	OHX	2	1980	-	0,6,6	-	-	-		
92	OHX	5	3460	85	0,6,6	-	-	-		
92	OHX	6	2005	-	0,6,6	-	-	-		
92	OHX	1	3625	-	0,6,6	-	-	-		
92	OHX	1	3633	-	0,6,6	-	-	-		
92	OHX	2	1942	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	19	201	-	0,6,6	-	-	-		
92	OHX	1	3445	-	0,6,6	-	-	-		
92	OHX	2	1982	-	0,6,6	-	-	-		
92	OHX	6	1942	80	0,6,6	-	-	-		
92	OHX	1	3635	-	0,6,6	-	-	-		
92	OHX	1	3438	-	0,6,6	-	-	-		
92	OHX	5	3509	85	0,6,6	-	-	-		
92	OHX	1	3607	-	0,6,6	-	-	-		
92	OHX	5	3615	85	0,6,6	-	-	-		
92	OHX	6	2003	-	0,6,6	-	-	-		
98	8AN	p	102	93,91	17,24,25	0.95	1 (5%)	13,35,38	1.80	5 (38%)
92	OHX	2	1912	-	0,6,6	-	-	-		
92	OHX	1	3515	-	0,6,6	-	-	-		
92	OHX	2	1935	-	0,6,6	-	-	-		
92	OHX	1	3626	-	0,6,6	-	-	-		
92	OHX	5	3641	-	0,6,6	-	-	-		
92	OHX	1	3558	-	0,6,6	-	-	-		
92	OHX	5	3607	-	0,6,6	-	-	-		
92	OHX	6	2037	80	0,6,6	-	-	-		
92	OHX	1	3687	-	0,6,6	-	-	-		
92	OHX	8	210	38	0,6,6	-	-	-		
92	OHX	1	3510	-	0,6,6	-	-	-		
92	OHX	2	1971	-	0,6,6	-	-	-		
92	OHX	1	3628	-	0,6,6	-	-	-		
92	OHX	1	3652	-	0,6,6	-	-	-		
92	OHX	6	2008	-	0,6,6	-	-	-		
92	OHX	6	1943	-	0,6,6	-	-	-		
92	OHX	5	3535	85	0,6,6	-	-	-		
92	OHX	5	3492	-	0,6,6	-	-	-		
92	OHX	1	3485	-	0,6,6	-	-	-		
92	OHX	5	3589	85	0,6,6	-	-	-		
92	OHX	1	3583	-	0,6,6	-	-	-		
92	OHX	M5	302	-	0,6,6	-	-	-		
92	OHX	2	1962	-	0,6,6	-	-	-		
92	OHX	8	216	38	0,6,6	-	-	-		
92	OHX	6	1962	80	0,6,6	-	-	-		
92	OHX	2	2003	-	0,6,6	-	-	-		
92	OHX	O4	201	-	0,6,6	-	-	-		
92	OHX	6	1995	-	0,6,6	-	-	-		
92	OHX	5	3729	85	0,6,6	-	-	-		
92	OHX	1	3511	-	0,6,6	-	-	-		
92	OHX	5	3471	85	0,6,6	-	-	-		
92	OHX	2	2045	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	3567	-	0,6,6	-	-	-		
92	OHX	5	3483	-	0,6,6	-	-	-		
92	OHX	1	3463	-	0,6,6	-	-	-		
92	OHX	1	3514	-	0,6,6	-	-	-		
92	OHX	q2	502	-	0,6,6	-	-	-		
92	OHX	1	3406	-	0,6,6	-	-	-		
92	OHX	1	3562	-	0,6,6	-	-	-		
92	OHX	5	3476	-	0,6,6	-	-	-		
92	OHX	8	212	38	0,6,6	-	-	-		
92	OHX	5	3545	-	0,6,6	-	-	-		
92	OHX	C8	201	36	0,6,6	-	-	-		
92	OHX	1	3642	-	0,6,6	-	-	-		
92	OHX	5	3477	85	0,6,6	-	-	-		
92	OHX	4	214	-	0,6,6	-	-	-		
92	OHX	1	3577	-	0,6,6	-	-	-		
92	OHX	2	2047	1	0,6,6	-	-	-		
92	OHX	1	3407	-	0,6,6	-	-	-		
92	OHX	1	3640	-	0,6,6	-	-	-		
92	OHX	5	3540	85	0,6,6	-	-	-		
92	OHX	5	3719	-	0,6,6	-	-	-		
92	OHX	6	1915	80	0,6,6	-	-	-		
92	OHX	5	3661	-	0,6,6	-	-	-		
92	OHX	2	1927	-	0,6,6	-	-	-		
92	OHX	1	3454	-	0,6,6	-	-	-		
92	OHX	3	204	-	0,6,6	-	-	-		
92	OHX	2	1925	-	0,6,6	-	-	-		
92	OHX	4	211	-	0,6,6	-	-	-		
92	OHX	6	1967	80	0,6,6	-	-	-		
92	OHX	5	3452	-	0,6,6	-	-	-		
92	OHX	4	218	-	0,6,6	-	-	-		
92	OHX	8	215	38	0,6,6	-	-	-		
92	OHX	6	1925	-	0,6,6	-	-	-		
92	OHX	6	1955	80	0,6,6	-	-	-		
92	OHX	8	213	-	0,6,6	-	-	-		
92	OHX	5	3739	-	0,6,6	-	-	-		
92	OHX	1	3439	-	0,6,6	-	-	-		
92	OHX	6	2044	-	0,6,6	-	-	-		
92	OHX	1	3529	36	0,6,6	-	-	-		
92	OHX	5	3644	-	0,6,6	-	-	-		
92	OHX	5	3683	85	0,6,6	-	-	-		
92	OHX	4	215	38	0,6,6	-	-	-		
92	OHX	1	3594	-	0,6,6	-	-	-		
92	OHX	1	3639	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	2	1967	-	0,6,6	-	-	-		
92	OHX	L6	202	-	0,6,6	-	-	-		
92	OHX	5	3539	85	0,6,6	-	-	-		
92	OHX	7	211	-	0,6,6	-	-	-		
92	OHX	6	1980	-	0,6,6	-	-	-		
92	OHX	1	3668	-	0,6,6	-	-	-		
92	OHX	2	1944	-	0,6,6	-	-	-		
92	OHX	1	3537	-	0,6,6	-	-	-		
92	OHX	6	2021	-	0,6,6	-	-	-		
92	OHX	5	3568	-	0,6,6	-	-	-		
92	OHX	2	2019	-	0,6,6	-	-	-		
92	OHX	5	3556	85	0,6,6	-	-	-		
92	OHX	6	1944	80	0,6,6	-	-	-		
92	OHX	6	2019	80	0,6,6	-	-	-		
92	OHX	5	3727	-	0,6,6	-	-	-		
92	OHX	1	3446	-	0,6,6	-	-	-		
92	OHX	6	1950	-	0,6,6	-	-	-		
92	OHX	6	1922	80	0,6,6	-	-	-		
92	OHX	6	1987	80	0,6,6	-	-	-		
92	OHX	2	1907	-	0,6,6	-	-	-		
92	OHX	2	1994	-	0,6,6	-	-	-		
92	OHX	1	3420	-	0,6,6	-	-	-		
92	OHX	5	3606	85	0,6,6	-	-	-		
92	OHX	5	3446	-	0,6,6	-	-	-		
92	OHX	5	3672	-	0,6,6	-	-	-		
92	OHX	5	3684	85	0,6,6	-	-	-		
92	OHX	5	3691	-	0,6,6	-	-	-		
92	OHX	5	3748	-	0,6,6	-	-	-		
92	OHX	5	3420	-	0,6,6	-	-	-		
92	OHX	5	3473	85	0,6,6	-	-	-		
92	OHX	1	3494	36	0,6,6	-	-	-		
92	OHX	1	3667	-	0,6,6	-	-	-		
92	OHX	5	3497	85	0,6,6	-	-	-		
92	OHX	1	3610	-	0,6,6	-	-	-		
92	OHX	3	208	-	0,6,6	-	-	-		
92	OHX	2	2036	-	0,6,6	-	-	-		
92	OHX	1	3600	-	0,6,6	-	-	-		
92	OHX	2	1922	-	0,6,6	-	-	-		
92	OHX	2	1993	-	0,6,6	-	-	-		
92	OHX	6	2010	80	0,6,6	-	-	-		
92	OHX	5	3610	-	0,6,6	-	-	-		
92	OHX	5	3618	-	0,6,6	-	-	-		
92	OHX	1	3440	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	L3	402	-	0,6,6	-	-	-		
92	OHX	m6	201	-	0,6,6	-	-	-		
92	OHX	1	3638	-	0,6,6	-	-	-		
92	OHX	2	1924	-	0,6,6	-	-	-		
92	OHX	5	3519	-	0,6,6	-	-	-		
92	OHX	1	3611	-	0,6,6	-	-	-		
95	PHE	5	3401	-	10,11,12	1.42	2 (20%)	8,13,15	0.71	0
92	OHX	6	2035	-	0,6,6	-	-	-		
92	OHX	1	3627	36	0,6,6	-	-	-		
92	OHX	6	2041	-	0,6,6	-	-	-		
92	OHX	1	3593	-	0,6,6	-	-	-		
92	OHX	5	3551	85	0,6,6	-	-	-		
92	OHX	1	3724	-	0,6,6	-	-	-		
92	OHX	2	1931	-	0,6,6	-	-	-		
92	OHX	1	3673	-	0,6,6	-	-	-		
92	OHX	1	3683	36	0,6,6	-	-	-		
92	OHX	1	3546	-	0,6,6	-	-	-		
92	OHX	6	1912	-	0,6,6	-	-	-		
92	OHX	5	3604	85	0,6,6	-	-	-		
92	OHX	5	3737	85	0,6,6	-	-	-		
92	OHX	2	1981	-	0,6,6	-	-	-		
92	OHX	2	1926	-	0,6,6	-	-	-		
92	OHX	5	3501	85	0,6,6	-	-	-		
92	OHX	1	3560	-	0,6,6	-	-	-		
92	OHX	m5	302	-	0,6,6	-	-	-		
92	OHX	5	3440	-	0,6,6	-	-	-		
92	OHX	1	3666	-	0,6,6	-	-	-		
92	OHX	5	3436	85	0,6,6	-	-	-		
92	OHX	S8	301	-	0,6,6	-	-	-		
92	OHX	1	3591	-	0,6,6	-	-	-		
92	OHX	l5	301	-	0,6,6	-	-	-		
92	OHX	1	3453	-	0,6,6	-	-	-		
92	OHX	5	3746	85	0,6,6	-	-	-		
92	OHX	1	3419	36	0,6,6	-	-	-		
92	OHX	5	3591	-	0,6,6	-	-	-		
92	OHX	1	3550	-	0,6,6	-	-	-		
92	OHX	c3	201	-	0,6,6	-	-	-		
92	OHX	5	3718	85	0,6,6	-	-	-		
92	OHX	1	3492	-	0,6,6	-	-	-		
92	OHX	D9	102	-	0,6,6	-	-	-		
92	OHX	2	1908	-	0,6,6	-	-	-		
92	OHX	5	3531	85	0,6,6	-	-	-		
92	OHX	O7	102	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	6	1940	80	0,6,6	-	-	-		
92	OHX	1	3467	-	0,6,6	-	-	-		
92	OHX	1	3723	-	0,6,6	-	-	-		
92	OHX	5	3425	-	0,6,6	-	-	-		
92	OHX	6	2025	80	0,6,6	-	-	-		
92	OHX	1	3571	-	0,6,6	-	-	-		
92	OHX	5	3481	-	0,6,6	-	-	-		
92	OHX	1	3443	-	0,6,6	-	-	-		
92	OHX	5	3500	-	0,6,6	-	-	-		
92	OHX	5	3537	-	0,6,6	-	-	-		
92	OHX	5	3597	85	0,6,6	-	-	-		
92	OHX	5	3557	-	0,6,6	-	-	-		
92	OHX	2	1903	-	0,6,6	-	-	-		
92	OHX	2	2032	-	0,6,6	-	-	-		
92	OHX	1	3720	-	0,6,6	-	-	-		
92	OHX	1	3482	-	0,6,6	-	-	-		
92	OHX	6	1921	80	0,6,6	-	-	-		
92	OHX	5	3671	85	0,6,6	-	-	-		
92	OHX	5	3559	-	0,6,6	-	-	-		
92	OHX	1	3526	-	0,6,6	-	-	-		
92	OHX	1	3585	-	0,6,6	-	-	-		
92	OHX	5	3552	85	0,6,6	-	-	-		
92	OHX	1	3592	-	0,6,6	-	-	-		
92	OHX	1	3503	-	0,6,6	-	-	-		
92	OHX	7	202	-	0,6,6	-	-	-		
92	OHX	5	3484	85	0,6,6	-	-	-		
92	OHX	5	3585	85	0,6,6	-	-	-		
92	OHX	1	3704	-	0,6,6	-	-	-		
92	OHX	1	3549	-	0,6,6	-	-	-		
92	OHX	1	3566	36	0,6,6	-	-	-		
92	OHX	5	3564	85	0,6,6	-	-	-		
92	OHX	1	3632	-	0,6,6	-	-	-		
92	OHX	1	3718	-	0,6,6	-	-	-		
92	OHX	5	3542	85	0,6,6	-	-	-		
92	OHX	2	2011	1	0,6,6	-	-	-		
92	OHX	5	3566	-	0,6,6	-	-	-		
92	OHX	5	3616	-	0,6,6	-	-	-		
92	OHX	5	3622	85	0,6,6	-	-	-		
92	OHX	1	3689	-	0,6,6	-	-	-		
92	OHX	5	3710	-	0,6,6	-	-	-		
92	OHX	2	1932	-	0,6,6	-	-	-		
92	OHX	2	2001	-	0,6,6	-	-	-		
92	OHX	1	3535	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	2	2020	-	0,6,6	-	-	-		
92	OHX	4	219	-	0,6,6	-	-	-		
92	OHX	1	3524	-	0,6,6	-	-	-		
92	OHX	6	1903	-	0,6,6	-	-	-		
92	OHX	1	3489	-	0,6,6	-	-	-		
92	OHX	6	1917	80	0,6,6	-	-	-		
92	OHX	6	1945	80	0,6,6	-	-	-		
92	OHX	6	1999	80	0,6,6	-	-	-		
92	OHX	6	2022	-	0,6,6	-	-	-		
92	OHX	4	202	-	0,6,6	-	-	-		
92	OHX	6	1909	80	0,6,6	-	-	-		
92	OHX	5	3437	85	0,6,6	-	-	-		
92	OHX	2	1983	-	0,6,6	-	-	-		
92	OHX	2	2022	-	0,6,6	-	-	-		
92	OHX	5	3505	-	0,6,6	-	-	-		
92	OHX	1	3702	-	0,6,6	-	-	-		
92	OHX	5	3679	-	0,6,6	-	-	-		
92	OHX	2	1937	-	0,6,6	-	-	-		
92	OHX	1	3557	-	0,6,6	-	-	-		
92	OHX	5	3717	85	0,6,6	-	-	-		
92	OHX	m0	301	-	0,6,6	-	-	-		
92	OHX	2	1990	-	0,6,6	-	-	-		
92	OHX	7	207	37	0,6,6	-	-	-		
92	OHX	2	1977	-	0,6,6	-	-	-		
92	OHX	5	3677	85	0,6,6	-	-	-		
92	OHX	5	3670	85	0,6,6	-	-	-		
92	OHX	1	3502	-	0,6,6	-	-	-		
92	OHX	5	3725	-	0,6,6	-	-	-		
92	OHX	6	1970	80	0,6,6	-	-	-		
92	OHX	8	205	-	0,6,6	-	-	-		
92	OHX	1	3457	-	0,6,6	-	-	-		
92	OHX	1	3574	-	0,6,6	-	-	-		
92	OHX	s4	301	-	0,6,6	-	-	-		
92	OHX	5	3429	85	0,6,6	-	-	-		
92	OHX	1	3624	-	0,6,6	-	-	-		
92	OHX	1	3708	-	0,6,6	-	-	-		
92	OHX	1	3448	36	0,6,6	-	-	-		
92	OHX	2	1988	-	0,6,6	-	-	-		
92	OHX	5	3455	-	0,6,6	-	-	-		
92	OHX	M8	201	-	0,6,6	-	-	-		
92	OHX	6	2058	-	0,6,6	-	-	-		
92	OHX	5	3699	-	0,6,6	-	-	-		
92	OHX	5	3701	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	8	204	-	0,6,6	-	-	-		
92	OHX	5	3716	-	0,6,6	-	-	-		
92	OHX	6	1994	-	0,6,6	-	-	-		
92	OHX	5	3494	-	0,6,6	-	-	-		
92	OHX	1	3711	-	0,6,6	-	-	-		
92	OHX	5	3738	85	0,6,6	-	-	-		
92	OHX	5	3743	-	0,6,6	-	-	-		
92	OHX	2	2028	-	0,6,6	-	-	-		
92	OHX	2	2014	-	0,6,6	-	-	-		
92	OHX	o7	503	-	0,6,6	-	-	-		
92	OHX	5	3405	85	0,6,6	-	-	-		
92	OHX	1	3528	-	0,6,6	-	-	-		
92	OHX	1	3513	-	0,6,6	-	-	-		
92	OHX	3	206	-	0,6,6	-	-	-		
92	OHX	1	3567	-	0,6,6	-	-	-		
92	OHX	2	1902	-	0,6,6	-	-	-		
92	OHX	3	205	-	0,6,6	-	-	-		
92	OHX	1	3442	-	0,6,6	-	-	-		
92	OHX	Q2	502	-	0,6,6	-	-	-		
92	OHX	7	209	-	0,6,6	-	-	-		
92	OHX	5	3404	-	0,6,6	-	-	-		
92	OHX	6	1961	-	0,6,6	-	-	-		
92	OHX	1	3662	-	0,6,6	-	-	-		
92	OHX	6	1963	-	0,6,6	-	-	-		
92	OHX	1	3542	-	0,6,6	-	-	-		
92	OHX	5	3461	85	0,6,6	-	-	-		
92	OHX	1	3468	-	0,6,6	-	-	-		
92	OHX	5	3645	-	0,6,6	-	-	-		
92	OHX	5	3709	-	0,6,6	-	-	-		
92	OHX	6	1906	-	0,6,6	-	-	-		
92	OHX	1	3669	-	0,6,6	-	-	-		
92	OHX	1	3460	-	0,6,6	-	-	-		
92	OHX	c5	201	-	0,6,6	-	-	-		
92	OHX	6	1954	-	0,6,6	-	-	-		
92	OHX	5	3593	-	0,6,6	-	-	-		
92	OHX	2	1974	-	0,6,6	-	-	-		
92	OHX	5	3745	-	0,6,6	-	-	-		
92	OHX	5	3703	-	0,6,6	-	-	-		
92	OHX	1	3604	-	0,6,6	-	-	-		
92	OHX	5	3633	-	0,6,6	-	-	-		
92	OHX	2	1953	-	0,6,6	-	-	-		
92	OHX	5	3458	85	0,6,6	-	-	-		
92	OHX	1	3504	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	1	3408	-	0,6,6	-	-	-		
92	OHX	5	3490	85	0,6,6	-	-	-		
92	OHX	1	3712	36	0,6,6	-	-	-		
92	OHX	1	3620	-	0,6,6	-	-	-		
92	OHX	1	3656	-	0,6,6	-	-	-		
92	OHX	6	2023	80	0,6,6	-	-	-		
92	OHX	6	1931	80	0,6,6	-	-	-		
92	OHX	6	1947	-	0,6,6	-	-	-		
92	OHX	5	3408	85	0,6,6	-	-	-		
92	OHX	6	1933	-	0,6,6	-	-	-		
92	OHX	5	3594	-	0,6,6	-	-	-		
92	OHX	2	2044	-	0,6,6	-	-	-		
92	OHX	1	3459	-	0,6,6	-	-	-		
92	OHX	5	3513	85	0,6,6	-	-	-		
92	OHX	5	3631	85	0,6,6	-	-	-		
92	OHX	1	3677	-	0,6,6	-	-	-		
92	OHX	8	207	38	0,6,6	-	-	-		
92	OHX	5	3660	85	0,6,6	-	-	-		
92	OHX	5	3650	-	0,6,6	-	-	-		
92	OHX	5	3613	-	0,6,6	-	-	-		
92	OHX	5	3487	-	0,6,6	-	-	-		
92	OHX	5	3700	85	0,6,6	-	-	-		
92	OHX	1	3465	-	0,6,6	-	-	-		
92	OHX	5	3522	-	0,6,6	-	-	-		
92	OHX	5	3617	-	0,6,6	-	-	-		
92	OHX	5	3468	-	0,6,6	-	-	-		
92	OHX	1	3581	-	0,6,6	-	-	-		
92	OHX	1	3722	-	0,6,6	-	-	-		
92	OHX	2	2007	-	0,6,6	-	-	-		
92	OHX	1	3415	-	0,6,6	-	-	-		
92	OHX	6	1938	-	0,6,6	-	-	-		
92	OHX	5	3706	-	0,6,6	-	-	-		
92	OHX	1	3556	-	0,6,6	-	-	-		
92	OHX	5	3675	-	0,6,6	-	-	-		
92	OHX	5	3415	-	0,6,6	-	-	-		
92	OHX	5	3510	85	0,6,6	-	-	-		
92	OHX	1	3433	-	0,6,6	-	-	-		
92	OHX	2	2050	1	0,6,6	-	-	-		
92	OHX	1	3470	-	0,6,6	-	-	-		
92	OHX	1	3634	-	0,6,6	-	-	-		
92	OHX	5	3530	-	0,6,6	-	-	-		
92	OHX	5	3553	85	0,6,6	-	-	-		
92	OHX	1	3715	36	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	6	2050	80	0,6,6	-	-	-		
92	OHX	5	3433	-	0,6,6	-	-	-		
92	OHX	5	3470	-	0,6,6	-	-	-		
92	OHX	1	3527	-	0,6,6	-	-	-		
92	OHX	1	3500	-	0,6,6	-	-	-		
92	OHX	6	1976	80	0,6,6	-	-	-		
92	OHX	sR	401	-	0,6,6	-	-	-		
92	OHX	5	3457	-	0,6,6	-	-	-		
92	OHX	5	3527	85	0,6,6	-	-	-		
92	OHX	5	3685	-	0,6,6	-	-	-		
92	OHX	6	1910	-	0,6,6	-	-	-		
92	OHX	6	2032	-	0,6,6	-	-	-		
92	OHX	1	3519	-	0,6,6	-	-	-		
92	OHX	6	2056	80	0,6,6	-	-	-		
92	OHX	1	3563	-	0,6,6	-	-	-		
92	OHX	5	3663	-	0,6,6	-	-	-		
92	OHX	2	1934	-	0,6,6	-	-	-		
92	OHX	2	2005	-	0,6,6	-	-	-		
92	OHX	5	3507	-	0,6,6	-	-	-		
92	OHX	5	3713	85	0,6,6	-	-	-		
92	OHX	1	3664	-	0,6,6	-	-	-		
92	OHX	1	3645	-	0,6,6	-	-	-		
92	OHX	6	1972	80	0,6,6	-	-	-		
92	OHX	1	3705	-	0,6,6	-	-	-		
92	OHX	5	3427	-	0,6,6	-	-	-		
92	OHX	1	3538	-	0,6,6	-	-	-		
92	OHX	1	3426	-	0,6,6	-	-	-		
92	OHX	1	3589	-	0,6,6	-	-	-		
92	OHX	5	3705	-	0,6,6	-	-	-		
92	OHX	6	2013	80	0,6,6	-	-	-		
92	OHX	6	1998	80	0,6,6	-	-	-		
92	OHX	1	3615	-	0,6,6	-	-	-		
92	OHX	6	1974	80	0,6,6	-	-	-		
92	OHX	6	2031	80	0,6,6	-	-	-		
92	OHX	5	3609	-	0,6,6	-	-	-		
92	OHX	5	3456	85	0,6,6	-	-	-		
95	PHE	1	3401	-	10,11,12	1.42	2 (20%)	8,13,15	0.71	0
92	OHX	5	3548	85	0,6,6	-	-	-		
92	OHX	1	3434	-	0,6,6	-	-	-		
92	OHX	2	1914	-	0,6,6	-	-	-		
92	OHX	5	3647	-	0,6,6	-	-	-		
92	OHX	1	3496	-	0,6,6	-	-	-		
92	OHX	n9	101	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	3635	85	0,6,6	-	-	-		
92	OHX	7	203	37	0,6,6	-	-	-		
96	LEU	1	3402	-	5,7,8	0.44	0	6,8,10	0.83	0
92	OHX	5	3654	-	0,6,6	-	-	-		
92	OHX	5	3669	85	0,6,6	-	-	-		
92	OHX	6	1990	-	0,6,6	-	-	-		
92	OHX	5	3619	-	0,6,6	-	-	-		
92	OHX	1	3728	-	0,6,6	-	-	-		
92	OHX	1	3680	-	0,6,6	-	-	-		
92	OHX	2	2009	1	0,6,6	-	-	-		
92	OHX	1	3569	-	0,6,6	-	-	-		
92	OHX	1	3576	36	0,6,6	-	-	-		
92	OHX	2	1943	-	0,6,6	-	-	-		
92	OHX	3	203	-	0,6,6	-	-	-		
92	OHX	6	2045	-	0,6,6	-	-	-		
92	OHX	5	3416	85	0,6,6	-	-	-		
92	OHX	5	3680	-	0,6,6	-	-	-		
92	OHX	m0	302	-	0,6,6	-	-	-		
92	OHX	5	3410	-	0,6,6	-	-	-		
92	OHX	7	205	-	0,6,6	-	-	-		
92	OHX	2	2006	-	0,6,6	-	-	-		
92	OHX	1	3691	-	0,6,6	-	-	-		
92	OHX	6	2027	-	0,6,6	-	-	-		
92	OHX	5	3534	85	0,6,6	-	-	-		
92	OHX	2	1961	-	0,6,6	-	-	-		
92	OHX	2	2025	-	0,6,6	-	-	-		
92	OHX	2	1940	-	0,6,6	-	-	-		
92	OHX	1	3518	-	0,6,6	-	-	-		
92	OHX	2	1964	-	0,6,6	-	-	-		
92	OHX	1	3561	-	0,6,6	-	-	-		
92	OHX	1	3721	-	0,6,6	-	-	-		
92	OHX	6	1957	80	0,6,6	-	-	-		
92	OHX	5	3747	85	0,6,6	-	-	-		
92	OHX	2	2010	-	0,6,6	-	-	-		
92	OHX	1	3497	-	0,6,6	-	-	-		
92	OHX	1	3403	-	0,6,6	-	-	-		
92	OHX	1	3545	-	0,6,6	-	-	-		
92	OHX	7	204	37	0,6,6	-	-	-		
92	OHX	o3	201	-	0,6,6	-	-	-		
92	OHX	5	3612	-	0,6,6	-	-	-		
92	OHX	5	3744	-	0,6,6	-	-	-		
92	OHX	1	3682	-	0,6,6	-	-	-		
92	OHX	5	3413	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	1	3509	36	0,6,6	-	-	-		
92	OHX	2	1973	-	0,6,6	-	-	-		
92	OHX	1	3629	36	0,6,6	-	-	-		
92	OHX	2	1986	1	0,6,6	-	-	-		
92	OHX	4	210	-	0,6,6	-	-	-		
92	OHX	2	1945	-	0,6,6	-	-	-		
92	OHX	6	2014	80	0,6,6	-	-	-		
92	OHX	6	2015	-	0,6,6	-	-	-		
92	OHX	1	3663	-	0,6,6	-	-	-		
92	OHX	C3	201	-	0,6,6	-	-	-		
92	OHX	5	3521	85	0,6,6	-	-	-		
92	OHX	6	1986	-	0,6,6	-	-	-		
92	OHX	2	1972	1	0,6,6	-	-	-		
92	OHX	1	3478	-	0,6,6	-	-	-		
92	OHX	1	3690	-	0,6,6	-	-	-		
92	OHX	1	3423	-	0,6,6	-	-	-		
92	OHX	5	3629	85	0,6,6	-	-	-		
92	OHX	5	3741	-	0,6,6	-	-	-		
92	OHX	5	3694	-	0,6,6	-	-	-		
92	OHX	1	3671	-	0,6,6	-	-	-		
92	OHX	5	3690	-	0,6,6	-	-	-		
92	OHX	5	3423	85	0,6,6	-	-	-		
92	OHX	6	1920	80	0,6,6	-	-	-		
92	OHX	1	3651	-	0,6,6	-	-	-		
92	OHX	6	2009	-	0,6,6	-	-	-		
92	OHX	6	2043	-	0,6,6	-	-	-		
92	OHX	1	3674	-	0,6,6	-	-	-		
92	OHX	5	3432	-	0,6,6	-	-	-		
92	OHX	1	3512	36	0,6,6	-	-	-		
92	OHX	1	3641	-	0,6,6	-	-	-		
92	OHX	1	3456	-	0,6,6	-	-	-		
92	OHX	1	3578	-	0,6,6	-	-	-		
92	OHX	1	3598	-	0,6,6	-	-	-		
92	OHX	3	207	-	0,6,6	-	-	-		
92	OHX	5	3640	85	0,6,6	-	-	-		
92	OHX	1	3622	-	0,6,6	-	-	-		
92	OHX	2	1968	-	0,6,6	-	-	-		
92	OHX	5	3578	85	0,6,6	-	-	-		
92	OHX	5	3693	-	0,6,6	-	-	-		
92	OHX	1	3643	-	0,6,6	-	-	-		
92	OHX	2	2042	-	0,6,6	-	-	-		
92	OHX	5	3511	85	0,6,6	-	-	-		
92	OHX	8	209	38	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	15	302	-	0,6,6	-	-	-		
92	OHX	5	3653	85	0,6,6	-	-	-		
92	OHX	2	2021	-	0,6,6	-	-	-		
92	OHX	5	3448	-	0,6,6	-	-	-		
92	OHX	5	3614	-	0,6,6	-	-	-		
92	OHX	6	2012	-	0,6,6	-	-	-		
92	OHX	5	3571	-	0,6,6	-	-	-		
92	OHX	5	3736	85	0,6,6	-	-	-		
92	OHX	c8	201	-	0,6,6	-	-	-		
92	OHX	5	3666	85	0,6,6	-	-	-		
92	OHX	5	3430	-	0,6,6	-	-	-		
92	OHX	4	209	-	0,6,6	-	-	-		
92	OHX	O3	201	-	0,6,6	-	-	-		
92	OHX	2	1995	-	0,6,6	-	-	-		
92	OHX	5	3708	-	0,6,6	-	-	-		
92	OHX	6	2042	80	0,6,6	-	-	-		
92	OHX	5	3554	-	0,6,6	-	-	-		
92	OHX	6	2007	80	0,6,6	-	-	-		
92	OHX	1	3432	-	0,6,6	-	-	-		
92	OHX	6	2026	80	0,6,6	-	-	-		
92	OHX	4	212	-	0,6,6	-	-	-		
92	OHX	1	3429	-	0,6,6	-	-	-		
92	OHX	1	3623	-	0,6,6	-	-	-		
92	OHX	3	201	-	0,6,6	-	-	-		
92	OHX	7	206	37	0,6,6	-	-	-		
92	OHX	1	3476	-	0,6,6	-	-	-		
92	OHX	6	1989	80	0,6,6	-	-	-		
92	OHX	5	3603	-	0,6,6	-	-	-		
92	OHX	5	3696	85	0,6,6	-	-	-		
92	OHX	6	2048	80	0,6,6	-	-	-		
92	OHX	6	2011	-	0,6,6	-	-	-		
92	OHX	4	220	-	0,6,6	-	-	-		
92	OHX	6	1991	80	0,6,6	-	-	-		
92	OHX	2	2035	1	0,6,6	-	-	-		
92	OHX	5	3667	-	0,6,6	-	-	-		
92	OHX	5	3547	-	0,6,6	-	-	-		
92	OHX	2	2024	-	0,6,6	-	-	-		
92	OHX	1	3405	-	0,6,6	-	-	-		
92	OHX	2	1915	-	0,6,6	-	-	-		
92	OHX	5	3538	-	0,6,6	-	-	-		
92	OHX	5	3600	85	0,6,6	-	-	-		
92	OHX	2	1978	-	0,6,6	-	-	-		
92	OHX	2	1989	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	1	3676	-	0,6,6	-	-	-		
92	OHX	1	3698	36	0,6,6	-	-	-		
92	OHX	6	2030	80	0,6,6	-	-	-		
92	OHX	2	2043	1	0,6,6	-	-	-		
92	OHX	5	3733	-	0,6,6	-	-	-		
92	OHX	6	2038	-	0,6,6	-	-	-		
92	OHX	6	1919	80	0,6,6	-	-	-		
92	OHX	5	3698	-	0,6,6	-	-	-		
92	OHX	2	1958	-	0,6,6	-	-	-		
92	OHX	1	3565	-	0,6,6	-	-	-		
92	OHX	2	1979	-	0,6,6	-	-	-		
92	OHX	1	3411	-	0,6,6	-	-	-		
92	OHX	5	3546	-	0,6,6	-	-	-		
92	OHX	1	3588	36	0,6,6	-	-	-		
92	OHX	2	1911	-	0,6,6	-	-	-		
92	OHX	1	3436	-	0,6,6	-	-	-		
92	OHX	6	1914	80	0,6,6	-	-	-		
92	OHX	6	1981	80	0,6,6	-	-	-		
92	OHX	4	204	-	0,6,6	-	-	-		
92	OHX	5	3579	-	0,6,6	-	-	-		
92	OHX	2	1950	1	0,6,6	-	-	-		
92	OHX	5	3584	85	0,6,6	-	-	-		
92	OHX	1	3617	-	0,6,6	-	-	-		
92	OHX	5	3422	85	0,6,6	-	-	-		
92	OHX	1	3570	-	0,6,6	-	-	-		
92	OHX	1	3472	-	0,6,6	-	-	-		
92	OHX	5	3598	85	0,6,6	-	-	-		
92	OHX	5	3630	-	0,6,6	-	-	-		
92	OHX	6	2057	80	0,6,6	-	-	-		
92	OHX	5	3417	-	0,6,6	-	-	-		
92	OHX	5	3570	-	0,6,6	-	-	-		
92	OHX	1	3455	-	0,6,6	-	-	-		
92	OHX	2	2026	-	0,6,6	-	-	-		
92	OHX	1	3701	36	0,6,6	-	-	-		
92	OHX	SR	401	-	0,6,6	-	-	-		
92	OHX	1	3684	-	0,6,6	-	-	-		
92	OHX	1	3487	-	0,6,6	-	-	-		
92	OHX	2	1957	-	0,6,6	-	-	-		
92	OHX	L4	401	-	0,6,6	-	-	-		
92	OHX	C5	201	-	0,6,6	-	-	-		
92	OHX	1	3444	-	0,6,6	-	-	-		
92	OHX	1	3532	-	0,6,6	-	-	-		
92	OHX	6	2006	80	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	3659	-	0,6,6	-	-	-		
92	OHX	6	1928	80	0,6,6	-	-	-		
92	OHX	2	1996	-	0,6,6	-	-	-		
92	OHX	1	3491	-	0,6,6	-	-	-		
92	OHX	1	3710	36	0,6,6	-	-	-		
92	OHX	1	3618	-	0,6,6	-	-	-		
92	OHX	6	2029	80	0,6,6	-	-	-		
92	OHX	5	3406	-	0,6,6	-	-	-		
92	OHX	5	3506	-	0,6,6	-	-	-		
92	OHX	5	3582	-	0,6,6	-	-	-		
92	OHX	1	3435	-	0,6,6	-	-	-		
92	OHX	1	3603	-	0,6,6	-	-	-		
92	OHX	6	1905	-	0,6,6	-	-	-		
92	OHX	1	3692	-	0,6,6	-	-	-		
92	OHX	3	202	-	0,6,6	-	-	-		
92	OHX	6	1904	-	0,6,6	-	-	-		
92	OHX	1	3413	-	0,6,6	-	-	-		
92	OHX	2	1969	1	0,6,6	-	-	-		
92	OHX	6	2049	-	0,6,6	-	-	-		
92	OHX	1	3536	-	0,6,6	-	-	-		
92	OHX	6	2046	-	0,6,6	-	-	-		
92	OHX	5	3475	85	0,6,6	-	-	-		
92	OHX	1	3520	-	0,6,6	-	-	-		
92	OHX	5	3563	85	0,6,6	-	-	-		
92	OHX	1	3543	-	0,6,6	-	-	-		
92	OHX	2	1921	-	0,6,6	-	-	-		
92	OHX	5	3536	-	0,6,6	-	-	-		
92	OHX	6	1984	-	0,6,6	-	-	-		
92	OHX	5	3543	85	0,6,6	-	-	-		
92	OHX	1	3688	36	0,6,6	-	-	-		
92	OHX	5	3668	85	0,6,6	-	-	-		
92	OHX	1	3713	-	0,6,6	-	-	-		
92	OHX	5	3503	-	0,6,6	-	-	-		
92	OHX	6	1973	80	0,6,6	-	-	-		
92	OHX	1	3505	-	0,6,6	-	-	-		
92	OHX	5	3498	85	0,6,6	-	-	-		
92	OHX	1	3678	36	0,6,6	-	-	-		
92	OHX	5	3595	85	0,6,6	-	-	-		
92	OHX	1	3412	-	0,6,6	-	-	-		
92	OHX	5	3573	-	0,6,6	-	-	-		
92	OHX	s8	301	-	0,6,6	-	-	-		
92	OHX	5	3450	85	0,6,6	-	-	-		
92	OHX	6	2001	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	1	3447	-	0,6,6	-	-	-		
92	OHX	1	3548	-	0,6,6	-	-	-		
92	OHX	5	3489	-	0,6,6	-	-	-		
92	OHX	1	3725	-	0,6,6	-	-	-		
92	OHX	2	1970	-	0,6,6	-	-	-		
92	OHX	3	209	-	0,6,6	-	-	-		
92	OHX	2	1919	-	0,6,6	-	-	-		
92	OHX	1	3630	-	0,6,6	-	-	-		
92	OHX	2	1960	-	0,6,6	-	-	-		
92	OHX	5	3587	-	0,6,6	-	-	-		
92	OHX	5	3623	-	0,6,6	-	-	-		
92	OHX	2	2004	-	0,6,6	-	-	-		
92	OHX	1	3655	-	0,6,6	-	-	-		
92	OHX	1	3483	-	0,6,6	-	-	-		
92	OHX	1	3686	-	0,6,6	-	-	-		
92	OHX	6	2040	80	0,6,6	-	-	-		
92	OHX	1	3670	-	0,6,6	-	-	-		
92	OHX	l3	402	-	0,6,6	-	-	-		
92	OHX	5	3655	-	0,6,6	-	-	-		
92	OHX	1	3464	-	0,6,6	-	-	-		
92	OHX	5	3686	-	0,6,6	-	-	-		
92	OHX	1	3416	-	0,6,6	-	-	-		
92	OHX	1	3451	-	0,6,6	-	-	-		
92	OHX	5	3561	85	0,6,6	-	-	-		
92	OHX	2	1938	-	0,6,6	-	-	-		
92	OHX	5	3692	-	0,6,6	-	-	-		
92	OHX	5	3721	85	0,6,6	-	-	-		
92	OHX	5	3431	85	0,6,6	-	-	-		
92	OHX	1	3616	36	0,6,6	-	-	-		
92	OHX	5	3451	-	0,6,6	-	-	-		
92	OHX	2	2002	-	0,6,6	-	-	-		
92	OHX	2	1913	-	0,6,6	-	-	-		
92	OHX	5	3403	85	0,6,6	-	-	-		
92	OHX	2	1920	-	0,6,6	-	-	-		
92	OHX	1	3458	-	0,6,6	-	-	-		
92	OHX	1	3697	36	0,6,6	-	-	-		
92	OHX	d4	201	-	0,6,6	-	-	-		
92	OHX	2	1904	1	0,6,6	-	-	-		
92	OHX	1	3441	-	0,6,6	-	-	-		
92	OHX	2	1965	-	0,6,6	-	-	-		
92	OHX	1	3564	36	0,6,6	-	-	-		
92	OHX	5	3735	-	0,6,6	-	-	-		
92	OHX	4	203	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	3646	-	0,6,6	-	-	-		
92	OHX	2	1906	-	0,6,6	-	-	-		
92	OHX	5	3496	-	0,6,6	-	-	-		
92	OHX	6	2047	-	0,6,6	-	-	-		
92	OHX	1	3601	-	0,6,6	-	-	-		
92	OHX	2	2037	1	0,6,6	-	-	-		
92	OHX	5	3637	85	0,6,6	-	-	-		
92	OHX	5	3648	-	0,6,6	-	-	-		
92	OHX	1	3613	-	0,6,6	-	-	-		
92	OHX	1	3636	-	0,6,6	-	-	-		
92	OHX	5	3418	-	0,6,6	-	-	-		
92	OHX	5	3558	-	0,6,6	-	-	-		
92	OHX	1	3700	-	0,6,6	-	-	-		
92	OHX	4	221	-	0,6,6	-	-	-		
92	OHX	2	1901	-	0,6,6	-	-	-		
92	OHX	6	1913	80	0,6,6	-	-	-		
92	OHX	6	1978	-	0,6,6	-	-	-		
92	OHX	2	1959	-	0,6,6	-	-	-		
92	OHX	1	3473	-	0,6,6	-	-	-		
92	OHX	5	3565	85	0,6,6	-	-	-		
92	OHX	6	1971	80	0,6,6	-	-	-		
92	OHX	5	3621	-	0,6,6	-	-	-		
92	OHX	6	1956	-	0,6,6	-	-	-		
92	OHX	5	3625	85	0,6,6	-	-	-		
92	OHX	2	1936	1	0,6,6	-	-	-		
92	OHX	5	3588	85	0,6,6	-	-	-		
92	OHX	8	211	-	0,6,6	-	-	-		
92	OHX	5	3712	85	0,6,6	-	-	-		
92	OHX	5	3620	-	0,6,6	-	-	-		
92	OHX	1	3409	-	0,6,6	-	-	-		
92	OHX	2	1966	1	0,6,6	-	-	-		
92	OHX	1	3679	-	0,6,6	-	-	-		
92	OHX	1	3572	36	0,6,6	-	-	-		
92	OHX	2	1918	-	0,6,6	-	-	-		
92	OHX	5	3601	-	0,6,6	-	-	-		
92	OHX	1	3650	-	0,6,6	-	-	-		
92	OHX	5	3515	-	0,6,6	-	-	-		
92	OHX	1	3644	-	0,6,6	-	-	-		
92	OHX	1	3693	-	0,6,6	-	-	-		
92	OHX	2	1987	1	0,6,6	-	-	-		
92	OHX	1	3466	-	0,6,6	-	-	-		
92	OHX	5	3695	-	0,6,6	-	-	-		
92	OHX	6	1901	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	6	2053	80	0,6,6	-	-	-		
92	OHX	5	3656	-	0,6,6	-	-	-		
92	OHX	1	3449	36	0,6,6	-	-	-		
92	OHX	1	3614	-	0,6,6	-	-	-		
92	OHX	5	3466	-	0,6,6	-	-	-		
92	OHX	5	3525	85	0,6,6	-	-	-		
92	OHX	1	3657	-	0,6,6	-	-	-		
92	OHX	5	3459	85	0,6,6	-	-	-		
92	OHX	5	3605	-	0,6,6	-	-	-		
92	OHX	5	3636	-	0,6,6	-	-	-		
92	OHX	5	3722	85	0,6,6	-	-	-		
92	OHX	6	1952	80	0,6,6	-	-	-		
92	OHX	1	3417	-	0,6,6	-	-	-		
92	OHX	2	1916	-	0,6,6	-	-	-		
92	OHX	5	3562	-	0,6,6	-	-	-		
92	OHX	5	3576	-	0,6,6	-	-	-		
92	OHX	5	3720	85	0,6,6	-	-	-		
92	OHX	5	3482	85	0,6,6	-	-	-		
92	OHX	6	1916	-	0,6,6	-	-	-		
92	OHX	5	3523	-	0,6,6	-	-	-		
92	OHX	1	3612	-	0,6,6	-	-	-		
92	OHX	2	1955	-	0,6,6	-	-	-		
92	OHX	1	3621	36	0,6,6	-	-	-		
92	OHX	5	3731	-	0,6,6	-	-	-		
92	OHX	5	3665	85	0,6,6	-	-	-		
92	OHX	1	3424	-	0,6,6	-	-	-		
92	OHX	1	3706	-	0,6,6	-	-	-		
92	OHX	2	1949	-	0,6,6	-	-	-		
92	OHX	2	2017	-	0,6,6	-	-	-		
92	OHX	1	3554	-	0,6,6	-	-	-		
92	OHX	5	3657	85	0,6,6	-	-	-		
92	OHX	1	3703	-	0,6,6	-	-	-		
92	OHX	1	3647	-	0,6,6	-	-	-		
92	OHX	6	1949	-	0,6,6	-	-	-		
92	OHX	s1	301	-	0,6,6	-	-	-		
92	OHX	5	3634	-	0,6,6	-	-	-		
92	OHX	5	3469	85	0,6,6	-	-	-		
92	OHX	6	1927	80	0,6,6	-	-	-		
92	OHX	2	1963	1	0,6,6	-	-	-		
92	OHX	6	1969	-	0,6,6	-	-	-		
92	OHX	5	3555	-	0,6,6	-	-	-		
92	OHX	1	3649	-	0,6,6	-	-	-		
92	OHX	5	3599	85	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	2	1956	-	0,6,6	-	-	-		
97	SPS	p	101	93	20,23,23	3.43	9 (45%)	18,30,30	4.56	13 (72%)
92	OHX	2	2051	-	0,6,6	-	-	-		
92	OHX	1	3516	-	0,6,6	-	-	-		
92	OHX	1	3580	-	0,6,6	-	-	-		
92	OHX	4	206	38	0,6,6	-	-	-		
92	OHX	6	1985	-	0,6,6	-	-	-		
92	OHX	1	3714	-	0,6,6	-	-	-		
92	OHX	2	2018	-	0,6,6	-	-	-		
92	OHX	6	2017	80	0,6,6	-	-	-		
92	OHX	5	3544	85	0,6,6	-	-	-		
92	OHX	5	3412	-	0,6,6	-	-	-		
92	OHX	5	3516	85	0,6,6	-	-	-		
92	OHX	6	2052	80	0,6,6	-	-	-		
92	OHX	6	2018	80	0,6,6	-	-	-		
92	OHX	6	1992	-	0,6,6	-	-	-		
92	OHX	5	3714	85	0,6,6	-	-	-		
92	OHX	8	203	-	0,6,6	-	-	-		
92	OHX	5	3426	-	0,6,6	-	-	-		
92	OHX	5	3445	-	0,6,6	-	-	-		
92	OHX	6	1966	80	0,6,6	-	-	-		
92	OHX	6	1983	-	0,6,6	-	-	-		
92	OHX	5	3439	-	0,6,6	-	-	-		
92	OHX	1	3602	-	0,6,6	-	-	-		
92	OHX	1	3660	-	0,6,6	-	-	-		
92	OHX	6	2054	-	0,6,6	-	-	-		
92	OHX	5	3434	-	0,6,6	-	-	-		
92	OHX	5	3488	85	0,6,6	-	-	-		
92	OHX	6	1977	80	0,6,6	-	-	-		
92	OHX	o7	502	-	0,6,6	-	-	-		
92	OHX	6	1968	80	0,6,6	-	-	-		
92	OHX	5	3687	-	0,6,6	-	-	-		
92	OHX	2	2039	1	0,6,6	-	-	-		
92	OHX	6	1907	80	0,6,6	-	-	-		
92	OHX	1	3579	-	0,6,6	-	-	-		
92	OHX	6	1960	80	0,6,6	-	-	-		
92	OHX	1	3685	-	0,6,6	-	-	-		
92	OHX	5	3707	-	0,6,6	-	-	-		
92	OHX	1	3716	-	0,6,6	-	-	-		
92	OHX	5	3541	-	0,6,6	-	-	-		
92	OHX	5	3732	-	0,6,6	-	-	-		
92	OHX	1	3507	-	0,6,6	-	-	-		
92	OHX	5	3485	85	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	6	1930	80	0,6,6	-	-	-		
92	OHX	2	1992	-	0,6,6	-	-	-		
92	OHX	5	3704	85	0,6,6	-	-	-		
92	OHX	1	3661	-	0,6,6	-	-	-		
92	OHX	6	1993	80	0,6,6	-	-	-		
92	OHX	2	1984	-	0,6,6	-	-	-		
92	OHX	1	3427	36	0,6,6	-	-	-		
92	OHX	1	3452	-	0,6,6	-	-	-		
92	OHX	2	1923	1	0,6,6	-	-	-		
92	OHX	5	3638	85	0,6,6	-	-	-		
92	OHX	2	2030	1	0,6,6	-	-	-		
92	OHX	1	3541	-	0,6,6	-	-	-		
92	OHX	6	1923	80	0,6,6	-	-	-		
92	OHX	6	1932	80	0,6,6	-	-	-		
92	OHX	5	3730	-	0,6,6	-	-	-		
92	OHX	13	401	-	0,6,6	-	-	-		
92	OHX	5	3438	-	0,6,6	-	-	-		
92	OHX	5	3441	85	0,6,6	-	-	-		
92	OHX	5	3407	-	0,6,6	-	-	-		
92	OHX	4	216	-	0,6,6	-	-	-		
92	OHX	1	3508	-	0,6,6	-	-	-		
92	OHX	5	3676	-	0,6,6	-	-	-		
92	OHX	4	217	-	0,6,6	-	-	-		
92	OHX	1	3517	-	0,6,6	-	-	-		
92	OHX	5	3508	-	0,6,6	-	-	-		
92	OHX	6	1975	-	0,6,6	-	-	-		
92	OHX	8	202	38	0,6,6	-	-	-		
92	OHX	5	3517	-	0,6,6	-	-	-		
92	OHX	6	2039	80	0,6,6	-	-	-		
92	OHX	5	3674	85	0,6,6	-	-	-		
92	OHX	5	3577	85	0,6,6	-	-	-		
92	OHX	1	3430	-	0,6,6	-	-	-		
92	OHX	1	3544	-	0,6,6	-	-	-		
92	OHX	5	3652	-	0,6,6	-	-	-		
92	OHX	2	2033	1	0,6,6	-	-	-		
92	OHX	2	1946	-	0,6,6	-	-	-		
92	OHX	2	1952	1	0,6,6	-	-	-		
92	OHX	2	1975	-	0,6,6	-	-	-		
92	OHX	6	2024	-	0,6,6	-	-	-		
92	OHX	6	1964	80	0,6,6	-	-	-		
92	OHX	6	2033	80	0,6,6	-	-	-		
92	OHX	5	3651	-	0,6,6	-	-	-		
92	OHX	5	3678	85	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	3454	-	0,6,6	-	-	-		
92	OHX	1	3534	-	0,6,6	-	-	-		
92	OHX	6	2034	-	0,6,6	-	-	-		
92	OHX	5	3512	-	0,6,6	-	-	-		
92	OHX	5	3520	-	0,6,6	-	-	-		
92	OHX	1	3498	36	0,6,6	-	-	-		
92	OHX	5	3628	-	0,6,6	-	-	-		
92	OHX	7	208	37	0,6,6	-	-	-		
92	OHX	5	3649	-	0,6,6	-	-	-		
92	OHX	5	3724	85	0,6,6	-	-	-		
92	OHX	1	3619	-	0,6,6	-	-	-		
92	OHX	2	1985	-	0,6,6	-	-	-		
92	OHX	6	1908	80	0,6,6	-	-	-		
92	OHX	5	3411	-	0,6,6	-	-	-		
92	OHX	5	3462	-	0,6,6	-	-	-		
92	OHX	5	3529	85	0,6,6	-	-	-		
92	OHX	1	3606	-	0,6,6	-	-	-		
92	OHX	1	3672	-	0,6,6	-	-	-		
92	OHX	O9	101	-	0,6,6	-	-	-		
92	OHX	6	1911	-	0,6,6	-	-	-		
92	OHX	1	3646	-	0,6,6	-	-	-		
92	OHX	4	213	-	0,6,6	-	-	-		
92	OHX	2	2034	-	0,6,6	-	-	-		
92	OHX	1	3695	36	0,6,6	-	-	-		
92	OHX	2	1930	-	0,6,6	-	-	-		
92	OHX	1	3474	-	0,6,6	-	-	-		
92	OHX	2	2027	-	0,6,6	-	-	-		
92	OHX	5	3575	-	0,6,6	-	-	-		
92	OHX	5	3453	85	0,6,6	-	-	-		
92	OHX	2	1910	-	0,6,6	-	-	-		
92	OHX	5	3419	85	0,6,6	-	-	-		
92	OHX	2	2046	-	0,6,6	-	-	-		
92	OHX	1	3694	-	0,6,6	-	-	-		
92	OHX	1	3587	-	0,6,6	-	-	-		
92	OHX	2	1951	-	0,6,6	-	-	-		
92	OHX	1	3729	-	0,6,6	-	-	-		
92	OHX	1	3495	-	0,6,6	-	-	-		
92	OHX	1	3582	36	0,6,6	-	-	-		
92	OHX	1	3696	-	0,6,6	-	-	-		
92	OHX	1	3590	-	0,6,6	-	-	-		
92	OHX	6	2036	80	0,6,6	-	-	-		
92	OHX	2	1999	-	0,6,6	-	-	-		
92	OHX	5	3424	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	3592	85	0,6,6	-	-	-		
92	OHX	5	3682	85	0,6,6	-	-	-		
92	OHX	5	3715	85	0,6,6	-	-	-		
92	OHX	5	3590	85	0,6,6	-	-	-		
92	OHX	2	1991	-	0,6,6	-	-	-		
92	OHX	5	3626	85	0,6,6	-	-	-		
92	OHX	5	3549	-	0,6,6	-	-	-		
92	OHX	1	3418	-	0,6,6	-	-	-		
92	OHX	5	3435	-	0,6,6	-	-	-		
92	OHX	6	1941	80	0,6,6	-	-	-		
92	OHX	1	3477	-	0,6,6	-	-	-		
92	OHX	1	3540	-	0,6,6	-	-	-		
92	OHX	1	3719	-	0,6,6	-	-	-		
92	OHX	1	3709	-	0,6,6	-	-	-		
92	OHX	6	2000	80	0,6,6	-	-	-		
92	OHX	6	1982	80	0,6,6	-	-	-		
92	OHX	5	3524	85	0,6,6	-	-	-		
92	OHX	1	3584	-	0,6,6	-	-	-		
92	OHX	4	205	38	0,6,6	-	-	-		
92	OHX	1	3437	-	0,6,6	-	-	-		
92	OHX	1	3726	-	0,6,6	-	-	-		
92	OHX	2	1933	-	0,6,6	-	-	-		
92	OHX	1	3595	-	0,6,6	-	-	-		
92	OHX	5	3740	-	0,6,6	-	-	-		
92	OHX	1	3573	36	0,6,6	-	-	-		
92	OHX	5	3726	85	0,6,6	-	-	-		
92	OHX	6	1937	-	0,6,6	-	-	-		
92	OHX	1	3596	-	0,6,6	-	-	-		
97	SPS	P	101	93	20,23,23	3.42	9 (45%)	18,30,30	5.37	12 (66%)
92	OHX	1	3531	-	0,6,6	-	-	-		
92	OHX	1	3631	-	0,6,6	-	-	-		
92	OHX	6	1958	80	0,6,6	-	-	-		
92	OHX	5	3627	-	0,6,6	-	-	-		
92	OHX	5	3596	85	0,6,6	-	-	-		
92	OHX	2	1928	-	0,6,6	-	-	-		
92	OHX	2	1939	-	0,6,6	-	-	-		
92	OHX	6	2059	-	0,6,6	-	-	-		
92	OHX	5	3689	-	0,6,6	-	-	-		
92	OHX	1	3551	-	0,6,6	-	-	-		
92	OHX	5	3409	-	0,6,6	-	-	-		
92	OHX	1	3481	-	0,6,6	-	-	-		
92	OHX	2	2012	1	0,6,6	-	-	-		
92	OHX	1	3462	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	1	3608	-	0,6,6	-	-	-		
92	OHX	1	3597	-	0,6,6	-	-	-		
92	OHX	5	3493	85	0,6,6	-	-	-		
92	OHX	S9	201	-	0,6,6	-	-	-		
92	OHX	1	3539	-	0,6,6	-	-	-		
92	OHX	5	3734	-	0,6,6	-	-	-		
92	OHX	5	3463	-	0,6,6	-	-	-		
92	OHX	5	3608	-	0,6,6	-	-	-		
92	OHX	4	207	-	0,6,6	-	-	-		
92	OHX	6	2051	80	0,6,6	-	-	-		
92	OHX	5	3681	85	0,6,6	-	-	-		
92	OHX	5	3702	-	0,6,6	-	-	-		
92	OHX	1	3471	-	0,6,6	-	-	-		
92	OHX	5	3472	85	0,6,6	-	-	-		
92	OHX	7	210	37	0,6,6	-	-	-		
92	OHX	2	2015	-	0,6,6	-	-	-		
92	OHX	1	3499	-	0,6,6	-	-	-		
92	OHX	5	3602	-	0,6,6	-	-	-		
92	OHX	5	3642	85	0,6,6	-	-	-		
92	OHX	1	3486	-	0,6,6	-	-	-		
92	OHX	5	3499	85	0,6,6	-	-	-		
92	OHX	1	3422	-	0,6,6	-	-	-		
92	OHX	5	3502	-	0,6,6	-	-	-		
92	OHX	6	2016	80	0,6,6	-	-	-		
92	OHX	6	2028	80	0,6,6	-	-	-		
92	OHX	5	3444	-	0,6,6	-	-	-		
92	OHX	6	1965	-	0,6,6	-	-	-		
92	OHX	5	3518	-	0,6,6	-	-	-		
92	OHX	2	2041	-	0,6,6	-	-	-		
92	OHX	1	3525	-	0,6,6	-	-	-		
92	OHX	2	1976	-	0,6,6	-	-	-		
92	OHX	6	1918	80	0,6,6	-	-	-		
92	OHX	5	3528	-	0,6,6	-	-	-		
92	OHX	5	3611	-	0,6,6	-	-	-		
92	OHX	2	1905	-	0,6,6	-	-	-		
92	OHX	5	3624	-	0,6,6	-	-	-		
92	OHX	1	3484	-	0,6,6	-	-	-		
92	OHX	M6	201	-	0,6,6	-	-	-		
92	OHX	2	2016	-	0,6,6	-	-	-		
92	OHX	2	1909	-	0,6,6	-	-	-		
92	OHX	2	2048	-	0,6,6	-	-	-		
92	OHX	5	3532	85	0,6,6	-	-	-		
92	OHX	5	3491	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	3711	-	0,6,6	-	-	-		
92	OHX	1	3410	-	0,6,6	-	-	-		
92	OHX	1	3547	-	0,6,6	-	-	-		
92	OHX	2	1998	-	0,6,6	-	-	-		
92	OHX	1	3586	-	0,6,6	-	-	-		
92	OHX	5	3574	-	0,6,6	-	-	-		
92	OHX	6	2002	80	0,6,6	-	-	-		
92	OHX	5	3586	85	0,6,6	-	-	-		
92	OHX	2	2000	-	0,6,6	-	-	-		
92	OHX	1	3501	-	0,6,6	-	-	-		
92	OHX	6	2020	-	0,6,6	-	-	-		
92	OHX	1	3469	-	0,6,6	-	-	-		
92	OHX	2	2038	-	0,6,6	-	-	-		
92	OHX	2	2008	-	0,6,6	-	-	-		
92	OHX	5	3673	85	0,6,6	-	-	-		
92	OHX	5	3643	85	0,6,6	-	-	-		
92	OHX	5	3580	-	0,6,6	-	-	-		
92	OHX	2	2040	-	0,6,6	-	-	-		
92	OHX	6	1946	-	0,6,6	-	-	-		
92	OHX	1	3717	-	0,6,6	-	-	-		
92	OHX	2	1997	-	0,6,6	-	-	-		
92	OHX	1	3555	-	0,6,6	-	-	-		
92	OHX	1	3665	-	0,6,6	-	-	-		
92	OHX	N9	101	-	0,6,6	-	-	-		
92	OHX	6	1997	-	0,6,6	-	-	-		
92	OHX	1	3568	-	0,6,6	-	-	-		
92	OHX	1	3653	-	0,6,6	-	-	-		
92	OHX	1	3699	-	0,6,6	-	-	-		
92	OHX	m8	201	-	0,6,6	-	-	-		
92	OHX	1	3707	-	0,6,6	-	-	-		
92	OHX	5	3688	-	0,6,6	-	-	-		
92	OHX	5	3428	85	0,6,6	-	-	-		
92	OHX	m5	301	-	0,6,6	-	-	-		
92	OHX	5	3467	-	0,6,6	-	-	-		
92	OHX	1	3493	36	0,6,6	-	-	-		
92	OHX	5	3504	-	0,6,6	-	-	-		
92	OHX	8	214	38	0,6,6	-	-	-		
92	OHX	5	3572	85	0,6,6	-	-	-		
92	OHX	1	3681	-	0,6,6	-	-	-		
92	OHX	6	1926	80	0,6,6	-	-	-		
92	OHX	C7	201	-	0,6,6	-	-	-		
92	OHX	5	3723	85	0,6,6	-	-	-		
92	OHX	1	3559	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	3447	85	0,6,6	-	-	-		
92	OHX	2	2049	-	0,6,6	-	-	-		
92	OHX	1	3553	-	0,6,6	-	-	-		
92	OHX	5	3474	85	0,6,6	-	-	-		
92	OHX	5	3486	-	0,6,6	-	-	-		
92	OHX	1	3488	-	0,6,6	-	-	-		
92	OHX	5	3443	37	0,6,6	-	-	-		
92	OHX	6	1924	80	0,6,6	-	-	-		
92	OHX	1	3659	-	0,6,6	-	-	-		
92	OHX	m0	303	-	0,6,6	-	-	-		
92	OHX	1	3648	-	0,6,6	-	-	-		
92	OHX	6	1959	-	0,6,6	-	-	-		
92	OHX	1	3461	-	0,6,6	-	-	-		
92	OHX	5	3465	-	0,6,6	-	-	-		
92	OHX	1	3521	-	0,6,6	-	-	-		
92	OHX	6	2004	-	0,6,6	-	-	-		
92	OHX	5	3495	85	0,6,6	-	-	-		
92	OHX	7	212	-	0,6,6	-	-	-		
92	OHX	L3	401	-	0,6,6	-	-	-		
92	OHX	5	3581	-	0,6,6	-	-	-		
92	OHX	2	2029	-	0,6,6	-	-	-		
92	OHX	1	3479	-	0,6,6	-	-	-		
92	OHX	1	3506	-	0,6,6	-	-	-		
92	OHX	2	1917	-	0,6,6	-	-	-		
92	OHX	2	1941	-	0,6,6	-	-	-		
92	OHX	6	1935	80	0,6,6	-	-	-		
92	OHX	5	3479	-	0,6,6	-	-	-		
92	OHX	5	3464	85	0,6,6	-	-	-		
92	OHX	8	201	-	0,6,6	-	-	-		
92	OHX	5	3742	-	0,6,6	-	-	-		
92	OHX	1	3404	-	0,6,6	-	-	-		
92	OHX	1	3475	-	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
95	PHE	1	3401	-	-	3/5/6/8	0/1/1/1
96	LEU	5	3402	-	-	4/5/6/8	-
97	SPS	p	101	93	-	3/15/18/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
97	SPS	P	101	93	-	1/15/18/18	0/1/1/1
98	8AN	p	102	93,91	-	1/3/25/26	0/3/3/3
95	PHE	5	3401	-	-	3/5/6/8	0/1/1/1
98	8AN	P	102	93,91	-	1/3/25/26	0/3/3/3
96	LEU	1	3402	-	-	4/5/6/8	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
97	P	101	SPS	C9-C8	8.45	1.54	1.33
97	p	101	SPS	C9-C8	7.87	1.53	1.33
97	p	101	SPS	C9-C10	-7.33	1.32	1.48
97	P	101	SPS	C9-C10	-5.91	1.35	1.48
97	P	101	SPS	C10-N11	5.65	1.46	1.34

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
97	P	101	SPS	C3-N2-C1	12.87	125.96	115.09
97	P	101	SPS	O15-S15-C16	-11.93	92.28	106.47
97	p	101	SPS	C3-N2-C1	10.04	123.57	115.09
97	P	101	SPS	O13-C13-C12	7.76	131.24	111.73
97	P	101	SPS	C6-C1-N2	-6.74	117.79	124.68

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

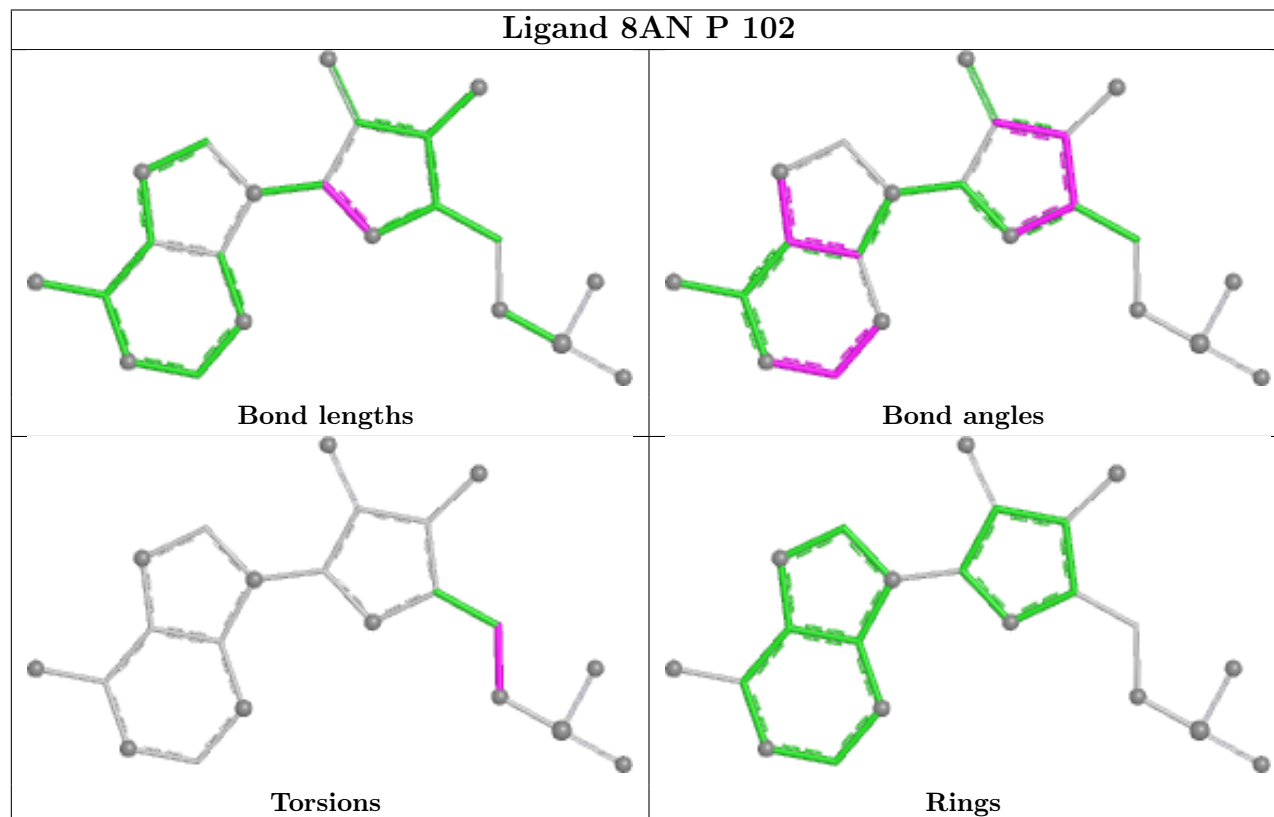
Mol	Chain	Res	Type	Atoms
95	1	3401	PHE	O-C-CA-CB
95	5	3401	PHE	O-C-CA-CB
96	1	3402	LEU	C-CA-CB-CG
96	5	3402	LEU	C-CA-CB-CG
97	P	101	SPS	N11-C12-C14-S15

There are no ring outliers.

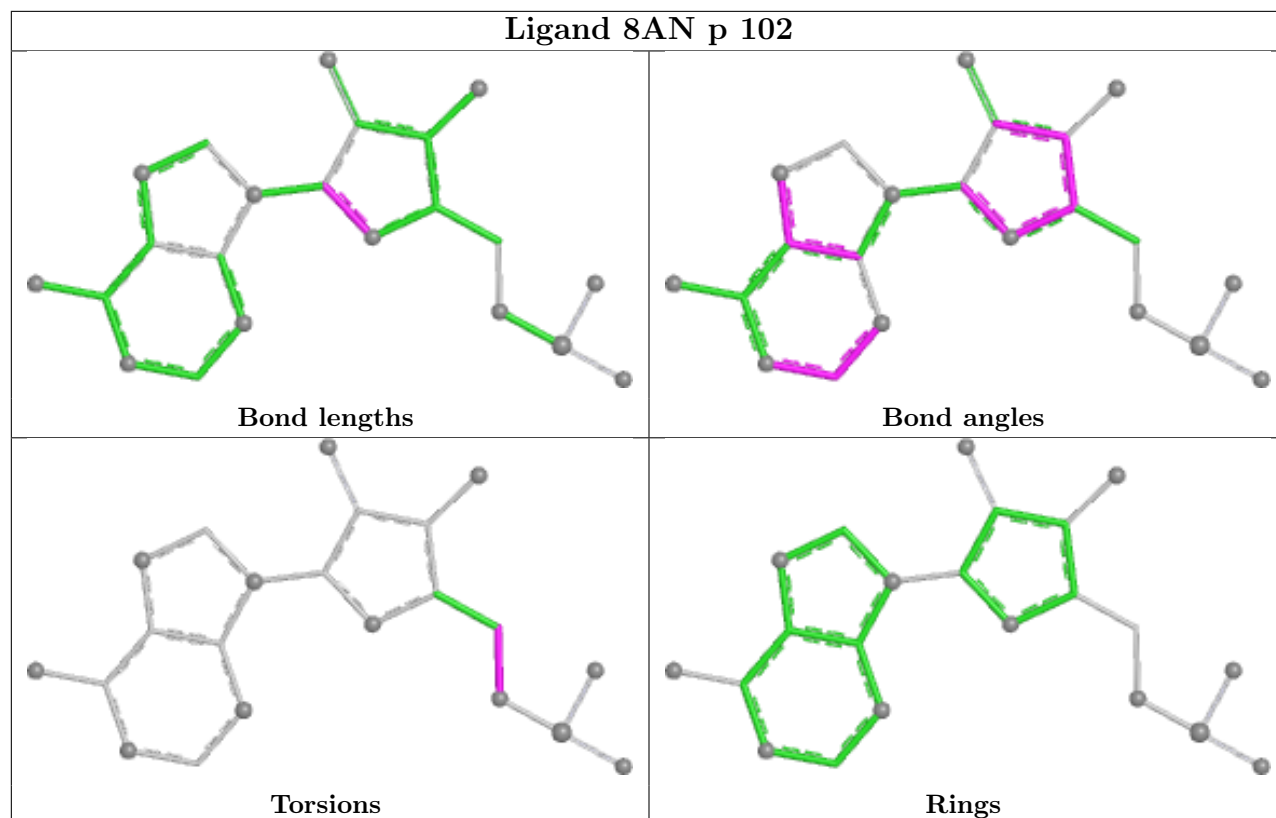
No monomer is involved in short contacts.

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

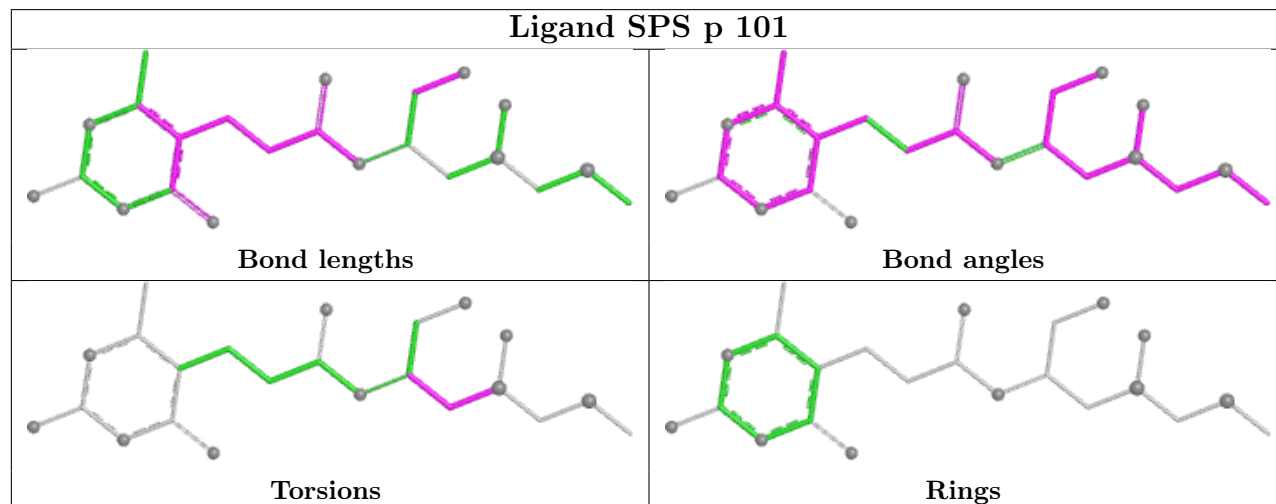
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

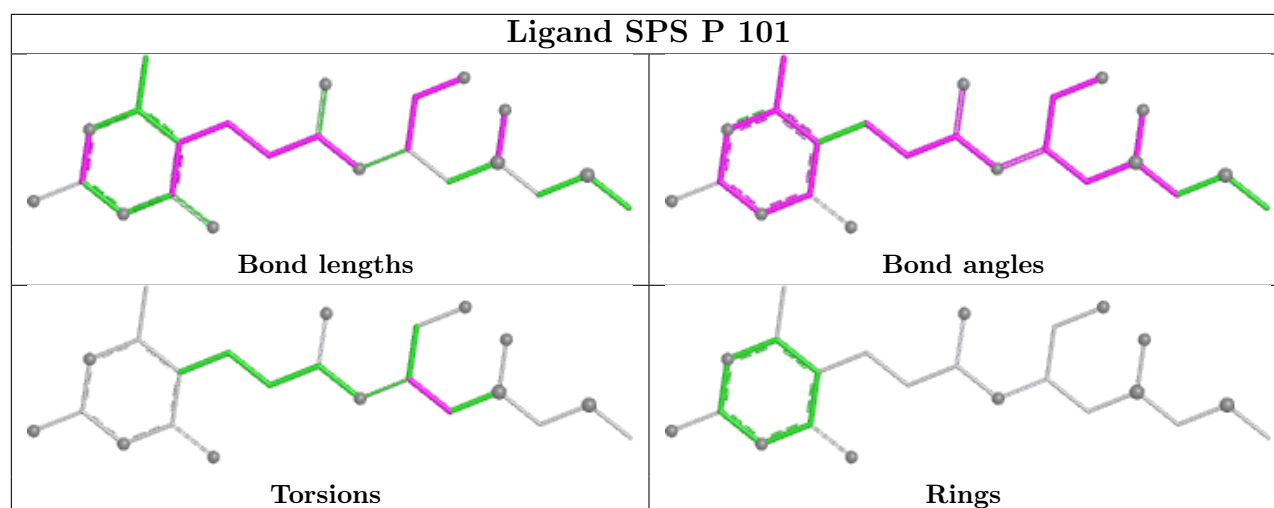


Ligand 8AN p 102



Ligand SPS p 101





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
36	1	3
85	5	3
1	2	2
84	sM	2
87	m2	2
41	l4	2
35	SM	1
10	s8	1
10	S8	1
89	p0	1
81	c0	1
19	C7	1
82	c7	1
13	C1	1
57	n1	1
68	O2	1
40	l3	1
6	S4	1

The worst 5 of 26 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1781:U	O3'	1782:C	P	145.43
1	sM	85:SER	C	119:UNK	N	43.83
1	sM	139:UNK	C	155:UNK	N	38.91
1	1	1955:U	O3'	2093:A	P	25.58
1	SM	141:ALA	C	151:UNK	N	25.40

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	2	1781/1812 (98%)	1.06	192 (10%) 12 10	38, 89, 120, 149	1 (0%)
2	S0	206/206 (100%)	0.97	22 (10%) 12 10	93, 99, 105, 107	0
2	s0	206/206 (100%)	0.68	11 (5%) 33 24	77, 83, 89, 90	0
3	S1	214/216 (99%)	1.06	20 (9%) 16 12	95, 106, 113, 113	0
3	s1	216/216 (100%)	0.54	4 (1%) 66 46	70, 75, 81, 84	0
4	S2	217/217 (100%)	0.87	18 (8%) 19 14	81, 88, 96, 99	0
4	s2	217/217 (100%)	0.82	26 (11%) 10 8	67, 73, 79, 81	0
5	S3	223/223 (100%)	0.83	19 (8%) 18 14	85, 96, 110, 115	0
5	s3	223/223 (100%)	0.71	12 (5%) 32 23	91, 102, 113, 114	0
6	S4	260/260 (100%)	1.00	23 (8%) 17 13	75, 88, 91, 93	0
6	s4	260/260 (100%)	0.70	9 (3%) 47 32	59, 73, 78, 80	0
7	S5	206/206 (100%)	1.43	41 (19%) 3 3	97, 105, 111, 113	0
7	s5	206/206 (100%)	1.09	27 (13%) 8 7	90, 95, 101, 103	0
8	S6	226/226 (100%)	1.01	30 (13%) 8 7	62, 76, 96, 101	0
8	s6	218/226 (96%)	0.53	8 (3%) 45 30	55, 63, 82, 86	0
9	S7	184/186 (98%)	1.18	24 (13%) 9 7	92, 102, 108, 109	0
9	s7	186/186 (100%)	0.97	17 (9%) 16 13	75, 90, 101, 104	0
10	S8	188/188 (100%)	0.86	12 (6%) 27 20	72, 78, 92, 95	0
10	s8	188/188 (100%)	0.93	16 (8%) 18 14	57, 68, 89, 95	0
11	S9	185/185 (100%)	1.03	18 (9%) 15 11	81, 89, 99, 103	0
11	s9	185/185 (100%)	0.62	7 (3%) 44 30	63, 74, 82, 84	0
12	C0	83/96 (86%)	0.65	3 (3%) 46 31	94, 100, 105, 107	0
13	C1	146/155 (94%)	1.13	18 (12%) 9 8	75, 79, 85, 89	0
13	c1	146/155 (94%)	1.18	20 (13%) 8 7	62, 67, 81, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	C2	119/124 (95%)	1.10	14 (11%) 10 9	111, 116, 118, 119	0
14	c2	119/124 (95%)	1.52	29 (24%) 2 2	133, 142, 148, 149	0
15	C3	150/150 (100%)	0.96	10 (6%) 25 19	80, 88, 92, 94	0
15	c3	150/150 (100%)	0.81	7 (4%) 37 26	65, 75, 80, 82	0
16	C4	127/128 (99%)	1.50	32 (25%) 2 2	82, 105, 111, 112	0
16	c4	128/128 (100%)	0.75	7 (5%) 32 23	63, 74, 79, 80	0
17	C5	122/135 (90%)	0.82	7 (5%) 30 23	80, 90, 96, 101	0
17	c5	125/135 (92%)	1.23	22 (17%) 4 4	65, 91, 98, 100	0
18	C6	141/142 (99%)	1.44	30 (21%) 3 3	88, 105, 109, 110	0
18	c6	142/142 (100%)	1.30	24 (16%) 5 5	90, 98, 102, 104	0
19	C7	120/120 (100%)	0.88	6 (5%) 35 25	98, 104, 108, 109	0
20	C8	145/145 (100%)	0.62	2 (1%) 73 53	83, 95, 107, 110	0
20	c8	145/145 (100%)	0.70	4 (2%) 55 37	69, 86, 93, 97	0
21	C9	143/143 (100%)	1.09	14 (9%) 14 11	92, 101, 106, 108	0
21	c9	143/143 (100%)	0.83	11 (7%) 21 16	87, 92, 96, 98	0
22	D0	107/110 (97%)	1.09	17 (15%) 6 6	87, 100, 105, 106	0
22	d0	110/110 (100%)	0.75	7 (6%) 27 20	92, 104, 110, 111	0
23	D1	87/87 (100%)	0.70	5 (5%) 30 23	90, 94, 102, 106	0
23	d1	87/87 (100%)	0.58	1 (1%) 77 59	74, 78, 86, 89	0
24	D2	129/129 (100%)	1.24	20 (15%) 6 6	82, 88, 92, 98	0
24	d2	129/129 (100%)	0.78	4 (3%) 51 35	67, 72, 75, 76	0
25	D3	144/144 (100%)	1.33	28 (19%) 4 3	71, 76, 79, 80	0
25	d3	144/144 (100%)	0.91	19 (13%) 8 7	57, 59, 64, 66	0
26	D4	134/134 (100%)	0.74	5 (3%) 45 30	76, 88, 92, 94	0
26	d4	134/134 (100%)	0.66	11 (8%) 19 15	60, 71, 74, 76	0
27	D5	70/70 (100%)	0.84	2 (2%) 54 36	104, 108, 111, 112	0
27	d5	69/70 (98%)	0.90	3 (4%) 40 27	93, 97, 100, 101	0
28	D6	97/97 (100%)	1.32	14 (14%) 7 6	84, 91, 112, 113	0
28	d6	97/97 (100%)	0.92	10 (10%) 13 11	65, 72, 81, 83	0
29	D7	81/81 (100%)	0.87	4 (4%) 36 25	90, 94, 99, 100	0
29	d7	81/81 (100%)	0.79	3 (3%) 45 30	74, 80, 88, 89	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
30	D8	63/63 (100%)	1.37	9 (14%)	7 6	98, 107, 112, 113	0
30	d8	63/63 (100%)	0.96	5 (7%)	20 16	90, 95, 99, 100	0
31	D9	53/53 (100%)	1.02	9 (16%)	5 5	89, 91, 96, 97	0
31	d9	53/53 (100%)	1.47	15 (28%)	1 2	93, 97, 113, 120	0
32	E0	60/62 (96%)	1.25	11 (18%)	4 4	72, 87, 97, 101	0
32	e0	62/62 (100%)	0.51	3 (4%)	36 26	58, 72, 77, 80	0
33	E1	71/76 (93%)	1.40	13 (18%)	4 4	92, 108, 113, 113	0
33	e1	76/76 (100%)	2.04	35 (46%)	1 1	99, 127, 139, 140	0
34	SR	318/318 (100%)	1.03	28 (8%)	17 13	104, 111, 118, 122	0
35	SM	121/159 (76%)	0.68	8 (6%)	26 19	55, 83, 96, 98	0
36	1	3149/3149 (100%)	0.48	169 (5%)	32 23	31, 49, 82, 154	0
37	3	121/121 (100%)	0.13	1 (0%)	82 67	41, 59, 64, 65	0
37	7	121/121 (100%)	0.24	2 (1%)	69 49	36, 47, 51, 54	0
38	4	158/158 (100%)	0.11	2 (1%)	74 56	33, 45, 63, 84	0
38	8	158/158 (100%)	0.25	7 (4%)	39 27	36, 49, 68, 76	0
39	L2	252/252 (100%)	0.61	9 (3%)	46 31	40, 52, 61, 73	0
39	l2	252/252 (100%)	0.68	18 (7%)	23 18	39, 53, 62, 66	0
40	L3	386/386 (100%)	0.46	19 (4%)	36 25	38, 50, 58, 62	0
40	l3	386/386 (100%)	0.33	13 (3%)	48 32	32, 39, 47, 58	0
41	L4	361/361 (100%)	0.16	9 (2%)	58 40	31, 37, 47, 51	0
41	l4	361/361 (100%)	0.24	16 (4%)	39 27	33, 41, 48, 58	0
42	L5	296/296 (100%)	0.30	7 (2%)	59 41	50, 60, 67, 69	0
42	l5	294/296 (99%)	0.24	5 (1%)	69 49	43, 49, 57, 66	0
43	L6	156/175 (89%)	0.34	8 (5%)	34 25	38, 46, 49, 55	0
43	l6	157/175 (89%)	0.45	9 (5%)	30 23	40, 46, 49, 52	0
44	L7	222/223 (99%)	0.31	3 (1%)	73 53	36, 40, 48, 50	0
44	l7	223/223 (100%)	0.18	2 (0%)	81 64	34, 38, 48, 54	0
45	L8	233/233 (100%)	0.50	3 (1%)	74 56	54, 60, 74, 77	0
46	L9	191/191 (100%)	0.19	2 (1%)	79 61	48, 51, 53, 59	0
46	l9	191/191 (100%)	0.28	4 (2%)	63 44	39, 44, 52, 63	0
47	M0	211/220 (95%)	0.29	2 (0%)	81 64	39, 48, 61, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
47	m0	213/220 (96%)	0.33	4 (1%) 66 46	36, 42, 57, 67	0
48	M1	169/169 (100%)	0.39	1 (0%) 85 72	57, 67, 73, 76	0
48	m1	169/169 (100%)	0.19	2 (1%) 76 57	44, 54, 59, 63	0
49	M3	193/194 (99%)	0.13	2 (1%) 79 61	33, 46, 59, 74	0
49	m3	194/194 (100%)	0.27	1 (0%) 87 75	35, 50, 61, 70	0
50	M4	136/137 (99%)	0.37	6 (4%) 39 27	45, 49, 54, 56	0
50	m4	137/137 (100%)	0.16	3 (2%) 62 43	39, 43, 52, 60	0
51	M5	203/203 (100%)	0.34	2 (0%) 79 61	35, 46, 54, 56	0
51	m5	203/203 (100%)	0.38	2 (0%) 79 61	38, 50, 57, 59	0
52	M6	197/197 (100%)	0.38	8 (4%) 42 28	39, 42, 50, 52	0
52	m6	197/197 (100%)	0.19	7 (3%) 46 31	32, 36, 49, 50	0
53	M7	183/183 (100%)	0.51	18 (9%) 14 11	38, 43, 58, 62	0
53	m7	155/183 (84%)	0.11	2 (1%) 74 56	34, 37, 40, 43	0
54	M8	185/185 (100%)	0.45	6 (3%) 50 34	36, 44, 54, 61	0
54	m8	185/185 (100%)	0.33	6 (3%) 50 34	35, 44, 48, 50	0
55	M9	188/188 (100%)	0.59	14 (7%) 22 17	49, 61, 103, 111	0
55	m9	188/188 (100%)	0.52	10 (5%) 33 24	43, 55, 98, 106	0
56	N0	172/172 (100%)	0.21	3 (1%) 69 49	42, 46, 51, 53	0
56	n0	172/172 (100%)	0.12	2 (1%) 76 57	36, 39, 44, 48	0
57	N1	159/159 (100%)	0.33	1 (0%) 85 72	40, 47, 56, 57	0
57	n1	159/159 (100%)	0.18	2 (1%) 74 56	36, 42, 53, 55	0
58	N2	100/100 (100%)	0.57	2 (2%) 64 45	65, 69, 72, 73	0
58	n2	98/100 (98%)	0.25	0 100 100	56, 59, 60, 61	0
59	N3	136/136 (100%)	0.59	9 (6%) 26 19	43, 49, 52, 54	0
59	n3	136/136 (100%)	0.29	2 (1%) 71 53	33, 37, 41, 43	0
60	N4	98/98 (100%)	1.33	20 (20%) 3 3	49, 59, 89, 91	0
61	N5	121/121 (100%)	0.14	0 100 100	43, 45, 62, 72	0
61	n5	120/121 (99%)	0.29	1 (0%) 82 67	44, 48, 65, 67	0
62	N6	126/126 (100%)	0.13	2 (1%) 70 51	35, 41, 44, 45	0
62	n6	126/126 (100%)	0.11	4 (3%) 50 34	38, 45, 49, 50	0
63	N7	135/135 (100%)	0.38	3 (2%) 62 43	62, 67, 76, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
63	n7	135/135 (100%)	0.51	2 (1%) 71 53	65, 71, 78, 83	0
64	N8	148/148 (100%)	0.10	0 100 100	31, 43, 50, 57	0
64	n8	148/148 (100%)	0.10	3 (2%) 64 45	31, 45, 48, 50	0
65	N9	58/58 (100%)	0.38	2 (3%) 48 32	36, 49, 66, 71	0
65	n9	58/58 (100%)	0.16	2 (3%) 48 32	34, 45, 52, 53	0
66	O0	97/100 (97%)	0.28	1 (1%) 79 61	60, 64, 70, 71	0
66	o0	100/100 (100%)	0.34	3 (3%) 52 35	61, 66, 73, 75	0
67	O1	109/109 (100%)	0.61	2 (1%) 67 48	51, 55, 59, 67	0
67	o1	109/109 (100%)	0.27	2 (1%) 67 48	41, 43, 47, 49	0
68	O2	127/127 (100%)	0.45	9 (7%) 23 18	32, 39, 41, 43	0
68	o2	127/127 (100%)	0.22	1 (0%) 82 67	31, 40, 43, 44	0
69	O3	106/106 (100%)	0.35	4 (3%) 44 30	37, 42, 50, 52	0
69	o3	106/106 (100%)	0.37	3 (2%) 55 37	34, 40, 50, 51	0
70	O4	112/112 (100%)	0.64	4 (3%) 46 31	47, 60, 70, 73	0
70	o4	112/112 (100%)	0.59	7 (6%) 27 20	46, 62, 70, 72	0
71	O5	119/119 (100%)	0.05	1 (0%) 82 67	42, 44, 56, 58	0
71	o5	119/119 (100%)	0.26	1 (0%) 82 67	46, 48, 60, 64	0
72	O6	99/99 (100%)	0.28	3 (3%) 52 35	44, 54, 62, 66	0
72	o6	99/99 (100%)	0.30	0 100 100	48, 57, 62, 66	0
73	O7	87/87 (100%)	0.23	1 (1%) 77 59	35, 41, 46, 49	0
73	o7	87/87 (100%)	0.29	4 (4%) 38 27	37, 42, 51, 58	0
74	O8	77/77 (100%)	0.26	1 (1%) 74 56	57, 60, 66, 66	0
74	o8	77/77 (100%)	0.41	2 (2%) 57 39	59, 63, 66, 68	0
75	O9	50/50 (100%)	0.23	1 (2%) 64 45	40, 42, 44, 45	0
75	o9	50/50 (100%)	0.20	0 100 100	40, 44, 46, 49	0
76	Q0	52/52 (100%)	0.03	1 (1%) 66 46	46, 49, 50, 52	0
76	q0	52/52 (100%)	-0.06	0 100 100	38, 39, 43, 45	0
77	Q1	25/25 (100%)	1.19	4 (16%) 6 5	60, 70, 78, 78	0
77	q1	25/25 (100%)	0.69	2 (8%) 20 15	49, 56, 59, 60	0
78	Q2	105/105 (100%)	0.12	1 (0%) 79 61	38, 49, 58, 66	0
78	q2	105/105 (100%)	0.20	0 100 100	37, 44, 49, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
79	Q3	91/91 (100%)	0.48	1 (1%) 77 59	49, 53, 57, 58	0
79	q3	91/91 (100%)	0.48	4 (4%) 39 27	45, 53, 60, 64	0
80	6	1795/1800 (99%)	0.89	152 (8%) 18 14	30, 75, 111, 134	1 (0%)
81	c0	79/96 (82%)	0.92	8 (10%) 14 11	105, 116, 121, 122	0
82	c7	117/121 (96%)	0.69	7 (5%) 29 22	86, 94, 99, 100	0
83	sR	318/318 (100%)	1.15	36 (11%) 11 9	90, 107, 111, 114	0
84	sM	63/104 (60%)	0.83	9 (14%) 7 6	45, 78, 89, 91	0
85	5	3150/3150 (100%)	0.41	139 (4%) 39 27	31, 45, 82, 107	0
86	l8	225/231 (97%)	0.66	12 (5%) 33 24	58, 64, 78, 81	0
87	m2	0/150	-	-	-	-
88	n4	135/135 (100%)	0.69	10 (7%) 22 17	37, 62, 81, 82	0
89	p0	120/143 (83%)	0.55	5 (4%) 41 28	78, 91, 98, 104	0
90	p1	0/47	-	-	-	-
90	p2	0/47	-	-	-	-
91	P	2/2 (100%)	0.08	0 100 100	38, 38, 38, 40	0
91	p	2/2 (100%)	1.81	1 (50%) 0 0	34, 34, 34, 38	0
All	All	32929/33519 (98%)	0.61	2011 (6%) 28 21	30, 60, 107, 154	2 (0%)

The worst 5 of 2011 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	N4	88	ASP	9.1
7	S5	152	GLY	8.9
1	2	1805	C	8.1
1	2	1804	U	7.7
7	S5	37	GLN	7.6

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(Å ²)	Q<0.9
93	MG	2	2141	1/1	-0.15	0.33	79,79,79,79	0
93	MG	6	2166	1/1	-0.09	0.40	114,114,114,114	0
93	MG	1	4062	1/1	0.01	0.32	105,105,105,105	0
93	MG	1	3735	1/1	0.01	0.42	125,125,125,125	0
93	MG	6	2133	1/1	0.13	0.29	94,94,94,94	0
93	MG	6	2153	1/1	0.19	0.35	86,86,86,86	0
93	MG	1	3914	1/1	0.19	0.45	50,50,50,50	0
93	MG	2	2059	1/1	0.21	0.36	86,86,86,86	0
93	MG	6	2136	1/1	0.22	0.27	75,75,75,75	0
93	MG	2	2112	1/1	0.24	0.55	83,83,83,83	0
93	MG	6	2068	1/1	0.30	0.37	105,105,105,105	0
93	MG	2	2097	1/1	0.31	0.23	118,118,118,118	0
93	MG	2	2108	1/1	0.32	0.33	92,92,92,92	0
93	MG	5	3988	1/1	0.32	0.52	35,35,35,35	0
93	MG	6	2124	1/1	0.36	0.24	89,89,89,89	0
93	MG	2	2111	1/1	0.36	0.33	78,78,78,78	0
93	MG	C9	201	1/1	0.36	0.58	96,96,96,96	0
93	MG	6	2098	1/1	0.37	0.45	99,99,99,99	0
93	MG	5	4155	1/1	0.37	0.13	72,72,72,72	0
93	MG	1	3938	1/1	0.38	0.19	54,54,54,54	0
93	MG	2	2099	1/1	0.38	0.48	80,80,80,80	0
93	MG	4	234	1/1	0.38	0.18	43,43,43,43	0
93	MG	2	2117	1/1	0.38	0.45	94,94,94,94	0
93	MG	2	2078	1/1	0.41	0.39	92,92,92,92	0
93	MG	2	2084	1/1	0.42	0.42	88,88,88,88	0
93	MG	2	2139	1/1	0.42	0.19	93,93,93,93	0
93	MG	2	2064	1/1	0.42	0.35	85,85,85,85	0
93	MG	6	2154	1/1	0.43	0.33	94,94,94,94	0
93	MG	2	2103	1/1	0.44	0.36	74,74,74,74	0
93	MG	6	2180	1/1	0.44	0.45	98,98,98,98	0
93	MG	5	3807	1/1	0.44	0.34	88,88,88,88	0
93	MG	2	2062	1/1	0.44	0.38	98,98,98,98	0
93	MG	2	2109	1/1	0.44	0.34	80,80,80,80	0
93	MG	6	2079	1/1	0.46	0.43	72,72,72,72	0
93	MG	2	2101	1/1	0.46	0.41	79,79,79,79	0
93	MG	2	2073	1/1	0.46	0.34	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	6	2075	1/1	0.46	0.44	71,71,71,71	0
93	MG	1	4031	1/1	0.47	0.22	34,34,34,34	0
93	MG	6	2137	1/1	0.47	0.38	85,85,85,85	0
93	MG	6	2159	1/1	0.47	0.23	88,88,88,88	0
93	MG	6	2141	1/1	0.47	0.36	95,95,95,95	0
93	MG	2	2126	1/1	0.48	0.36	78,78,78,78	0
93	MG	2	2056	1/1	0.48	0.22	74,74,74,74	0
93	MG	2	2054	1/1	0.48	0.40	81,81,81,81	0
93	MG	5	3762	1/1	0.49	0.26	50,50,50,50	0
93	MG	6	2082	1/1	0.49	0.31	87,87,87,87	0
93	MG	2	2083	1/1	0.49	0.38	83,83,83,83	0
93	MG	2	2082	1/1	0.49	0.40	74,74,74,74	0
93	MG	2	2100	1/1	0.50	0.35	102,102,102,102	0
93	MG	5	3969	1/1	0.50	0.46	73,73,73,73	0
93	MG	2	2094	1/1	0.51	0.34	81,81,81,81	0
93	MG	6	2138	1/1	0.51	0.31	82,82,82,82	0
93	MG	6	2109	1/1	0.51	0.59	90,90,90,90	0
93	MG	6	2063	1/1	0.51	0.30	89,89,89,89	0
93	MG	1	3749	1/1	0.51	0.37	55,55,55,55	0
93	MG	6	2093	1/1	0.51	0.26	90,90,90,90	0
93	MG	6	2163	1/1	0.51	0.40	66,66,66,66	0
93	MG	6	2108	1/1	0.52	0.37	63,63,63,63	0
93	MG	2	2105	1/1	0.53	0.34	96,96,96,96	0
93	MG	2	2079	1/1	0.54	0.38	85,85,85,85	0
93	MG	6	2182	1/1	0.54	0.30	66,66,66,66	0
93	MG	2	2124	1/1	0.54	0.25	87,87,87,87	0
93	MG	2	2125	1/1	0.54	0.38	78,78,78,78	0
93	MG	2	2106	1/1	0.54	0.29	96,96,96,96	0
93	MG	1	3854	1/1	0.54	0.50	56,56,56,56	0
93	MG	2	2075	1/1	0.54	0.21	96,96,96,96	0
93	MG	2	2093	1/1	0.55	0.37	81,81,81,81	0
93	MG	1	3874	1/1	0.56	0.42	44,44,44,44	0
93	MG	2	2118	1/1	0.56	0.39	92,92,92,92	0
93	MG	2	2128	1/1	0.56	0.35	89,89,89,89	0
93	MG	6	2084	1/1	0.57	0.37	60,60,60,60	0
93	MG	2	2076	1/1	0.57	0.31	86,86,86,86	0
93	MG	3	215	1/1	0.57	0.27	59,59,59,59	0
93	MG	6	2104	1/1	0.57	0.36	90,90,90,90	0
93	MG	5	4104	1/1	0.58	0.16	93,93,93,93	0
93	MG	2	2067	1/1	0.58	0.41	78,78,78,78	0
93	MG	1	3937	1/1	0.59	0.26	57,57,57,57	0
93	MG	1	3748	1/1	0.59	0.33	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	6	2115	1/1	0.60	0.34	69,69,69,69	0
93	MG	6	2118	1/1	0.60	0.37	96,96,96,96	0
93	MG	6	2102	1/1	0.60	0.42	96,96,96,96	0
93	MG	5	3936	1/1	0.60	0.49	38,38,38,38	0
93	MG	1	4052	1/1	0.60	0.19	59,59,59,59	0
93	MG	1	4023	1/1	0.60	0.38	60,60,60,60	0
93	MG	1	3956	1/1	0.60	0.27	56,56,56,56	0
93	MG	6	2114	1/1	0.60	0.49	89,89,89,89	0
93	MG	5	3838	1/1	0.61	0.17	45,45,45,45	0
93	MG	6	2128	1/1	0.61	0.30	88,88,88,88	0
93	MG	2	2065	1/1	0.61	0.33	88,88,88,88	0
93	MG	5	3971	1/1	0.61	0.29	84,84,84,84	0
93	MG	1	3946	1/1	0.61	0.39	98,98,98,98	0
93	MG	4	225	1/1	0.61	0.45	47,47,47,47	0
93	MG	C1	201	1/1	0.61	0.27	76,76,76,76	0
93	MG	1	3785	1/1	0.62	0.42	51,51,51,51	0
93	MG	2	2121	1/1	0.62	0.29	68,68,68,68	0
93	MG	2	2070	1/1	0.62	0.51	71,71,71,71	0
93	MG	1	3912	1/1	0.62	0.40	43,43,43,43	0
93	MG	2	2058	1/1	0.62	0.32	81,81,81,81	0
93	MG	1	3755	1/1	0.62	0.35	54,54,54,54	0
93	MG	5	3963	1/1	0.63	0.16	36,36,36,36	0
93	MG	1	3852	1/1	0.63	0.41	52,52,52,52	0
93	MG	1	3911	1/1	0.63	0.52	52,52,52,52	0
93	MG	5	3815	1/1	0.63	0.25	46,46,46,46	0
93	MG	1	3808	1/1	0.63	0.26	37,37,37,37	0
93	MG	1	4069	1/1	0.63	0.16	46,46,46,46	0
93	MG	5	3937	1/1	0.64	0.45	43,43,43,43	0
93	MG	2	2086	1/1	0.64	0.37	71,71,71,71	0
93	MG	5	3782	1/1	0.64	0.33	42,42,42,42	0
93	MG	2	2131	1/1	0.64	0.19	80,80,80,80	0
93	MG	6	2073	1/1	0.64	0.26	91,91,91,91	0
93	MG	2	2132	1/1	0.64	0.48	76,76,76,76	0
93	MG	2	2136	1/1	0.64	0.24	90,90,90,90	0
93	MG	7	213	1/1	0.64	0.48	46,46,46,46	0
93	MG	8	219	1/1	0.64	0.32	46,46,46,46	0
93	MG	5	3820	1/1	0.65	0.26	54,54,54,54	0
93	MG	6	2092	1/1	0.65	0.24	88,88,88,88	0
93	MG	2	2140	1/1	0.65	0.18	83,83,83,83	0
93	MG	6	2169	1/1	0.65	0.35	97,97,97,97	0
93	MG	2	2130	1/1	0.66	0.18	85,85,85,85	0
93	MG	6	2143	1/1	0.66	0.31	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	6	2145	1/1	0.66	0.18	89,89,89,89	0
93	MG	c8	202	1/1	0.66	0.47	84,84,84,84	0
93	MG	2	2113	1/1	0.66	0.18	101,101,101,101	0
93	MG	6	2110	1/1	0.66	0.27	91,91,91,91	0
93	MG	6	2155	1/1	0.66	0.22	76,76,76,76	0
93	MG	1	4058	1/1	0.66	0.15	38,38,38,38	0
93	MG	2	2060	1/1	0.66	0.49	74,74,74,74	0
93	MG	1	3896	1/1	0.66	0.50	44,44,44,44	0
93	MG	o9	101	1/1	0.66	0.22	41,41,41,41	0
93	MG	5	4048	1/1	0.67	0.15	57,57,57,57	0
93	MG	1	3788	1/1	0.67	0.42	39,39,39,39	0
93	MG	2	2104	1/1	0.67	0.37	97,97,97,97	0
93	MG	5	4172	1/1	0.67	0.20	81,81,81,81	0
93	MG	6	2117	1/1	0.67	0.41	55,55,55,55	0
93	MG	1	3839	1/1	0.67	0.46	42,42,42,42	0
93	MG	6	2089	1/1	0.67	0.16	70,70,70,70	0
93	MG	2	2071	1/1	0.68	0.41	79,79,79,79	0
93	MG	5	3754	1/1	0.68	0.17	45,45,45,45	0
93	MG	1	3883	1/1	0.68	0.50	42,42,42,42	0
93	MG	5	3766	1/1	0.68	0.32	46,46,46,46	0
93	MG	2	2089	1/1	0.68	0.34	85,85,85,85	0
93	MG	6	2083	1/1	0.68	0.48	56,56,56,56	0
93	MG	1	3822	1/1	0.68	0.37	44,44,44,44	0
93	MG	6	2067	1/1	0.68	0.24	57,57,57,57	0
93	MG	1	4109	1/1	0.68	0.15	43,43,43,43	0
93	MG	6	2070	1/1	0.68	0.27	94,94,94,94	0
93	MG	3	211	1/1	0.68	0.27	60,60,60,60	0
95	PHE	5	3401	11/12	0.68	0.36	31,31,41,41	0
93	MG	5	3982	1/1	0.69	0.26	41,41,41,41	0
93	MG	2	2102	1/1	0.69	0.28	98,98,98,98	0
93	MG	5	4015	1/1	0.69	0.48	66,66,66,66	0
93	MG	5	4019	1/1	0.69	0.43	50,50,50,50	0
93	MG	O7	103	1/1	0.69	0.30	42,42,42,42	0
93	MG	5	4102	1/1	0.69	0.37	43,43,43,43	0
93	MG	6	2061	1/1	0.69	0.26	69,69,69,69	0
93	MG	5	4107	1/1	0.69	0.38	42,42,42,42	0
93	MG	5	3931	1/1	0.69	0.49	31,31,31,31	0
93	MG	6	2086	1/1	0.69	0.19	75,75,75,75	0
93	MG	5	3765	1/1	0.69	0.43	31,31,31,31	0
93	MG	7	226	1/1	0.69	0.45	44,44,44,44	0
93	MG	6	2087	1/1	0.69	0.27	66,66,66,66	0
93	MG	2	2091	1/1	0.69	0.31	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	S4	301	1/1	0.69	0.18	83,83,83,83	0
93	MG	1	3907	1/1	0.70	0.37	53,53,53,53	0
93	MG	D9	103	1/1	0.70	0.32	92,92,92,92	0
93	MG	1	4015	1/1	0.70	0.50	49,49,49,49	0
93	MG	5	3793	1/1	0.70	0.25	62,62,62,62	0
93	MG	2	2115	1/1	0.70	0.52	84,84,84,84	0
93	MG	3	213	1/1	0.70	0.42	39,39,39,39	0
93	MG	1	3764	1/1	0.70	0.30	42,42,42,42	0
93	MG	1	3827	1/1	0.70	0.42	50,50,50,50	0
93	MG	5	3850	1/1	0.70	0.36	41,41,41,41	0
93	MG	2	2057	1/1	0.70	0.41	73,73,73,73	0
93	MG	1	3955	1/1	0.71	0.23	50,50,50,50	0
93	MG	1	3908	1/1	0.71	0.45	41,41,41,41	0
93	MG	5	3999	1/1	0.71	0.37	45,45,45,45	0
93	MG	2	2129	1/1	0.71	0.20	80,80,80,80	0
93	MG	2	2088	1/1	0.71	0.35	77,77,77,77	0
93	MG	1	3756	1/1	0.71	0.30	43,43,43,43	0
93	MG	6	2189	1/1	0.71	0.24	90,90,90,90	0
93	MG	5	3842	1/1	0.71	0.34	38,38,38,38	0
93	MG	2	2137	1/1	0.71	0.19	85,85,85,85	0
93	MG	5	4122	1/1	0.71	0.16	37,37,37,37	0
93	MG	5	3902	1/1	0.71	0.47	37,37,37,37	0
93	MG	6	2074	1/1	0.71	0.47	88,88,88,88	0
93	MG	1	3838	1/1	0.71	0.39	46,46,46,46	0
93	MG	M7	202	1/1	0.71	0.48	52,52,52,52	0
93	MG	2	2092	1/1	0.71	0.25	80,80,80,80	0
93	MG	5	3777	1/1	0.71	0.26	48,48,48,48	0
93	MG	5	3778	1/1	0.71	0.19	57,57,57,57	0
93	MG	1	3757	1/1	0.72	0.21	42,42,42,42	0
93	MG	5	3998	1/1	0.72	0.32	39,39,39,39	0
93	MG	2	2114	1/1	0.72	0.38	77,77,77,77	0
93	MG	1	3747	1/1	0.72	0.33	49,49,49,49	0
93	MG	2	2066	1/1	0.72	0.36	72,72,72,72	0
93	MG	5	4029	1/1	0.72	0.17	56,56,56,56	0
93	MG	6	2132	1/1	0.72	0.37	59,59,59,59	0
93	MG	sM	201	1/1	0.72	0.12	45,45,45,45	0
93	MG	1	4012	1/1	0.72	0.32	50,50,50,50	0
93	MG	2	2135	1/1	0.73	0.39	68,68,68,68	0
93	MG	1	4006	1/1	0.73	0.39	61,61,61,61	0
93	MG	1	4026	1/1	0.73	0.41	39,39,39,39	0
93	MG	5	3758	1/1	0.73	0.43	43,43,43,43	0
93	MG	5	3916	1/1	0.73	0.49	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	1	3867	1/1	0.73	0.31	44,44,44,44	0
93	MG	1	4082	1/1	0.73	0.27	54,54,54,54	0
93	MG	6	2094	1/1	0.73	0.25	77,77,77,77	0
93	MG	5	4021	1/1	0.73	0.20	33,33,33,33	0
93	MG	5	3959	1/1	0.73	0.22	41,41,41,41	0
93	MG	5	3828	1/1	0.73	0.15	35,35,35,35	0
93	MG	1	3817	1/1	0.74	0.26	51,51,51,51	0
93	MG	1	3906	1/1	0.74	0.32	49,49,49,49	0
93	MG	5	3750	1/1	0.74	0.34	60,60,60,60	0
93	MG	1	3766	1/1	0.74	0.31	36,36,36,36	0
93	MG	2	2127	1/1	0.74	0.43	77,77,77,77	0
93	MG	2	2098	1/1	0.74	0.19	87,87,87,87	0
93	MG	5	4115	1/1	0.74	0.18	63,63,63,63	0
93	MG	5	3976	1/1	0.74	0.40	40,40,40,40	0
93	MG	5	4140	1/1	0.74	0.36	39,39,39,39	0
93	MG	2	2074	1/1	0.74	0.49	80,80,80,80	0
93	MG	5	3983	1/1	0.74	0.25	41,41,41,41	0
93	MG	1	4124	1/1	0.74	0.32	49,49,49,49	0
93	MG	5	3858	1/1	0.74	0.34	39,39,39,39	0
93	MG	6	2144	1/1	0.74	0.31	94,94,94,94	0
93	MG	6	2088	1/1	0.74	0.33	65,65,65,65	0
93	MG	6	2152	1/1	0.74	0.20	62,62,62,62	0
93	MG	M3	1000	1/1	0.75	0.21	64,64,64,64	0
93	MG	6	2135	1/1	0.75	0.32	64,64,64,64	0
93	MG	5	3802	1/1	0.75	0.21	38,38,38,38	0
93	MG	5	4055	1/1	0.75	0.13	48,48,48,48	0
93	MG	5	4079	1/1	0.75	0.30	43,43,43,43	0
93	MG	1	4025	1/1	0.75	0.31	49,49,49,49	0
93	MG	6	2097	1/1	0.75	0.27	92,92,92,92	0
93	MG	1	3929	1/1	0.75	0.36	51,51,51,51	0
93	MG	5	4112	1/1	0.75	0.29	62,62,62,62	0
93	MG	6	2125	1/1	0.75	0.39	57,57,57,57	0
93	MG	6	2111	1/1	0.75	0.47	69,69,69,69	0
93	MG	6	2130	1/1	0.75	0.23	67,67,67,67	0
93	MG	1	3784	1/1	0.75	0.37	57,57,57,57	0
93	MG	5	3856	1/1	0.75	0.29	42,42,42,42	0
93	MG	6	2150	1/1	0.75	0.38	58,58,58,58	0
93	MG	5	3863	1/1	0.75	0.40	38,38,38,38	0
93	MG	5	3874	1/1	0.75	0.38	35,35,35,35	0
93	MG	5	3901	1/1	0.75	0.42	39,39,39,39	0
93	MG	6	2186	1/1	0.75	0.30	63,63,63,63	0
93	MG	5	4007	1/1	0.76	0.31	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	5	3788	1/1	0.76	0.17	34,34,34,34	0
93	MG	1	4105	1/1	0.76	0.13	54,54,54,54	0
93	MG	5	4020	1/1	0.76	0.22	65,65,65,65	0
93	MG	1	3824	1/1	0.76	0.40	38,38,38,38	0
93	MG	5	3929	1/1	0.76	0.42	32,32,32,32	0
93	MG	6	2099	1/1	0.76	0.21	65,65,65,65	0
93	MG	6	2101	1/1	0.76	0.35	53,53,53,53	0
93	MG	1	4123	1/1	0.76	0.24	46,46,46,46	0
93	MG	5	4084	1/1	0.76	0.13	34,34,34,34	0
93	MG	5	3942	1/1	0.76	0.27	40,40,40,40	0
93	MG	5	3949	1/1	0.76	0.34	33,33,33,33	0
93	MG	5	3957	1/1	0.76	0.21	38,38,38,38	0
93	MG	5	4108	1/1	0.76	0.43	32,32,32,32	0
93	MG	1	3962	1/1	0.76	0.36	54,54,54,54	0
93	MG	6	2066	1/1	0.76	0.15	89,89,89,89	0
93	MG	1	3880	1/1	0.76	0.30	41,41,41,41	0
93	MG	5	3846	1/1	0.76	0.35	50,50,50,50	0
93	MG	2	2072	1/1	0.76	0.34	83,83,83,83	0
93	MG	1	3837	1/1	0.76	0.42	39,39,39,39	0
93	MG	1	3954	1/1	0.76	0.20	57,57,57,57	0
93	MG	1	4076	1/1	0.76	0.27	51,51,51,51	0
93	MG	5	3866	1/1	0.76	0.43	33,33,33,33	0
93	MG	m6	205	1/1	0.76	0.32	37,37,37,37	0
93	MG	1	3815	1/1	0.76	0.26	41,41,41,41	0
93	MG	5	4001	1/1	0.76	0.19	37,37,37,37	0
93	MG	5	3767	1/1	0.77	0.34	36,36,36,36	0
93	MG	5	4000	1/1	0.77	0.22	40,40,40,40	0
93	MG	4	230	1/1	0.77	0.22	72,72,72,72	0
93	MG	1	4064	1/1	0.77	0.40	54,54,54,54	0
93	MG	L4	402	1/1	0.77	0.24	50,50,50,50	0
93	MG	5	4119	1/1	0.77	0.20	41,41,41,41	0
93	MG	1	3804	1/1	0.77	0.10	58,58,58,58	0
93	MG	d7	102	1/1	0.77	0.24	74,74,74,74	0
93	MG	6	2116	1/1	0.77	0.36	63,63,63,63	0
93	MG	6	2080	1/1	0.77	0.43	63,63,63,63	0
93	MG	6	2081	1/1	0.77	0.18	70,70,70,70	0
93	MG	6	2140	1/1	0.77	0.11	71,71,71,71	0
93	MG	5	4074	1/1	0.77	0.26	47,47,47,47	0
93	MG	6	2105	1/1	0.77	0.49	65,65,65,65	0
93	MG	1	3998	1/1	0.77	0.33	43,43,43,43	0
93	MG	2	2055	1/1	0.77	0.52	75,75,75,75	0
96	LEU	5	3402	8/9	0.77	0.31	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	5	3940	1/1	0.78	0.38	34,34,34,34	0
93	MG	1	3800	1/1	0.78	0.27	32,32,32,32	0
93	MG	1	3866	1/1	0.78	0.39	40,40,40,40	0
93	MG	5	4132	1/1	0.78	0.25	50,50,50,50	0
93	MG	5	3954	1/1	0.78	0.13	48,48,48,48	0
93	MG	6	2065	1/1	0.78	0.23	61,61,61,61	0
93	MG	1	3980	1/1	0.78	0.43	63,63,63,63	0
93	MG	5	4098	1/1	0.78	0.52	32,32,32,32	0
93	MG	M7	205	1/1	0.78	0.21	38,38,38,38	0
93	MG	O4	202	1/1	0.78	0.23	61,61,61,61	0
93	MG	m5	304	1/1	0.78	0.25	47,47,47,47	0
93	MG	5	3934	1/1	0.78	0.39	31,31,31,31	0
93	MG	1	3944	1/1	0.78	0.38	45,45,45,45	0
93	MG	6	2173	1/1	0.78	0.33	70,70,70,70	0
93	MG	5	4114	1/1	0.78	0.19	44,44,44,44	0
93	MG	5	3869	1/1	0.79	0.51	59,59,59,59	0
93	MG	6	2095	1/1	0.79	0.39	55,55,55,55	0
93	MG	5	3889	1/1	0.79	0.44	39,39,39,39	0
93	MG	5	3892	1/1	0.79	0.40	43,43,43,43	0
93	MG	1	3951	1/1	0.79	0.26	32,32,32,32	0
93	MG	1	4063	1/1	0.79	0.16	43,43,43,43	0
93	MG	5	3909	1/1	0.79	0.52	31,31,31,31	0
93	MG	5	3912	1/1	0.79	0.32	35,35,35,35	0
93	MG	1	3952	1/1	0.79	0.12	48,48,48,48	0
93	MG	5	3924	1/1	0.79	0.42	36,36,36,36	0
93	MG	6	2167	1/1	0.79	0.23	55,55,55,55	0
93	MG	1	4067	1/1	0.79	0.32	39,39,39,39	0
93	MG	5	4089	1/1	0.79	0.18	51,51,51,51	0
93	MG	1	4068	1/1	0.79	0.21	43,43,43,43	0
93	MG	5	3798	1/1	0.79	0.29	52,52,52,52	0
93	MG	1	3921	1/1	0.79	0.32	42,42,42,42	0
93	MG	5	3939	1/1	0.79	0.39	38,38,38,38	0
93	MG	5	3805	1/1	0.79	0.17	36,36,36,36	0
93	MG	1	3830	1/1	0.79	0.34	38,38,38,38	0
93	MG	5	3948	1/1	0.79	0.13	43,43,43,43	0
93	MG	N0	201	1/1	0.79	0.18	44,44,44,44	0
93	MG	1	4024	1/1	0.79	0.29	49,49,49,49	0
93	MG	5	3823	1/1	0.79	0.35	50,50,50,50	0
93	MG	1	3779	1/1	0.79	0.37	37,37,37,37	0
93	MG	5	3837	1/1	0.79	0.44	34,34,34,34	0
93	MG	5	4154	1/1	0.79	0.16	50,50,50,50	0
93	MG	5	3964	1/1	0.79	0.16	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	d3	201	1/1	0.79	0.41	55,55,55,55	0
93	MG	1	3825	1/1	0.79	0.35	49,49,49,49	0
93	MG	5	3845	1/1	0.79	0.43	32,32,32,32	0
93	MG	2	2087	1/1	0.79	0.29	77,77,77,77	0
93	MG	8	227	1/1	0.79	0.19	40,40,40,40	0
93	MG	1	4040	1/1	0.79	0.16	49,49,49,49	0
93	MG	1	4043	1/1	0.79	0.19	52,52,52,52	0
93	MG	1	3870	1/1	0.79	0.33	52,52,52,52	0
93	MG	1	4000	1/1	0.79	0.29	61,61,61,61	0
93	MG	6	2069	1/1	0.79	0.33	61,61,61,61	0
93	MG	1	4050	1/1	0.80	0.37	53,53,53,53	0
93	MG	L3	403	1/1	0.80	0.43	51,51,51,51	0
93	MG	1	4096	1/1	0.80	0.08	49,49,49,49	0
93	MG	5	3920	1/1	0.80	0.46	44,44,44,44	0
93	MG	6	2161	1/1	0.80	0.22	59,59,59,59	0
93	MG	5	3995	1/1	0.80	0.16	34,34,34,34	0
93	MG	1	3799	1/1	0.80	0.27	39,39,39,39	0
93	MG	1	3826	1/1	0.80	0.32	33,33,33,33	0
93	MG	6	2072	1/1	0.80	0.36	59,59,59,59	0
93	MG	6	2112	1/1	0.80	0.24	63,63,63,63	0
93	MG	5	3853	1/1	0.80	0.27	36,36,36,36	0
93	MG	6	2170	1/1	0.80	0.63	64,64,64,64	0
93	MG	1	3841	1/1	0.80	0.36	33,33,33,33	0
93	MG	5	4166	1/1	0.80	0.63	44,44,44,44	0
93	MG	1	3981	1/1	0.80	0.21	58,58,58,58	0
93	MG	2	2080	1/1	0.80	0.24	82,82,82,82	0
93	MG	7	221	1/1	0.80	0.20	48,48,48,48	0
93	MG	2	2138	1/1	0.80	0.10	87,87,87,87	0
93	MG	6	2060	1/1	0.80	0.35	63,63,63,63	0
93	MG	5	3886	1/1	0.80	0.39	61,61,61,61	0
93	MG	6	2147	1/1	0.80	0.25	66,66,66,66	0
93	MG	5	3962	1/1	0.80	0.33	46,46,46,46	0
93	MG	1	4032	1/1	0.80	0.26	47,47,47,47	0
93	MG	1	3831	1/1	0.80	0.35	31,31,31,31	0
93	MG	1	3743	1/1	0.80	0.25	52,52,52,52	0
93	MG	5	3818	1/1	0.81	0.33	31,31,31,31	0
93	MG	1	3953	1/1	0.81	0.12	55,55,55,55	0
93	MG	2	2119	1/1	0.81	0.17	87,87,87,87	0
93	MG	1	4117	1/1	0.81	0.22	43,43,43,43	0
93	MG	5	3966	1/1	0.81	0.15	49,49,49,49	0
93	MG	5	3935	1/1	0.81	0.37	34,34,34,34	0
93	MG	2	2095	1/1	0.81	0.18	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	d6	102	1/1	0.81	0.47	64,64,64,64	0
93	MG	5	3978	1/1	0.81	0.31	56,56,56,56	0
93	MG	5	4159	1/1	0.81	0.30	45,45,45,45	0
93	MG	5	4062	1/1	0.81	0.36	59,59,59,59	0
93	MG	1	3858	1/1	0.81	0.40	32,32,32,32	0
93	MG	1	3767	1/1	0.81	0.23	46,46,46,46	0
93	MG	5	3986	1/1	0.81	0.26	60,60,60,60	0
93	MG	5	4086	1/1	0.81	0.30	41,41,41,41	0
93	MG	6	2148	1/1	0.81	0.19	58,58,58,58	0
93	MG	5	4092	1/1	0.81	0.21	34,34,34,34	0
93	MG	l3	403	1/1	0.81	0.45	31,31,31,31	0
93	MG	5	3990	1/1	0.81	0.14	50,50,50,50	0
93	MG	1	3948	1/1	0.81	0.29	48,48,48,48	0
93	MG	1	3819	1/1	0.81	0.20	43,43,43,43	0
93	MG	1	3787	1/1	0.81	0.28	49,49,49,49	0
93	MG	6	2121	1/1	0.81	0.26	62,62,62,62	0
93	MG	5	3831	1/1	0.82	0.18	44,44,44,44	0
93	MG	6	2131	1/1	0.82	0.28	60,60,60,60	0
93	MG	6	2183	1/1	0.82	0.25	72,72,72,72	0
93	MG	6	2077	1/1	0.82	0.31	55,55,55,55	0
93	MG	5	3961	1/1	0.82	0.29	43,43,43,43	0
93	MG	1	3818	1/1	0.82	0.16	62,62,62,62	0
93	MG	5	4139	1/1	0.82	0.25	60,60,60,60	0
93	MG	2	2120	1/1	0.82	0.15	95,95,95,95	0
93	MG	5	3849	1/1	0.82	0.44	31,31,31,31	0
93	MG	1	3809	1/1	0.82	0.37	49,49,49,49	0
93	MG	5	3851	1/1	0.82	0.52	40,40,40,40	0
93	MG	1	4039	1/1	0.82	0.13	49,49,49,49	0
93	MG	5	4168	1/1	0.82	0.14	41,41,41,41	0
93	MG	5	3932	1/1	0.82	0.41	41,41,41,41	0
93	MG	5	4077	1/1	0.82	0.34	43,43,43,43	0
93	MG	1	3847	1/1	0.82	0.24	36,36,36,36	0
93	MG	1	3979	1/1	0.82	0.12	48,48,48,48	0
93	MG	8	218	1/1	0.82	0.13	49,49,49,49	0
93	MG	2	2110	1/1	0.82	0.40	76,76,76,76	0
93	MG	5	3985	1/1	0.82	0.37	42,42,42,42	0
93	MG	3	214	1/1	0.82	0.29	59,59,59,59	0
93	MG	m5	303	1/1	0.82	0.29	37,37,37,37	0
93	MG	1	3795	1/1	0.82	0.27	39,39,39,39	0
93	MG	6	2107	1/1	0.82	0.37	63,63,63,63	0
93	MG	1	4093	1/1	0.82	0.28	55,55,55,55	0
93	MG	5	3943	1/1	0.82	0.13	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	1	3987	1/1	0.82	0.20	35,35,35,35	0
93	MG	1	3738	1/1	0.83	0.34	37,37,37,37	0
93	MG	4	232	1/1	0.83	0.31	45,45,45,45	0
93	MG	1	3758	1/1	0.83	0.62	41,41,41,41	0
93	MG	1	3871	1/1	0.83	0.26	41,41,41,41	0
93	MG	5	3888	1/1	0.83	0.32	48,48,48,48	0
93	MG	6	2178	1/1	0.83	0.18	67,67,67,67	0
93	MG	5	3890	1/1	0.83	0.33	40,40,40,40	0
93	MG	2	2123	1/1	0.83	0.17	96,96,96,96	0
93	MG	6	2181	1/1	0.83	0.16	77,77,77,77	0
93	MG	1	3746	1/1	0.83	0.20	48,48,48,48	0
93	MG	1	3930	1/1	0.83	0.41	60,60,60,60	0
93	MG	1	3963	1/1	0.83	0.49	45,45,45,45	0
93	MG	1	3966	1/1	0.83	0.13	32,32,32,32	0
93	MG	5	3821	1/1	0.83	0.23	55,55,55,55	0
93	MG	5	3922	1/1	0.83	0.37	36,36,36,36	0
93	MG	s6	301	1/1	0.83	0.12	67,67,67,67	0
93	MG	5	3991	1/1	0.83	0.28	38,38,38,38	0
93	MG	1	4107	1/1	0.83	0.25	48,48,48,48	0
93	MG	2	2081	1/1	0.83	0.32	87,87,87,87	0
93	MG	1	3891	1/1	0.83	0.35	33,33,33,33	0
93	MG	1	4118	1/1	0.83	0.14	44,44,44,44	0
93	MG	5	4162	1/1	0.83	0.13	49,49,49,49	0
93	MG	6	2062	1/1	0.83	0.51	61,61,61,61	0
93	MG	1	3939	1/1	0.83	0.25	54,54,54,54	0
93	MG	6	2091	1/1	0.83	0.52	66,66,66,66	0
93	MG	5	3756	1/1	0.83	0.41	44,44,44,44	0
93	MG	7	220	1/1	0.83	0.34	45,45,45,45	0
93	MG	1	3983	1/1	0.83	0.32	37,37,37,37	0
93	MG	7	222	1/1	0.83	0.13	47,47,47,47	0
93	MG	2	2133	1/1	0.83	0.11	85,85,85,85	0
93	MG	5	4024	1/1	0.83	0.16	49,49,49,49	0
93	MG	5	4025	1/1	0.83	0.24	39,39,39,39	0
93	MG	5	3852	1/1	0.83	0.49	31,31,31,31	0
93	MG	5	4036	1/1	0.83	0.15	41,41,41,41	0
93	MG	1	3997	1/1	0.83	0.29	43,43,43,43	0
92	OHX	2	1994	7/7	0.83	0.24	98,98,98,98	0
93	MG	m6	202	1/1	0.83	0.34	29,29,29,29	0
93	MG	5	4060	1/1	0.83	0.14	48,48,48,48	0
93	MG	m7	202	1/1	0.83	0.28	36,36,36,36	0
93	MG	1	3733	1/1	0.83	0.40	39,39,39,39	0
93	MG	5	3956	1/1	0.83	0.28	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	2	2069	1/1	0.83	0.31	79,79,79,79	0
93	MG	5	3881	1/1	0.84	0.59	35,35,35,35	0
93	MG	5	3885	1/1	0.84	0.33	34,34,34,34	0
93	MG	5	4096	1/1	0.84	0.15	45,45,45,45	0
93	MG	1	3934	1/1	0.84	0.34	37,37,37,37	0
93	MG	1	3882	1/1	0.84	0.33	44,44,44,44	0
93	MG	1	3760	1/1	0.84	0.27	45,45,45,45	0
93	MG	1	3887	1/1	0.84	0.23	35,35,35,35	0
93	MG	5	3891	1/1	0.84	0.29	43,43,43,43	0
93	MG	5	3979	1/1	0.84	0.09	50,50,50,50	0
93	MG	6	2096	1/1	0.84	0.42	59,59,59,59	0
93	MG	3	212	1/1	0.84	0.44	59,59,59,59	0
93	MG	2	2134	1/1	0.84	0.43	59,59,59,59	0
93	MG	5	3809	1/1	0.84	0.24	39,39,39,39	0
93	MG	5	3911	1/1	0.84	0.48	37,37,37,37	0
93	MG	2	2107	1/1	0.84	0.21	81,81,81,81	0
93	MG	1	3947	1/1	0.84	0.24	43,43,43,43	0
93	MG	6	2185	1/1	0.84	0.12	92,92,92,92	0
93	MG	1	3862	1/1	0.84	0.19	36,36,36,36	0
93	MG	6	2103	1/1	0.84	0.50	62,62,62,62	0
93	MG	1	4004	1/1	0.84	0.16	40,40,40,40	0
93	MG	2	2116	1/1	0.84	0.19	85,85,85,85	0
93	MG	1	3823	1/1	0.84	0.33	37,37,37,37	0
93	MG	5	4010	1/1	0.84	0.18	44,44,44,44	0
93	MG	1	3869	1/1	0.84	0.21	49,49,49,49	0
93	MG	1	4017	1/1	0.84	0.31	61,61,61,61	0
93	MG	1	3793	1/1	0.84	0.23	39,39,39,39	0
93	MG	1	4089	1/1	0.84	0.32	31,31,31,31	0
93	MG	5	3751	1/1	0.84	0.20	45,45,45,45	0
93	MG	6	2151	1/1	0.84	0.32	64,64,64,64	0
93	MG	1	3814	1/1	0.84	0.18	50,50,50,50	0
93	MG	5	3757	1/1	0.84	0.42	42,42,42,42	0
93	MG	1	3920	1/1	0.84	0.57	34,34,34,34	0
93	MG	N3	201	1/1	0.84	0.35	41,41,41,41	0
93	MG	5	3951	1/1	0.84	0.35	39,39,39,39	0
93	MG	N8	203	1/1	0.84	0.77	32,32,32,32	0
93	MG	5	3860	1/1	0.84	0.32	32,32,32,32	0
93	MG	1	3873	1/1	0.84	0.24	33,33,33,33	0
93	MG	2	2096	1/1	0.84	0.21	75,75,75,75	0
93	MG	1	3850	1/1	0.84	0.32	33,33,33,33	0
93	MG	1	4035	1/1	0.84	0.33	37,37,37,37	0
93	MG	5	3973	1/1	0.85	0.18	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	5	3903	1/1	0.85	0.40	32,32,32,32	0
93	MG	1	3789	1/1	0.85	0.30	33,33,33,33	0
93	MG	5	3910	1/1	0.85	0.28	34,34,34,34	0
93	MG	1	3846	1/1	0.85	0.26	33,33,33,33	0
93	MG	1	3750	1/1	0.85	0.34	39,39,39,39	0
93	MG	1	3765	1/1	0.85	0.35	47,47,47,47	0
93	MG	5	3759	1/1	0.85	0.26	32,32,32,32	0
93	MG	5	3844	1/1	0.85	0.27	45,45,45,45	0
93	MG	6	2175	1/1	0.85	0.26	64,64,64,64	0
92	OHX	2	2044	7/7	0.85	0.35	88,88,88,88	0
93	MG	5	3994	1/1	0.85	0.37	31,31,31,31	0
93	MG	N6	201	1/1	0.85	0.30	40,40,40,40	0
93	MG	1	4075	1/1	0.85	0.13	59,59,59,59	0
93	MG	5	3770	1/1	0.85	0.24	41,41,41,41	0
93	MG	6	2078	1/1	0.85	0.30	58,58,58,58	0
93	MG	2	2061	1/1	0.85	0.32	83,83,83,83	0
93	MG	5	4156	1/1	0.85	0.25	39,39,39,39	0
93	MG	5	4158	1/1	0.85	0.23	57,57,57,57	0
93	MG	1	3857	1/1	0.85	0.15	35,35,35,35	0
93	MG	1	4084	1/1	0.85	0.14	33,33,33,33	0
93	MG	6	2187	1/1	0.85	0.26	90,90,90,90	0
93	MG	5	3941	1/1	0.85	0.19	41,41,41,41	0
93	MG	1	3879	1/1	0.85	0.28	41,41,41,41	0
93	MG	5	4174	1/1	0.85	0.11	36,36,36,36	0
93	MG	4	227	1/1	0.85	0.29	36,36,36,36	0
93	MG	1	3772	1/1	0.85	0.15	57,57,57,57	0
93	MG	6	2157	1/1	0.85	0.14	57,57,57,57	0
93	MG	5	3876	1/1	0.85	0.17	45,45,45,45	0
93	MG	5	4035	1/1	0.85	0.18	40,40,40,40	0
93	MG	5	3808	1/1	0.85	0.18	37,37,37,37	0
93	MG	1	4016	1/1	0.85	0.14	52,52,52,52	0
93	MG	5	3811	1/1	0.85	0.26	44,44,44,44	0
93	MG	1	3840	1/1	0.85	0.36	41,41,41,41	0
93	MG	5	3817	1/1	0.85	0.27	43,43,43,43	0
93	MG	5	4068	1/1	0.85	0.23	40,40,40,40	0
93	MG	1	4019	1/1	0.85	0.19	49,49,49,49	0
93	MG	5	3819	1/1	0.85	0.22	41,41,41,41	0
93	MG	6	2165	1/1	0.85	0.20	69,69,69,69	0
93	MG	5	3894	1/1	0.85	0.45	33,33,33,33	0
93	MG	1	3863	1/1	0.85	0.34	30,30,30,30	0
93	MG	5	3752	1/1	0.85	0.28	32,32,32,32	0
93	MG	1	4057	1/1	0.86	0.88	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	5	4009	1/1	0.86	0.39	43,43,43,43	0
93	MG	1	3900	1/1	0.86	0.27	31,31,31,31	0
92	OHX	2	1976	7/7	0.86	0.33	110,110,110,110	0
93	MG	6	2119	1/1	0.86	0.24	59,59,59,59	0
93	MG	6	2120	1/1	0.86	0.15	102,102,102,102	0
92	OHX	1	3707	7/7	0.86	0.18	114,114,114,114	0
93	MG	6	2122	1/1	0.86	0.15	74,74,74,74	0
93	MG	1	3875	1/1	0.86	0.44	45,45,45,45	0
93	MG	6	2076	1/1	0.86	0.30	70,70,70,70	0
93	MG	1	3773	1/1	0.86	0.32	51,51,51,51	0
93	MG	5	3968	1/1	0.86	0.22	40,40,40,40	0
93	MG	5	4037	1/1	0.86	0.24	39,39,39,39	0
93	MG	5	3919	1/1	0.86	0.23	34,34,34,34	0
93	MG	5	3855	1/1	0.86	0.38	31,31,31,31	0
93	MG	1	4126	1/1	0.86	0.18	42,42,42,42	0
93	MG	1	3982	1/1	0.86	0.39	48,48,48,48	0
93	MG	5	3859	1/1	0.86	0.42	30,30,30,30	0
93	MG	7	215	1/1	0.86	0.32	47,47,47,47	0
93	MG	1	3865	1/1	0.86	0.33	31,31,31,31	0
93	MG	5	3812	1/1	0.86	0.20	42,42,42,42	0
93	MG	1	3774	1/1	0.86	0.31	44,44,44,44	0
93	MG	1	3833	1/1	0.86	0.36	39,39,39,39	0
93	MG	8	217	1/1	0.86	0.29	37,37,37,37	0
93	MG	1	3731	1/1	0.86	0.28	47,47,47,47	0
93	MG	3	216	1/1	0.86	0.20	59,59,59,59	0
93	MG	1	4083	1/1	0.86	0.34	56,56,56,56	0
93	MG	5	4095	1/1	0.86	0.33	34,34,34,34	0
93	MG	1	3890	1/1	0.86	0.27	40,40,40,40	0
93	MG	5	3822	1/1	0.86	0.20	42,42,42,42	0
93	MG	5	4100	1/1	0.86	0.18	40,40,40,40	0
92	OHX	7	211	7/7	0.86	0.27	91,91,91,91	0
93	MG	1	3797	1/1	0.86	0.11	51,51,51,51	0
93	MG	5	3946	1/1	0.86	0.10	61,61,61,61	0
93	MG	p	103	1/1	0.86	0.36	35,35,35,35	0
93	MG	1	3960	1/1	0.86	0.24	40,40,40,40	0
93	MG	1	3899	1/1	0.86	0.30	33,33,33,33	0
92	OHX	1	3682	7/7	0.87	0.27	87,87,87,87	0
93	MG	1	3977	1/1	0.87	0.41	65,65,65,65	0
93	MG	1	3811	1/1	0.87	0.30	40,40,40,40	0
93	MG	1	3888	1/1	0.87	0.41	39,39,39,39	0
93	MG	N8	202	1/1	0.87	0.28	31,31,31,31	0
92	OHX	6	1970	7/7	0.87	0.38	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	2	2090	1/1	0.87	0.18	83,83,83,83	0
93	MG	5	3996	1/1	0.87	0.27	35,35,35,35	0
93	MG	5	3789	1/1	0.87	0.38	36,36,36,36	0
93	MG	5	3792	1/1	0.87	0.21	39,39,39,39	0
93	MG	5	4128	1/1	0.87	0.15	33,33,33,33	0
93	MG	5	4129	1/1	0.87	0.14	40,40,40,40	0
93	MG	6	2085	1/1	0.87	0.39	58,58,58,58	0
93	MG	1	3894	1/1	0.87	0.31	42,42,42,42	0
93	MG	5	3857	1/1	0.87	0.33	32,32,32,32	0
93	MG	5	3800	1/1	0.87	0.23	48,48,48,48	0
93	MG	2	2077	1/1	0.87	0.50	59,59,59,59	0
93	MG	1	4071	1/1	0.87	0.29	34,34,34,34	0
93	MG	1	3768	1/1	0.87	0.36	36,36,36,36	0
93	MG	1	3805	1/1	0.87	0.35	52,52,52,52	0
93	MG	1	4080	1/1	0.87	0.40	33,33,33,33	0
93	MG	5	3870	1/1	0.87	0.28	33,33,33,33	0
93	MG	4	223	1/1	0.87	0.32	49,49,49,49	0
93	MG	6	2156	1/1	0.87	0.21	68,68,68,68	0
93	MG	5	3814	1/1	0.87	0.16	38,38,38,38	0
93	MG	1	4036	1/1	0.87	0.19	56,56,56,56	0
93	MG	5	3816	1/1	0.87	0.21	43,43,43,43	0
93	MG	1	4037	1/1	0.87	0.36	46,46,46,46	0
93	MG	4	229	1/1	0.87	0.16	46,46,46,46	0
93	MG	5	4059	1/1	0.87	0.28	33,33,33,33	0
93	MG	1	3904	1/1	0.87	0.31	38,38,38,38	0
93	MG	1	3959	1/1	0.87	0.17	41,41,41,41	0
93	MG	1	3849	1/1	0.87	0.25	39,39,39,39	0
93	MG	5	3967	1/1	0.87	0.14	40,40,40,40	0
93	MG	8	225	1/1	0.87	0.08	51,51,51,51	0
93	MG	1	3794	1/1	0.87	0.27	58,58,58,58	0
93	MG	12	303	1/1	0.87	0.59	44,44,44,44	0
93	MG	1	4097	1/1	0.87	0.26	41,41,41,41	0
93	MG	19	202	1/1	0.87	0.18	41,41,41,41	0
93	MG	5	3826	1/1	0.87	0.24	43,43,43,43	0
93	MG	5	3760	1/1	0.87	0.20	42,42,42,42	0
93	MG	5	3761	1/1	0.87	0.33	33,33,33,33	0
93	MG	5	3833	1/1	0.87	0.22	40,40,40,40	0
93	MG	5	4093	1/1	0.87	0.11	35,35,35,35	0
93	MG	n3	201	1/1	0.87	0.33	32,32,32,32	0
93	MG	5	3835	1/1	0.87	0.25	34,34,34,34	0
93	MG	1	3940	1/1	0.87	0.16	51,51,51,51	0
93	MG	5	4097	1/1	0.87	0.20	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	1	4055	1/1	0.87	1.08	32,32,32,32	0
98	8AN	P	102	22/23	0.87	0.16	37,38,38,38	0
93	MG	5	4125	1/1	0.88	0.10	41,41,41,41	0
93	MG	5	4126	1/1	0.88	0.12	57,57,57,57	0
93	MG	1	3782	1/1	0.88	0.30	41,41,41,41	0
93	MG	6	2126	1/1	0.88	0.35	62,62,62,62	0
93	MG	5	4027	1/1	0.88	0.14	40,40,40,40	0
93	MG	5	4133	1/1	0.88	0.11	47,47,47,47	0
92	OHX	2	2045	7/7	0.88	0.38	100,100,100,100	0
93	MG	5	3915	1/1	0.88	0.34	36,36,36,36	0
93	MG	5	4151	1/1	0.88	0.11	46,46,46,46	0
93	MG	5	4153	1/1	0.88	0.14	52,52,52,52	0
93	MG	5	3810	1/1	0.88	0.24	89,89,89,89	0
92	OHX	1	3699	7/7	0.88	0.47	80,80,80,80	0
93	MG	5	4044	1/1	0.88	0.21	47,47,47,47	0
93	MG	1	3922	1/1	0.88	0.28	34,34,34,34	0
93	MG	5	3813	1/1	0.88	0.17	40,40,40,40	0
92	OHX	2	2051	7/7	0.88	0.29	105,105,105,105	0
93	MG	1	3872	1/1	0.88	0.28	41,41,41,41	0
93	MG	M7	206	1/1	0.88	0.39	37,37,37,37	0
93	MG	5	4063	1/1	0.88	0.20	38,38,38,38	0
93	MG	5	4065	1/1	0.88	0.11	37,37,37,37	0
93	MG	5	3980	1/1	0.88	0.30	43,43,43,43	0
93	MG	5	3861	1/1	0.88	0.38	39,39,39,39	0
93	MG	1	3898	1/1	0.88	0.31	34,34,34,34	0
93	MG	1	3832	1/1	0.88	0.27	39,39,39,39	0
93	MG	5	4081	1/1	0.88	0.14	32,32,32,32	0
93	MG	1	3803	1/1	0.88	0.28	46,46,46,46	0
93	MG	1	3902	1/1	0.88	0.38	40,40,40,40	0
93	MG	1	4129	1/1	0.88	0.13	39,39,39,39	0
93	MG	6	2142	1/1	0.88	0.27	48,48,48,48	0
93	MG	8	222	1/1	0.88	0.09	53,53,53,53	0
93	MG	8	223	1/1	0.88	0.21	62,62,62,62	0
93	MG	8	224	1/1	0.88	0.34	53,53,53,53	0
93	MG	1	3903	1/1	0.88	0.18	48,48,48,48	0
93	MG	1	3943	1/1	0.88	0.23	47,47,47,47	0
93	MG	1	4074	1/1	0.88	0.22	54,54,54,54	0
93	MG	1	3834	1/1	0.88	0.39	35,35,35,35	0
93	MG	l3	404	1/1	0.88	0.17	32,32,32,32	0
93	MG	5	3787	1/1	0.88	0.26	32,32,32,32	0
93	MG	2	2068	1/1	0.88	0.56	75,75,75,75	0
93	MG	1	3744	1/1	0.88	0.29	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	5	4006	1/1	0.88	0.17	33,33,33,33	0
93	MG	1	3984	1/1	0.88	0.29	42,42,42,42	0
93	MG	1	3807	1/1	0.88	0.23	48,48,48,48	0
93	MG	5	4110	1/1	0.88	0.28	45,45,45,45	0
93	MG	o3	202	1/1	0.88	0.43	44,44,44,44	0
93	MG	1	3989	1/1	0.88	0.15	40,40,40,40	0
92	OHX	1	3721	7/7	0.88	0.44	62,62,62,62	0
94	ZN	d7	101	1/1	0.88	0.11	89,89,89,89	0
93	MG	5	3960	1/1	0.88	0.31	39,39,39,39	0
93	MG	1	3781	1/1	0.88	0.23	41,41,41,41	0
93	MG	1	4094	1/1	0.88	0.31	37,37,37,37	0
98	8AN	p	102	22/23	0.88	0.14	33,34,35,35	0
93	MG	4	231	1/1	0.89	0.16	44,44,44,44	0
93	MG	5	4008	1/1	0.89	0.13	56,56,56,56	0
93	MG	1	3821	1/1	0.89	0.21	40,40,40,40	0
93	MG	6	2172	1/1	0.89	0.46	64,64,64,64	0
92	OHX	5	3601	7/7	0.89	0.18	84,84,84,84	0
93	MG	5	4017	1/1	0.89	0.14	42,42,42,42	0
93	MG	4	235	1/1	0.89	0.20	31,31,31,31	0
92	OHX	5	3647	7/7	0.89	0.28	64,64,64,64	0
92	OHX	5	3664	7/7	0.89	0.27	92,92,92,92	0
93	MG	5	4149	1/1	0.89	0.32	34,34,34,34	0
93	MG	M0	302	1/1	0.89	0.11	46,46,46,46	0
93	MG	1	3752	1/1	0.89	0.28	40,40,40,40	0
93	MG	5	3950	1/1	0.89	0.25	34,34,34,34	0
93	MG	1	3876	1/1	0.89	0.45	43,43,43,43	0
93	MG	1	3780	1/1	0.89	0.27	52,52,52,52	0
92	OHX	S9	201	7/7	0.89	0.34	93,93,93,93	0
93	MG	1	4101	1/1	0.89	0.54	43,43,43,43	0
93	MG	5	4039	1/1	0.89	0.11	43,43,43,43	0
93	MG	6	2188	1/1	0.89	0.15	86,86,86,86	0
93	MG	5	4167	1/1	0.89	0.39	33,33,33,33	0
93	MG	1	4102	1/1	0.89	0.18	39,39,39,39	0
93	MG	5	4049	1/1	0.89	0.24	48,48,48,48	0
93	MG	5	4173	1/1	0.89	0.17	30,30,30,30	0
93	MG	N3	202	1/1	0.89	0.13	51,51,51,51	0
93	MG	N3	203	1/1	0.89	0.12	46,46,46,46	0
93	MG	1	4044	1/1	0.89	0.26	35,35,35,35	0
93	MG	1	4048	1/1	0.89	0.13	44,44,44,44	0
93	MG	1	3996	1/1	0.89	0.21	40,40,40,40	0
93	MG	1	3950	1/1	0.89	0.11	44,44,44,44	0
93	MG	1	4053	1/1	0.89	0.14	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	5	4071	1/1	0.89	0.09	35,35,35,35	0
93	MG	D9	104	1/1	0.89	0.11	89,89,89,89	0
93	MG	2	2122	1/1	0.89	0.24	74,74,74,74	0
93	MG	5	3972	1/1	0.89	0.38	37,37,37,37	0
93	MG	5	4080	1/1	0.89	0.36	40,40,40,40	0
93	MG	1	4001	1/1	0.89	0.21	52,52,52,52	0
93	MG	5	3906	1/1	0.89	0.39	33,33,33,33	0
93	MG	5	3908	1/1	0.89	0.41	44,44,44,44	0
93	MG	8	228	1/1	0.89	0.35	56,56,56,56	0
93	MG	1	3884	1/1	0.89	0.31	35,35,35,35	0
93	MG	1	3918	1/1	0.89	0.42	32,32,32,32	0
92	OHX	1	3666	7/7	0.89	0.30	81,81,81,81	0
92	OHX	2	2028	7/7	0.89	0.20	109,109,109,109	0
92	OHX	2	2047	7/7	0.89	0.30	105,105,105,105	0
92	OHX	2	2048	7/7	0.89	0.22	100,100,100,100	0
92	OHX	2	2049	7/7	0.89	0.25	108,108,108,108	0
93	MG	6	2071	1/1	0.89	0.38	63,63,63,63	0
93	MG	m7	201	1/1	0.89	0.27	34,34,34,34	0
93	MG	5	3921	1/1	0.89	0.32	31,31,31,31	0
93	MG	1	4073	1/1	0.89	0.31	41,41,41,41	0
93	MG	n6	201	1/1	0.89	0.16	46,46,46,46	0
93	MG	n8	201	1/1	0.89	0.23	43,43,43,43	0
93	MG	o2	202	1/1	0.89	0.24	32,32,32,32	0
93	MG	5	4105	1/1	0.89	0.23	34,34,34,34	0
93	MG	6	2113	1/1	0.89	0.45	55,55,55,55	0
93	MG	5	3768	1/1	0.89	0.27	51,51,51,51	0
94	ZN	D7	101	1/1	0.89	0.17	100,100,100,100	0
93	MG	1	3932	1/1	0.89	0.12	37,37,37,37	0
93	MG	4	226	1/1	0.89	0.38	40,40,40,40	0
92	OHX	2	2015	7/7	0.89	0.26	92,92,92,92	0
93	MG	1	3970	1/1	0.89	0.33	37,37,37,37	0
92	OHX	6	2047	7/7	0.89	0.33	87,87,87,87	0
93	MG	5	3893	1/1	0.90	0.47	47,47,47,47	0
93	MG	1	4028	1/1	0.90	0.22	43,43,43,43	0
93	MG	1	3961	1/1	0.90	0.27	31,31,31,31	0
93	MG	6	2171	1/1	0.90	0.18	68,68,68,68	0
93	MG	1	3915	1/1	0.90	0.38	34,34,34,34	0
92	OHX	6	2057	7/7	0.90	0.31	92,92,92,92	0
93	MG	6	2064	1/1	0.90	0.46	68,68,68,68	0
92	OHX	c5	201	7/7	0.90	0.21	99,99,99,99	0
93	MG	1	3967	1/1	0.90	0.38	51,51,51,51	0
93	MG	1	4038	1/1	0.90	0.38	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	1	4122	1/1	0.90	0.22	37,37,37,37	0
93	MG	5	3914	1/1	0.90	0.21	48,48,48,48	0
93	MG	1	3969	1/1	0.90	0.35	42,42,42,42	0
93	MG	5	4004	1/1	0.90	0.39	29,29,29,29	0
92	OHX	SR	401	7/7	0.90	0.16	121,121,121,121	0
93	MG	1	4125	1/1	0.90	0.26	32,32,32,32	0
93	MG	1	3783	1/1	0.90	0.31	39,39,39,39	0
93	MG	1	3925	1/1	0.90	0.27	39,39,39,39	0
93	MG	1	4046	1/1	0.90	0.31	43,43,43,43	0
93	MG	5	4011	1/1	0.90	0.35	32,32,32,32	0
92	OHX	5	3619	7/7	0.90	0.20	73,73,73,73	0
92	OHX	1	3663	7/7	0.90	0.35	73,73,73,73	0
93	MG	5	3930	1/1	0.90	0.45	37,37,37,37	0
93	MG	6	2129	1/1	0.90	0.15	61,61,61,61	0
93	MG	1	3851	1/1	0.90	0.46	36,36,36,36	0
93	MG	5	4023	1/1	0.90	0.29	41,41,41,41	0
92	OHX	2	2014	7/7	0.90	0.16	107,107,107,107	0
92	OHX	5	3730	7/7	0.90	0.20	97,97,97,97	0
92	OHX	2	2046	7/7	0.90	0.34	100,100,100,100	0
93	MG	1	3892	1/1	0.90	0.28	32,32,32,32	0
93	MG	5	4034	1/1	0.90	0.07	89,89,89,89	0
93	MG	1	3990	1/1	0.90	0.22	39,39,39,39	0
93	MG	1	3893	1/1	0.90	0.36	46,46,46,46	0
93	MG	1	3941	1/1	0.90	0.38	42,42,42,42	0
93	MG	6	2139	1/1	0.90	0.16	57,57,57,57	0
92	OHX	m9	201	7/7	0.90	0.31	89,89,89,89	0
93	MG	5	4045	1/1	0.90	0.12	41,41,41,41	0
93	MG	7	227	1/1	0.90	0.16	46,46,46,46	0
93	MG	1	3999	1/1	0.90	0.24	43,43,43,43	0
93	MG	2	2052	1/1	0.90	0.44	69,69,69,69	0
93	MG	5	4051	1/1	0.90	0.36	34,34,34,34	0
93	MG	5	4054	1/1	0.90	0.11	36,36,36,36	0
92	OHX	2	1980	7/7	0.90	0.12	140,140,140,140	0
93	MG	1	4072	1/1	0.90	0.33	37,37,37,37	0
92	OHX	2	1947	7/7	0.90	0.17	106,106,106,106	0
93	MG	1	3828	1/1	0.90	0.32	43,43,43,43	0
93	MG	5	3955	1/1	0.90	0.29	35,35,35,35	0
93	MG	L4	403	1/1	0.90	0.13	31,31,31,31	0
93	MG	1	4010	1/1	0.90	0.10	47,47,47,47	0
93	MG	5	4070	1/1	0.90	0.13	40,40,40,40	0
93	MG	l3	405	1/1	0.90	0.21	38,38,38,38	0
93	MG	l6	201	1/1	0.90	0.20	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	2	2032	7/7	0.90	0.29	106,106,106,106	0
93	MG	m4	201	1/1	0.90	0.10	42,42,42,42	0
93	MG	5	3771	1/1	0.90	0.20	38,38,38,38	0
93	MG	5	3774	1/1	0.90	0.20	33,33,33,33	0
93	MG	5	3776	1/1	0.90	0.32	40,40,40,40	0
93	MG	1	4079	1/1	0.90	0.18	54,54,54,54	0
93	MG	1	3868	1/1	0.90	0.12	41,41,41,41	0
92	OHX	1	3725	7/7	0.90	0.33	87,87,87,87	0
93	MG	n0	201	1/1	0.90	0.15	39,39,39,39	0
92	OHX	2	2039	7/7	0.90	0.15	133,133,133,133	0
93	MG	1	3742	1/1	0.90	0.25	41,41,41,41	0
93	MG	n6	202	1/1	0.90	0.27	42,42,42,42	0
93	MG	5	3877	1/1	0.90	0.33	37,37,37,37	0
93	MG	1	4020	1/1	0.90	0.25	39,39,39,39	0
93	MG	1	4092	1/1	0.90	0.33	33,33,33,33	0
92	OHX	6	1980	7/7	0.90	0.19	112,112,112,112	0
93	MG	5	3975	1/1	0.90	0.27	35,35,35,35	0
93	MG	5	3794	1/1	0.90	0.20	37,37,37,37	0
92	OHX	6	2045	7/7	0.90	0.31	94,94,94,94	0
93	MG	5	4101	1/1	0.90	0.50	60,60,60,60	0
93	MG	1	3776	1/1	0.90	0.30	47,47,47,47	0
92	OHX	2	2004	7/7	0.90	0.26	96,96,96,96	0
93	MG	1	4098	1/1	0.90	0.29	58,58,58,58	0
92	OHX	2	2050	7/7	0.91	0.17	115,115,115,115	0
92	OHX	1	3715	7/7	0.91	0.32	51,51,51,51	0
93	MG	1	3856	1/1	0.91	0.43	36,36,36,36	0
93	MG	1	4041	1/1	0.91	0.33	53,53,53,53	0
92	OHX	1	3718	7/7	0.91	0.33	83,83,83,83	0
93	MG	5	4099	1/1	0.91	0.18	33,33,33,33	0
93	MG	1	3761	1/1	0.91	0.31	46,46,46,46	0
92	OHX	5	3703	7/7	0.91	0.20	57,57,57,57	0
93	MG	1	3910	1/1	0.91	0.29	38,38,38,38	0
93	MG	1	4049	1/1	0.91	0.24	47,47,47,47	0
92	OHX	5	3706	7/7	0.91	0.50	76,76,76,76	0
93	MG	5	3865	1/1	0.91	0.32	44,44,44,44	0
92	OHX	5	3709	7/7	0.91	0.33	57,57,57,57	0
93	MG	5	3868	1/1	0.91	0.42	32,32,32,32	0
93	MG	5	3977	1/1	0.91	0.16	48,48,48,48	0
93	MG	5	3769	1/1	0.91	0.33	35,35,35,35	0
93	MG	3	218	1/1	0.91	0.48	43,43,43,43	0
93	MG	5	3871	1/1	0.91	0.24	33,33,33,33	0
93	MG	1	3913	1/1	0.91	0.42	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	5	3875	1/1	0.91	0.29	34,34,34,34	0
93	MG	5	3772	1/1	0.91	0.45	46,46,46,46	0
92	OHX	5	3718	7/7	0.91	0.20	102,102,102,102	0
93	MG	5	3878	1/1	0.91	0.52	37,37,37,37	0
93	MG	5	3775	1/1	0.91	0.15	32,32,32,32	0
93	MG	5	3883	1/1	0.91	0.32	32,32,32,32	0
92	OHX	2	2042	7/7	0.91	0.16	126,126,126,126	0
93	MG	1	3771	1/1	0.91	0.26	30,30,30,30	0
93	MG	5	4145	1/1	0.91	0.14	48,48,48,48	0
93	MG	5	4148	1/1	0.91	0.26	34,34,34,34	0
93	MG	1	3919	1/1	0.91	0.39	36,36,36,36	0
93	MG	5	3997	1/1	0.91	0.25	31,31,31,31	0
93	MG	5	3779	1/1	0.91	0.25	33,33,33,33	0
92	OHX	5	3738	7/7	0.91	0.39	69,69,69,69	0
92	OHX	2	2013	7/7	0.91	0.19	104,104,104,104	0
93	MG	1	3732	1/1	0.91	0.34	48,48,48,48	0
93	MG	1	3924	1/1	0.91	0.21	42,42,42,42	0
92	OHX	8	215	7/7	0.91	0.35	55,55,55,55	0
93	MG	5	3897	1/1	0.91	0.27	37,37,37,37	0
93	MG	1	3926	1/1	0.91	0.21	38,38,38,38	0
92	OHX	13	402	7/7	0.91	0.34	67,67,67,67	0
93	MG	5	3795	1/1	0.91	0.24	37,37,37,37	0
93	MG	1	3736	1/1	0.91	0.15	47,47,47,47	0
93	MG	5	3799	1/1	0.91	0.27	31,31,31,31	0
93	MG	5	4016	1/1	0.91	0.18	31,31,31,31	0
93	MG	5	4176	1/1	0.91	0.22	36,36,36,36	0
93	MG	6	2162	1/1	0.91	0.22	55,55,55,55	0
93	MG	5	4018	1/1	0.91	0.16	38,38,38,38	0
93	MG	L4	405	1/1	0.91	0.50	33,33,33,33	0
92	OHX	2	2030	7/7	0.91	0.31	95,95,95,95	0
93	MG	1	3740	1/1	0.91	0.25	48,48,48,48	0
93	MG	7	224	1/1	0.91	0.12	36,36,36,36	0
93	MG	1	3935	1/1	0.91	0.32	40,40,40,40	0
93	MG	6	2168	1/1	0.91	0.20	57,57,57,57	0
93	MG	M7	203	1/1	0.91	0.22	38,38,38,38	0
93	MG	5	3918	1/1	0.91	0.32	42,42,42,42	0
93	MG	1	4077	1/1	0.91	0.16	40,40,40,40	0
93	MG	8	220	1/1	0.91	0.22	43,43,43,43	0
93	MG	5	4030	1/1	0.91	0.23	33,33,33,33	0
93	MG	1	3741	1/1	0.91	0.30	35,35,35,35	0
92	OHX	1	3548	7/7	0.91	0.14	91,91,91,91	0
92	OHX	6	2022	7/7	0.91	0.34	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	6	2026	7/7	0.91	0.37	90,90,90,90	0
93	MG	5	3925	1/1	0.91	0.37	38,38,38,38	0
93	MG	1	3745	1/1	0.91	0.23	40,40,40,40	0
93	MG	6	2179	1/1	0.91	0.17	93,93,93,93	0
93	MG	5	4047	1/1	0.91	0.20	36,36,36,36	0
93	MG	1	4088	1/1	0.91	0.34	44,44,44,44	0
93	MG	l3	406	1/1	0.91	0.47	34,34,34,34	0
93	MG	l5	303	1/1	0.91	0.11	50,50,50,50	0
93	MG	1	3942	1/1	0.91	0.14	33,33,33,33	0
92	OHX	6	2042	7/7	0.91	0.21	94,94,94,94	0
92	OHX	1	3593	7/7	0.91	0.24	66,66,66,66	0
93	MG	1	3889	1/1	0.91	0.55	36,36,36,36	0
93	MG	5	4057	1/1	0.91	0.17	35,35,35,35	0
93	MG	1	4022	1/1	0.91	0.10	34,34,34,34	0
92	OHX	2	2031	7/7	0.91	0.23	103,103,103,103	0
93	MG	5	4061	1/1	0.91	0.26	39,39,39,39	0
92	OHX	6	2051	7/7	0.91	0.33	84,84,84,84	0
92	OHX	2	2024	7/7	0.91	0.20	103,103,103,103	0
93	MG	5	3832	1/1	0.91	0.46	41,41,41,41	0
93	MG	1	3842	1/1	0.91	0.33	38,38,38,38	0
93	MG	1	4103	1/1	0.91	0.10	39,39,39,39	0
92	OHX	2	2038	7/7	0.91	0.25	95,95,95,95	0
93	MG	d4	202	1/1	0.91	0.37	65,65,65,65	0
93	MG	5	4075	1/1	0.91	0.32	49,49,49,49	0
93	MG	5	3841	1/1	0.91	0.32	43,43,43,43	0
93	MG	P	103	1/1	0.91	0.38	39,39,39,39	0
93	MG	1	4106	1/1	0.91	0.21	39,39,39,39	0
93	MG	1	3753	1/1	0.91	0.21	45,45,45,45	0
93	MG	6	2127	1/1	0.91	0.08	54,54,54,54	0
93	MG	1	3802	1/1	0.91	0.18	36,36,36,36	0
92	OHX	5	3596	7/7	0.91	0.25	68,68,68,68	0
92	OHX	2	2027	7/7	0.91	0.25	93,93,93,93	0
93	MG	1	3957	1/1	0.91	0.22	39,39,39,39	0
93	MG	2	2085	1/1	0.92	0.50	76,76,76,76	0
92	OHX	c3	201	7/7	0.92	0.23	89,89,89,89	0
93	MG	1	3881	1/1	0.92	0.29	33,33,33,33	0
92	OHX	2	2023	7/7	0.92	0.25	91,91,91,91	0
92	OHX	sR	401	7/7	0.92	0.17	116,116,116,116	0
93	MG	1	3927	1/1	0.92	0.14	56,56,56,56	0
93	MG	5	3780	1/1	0.92	0.17	35,35,35,35	0
93	MG	5	3781	1/1	0.92	0.19	37,37,37,37	0
93	MG	5	4033	1/1	0.92	0.12	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	5	3947	1/1	0.92	0.10	40,40,40,40	0
93	MG	1	3759	1/1	0.92	0.41	45,45,45,45	0
93	MG	5	3785	1/1	0.92	0.26	33,33,33,33	0
92	OHX	1	3501	7/7	0.92	0.16	66,66,66,66	0
93	MG	5	4038	1/1	0.92	0.23	37,37,37,37	0
93	MG	1	4111	1/1	0.92	0.18	45,45,45,45	0
93	MG	5	3867	1/1	0.92	0.19	40,40,40,40	0
93	MG	5	4163	1/1	0.92	0.29	37,37,37,37	0
93	MG	1	4115	1/1	0.92	0.24	63,63,63,63	0
93	MG	1	3931	1/1	0.92	0.20	37,37,37,37	0
93	MG	1	3844	1/1	0.92	0.50	39,39,39,39	0
93	MG	1	4121	1/1	0.92	0.17	39,39,39,39	0
93	MG	5	4050	1/1	0.92	0.51	24,24,24,24	0
93	MG	2	2063	1/1	0.92	0.13	74,74,74,74	0
93	MG	5	4052	1/1	0.92	0.38	65,65,65,65	0
92	OHX	2	1986	7/7	0.92	0.32	107,107,107,107	0
93	MG	7	214	1/1	0.92	0.34	33,33,33,33	0
93	MG	1	4056	1/1	0.92	0.15	34,34,34,34	0
93	MG	7	219	1/1	0.92	0.10	37,37,37,37	0
93	MG	1	3848	1/1	0.92	0.17	34,34,34,34	0
92	OHX	1	3722	7/7	0.92	0.34	76,76,76,76	0
92	OHX	5	3633	7/7	0.92	0.43	70,70,70,70	0
92	OHX	2	2011	7/7	0.92	0.25	104,104,104,104	0
93	MG	5	3884	1/1	0.92	0.29	39,39,39,39	0
93	MG	1	3895	1/1	0.92	0.38	37,37,37,37	0
92	OHX	3	210	7/7	0.92	0.29	85,85,85,85	0
93	MG	1	3897	1/1	0.92	0.47	30,30,30,30	0
93	MG	5	4069	1/1	0.92	0.35	33,33,33,33	0
93	MG	1	3769	1/1	0.92	0.30	36,36,36,36	0
92	OHX	O4	201	7/7	0.92	0.41	73,73,73,73	0
93	MG	5	4073	1/1	0.92	0.21	34,34,34,34	0
92	OHX	1	3594	7/7	0.92	0.33	68,68,68,68	0
93	MG	4	222	1/1	0.92	0.32	48,48,48,48	0
93	MG	5	4076	1/1	0.92	0.11	61,61,61,61	0
93	MG	1	3901	1/1	0.92	0.41	37,37,37,37	0
92	OHX	1	3625	7/7	0.92	0.33	70,70,70,70	0
92	OHX	6	1989	7/7	0.92	0.32	97,97,97,97	0
93	MG	5	3900	1/1	0.92	0.14	49,49,49,49	0
93	MG	6	2134	1/1	0.92	0.22	57,57,57,57	0
93	MG	5	4085	1/1	0.92	0.32	49,49,49,49	0
92	OHX	6	2015	7/7	0.92	0.31	79,79,79,79	0
92	OHX	1	3637	7/7	0.92	0.11	145,145,145,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	1	4078	1/1	0.92	0.09	36,36,36,36	0
93	MG	5	3907	1/1	0.92	0.22	31,31,31,31	0
92	OHX	6	2023	7/7	0.92	0.29	91,91,91,91	0
92	OHX	2	2041	7/7	0.92	0.31	83,83,83,83	0
92	OHX	6	2035	7/7	0.92	0.36	84,84,84,84	0
93	MG	m6	204	1/1	0.92	0.27	36,36,36,36	0
92	OHX	2	1996	7/7	0.92	0.18	103,103,103,103	0
93	MG	4	236	1/1	0.92	0.23	42,42,42,42	0
93	MG	4	239	1/1	0.92	0.10	42,42,42,42	0
93	MG	m7	203	1/1	0.92	0.17	33,33,33,33	0
93	MG	6	2090	1/1	0.92	0.19	56,56,56,56	0
93	MG	n0	202	1/1	0.92	0.29	37,37,37,37	0
93	MG	1	3958	1/1	0.92	0.25	36,36,36,36	0
93	MG	6	2146	1/1	0.92	0.06	75,75,75,75	0
93	MG	1	4087	1/1	0.92	0.42	34,34,34,34	0
92	OHX	1	3673	7/7	0.92	0.35	73,73,73,73	0
92	OHX	2	1998	7/7	0.92	0.27	95,95,95,95	0
93	MG	5	3843	1/1	0.92	0.22	34,34,34,34	0
92	OHX	6	2050	7/7	0.92	0.39	68,68,68,68	0
92	OHX	2	1999	7/7	0.92	0.30	106,106,106,106	0
93	MG	1	3751	1/1	0.92	0.14	38,38,38,38	0
93	MG	5	3847	1/1	0.92	0.24	33,33,33,33	0
93	MG	5	3848	1/1	0.92	0.41	41,41,41,41	0
95	PHE	1	3401	11/12	0.92	0.19	34,34,44,44	0
93	MG	1	4095	1/1	0.92	0.11	52,52,52,52	0
92	OHX	D9	102	7/7	0.92	0.34	98,98,98,98	0
93	MG	5	4127	1/1	0.92	0.18	36,36,36,36	0
92	OHX	6	2059	7/7	0.92	0.23	103,103,103,103	0
92	OHX	6	1988	7/7	0.93	0.28	82,82,82,82	0
92	OHX	5	3716	7/7	0.93	0.24	84,84,84,84	0
93	MG	1	3994	1/1	0.93	0.10	46,46,46,46	0
92	OHX	2	1943	7/7	0.93	0.24	101,101,101,101	0
93	MG	1	3853	1/1	0.93	0.53	43,43,43,43	0
92	OHX	5	3721	7/7	0.93	0.20	99,99,99,99	0
93	MG	1	4086	1/1	0.93	0.10	41,41,41,41	0
93	MG	O7	104	1/1	0.93	0.19	46,46,46,46	0
93	MG	5	4111	1/1	0.93	0.22	35,35,35,35	0
92	OHX	5	3724	7/7	0.93	0.38	55,55,55,55	0
92	OHX	6	2003	7/7	0.93	0.20	89,89,89,89	0
93	MG	5	3880	1/1	0.93	0.33	37,37,37,37	0
93	MG	5	4116	1/1	0.93	0.27	44,44,44,44	0
93	MG	5	3989	1/1	0.93	0.15	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	C5	201	7/7	0.93	0.20	105,105,105,105	0
93	MG	1	3860	1/1	0.93	0.44	44,44,44,44	0
92	OHX	5	3748	7/7	0.93	0.27	87,87,87,87	0
93	MG	1	4007	1/1	0.93	0.19	51,51,51,51	0
93	MG	1	4008	1/1	0.93	0.19	34,34,34,34	0
93	MG	5	3784	1/1	0.93	0.31	37,37,37,37	0
93	MG	5	4131	1/1	0.93	0.14	35,35,35,35	0
93	MG	1	4009	1/1	0.93	0.15	37,37,37,37	0
92	OHX	2	1974	7/7	0.93	0.17	112,112,112,112	0
93	MG	5	4137	1/1	0.93	0.15	38,38,38,38	0
92	OHX	8	213	7/7	0.93	0.30	62,62,62,62	0
93	MG	1	4099	1/1	0.93	0.29	45,45,45,45	0
93	MG	5	4142	1/1	0.93	0.23	34,34,34,34	0
93	MG	5	4003	1/1	0.93	0.26	36,36,36,36	0
93	MG	5	3791	1/1	0.93	0.08	42,42,42,42	0
93	MG	1	4013	1/1	0.93	0.33	37,37,37,37	0
92	OHX	2	1975	7/7	0.93	0.15	77,77,77,77	0
93	MG	5	3898	1/1	0.93	0.37	39,39,39,39	0
93	MG	5	3899	1/1	0.93	0.23	32,32,32,32	0
92	OHX	6	2024	7/7	0.93	0.28	103,103,103,103	0
92	OHX	6	2025	7/7	0.93	0.33	70,70,70,70	0
93	MG	5	4013	1/1	0.93	0.26	38,38,38,38	0
93	MG	5	3797	1/1	0.93	0.22	38,38,38,38	0
93	MG	5	4161	1/1	0.93	0.19	39,39,39,39	0
92	OHX	1	3693	7/7	0.93	0.28	80,80,80,80	0
93	MG	5	3905	1/1	0.93	0.52	38,38,38,38	0
93	MG	1	3737	1/1	0.93	0.19	48,48,48,48	0
93	MG	1	4108	1/1	0.93	0.14	44,44,44,44	0
93	MG	1	3936	1/1	0.93	0.34	40,40,40,40	0
93	MG	5	4169	1/1	0.93	0.24	47,47,47,47	0
93	MG	5	3804	1/1	0.93	0.29	39,39,39,39	0
92	OHX	6	2027	7/7	0.93	0.27	91,91,91,91	0
93	MG	1	4112	1/1	0.93	0.12	59,59,59,59	0
92	OHX	6	2031	7/7	0.93	0.28	106,106,106,106	0
93	MG	5	4178	1/1	0.93	0.11	63,63,63,63	0
93	MG	7	201	1/1	0.93	0.12	43,43,43,43	0
93	MG	5	4026	1/1	0.93	0.14	33,33,33,33	0
93	MG	5	3913	1/1	0.93	0.39	30,30,30,30	0
93	MG	1	4116	1/1	0.93	0.12	76,76,76,76	0
93	MG	7	217	1/1	0.93	0.39	34,34,34,34	0
92	OHX	6	2032	7/7	0.93	0.21	92,92,92,92	0
93	MG	5	4032	1/1	0.93	0.34	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	1	3695	7/7	0.93	0.31	64,64,64,64	0
93	MG	6	2164	1/1	0.93	0.08	57,57,57,57	0
92	OHX	6	2037	7/7	0.93	0.32	77,77,77,77	0
93	MG	7	225	1/1	0.93	0.08	36,36,36,36	0
93	MG	1	4029	1/1	0.93	0.19	44,44,44,44	0
92	OHX	1	3495	7/7	0.93	0.17	56,56,56,56	0
92	OHX	6	2044	7/7	0.93	0.28	63,63,63,63	0
93	MG	1	4034	1/1	0.93	0.22	47,47,47,47	0
92	OHX	2	2017	7/7	0.93	0.25	88,88,88,88	0
92	OHX	2	2021	7/7	0.93	0.25	110,110,110,110	0
92	OHX	6	2048	7/7	0.93	0.25	77,77,77,77	0
92	OHX	1	3552	7/7	0.93	0.28	58,58,58,58	0
92	OHX	1	3720	7/7	0.93	0.31	61,61,61,61	0
92	OHX	6	2053	7/7	0.93	0.26	87,87,87,87	0
92	OHX	2	2036	7/7	0.93	0.26	112,112,112,112	0
92	OHX	2	2007	7/7	0.93	0.35	88,88,88,88	0
93	MG	3	217	1/1	0.93	0.26	39,39,39,39	0
92	OHX	s9	201	7/7	0.93	0.31	77,77,77,77	0
92	OHX	1	3604	7/7	0.93	0.45	43,43,43,43	0
93	MG	6	2184	1/1	0.93	0.12	57,57,57,57	0
92	OHX	1	3727	7/7	0.93	0.41	50,50,50,50	0
92	OHX	1	3730	7/7	0.93	0.14	94,94,94,94	0
93	MG	5	3944	1/1	0.93	0.24	35,35,35,35	0
93	MG	5	3945	1/1	0.93	0.29	32,32,32,32	0
92	OHX	1	3613	7/7	0.93	0.34	58,58,58,58	0
93	MG	5	4067	1/1	0.93	0.26	35,35,35,35	0
92	OHX	2	1945	7/7	0.93	0.15	90,90,90,90	0
93	MG	6	2106	1/1	0.93	0.39	60,60,60,60	0
93	MG	m6	203	1/1	0.93	0.12	34,34,34,34	0
92	OHX	6	1927	7/7	0.93	0.12	109,109,109,109	0
93	MG	1	3762	1/1	0.93	0.17	34,34,34,34	0
92	OHX	5	3622	7/7	0.93	0.21	59,59,59,59	0
92	OHX	5	3628	7/7	0.93	0.19	90,90,90,90	0
92	OHX	5	3632	7/7	0.93	0.30	65,65,65,65	0
93	MG	1	4060	1/1	0.93	0.10	37,37,37,37	0
93	MG	1	4061	1/1	0.93	0.12	32,32,32,32	0
92	OHX	6	1931	7/7	0.93	0.17	86,86,86,86	0
92	OHX	5	3636	7/7	0.93	0.21	63,63,63,63	0
92	OHX	2	2026	7/7	0.93	0.21	109,109,109,109	0
93	MG	5	4082	1/1	0.93	0.24	42,42,42,42	0
93	MG	1	3973	1/1	0.93	0.17	47,47,47,47	0
92	OHX	6	1973	7/7	0.93	0.20	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	1	3978	1/1	0.93	0.38	43,43,43,43	0
92	OHX	5	3685	7/7	0.93	0.26	73,73,73,73	0
93	MG	5	4090	1/1	0.93	0.11	37,37,37,37	0
92	OHX	5	3687	7/7	0.93	0.34	66,66,66,66	0
94	ZN	E1	501	1/1	0.93	0.06	109,109,109,109	0
93	MG	1	3845	1/1	0.93	0.28	38,38,38,38	0
92	OHX	5	3689	7/7	0.93	0.25	79,79,79,79	0
93	MG	5	3970	1/1	0.93	0.21	32,32,32,32	0
92	OHX	5	3699	7/7	0.93	0.33	63,63,63,63	0
97	SPS	P	101	23/23	0.93	0.13	37,37,48,51	0
92	OHX	1	3646	7/7	0.93	0.24	93,93,93,93	0
92	OHX	6	1987	7/7	0.93	0.21	89,89,89,89	0
92	OHX	4	220	7/7	0.94	0.31	66,66,66,66	0
92	OHX	M9	201	7/7	0.94	0.25	74,74,74,74	0
92	OHX	1	3590	7/7	0.94	0.17	92,92,92,92	0
92	OHX	2	2019	7/7	0.94	0.27	91,91,91,91	0
92	OHX	5	3700	7/7	0.94	0.35	53,53,53,53	0
93	MG	5	3749	1/1	0.94	0.19	36,36,36,36	0
92	OHX	2	2020	7/7	0.94	0.19	96,96,96,96	0
92	OHX	6	1949	7/7	0.94	0.16	81,81,81,81	0
92	OHX	5	3707	7/7	0.94	0.35	67,67,67,67	0
92	OHX	6	1959	7/7	0.94	0.17	67,67,67,67	0
92	OHX	6	1961	7/7	0.94	0.29	75,75,75,75	0
93	MG	1	3806	1/1	0.94	0.17	41,41,41,41	0
93	MG	1	4054	1/1	0.94	0.34	38,38,38,38	0
92	OHX	6	1967	7/7	0.94	0.17	78,78,78,78	0
92	OHX	1	3595	7/7	0.94	0.42	60,60,60,60	0
92	OHX	1	3601	7/7	0.94	0.32	62,62,62,62	0
93	MG	5	3917	1/1	0.94	0.34	32,32,32,32	0
93	MG	1	3923	1/1	0.94	0.22	41,41,41,41	0
93	MG	5	4088	1/1	0.94	0.14	42,42,42,42	0
93	MG	5	3764	1/1	0.94	0.13	34,34,34,34	0
92	OHX	5	3726	7/7	0.94	0.35	60,60,60,60	0
93	MG	1	3813	1/1	0.94	0.20	44,44,44,44	0
92	OHX	2	1909	7/7	0.94	0.13	97,97,97,97	0
93	MG	5	3923	1/1	0.94	0.32	38,38,38,38	0
92	OHX	6	1985	7/7	0.94	0.32	91,91,91,91	0
93	MG	1	3928	1/1	0.94	0.41	51,51,51,51	0
92	OHX	1	3612	7/7	0.94	0.22	87,87,87,87	0
92	OHX	2	2022	7/7	0.94	0.18	105,105,105,105	0
92	OHX	1	3614	7/7	0.94	0.21	77,77,77,77	0
92	OHX	6	1997	7/7	0.94	0.24	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	1	3933	1/1	0.94	0.12	51,51,51,51	0
92	OHX	6	2001	7/7	0.94	0.23	93,93,93,93	0
92	OHX	m8	201	7/7	0.94	0.30	60,60,60,60	0
93	MG	5	4106	1/1	0.94	0.26	37,37,37,37	0
92	OHX	2	1950	7/7	0.94	0.23	101,101,101,101	0
92	OHX	6	2009	7/7	0.94	0.22	88,88,88,88	0
93	MG	2	2053	1/1	0.94	0.41	70,70,70,70	0
92	OHX	1	3630	7/7	0.94	0.26	59,59,59,59	0
92	OHX	6	2017	7/7	0.94	0.22	99,99,99,99	0
92	OHX	6	2018	7/7	0.94	0.15	114,114,114,114	0
92	OHX	6	2019	7/7	0.94	0.28	75,75,75,75	0
92	OHX	2	2000	7/7	0.94	0.24	95,95,95,95	0
92	OHX	1	3645	7/7	0.94	0.32	57,57,57,57	0
93	MG	5	4121	1/1	0.94	0.23	33,33,33,33	0
93	MG	1	4085	1/1	0.94	0.21	39,39,39,39	0
93	MG	5	3790	1/1	0.94	0.27	31,31,31,31	0
92	OHX	2	2025	7/7	0.94	0.29	85,85,85,85	0
93	MG	1	3836	1/1	0.94	0.35	34,34,34,34	0
92	OHX	2	2002	7/7	0.94	0.32	86,86,86,86	0
93	MG	1	3949	1/1	0.94	0.24	36,36,36,36	0
92	OHX	2	2003	7/7	0.94	0.20	100,100,100,100	0
92	OHX	1	3672	7/7	0.94	0.34	67,67,67,67	0
92	OHX	6	2029	7/7	0.94	0.34	69,69,69,69	0
93	MG	5	4134	1/1	0.94	0.11	36,36,36,36	0
92	OHX	2	1978	7/7	0.94	0.18	103,103,103,103	0
93	MG	1	3734	1/1	0.94	0.33	53,53,53,53	0
93	MG	5	3801	1/1	0.94	0.29	32,32,32,32	0
93	MG	1	3843	1/1	0.94	0.27	36,36,36,36	0
92	OHX	1	3679	7/7	0.94	0.27	67,67,67,67	0
93	MG	5	4147	1/1	0.94	0.31	41,41,41,41	0
92	OHX	2	2029	7/7	0.94	0.30	79,79,79,79	0
92	OHX	6	2036	7/7	0.94	0.34	73,73,73,73	0
92	OHX	1	3684	7/7	0.94	0.29	65,65,65,65	0
92	OHX	6	2038	7/7	0.94	0.17	105,105,105,105	0
92	OHX	2	1957	7/7	0.94	0.30	85,85,85,85	0
92	OHX	6	2043	7/7	0.94	0.32	81,81,81,81	0
92	OHX	C7	201	7/7	0.94	0.19	106,106,106,106	0
93	MG	1	3964	1/1	0.94	0.23	51,51,51,51	0
92	OHX	1	3697	7/7	0.94	0.27	58,58,58,58	0
93	MG	1	4110	1/1	0.94	0.30	41,41,41,41	0
92	OHX	2	1959	7/7	0.94	0.18	98,98,98,98	0
93	MG	6	2123	1/1	0.94	0.05	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	5	4164	1/1	0.94	0.11	33,33,33,33	0
93	MG	5	4165	1/1	0.94	0.14	32,32,32,32	0
92	OHX	1	3700	7/7	0.94	0.21	87,87,87,87	0
93	MG	1	4114	1/1	0.94	0.13	34,34,34,34	0
93	MG	1	3855	1/1	0.94	0.22	32,32,32,32	0
93	MG	1	3971	1/1	0.94	0.16	44,44,44,44	0
93	MG	5	4171	1/1	0.94	0.15	31,31,31,31	0
92	OHX	6	2049	7/7	0.94	0.34	81,81,81,81	0
92	OHX	1	3703	7/7	0.94	0.26	82,82,82,82	0
93	MG	5	3825	1/1	0.94	0.26	35,35,35,35	0
93	MG	1	4119	1/1	0.94	0.26	58,58,58,58	0
92	OHX	2	1991	7/7	0.94	0.30	96,96,96,96	0
93	MG	1	3859	1/1	0.94	0.44	41,41,41,41	0
92	OHX	1	3709	7/7	0.94	0.45	47,47,47,47	0
92	OHX	6	2055	7/7	0.94	0.20	118,118,118,118	0
92	OHX	1	3481	7/7	0.94	0.14	66,66,66,66	0
92	OHX	2	1973	7/7	0.94	0.12	112,112,112,112	0
92	OHX	s4	301	7/7	0.94	0.23	90,90,90,90	0
93	MG	1	4130	1/1	0.94	0.18	40,40,40,40	0
92	OHX	2	1995	7/7	0.94	0.21	103,103,103,103	0
92	OHX	1	3535	7/7	0.94	0.17	50,50,50,50	0
92	OHX	2	1915	7/7	0.94	0.13	99,99,99,99	0
93	MG	1	3992	1/1	0.94	0.31	44,44,44,44	0
93	MG	1	3993	1/1	0.94	0.33	45,45,45,45	0
92	OHX	d4	201	7/7	0.94	0.28	84,84,84,84	0
93	MG	1	3995	1/1	0.94	0.17	47,47,47,47	0
92	OHX	1	3724	7/7	0.94	0.25	75,75,75,75	0
92	OHX	5	3475	7/7	0.94	0.19	42,42,42,42	0
92	OHX	5	3501	7/7	0.94	0.14	59,59,59,59	0
93	MG	4	224	1/1	0.94	0.40	49,49,49,49	0
92	OHX	5	3503	7/7	0.94	0.15	61,61,61,61	0
92	OHX	5	3518	7/7	0.94	0.16	78,78,78,78	0
92	OHX	5	3553	7/7	0.94	0.30	50,50,50,50	0
93	MG	8	226	1/1	0.94	0.18	47,47,47,47	0
93	MG	1	3877	1/1	0.94	0.20	39,39,39,39	0
93	MG	1	3878	1/1	0.94	0.40	33,33,33,33	0
93	MG	l2	302	1/1	0.94	0.25	41,41,41,41	0
92	OHX	2	2040	7/7	0.94	0.22	97,97,97,97	0
92	OHX	1	3726	7/7	0.94	0.28	69,69,69,69	0
92	OHX	5	3617	7/7	0.94	0.27	74,74,74,74	0
93	MG	5	3862	1/1	0.94	0.32	35,35,35,35	0
93	MG	6	2160	1/1	0.94	0.08	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	5	3864	1/1	0.94	0.47	39,39,39,39	0
93	MG	1	3770	1/1	0.94	0.08	41,41,41,41	0
92	OHX	1	3559	7/7	0.94	0.31	54,54,54,54	0
93	MG	4	238	1/1	0.94	0.31	42,42,42,42	0
92	OHX	1	3560	7/7	0.94	0.18	60,60,60,60	0
93	MG	5	4031	1/1	0.94	0.26	54,54,54,54	0
93	MG	1	4014	1/1	0.94	0.24	36,36,36,36	0
93	MG	1	3886	1/1	0.94	0.31	38,38,38,38	0
92	OHX	3	206	7/7	0.94	0.14	69,69,69,69	0
92	OHX	3	209	7/7	0.94	0.23	84,84,84,84	0
92	OHX	1	3587	7/7	0.94	0.15	81,81,81,81	0
93	MG	1	3777	1/1	0.94	0.12	31,31,31,31	0
92	OHX	4	217	7/7	0.94	0.31	69,69,69,69	0
92	OHX	5	3638	7/7	0.94	0.28	56,56,56,56	0
92	OHX	5	3641	7/7	0.94	0.26	72,72,72,72	0
92	OHX	4	218	7/7	0.94	0.30	67,67,67,67	0
92	OHX	5	3651	7/7	0.94	0.38	48,48,48,48	0
93	MG	1	4027	1/1	0.94	0.09	41,41,41,41	0
92	OHX	4	219	7/7	0.94	0.28	65,65,65,65	0
92	OHX	5	3668	7/7	0.94	0.27	60,60,60,60	0
93	MG	1	3786	1/1	0.94	0.23	33,33,33,33	0
93	MG	N8	201	1/1	0.94	0.14	31,31,31,31	0
93	MG	5	4053	1/1	0.94	0.33	43,43,43,43	0
92	OHX	5	3671	7/7	0.94	0.16	103,103,103,103	0
93	MG	1	4033	1/1	0.94	0.22	34,34,34,34	0
93	MG	5	4056	1/1	0.94	0.14	40,40,40,40	0
92	OHX	5	3681	7/7	0.94	0.27	61,61,61,61	0
92	OHX	5	3683	7/7	0.94	0.40	72,72,72,72	0
93	MG	1	3790	1/1	0.94	0.30	32,32,32,32	0
93	MG	Q2	503	1/1	0.94	0.23	48,48,48,48	0
93	MG	1	3791	1/1	0.94	0.18	35,35,35,35	0
97	SPS	p	101	23/23	0.94	0.13	33,34,45,47	0
93	MG	1	3792	1/1	0.94	0.22	38,38,38,38	0
93	MG	5	4064	1/1	0.94	0.52	31,31,31,31	0
92	OHX	1	3723	7/7	0.95	0.29	65,65,65,65	0
92	OHX	1	3578	7/7	0.95	0.31	59,59,59,59	0
92	OHX	2	1941	7/7	0.95	0.26	93,93,93,93	0
92	OHX	6	2046	7/7	0.95	0.26	93,93,93,93	0
92	OHX	2	2012	7/7	0.95	0.19	108,108,108,108	0
93	MG	5	4041	1/1	0.95	0.14	41,41,41,41	0
93	MG	5	4042	1/1	0.95	0.10	35,35,35,35	0
92	OHX	2	1982	7/7	0.95	0.22	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	1	3729	7/7	0.95	0.13	60,60,60,60	0
92	OHX	2	1984	7/7	0.95	0.22	83,83,83,83	0
92	OHX	2	1985	7/7	0.95	0.25	98,98,98,98	0
92	OHX	2	2043	7/7	0.95	0.30	85,85,85,85	0
92	OHX	6	2054	7/7	0.95	0.24	89,89,89,89	0
93	MG	5	3854	1/1	0.95	0.30	53,53,53,53	0
92	OHX	1	3603	7/7	0.95	0.31	62,62,62,62	0
92	OHX	6	2056	7/7	0.95	0.16	99,99,99,99	0
92	OHX	4	213	7/7	0.95	0.21	72,72,72,72	0
92	OHX	6	2058	7/7	0.95	0.21	100,100,100,100	0
92	OHX	2	2016	7/7	0.95	0.28	84,84,84,84	0
92	OHX	2	1958	7/7	0.95	0.15	109,109,109,109	0
93	MG	5	4058	1/1	0.95	0.27	47,47,47,47	0
92	OHX	2	2018	7/7	0.95	0.29	84,84,84,84	0
92	OHX	2	1918	7/7	0.95	0.11	83,83,83,83	0
92	OHX	4	221	7/7	0.95	0.31	61,61,61,61	0
93	MG	1	4100	1/1	0.95	0.15	37,37,37,37	0
92	OHX	1	3620	7/7	0.95	0.22	70,70,70,70	0
92	OHX	2	1993	7/7	0.95	0.22	96,96,96,96	0
92	OHX	5	3443	7/7	0.95	0.14	51,51,51,51	0
93	MG	5	4066	1/1	0.95	0.18	42,42,42,42	0
93	MG	1	3801	1/1	0.95	0.16	37,37,37,37	0
92	OHX	5	3462	7/7	0.95	0.13	48,48,48,48	0
93	MG	1	3945	1/1	0.95	0.11	39,39,39,39	0
92	OHX	1	3626	7/7	0.95	0.21	73,73,73,73	0
92	OHX	2	1960	7/7	0.95	0.21	100,100,100,100	0
92	OHX	6	1937	7/7	0.95	0.14	81,81,81,81	0
92	OHX	6	1939	7/7	0.95	0.12	102,102,102,102	0
92	OHX	5	3524	7/7	0.95	0.12	75,75,75,75	0
93	MG	1	4113	1/1	0.95	0.07	39,39,39,39	0
92	OHX	5	3534	7/7	0.95	0.17	53,53,53,53	0
93	MG	5	4078	1/1	0.95	0.16	32,32,32,32	0
93	MG	6	2149	1/1	0.95	0.05	73,73,73,73	0
92	OHX	5	3535	7/7	0.95	0.16	65,65,65,65	0
92	OHX	5	3536	7/7	0.95	0.20	73,73,73,73	0
92	OHX	5	3542	7/7	0.95	0.21	53,53,53,53	0
93	MG	5	4083	1/1	0.95	0.22	35,35,35,35	0
92	OHX	1	3633	7/7	0.95	0.24	66,66,66,66	0
93	MG	5	3887	1/1	0.95	0.16	36,36,36,36	0
92	OHX	5	3570	7/7	0.95	0.27	61,61,61,61	0
93	MG	1	4120	1/1	0.95	0.19	38,38,38,38	0
93	MG	1	3816	1/1	0.95	0.17	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	5	3577	7/7	0.95	0.32	50,50,50,50	0
92	OHX	5	3579	7/7	0.95	0.34	53,53,53,53	0
92	OHX	6	1953	7/7	0.95	0.13	109,109,109,109	0
92	OHX	5	3598	7/7	0.95	0.24	68,68,68,68	0
93	MG	5	3896	1/1	0.95	0.45	44,44,44,44	0
92	OHX	5	3600	7/7	0.95	0.26	44,44,44,44	0
93	MG	1	4127	1/1	0.95	0.28	41,41,41,41	0
93	MG	1	4128	1/1	0.95	0.11	37,37,37,37	0
92	OHX	6	1954	7/7	0.95	0.10	116,116,116,116	0
92	OHX	5	3613	7/7	0.95	0.18	71,71,71,71	0
92	OHX	5	3616	7/7	0.95	0.30	63,63,63,63	0
92	OHX	1	3635	7/7	0.95	0.30	59,59,59,59	0
92	OHX	6	1960	7/7	0.95	0.16	77,77,77,77	0
92	OHX	2	1968	7/7	0.95	0.30	86,86,86,86	0
92	OHX	5	3625	7/7	0.95	0.26	79,79,79,79	0
92	OHX	1	3644	7/7	0.95	0.31	61,61,61,61	0
93	MG	1	3974	1/1	0.95	0.29	35,35,35,35	0
93	MG	6	2174	1/1	0.95	0.16	60,60,60,60	0
93	MG	1	3976	1/1	0.95	0.24	36,36,36,36	0
93	MG	5	4113	1/1	0.95	0.38	35,35,35,35	0
93	MG	6	2176	1/1	0.95	0.27	58,58,58,58	0
92	OHX	2	1970	7/7	0.95	0.28	98,98,98,98	0
92	OHX	S8	301	7/7	0.95	0.21	96,96,96,96	0
92	OHX	6	1974	7/7	0.95	0.20	106,106,106,106	0
92	OHX	6	1975	7/7	0.95	0.14	93,93,93,93	0
92	OHX	1	3659	7/7	0.95	0.31	70,70,70,70	0
92	OHX	5	3643	7/7	0.95	0.26	48,48,48,48	0
92	OHX	5	3644	7/7	0.95	0.32	53,53,53,53	0
92	OHX	5	3645	7/7	0.95	0.31	56,56,56,56	0
93	MG	1	3985	1/1	0.95	0.14	42,42,42,42	0
93	MG	1	3986	1/1	0.95	0.26	43,43,43,43	0
93	MG	5	4130	1/1	0.95	0.33	32,32,32,32	0
92	OHX	5	3646	7/7	0.95	0.34	63,63,63,63	0
92	OHX	2	1997	7/7	0.95	0.19	96,96,96,96	0
92	OHX	5	3648	7/7	0.95	0.32	50,50,50,50	0
93	MG	5	3926	1/1	0.95	0.43	32,32,32,32	0
93	MG	5	4135	1/1	0.95	0.33	38,38,38,38	0
92	OHX	C3	201	7/7	0.95	0.17	96,96,96,96	0
92	OHX	5	3659	7/7	0.95	0.30	70,70,70,70	0
93	MG	L2	301	1/1	0.95	0.18	42,42,42,42	0
92	OHX	5	3660	7/7	0.95	0.34	58,58,58,58	0
92	OHX	2	1971	7/7	0.95	0.15	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	5	4146	1/1	0.95	0.06	37,37,37,37	0
92	OHX	2	1972	7/7	0.95	0.25	105,105,105,105	0
93	MG	L4	404	1/1	0.95	0.10	33,33,33,33	0
92	OHX	6	1993	7/7	0.95	0.15	99,99,99,99	0
93	MG	L7	301	1/1	0.95	0.19	37,37,37,37	0
92	OHX	5	3678	7/7	0.95	0.34	55,55,55,55	0
93	MG	5	3753	1/1	0.95	0.21	43,43,43,43	0
92	OHX	5	3679	7/7	0.95	0.30	67,67,67,67	0
92	OHX	1	3674	7/7	0.95	0.30	61,61,61,61	0
92	OHX	6	1998	7/7	0.95	0.31	65,65,65,65	0
93	MG	M7	204	1/1	0.95	0.34	38,38,38,38	0
93	MG	5	4160	1/1	0.95	0.23	44,44,44,44	0
93	MG	1	4003	1/1	0.95	0.27	39,39,39,39	0
92	OHX	6	1999	7/7	0.95	0.26	75,75,75,75	0
93	MG	1	4005	1/1	0.95	0.23	45,45,45,45	0
92	OHX	1	3678	7/7	0.95	0.25	84,84,84,84	0
92	OHX	6	2002	7/7	0.95	0.26	71,71,71,71	0
92	OHX	5	3695	7/7	0.95	0.20	92,92,92,92	0
92	OHX	5	3698	7/7	0.95	0.24	70,70,70,70	0
92	OHX	2	1926	7/7	0.95	0.14	91,91,91,91	0
93	MG	1	4011	1/1	0.95	0.07	50,50,50,50	0
92	OHX	6	2004	7/7	0.95	0.21	84,84,84,84	0
92	OHX	6	2007	7/7	0.95	0.33	82,82,82,82	0
92	OHX	5	3705	7/7	0.95	0.38	54,54,54,54	0
92	OHX	6	2008	7/7	0.95	0.22	100,100,100,100	0
93	MG	5	3773	1/1	0.95	0.16	33,33,33,33	0
93	MG	5	4177	1/1	0.95	0.49	35,35,35,35	0
92	OHX	2	1946	7/7	0.95	0.14	99,99,99,99	0
92	OHX	6	2013	7/7	0.95	0.25	72,72,72,72	0
93	MG	5	3965	1/1	0.95	0.20	35,35,35,35	0
93	MG	1	4018	1/1	0.95	0.25	36,36,36,36	0
93	MG	2	2142	1/1	0.95	0.10	94,94,94,94	0
92	OHX	5	3710	7/7	0.95	0.19	89,89,89,89	0
93	MG	7	218	1/1	0.95	0.21	33,33,33,33	0
92	OHX	5	3713	7/7	0.95	0.17	39,39,39,39	0
92	OHX	5	3714	7/7	0.95	0.21	95,95,95,95	0
92	OHX	5	3715	7/7	0.95	0.30	59,59,59,59	0
92	OHX	1	3464	7/7	0.95	0.13	66,66,66,66	0
92	OHX	5	3717	7/7	0.95	0.39	48,48,48,48	0
93	MG	5	3974	1/1	0.95	0.08	38,38,38,38	0
92	OHX	6	2016	7/7	0.95	0.23	95,95,95,95	0
92	OHX	2	1932	7/7	0.95	0.21	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	5	3722	7/7	0.95	0.28	62,62,62,62	0
92	OHX	1	3694	7/7	0.95	0.27	73,73,73,73	0
92	OHX	1	3488	7/7	0.95	0.19	47,47,47,47	0
92	OHX	5	3727	7/7	0.95	0.25	71,71,71,71	0
92	OHX	5	3729	7/7	0.95	0.23	74,74,74,74	0
92	OHX	2	1934	7/7	0.95	0.25	94,94,94,94	0
92	OHX	5	3733	7/7	0.95	0.19	91,91,91,91	0
92	OHX	5	3735	7/7	0.95	0.32	81,81,81,81	0
93	MG	1	3885	1/1	0.95	0.16	53,53,53,53	0
92	OHX	5	3737	7/7	0.95	0.12	56,56,56,56	0
92	OHX	2	2006	7/7	0.95	0.23	98,98,98,98	0
92	OHX	5	3739	7/7	0.95	0.33	55,55,55,55	0
92	OHX	5	3741	7/7	0.95	0.34	56,56,56,56	0
92	OHX	5	3742	7/7	0.95	0.29	70,70,70,70	0
93	MG	5	3803	1/1	0.95	0.23	34,34,34,34	0
93	MG	1	4045	1/1	0.95	0.18	40,40,40,40	0
92	OHX	5	3746	7/7	0.95	0.25	61,61,61,61	0
92	OHX	2	1954	7/7	0.95	0.13	89,89,89,89	0
92	OHX	7	208	7/7	0.95	0.16	59,59,59,59	0
93	MG	17	301	1/1	0.95	0.33	34,34,34,34	0
92	OHX	2	2033	7/7	0.95	0.18	123,123,123,123	0
93	MG	1	4051	1/1	0.95	0.20	33,33,33,33	0
92	OHX	7	212	7/7	0.95	0.26	69,69,69,69	0
92	OHX	8	211	7/7	0.95	0.26	60,60,60,60	0
93	MG	1	3754	1/1	0.95	0.21	35,35,35,35	0
92	OHX	1	3704	7/7	0.95	0.36	49,49,49,49	0
92	OHX	8	214	7/7	0.95	0.32	59,59,59,59	0
92	OHX	1	3550	7/7	0.95	0.18	75,75,75,75	0
92	OHX	8	216	7/7	0.95	0.33	60,60,60,60	0
93	MG	5	4012	1/1	0.95	0.13	35,35,35,35	0
92	OHX	1	3551	7/7	0.95	0.20	60,60,60,60	0
93	MG	5	4014	1/1	0.95	0.33	42,42,42,42	0
92	OHX	15	302	7/7	0.95	0.29	70,70,70,70	0
93	MG	6	2100	1/1	0.95	0.46	45,45,45,45	0
92	OHX	19	201	7/7	0.95	0.23	60,60,60,60	0
92	OHX	6	2030	7/7	0.95	0.29	74,74,74,74	0
92	OHX	2	2034	7/7	0.95	0.24	87,87,87,87	0
93	MG	n8	203	1/1	0.95	0.31	34,34,34,34	0
93	MG	1	4066	1/1	0.95	0.38	38,38,38,38	0
92	OHX	1	3716	7/7	0.95	0.34	65,65,65,65	0
93	MG	o3	203	1/1	0.95	0.29	36,36,36,36	0
93	MG	5	4022	1/1	0.95	0.21	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	q1	101	1/1	0.95	0.31	58,58,58,58	0
92	OHX	6	2034	7/7	0.95	0.20	99,99,99,99	0
92	OHX	2	2035	7/7	0.95	0.20	107,107,107,107	0
93	MG	p	104	1/1	0.95	0.32	40,40,40,40	0
93	MG	1	4070	1/1	0.95	0.26	35,35,35,35	0
92	OHX	1	3719	7/7	0.95	0.29	65,65,65,65	0
92	OHX	2	2009	7/7	0.95	0.18	117,117,117,117	0
93	MG	5	4028	1/1	0.95	0.11	36,36,36,36	0
93	MG	5	3836	1/1	0.95	0.12	37,37,37,37	0
96	LEU	1	3402	8/9	0.95	0.17	39,40,40,40	0
92	OHX	1	3568	7/7	0.95	0.30	63,63,63,63	0
92	OHX	6	2039	7/7	0.95	0.23	94,94,94,94	0
93	MG	5	3839	1/1	0.95	0.14	35,35,35,35	0
92	OHX	6	2040	7/7	0.95	0.31	72,72,72,72	0
92	OHX	1	3575	7/7	0.95	0.29	47,47,47,47	0
92	OHX	2	2001	7/7	0.96	0.20	99,99,99,99	0
92	OHX	1	3588	7/7	0.96	0.27	45,45,45,45	0
92	OHX	5	3655	7/7	0.96	0.18	71,71,71,71	0
93	MG	1	4042	1/1	0.96	0.26	43,43,43,43	0
92	OHX	5	3657	7/7	0.96	0.26	50,50,50,50	0
92	OHX	5	3658	7/7	0.96	0.30	58,58,58,58	0
93	MG	5	4043	1/1	0.96	0.24	41,41,41,41	0
92	OHX	6	2005	7/7	0.96	0.18	79,79,79,79	0
92	OHX	6	2006	7/7	0.96	0.21	72,72,72,72	0
93	MG	1	4047	1/1	0.96	0.26	43,43,43,43	0
92	OHX	5	3661	7/7	0.96	0.39	51,51,51,51	0
92	OHX	5	3663	7/7	0.96	0.27	71,71,71,71	0
92	OHX	2	1952	7/7	0.96	0.18	104,104,104,104	0
92	OHX	5	3666	7/7	0.96	0.23	51,51,51,51	0
92	OHX	5	3667	7/7	0.96	0.18	72,72,72,72	0
92	OHX	1	3592	7/7	0.96	0.15	86,86,86,86	0
92	OHX	5	3670	7/7	0.96	0.32	40,40,40,40	0
92	OHX	2	1953	7/7	0.96	0.23	83,83,83,83	0
92	OHX	5	3672	7/7	0.96	0.23	76,76,76,76	0
92	OHX	5	3675	7/7	0.96	0.30	59,59,59,59	0
92	OHX	6	2012	7/7	0.96	0.29	76,76,76,76	0
92	OHX	1	3701	7/7	0.96	0.31	38,38,38,38	0
92	OHX	5	3680	7/7	0.96	0.35	45,45,45,45	0
92	OHX	1	3702	7/7	0.96	0.37	49,49,49,49	0
92	OHX	2	1935	7/7	0.96	0.12	82,82,82,82	0
92	OHX	2	2005	7/7	0.96	0.24	84,84,84,84	0
93	MG	1	4065	1/1	0.96	0.39	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	1	3705	7/7	0.96	0.27	74,74,74,74	0
92	OHX	5	3688	7/7	0.96	0.37	59,59,59,59	0
92	OHX	1	3597	7/7	0.96	0.15	78,78,78,78	0
92	OHX	5	3692	7/7	0.96	0.22	70,70,70,70	0
92	OHX	6	2020	7/7	0.96	0.22	94,94,94,94	0
92	OHX	5	3697	7/7	0.96	0.37	59,59,59,59	0
92	OHX	1	3598	7/7	0.96	0.35	50,50,50,50	0
93	MG	5	4072	1/1	0.96	0.18	37,37,37,37	0
92	OHX	1	3712	7/7	0.96	0.33	58,58,58,58	0
92	OHX	1	3713	7/7	0.96	0.32	72,72,72,72	0
92	OHX	1	3714	7/7	0.96	0.21	82,82,82,82	0
92	OHX	5	3704	7/7	0.96	0.35	59,59,59,59	0
92	OHX	2	1977	7/7	0.96	0.17	99,99,99,99	0
92	OHX	1	3602	7/7	0.96	0.22	74,74,74,74	0
92	OHX	1	3717	7/7	0.96	0.30	64,64,64,64	0
92	OHX	5	3708	7/7	0.96	0.29	68,68,68,68	0
92	OHX	2	1955	7/7	0.96	0.17	96,96,96,96	0
93	MG	1	3905	1/1	0.96	0.26	35,35,35,35	0
92	OHX	2	2008	7/7	0.96	0.12	106,106,106,106	0
92	OHX	1	3607	7/7	0.96	0.21	63,63,63,63	0
92	OHX	6	2033	7/7	0.96	0.32	78,78,78,78	0
92	OHX	1	3608	7/7	0.96	0.20	71,71,71,71	0
92	OHX	1	3609	7/7	0.96	0.28	66,66,66,66	0
92	OHX	2	1956	7/7	0.96	0.21	92,92,92,92	0
92	OHX	1	3446	7/7	0.96	0.15	53,53,53,53	0
92	OHX	5	3719	7/7	0.96	0.30	67,67,67,67	0
92	OHX	2	2010	7/7	0.96	0.21	85,85,85,85	0
93	MG	1	3917	1/1	0.96	0.48	32,32,32,32	0
92	OHX	1	3617	7/7	0.96	0.29	68,68,68,68	0
92	OHX	5	3723	7/7	0.96	0.33	36,36,36,36	0
92	OHX	2	1939	7/7	0.96	0.12	92,92,92,92	0
93	MG	5	3895	1/1	0.96	0.17	48,48,48,48	0
92	OHX	5	3725	7/7	0.96	0.21	90,90,90,90	0
92	OHX	6	2041	7/7	0.96	0.30	79,79,79,79	0
92	OHX	1	3728	7/7	0.96	0.34	55,55,55,55	0
93	MG	5	4103	1/1	0.96	0.09	38,38,38,38	0
92	OHX	5	3728	7/7	0.96	0.34	49,49,49,49	0
92	OHX	1	3624	7/7	0.96	0.17	69,69,69,69	0
93	MG	1	4104	1/1	0.96	0.40	54,54,54,54	0
92	OHX	1	3484	7/7	0.96	0.10	78,78,78,78	0
92	OHX	5	3731	7/7	0.96	0.33	65,65,65,65	0
93	MG	5	4109	1/1	0.96	0.08	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	5	3904	1/1	0.96	0.41	32,32,32,32	0
92	OHX	5	3732	7/7	0.96	0.22	74,74,74,74	0
92	OHX	3	203	7/7	0.96	0.15	59,59,59,59	0
92	OHX	5	3734	7/7	0.96	0.30	70,70,70,70	0
92	OHX	2	1983	7/7	0.96	0.21	81,81,81,81	0
92	OHX	3	207	7/7	0.96	0.14	68,68,68,68	0
92	OHX	3	208	7/7	0.96	0.17	81,81,81,81	0
93	MG	5	4117	1/1	0.96	0.05	43,43,43,43	0
93	MG	5	4118	1/1	0.96	0.17	35,35,35,35	0
92	OHX	2	1906	7/7	0.96	0.11	89,89,89,89	0
92	OHX	1	3497	7/7	0.96	0.13	74,74,74,74	0
92	OHX	4	209	7/7	0.96	0.28	56,56,56,56	0
92	OHX	5	3743	7/7	0.96	0.28	72,72,72,72	0
92	OHX	5	3744	7/7	0.96	0.18	59,59,59,59	0
92	OHX	6	2052	7/7	0.96	0.14	65,65,65,65	0
92	OHX	5	3747	7/7	0.96	0.11	92,92,92,92	0
92	OHX	2	1942	7/7	0.96	0.25	84,84,84,84	0
92	OHX	1	3636	7/7	0.96	0.17	75,75,75,75	0
92	OHX	1	3527	7/7	0.96	0.31	52,52,52,52	0
92	OHX	1	3641	7/7	0.96	0.23	64,64,64,64	0
92	OHX	8	209	7/7	0.96	0.20	78,78,78,78	0
93	MG	1	3778	1/1	0.96	0.24	37,37,37,37	0
92	OHX	1	3643	7/7	0.96	0.28	48,48,48,48	0
92	OHX	8	212	7/7	0.96	0.26	76,76,76,76	0
92	OHX	2	1930	7/7	0.96	0.10	95,95,95,95	0
92	OHX	L4	401	7/7	0.96	0.27	54,54,54,54	0
92	OHX	L6	202	7/7	0.96	0.31	62,62,62,62	0
93	MG	5	4144	1/1	0.96	0.10	33,33,33,33	0
92	OHX	M0	301	7/7	0.96	0.24	55,55,55,55	0
92	OHX	M8	201	7/7	0.96	0.29	65,65,65,65	0
93	MG	5	3933	1/1	0.96	0.37	31,31,31,31	0
92	OHX	l5	301	7/7	0.96	0.14	77,77,77,77	0
92	OHX	1	3536	7/7	0.96	0.27	61,61,61,61	0
92	OHX	c8	201	7/7	0.96	0.15	96,96,96,96	0
93	MG	5	4152	1/1	0.96	0.15	40,40,40,40	0
92	OHX	m0	303	7/7	0.96	0.38	53,53,53,53	0
92	OHX	1	3541	7/7	0.96	0.20	60,60,60,60	0
92	OHX	O9	101	7/7	0.96	0.37	49,49,49,49	0
92	OHX	o7	503	7/7	0.96	0.14	59,59,59,59	0
92	OHX	1	3647	7/7	0.96	0.37	55,55,55,55	0
92	OHX	1	3650	7/7	0.96	0.21	57,57,57,57	0
92	OHX	6	1932	7/7	0.96	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
93	MG	1	3796	1/1	0.96	0.23	35,35,35,35	0
93	MG	1	3965	1/1	0.96	0.36	44,44,44,44	0
92	OHX	5	3476	7/7	0.96	0.13	56,56,56,56	0
92	OHX	5	3490	7/7	0.96	0.15	64,64,64,64	0
92	OHX	5	3497	7/7	0.96	0.19	62,62,62,62	0
92	OHX	1	3652	7/7	0.96	0.28	57,57,57,57	0
93	MG	4	233	1/1	0.96	0.08	41,41,41,41	0
93	MG	5	3952	1/1	0.96	0.32	41,41,41,41	0
92	OHX	1	3653	7/7	0.96	0.32	60,60,60,60	0
93	MG	5	4170	1/1	0.96	0.34	42,42,42,42	0
93	MG	1	3972	1/1	0.96	0.10	43,43,43,43	0
92	OHX	1	3654	7/7	0.96	0.29	55,55,55,55	0
93	MG	4	237	1/1	0.96	0.09	43,43,43,43	0
92	OHX	6	1951	7/7	0.96	0.11	119,119,119,119	0
92	OHX	5	3526	7/7	0.96	0.27	47,47,47,47	0
92	OHX	5	3527	7/7	0.96	0.23	46,46,46,46	0
93	MG	L2	302	1/1	0.96	0.21	42,42,42,42	0
93	MG	5	3763	1/1	0.96	0.22	34,34,34,34	0
92	OHX	5	3530	7/7	0.96	0.26	55,55,55,55	0
93	MG	L3	404	1/1	0.96	0.11	41,41,41,41	0
92	OHX	1	3657	7/7	0.96	0.30	65,65,65,65	0
93	MG	7	216	1/1	0.96	0.20	36,36,36,36	0
92	OHX	1	3658	7/7	0.96	0.25	73,73,73,73	0
93	MG	1	3810	1/1	0.96	0.22	40,40,40,40	0
92	OHX	6	1958	7/7	0.96	0.17	89,89,89,89	0
92	OHX	5	3540	7/7	0.96	0.10	93,93,93,93	0
92	OHX	5	3541	7/7	0.96	0.22	57,57,57,57	0
92	OHX	1	3542	7/7	0.96	0.23	69,69,69,69	0
93	MG	7	223	1/1	0.96	0.17	35,35,35,35	0
93	MG	M5	303	1/1	0.96	0.15	37,37,37,37	0
92	OHX	5	3547	7/7	0.96	0.25	61,61,61,61	0
92	OHX	5	3549	7/7	0.96	0.14	79,79,79,79	0
93	MG	1	3988	1/1	0.96	0.35	59,59,59,59	0
92	OHX	1	3660	7/7	0.96	0.23	77,77,77,77	0
92	OHX	5	3555	7/7	0.96	0.32	55,55,55,55	0
93	MG	1	3820	1/1	0.96	0.17	49,49,49,49	0
92	OHX	5	3559	7/7	0.96	0.14	79,79,79,79	0
93	MG	5	3981	1/1	0.96	0.22	35,35,35,35	0
92	OHX	5	3562	7/7	0.96	0.18	70,70,70,70	0
92	OHX	5	3568	7/7	0.96	0.17	62,62,62,62	0
93	MG	5	3984	1/1	0.96	0.05	49,49,49,49	0
92	OHX	5	3569	7/7	0.96	0.22	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	2	1961	7/7	0.96	0.20	103,103,103,103	0
93	MG	5	3987	1/1	0.96	0.10	38,38,38,38	0
92	OHX	6	1966	7/7	0.96	0.26	69,69,69,69	0
92	OHX	1	3665	7/7	0.96	0.23	87,87,87,87	0
93	MG	N8	206	1/1	0.96	0.09	37,37,37,37	0
92	OHX	5	3580	7/7	0.96	0.35	55,55,55,55	0
93	MG	5	3992	1/1	0.96	0.31	40,40,40,40	0
93	MG	5	3993	1/1	0.96	0.19	41,41,41,41	0
92	OHX	5	3588	7/7	0.96	0.25	46,46,46,46	0
93	MG	1	4002	1/1	0.96	0.24	41,41,41,41	0
92	OHX	5	3593	7/7	0.96	0.21	74,74,74,74	0
92	OHX	5	3594	7/7	0.96	0.17	76,76,76,76	0
92	OHX	6	1968	7/7	0.96	0.29	74,74,74,74	0
93	MG	5	3796	1/1	0.96	0.41	42,42,42,42	0
92	OHX	5	3597	7/7	0.96	0.31	51,51,51,51	0
93	MG	1	3835	1/1	0.96	0.43	32,32,32,32	0
92	OHX	2	1963	7/7	0.96	0.24	73,73,73,73	0
92	OHX	5	3599	7/7	0.96	0.14	83,83,83,83	0
92	OHX	1	3667	7/7	0.96	0.27	92,92,92,92	0
92	OHX	1	3670	7/7	0.96	0.32	65,65,65,65	0
92	OHX	5	3604	7/7	0.96	0.26	46,46,46,46	0
92	OHX	5	3606	7/7	0.96	0.30	59,59,59,59	0
92	OHX	2	1964	7/7	0.96	0.14	97,97,97,97	0
93	MG	5	3806	1/1	0.96	0.25	50,50,50,50	0
92	OHX	6	1977	7/7	0.96	0.19	97,97,97,97	0
92	OHX	6	1978	7/7	0.96	0.23	90,90,90,90	0
92	OHX	5	3618	7/7	0.96	0.28	68,68,68,68	0
92	OHX	2	1965	7/7	0.96	0.16	84,84,84,84	0
92	OHX	5	3621	7/7	0.96	0.16	73,73,73,73	0
93	MG	o2	201	1/1	0.96	0.14	32,32,32,32	0
92	OHX	6	1984	7/7	0.96	0.31	87,87,87,87	0
92	OHX	2	1931	7/7	0.96	0.22	95,95,95,95	0
92	OHX	5	3626	7/7	0.96	0.16	84,84,84,84	0
92	OHX	5	3627	7/7	0.96	0.16	60,60,60,60	0
92	OHX	1	3675	7/7	0.96	0.27	64,64,64,64	0
92	OHX	5	3631	7/7	0.96	0.33	51,51,51,51	0
92	OHX	2	1903	7/7	0.96	0.12	95,95,95,95	0
92	OHX	2	1933	7/7	0.96	0.12	91,91,91,91	0
92	OHX	6	1992	7/7	0.96	0.21	88,88,88,88	0
92	OHX	1	3680	7/7	0.96	0.23	76,76,76,76	0
92	OHX	6	1994	7/7	0.96	0.22	98,98,98,98	0
94	ZN	e1	501	1/1	0.96	0.07	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	1	3681	7/7	0.96	0.20	84,84,84,84	0
93	MG	5	3824	1/1	0.96	0.16	45,45,45,45	0
92	OHX	2	1948	7/7	0.96	0.19	80,80,80,80	0
92	OHX	2	1921	7/7	0.96	0.19	97,97,97,97	0
92	OHX	1	3686	7/7	0.96	0.27	67,67,67,67	0
93	MG	5	3830	1/1	0.96	0.23	35,35,35,35	0
93	MG	1	3864	1/1	0.96	0.33	49,49,49,49	0
92	OHX	1	3583	7/7	0.96	0.29	78,78,78,78	0
92	OHX	1	3468	7/7	0.97	0.12	56,56,56,56	0
92	OHX	1	3687	7/7	0.97	0.32	58,58,58,58	0
92	OHX	6	1995	7/7	0.97	0.27	79,79,79,79	0
92	OHX	6	1996	7/7	0.97	0.24	78,78,78,78	0
92	OHX	1	3688	7/7	0.97	0.27	65,65,65,65	0
92	OHX	1	3691	7/7	0.97	0.24	80,80,80,80	0
92	OHX	5	3654	7/7	0.97	0.33	62,62,62,62	0
92	OHX	1	3469	7/7	0.97	0.10	82,82,82,82	0
92	OHX	5	3656	7/7	0.97	0.27	64,64,64,64	0
92	OHX	1	3589	7/7	0.97	0.32	53,53,53,53	0
93	MG	5	3783	1/1	0.97	0.25	33,33,33,33	0
92	OHX	1	3471	7/7	0.97	0.11	62,62,62,62	0
93	MG	4	228	1/1	0.97	0.14	46,46,46,46	0
92	OHX	1	3696	7/7	0.97	0.16	46,46,46,46	0
92	OHX	1	3591	7/7	0.97	0.23	65,65,65,65	0
92	OHX	1	3698	7/7	0.97	0.29	60,60,60,60	0
92	OHX	1	3475	7/7	0.97	0.11	62,62,62,62	0
92	OHX	1	3476	7/7	0.97	0.15	59,59,59,59	0
92	OHX	5	3665	7/7	0.97	0.24	55,55,55,55	0
92	OHX	1	3479	7/7	0.97	0.10	67,67,67,67	0
92	OHX	2	1989	7/7	0.97	0.17	93,93,93,93	0
92	OHX	6	2010	7/7	0.97	0.20	91,91,91,91	0
92	OHX	5	3669	7/7	0.97	0.31	50,50,50,50	0
92	OHX	6	2011	7/7	0.97	0.29	72,72,72,72	0
92	OHX	1	3596	7/7	0.97	0.29	56,56,56,56	0
92	OHX	2	1990	7/7	0.97	0.18	99,99,99,99	0
92	OHX	5	3673	7/7	0.97	0.34	56,56,56,56	0
92	OHX	6	2014	7/7	0.97	0.27	64,64,64,64	0
92	OHX	5	3677	7/7	0.97	0.28	60,60,60,60	0
92	OHX	1	3485	7/7	0.97	0.13	69,69,69,69	0
92	OHX	1	3706	7/7	0.97	0.09	97,97,97,97	0
92	OHX	1	3599	7/7	0.97	0.33	58,58,58,58	0
93	MG	5	4040	1/1	0.97	0.06	54,54,54,54	0
92	OHX	1	3487	7/7	0.97	0.13	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	1	3710	7/7	0.97	0.27	56,56,56,56	0
92	OHX	1	3711	7/7	0.97	0.31	58,58,58,58	0
92	OHX	5	3686	7/7	0.97	0.34	58,58,58,58	0
92	OHX	6	2021	7/7	0.97	0.24	84,84,84,84	0
93	MG	5	4046	1/1	0.97	0.11	40,40,40,40	0
92	OHX	2	1917	7/7	0.97	0.15	83,83,83,83	0
92	OHX	1	3491	7/7	0.97	0.11	66,66,66,66	0
92	OHX	1	3492	7/7	0.97	0.22	61,61,61,61	0
92	OHX	5	3693	7/7	0.97	0.24	63,63,63,63	0
92	OHX	5	3694	7/7	0.97	0.27	55,55,55,55	0
92	OHX	2	1992	7/7	0.97	0.16	95,95,95,95	0
92	OHX	5	3696	7/7	0.97	0.26	70,70,70,70	0
92	OHX	2	1927	7/7	0.97	0.14	85,85,85,85	0
92	OHX	1	3498	7/7	0.97	0.14	50,50,50,50	0
93	MG	N6	202	1/1	0.97	0.28	37,37,37,37	0
92	OHX	6	2028	7/7	0.97	0.28	62,62,62,62	0
93	MG	1	3968	1/1	0.97	0.18	42,42,42,42	0
92	OHX	1	3610	7/7	0.97	0.26	64,64,64,64	0
93	MG	N8	204	1/1	0.97	0.13	44,44,44,44	0
93	MG	N8	205	1/1	0.97	0.28	35,35,35,35	0
93	MG	1	3763	1/1	0.97	0.06	50,50,50,50	0
93	MG	5	3827	1/1	0.97	0.49	31,31,31,31	0
92	OHX	5	3702	7/7	0.97	0.24	52,52,52,52	0
93	MG	5	3829	1/1	0.97	0.23	41,41,41,41	0
92	OHX	1	3500	7/7	0.97	0.14	62,62,62,62	0
92	OHX	2	1979	7/7	0.97	0.22	82,82,82,82	0
92	OHX	1	3503	7/7	0.97	0.13	75,75,75,75	0
93	MG	1	3975	1/1	0.97	0.17	53,53,53,53	0
93	MG	5	3834	1/1	0.97	0.21	41,41,41,41	0
92	OHX	1	3615	7/7	0.97	0.19	64,64,64,64	0
92	OHX	1	3508	7/7	0.97	0.11	67,67,67,67	0
92	OHX	1	3618	7/7	0.97	0.27	59,59,59,59	0
92	OHX	1	3509	7/7	0.97	0.15	60,60,60,60	0
92	OHX	1	3623	7/7	0.97	0.17	81,81,81,81	0
93	MG	5	3840	1/1	0.97	0.11	35,35,35,35	0
92	OHX	5	3711	7/7	0.97	0.32	48,48,48,48	0
92	OHX	5	3712	7/7	0.97	0.25	53,53,53,53	0
93	MG	1	3775	1/1	0.97	0.06	44,44,44,44	0
92	OHX	1	3517	7/7	0.97	0.17	57,57,57,57	0
92	OHX	1	3522	7/7	0.97	0.17	58,58,58,58	0
92	OHX	1	3523	7/7	0.97	0.26	59,59,59,59	0
92	OHX	1	3524	7/7	0.97	0.26	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	1	3631	7/7	0.97	0.22	88,88,88,88	0
92	OHX	3	205	7/7	0.97	0.14	69,69,69,69	0
92	OHX	1	3632	7/7	0.97	0.22	72,72,72,72	0
93	MG	5	4087	1/1	0.97	0.11	41,41,41,41	0
93	MG	1	3991	1/1	0.97	0.27	45,45,45,45	0
92	OHX	2	2037	7/7	0.97	0.20	98,98,98,98	0
92	OHX	1	3533	7/7	0.97	0.22	55,55,55,55	0
92	OHX	1	3534	7/7	0.97	0.12	70,70,70,70	0
92	OHX	2	1944	7/7	0.97	0.15	83,83,83,83	0
92	OHX	4	208	7/7	0.97	0.20	69,69,69,69	0
92	OHX	1	3638	7/7	0.97	0.28	67,67,67,67	0
92	OHX	4	211	7/7	0.97	0.22	63,63,63,63	0
92	OHX	1	3639	7/7	0.97	0.28	63,63,63,63	0
92	OHX	4	215	7/7	0.97	0.37	48,48,48,48	0
92	OHX	4	216	7/7	0.97	0.27	57,57,57,57	0
92	OHX	1	3640	7/7	0.97	0.23	70,70,70,70	0
92	OHX	2	1981	7/7	0.97	0.17	75,75,75,75	0
92	OHX	1	3537	7/7	0.97	0.22	66,66,66,66	0
92	OHX	1	3540	7/7	0.97	0.20	66,66,66,66	0
92	OHX	2	1911	7/7	0.97	0.09	98,98,98,98	0
93	MG	1	3798	1/1	0.97	0.26	34,34,34,34	0
92	OHX	5	3736	7/7	0.97	0.23	85,85,85,85	0
92	OHX	L3	401	7/7	0.97	0.22	65,65,65,65	0
92	OHX	s8	301	7/7	0.97	0.21	96,96,96,96	0
92	OHX	L3	402	7/7	0.97	0.17	62,62,62,62	0
93	MG	5	3872	1/1	0.97	0.40	31,31,31,31	0
92	OHX	5	3740	7/7	0.97	0.12	59,59,59,59	0
92	OHX	2	1936	7/7	0.97	0.14	102,102,102,102	0
92	OHX	1	3545	7/7	0.97	0.23	68,68,68,68	0
92	OHX	1	3648	7/7	0.97	0.24	65,65,65,65	0
92	OHX	M5	302	7/7	0.97	0.22	61,61,61,61	0
93	MG	5	3879	1/1	0.97	0.36	36,36,36,36	0
92	OHX	M7	201	7/7	0.97	0.29	62,62,62,62	0
92	OHX	2	1908	7/7	0.97	0.09	95,95,95,95	0
93	MG	5	4120	1/1	0.97	0.10	34,34,34,34	0
93	MG	5	3882	1/1	0.97	0.23	30,30,30,30	0
92	OHX	5	3451	7/7	0.97	0.09	63,63,63,63	0
93	MG	5	4124	1/1	0.97	0.13	40,40,40,40	0
92	OHX	7	204	7/7	0.97	0.13	48,48,48,48	0
93	MG	1	4021	1/1	0.97	0.10	83,83,83,83	0
92	OHX	5	3454	7/7	0.97	0.12	58,58,58,58	0
92	OHX	7	209	7/7	0.97	0.24	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	5	3457	7/7	0.97	0.12	57,57,57,57	0
92	OHX	5	3458	7/7	0.97	0.10	64,64,64,64	0
92	OHX	8	203	7/7	0.97	0.18	56,56,56,56	0
92	OHX	8	205	7/7	0.97	0.13	75,75,75,75	0
92	OHX	8	206	7/7	0.97	0.15	57,57,57,57	0
92	OHX	8	208	7/7	0.97	0.17	66,66,66,66	0
92	OHX	5	3460	7/7	0.97	0.11	48,48,48,48	0
93	MG	5	4136	1/1	0.97	0.06	38,38,38,38	0
92	OHX	8	210	7/7	0.97	0.31	57,57,57,57	0
93	MG	5	4138	1/1	0.97	0.07	43,43,43,43	0
92	OHX	2	1925	7/7	0.97	0.12	85,85,85,85	0
92	OHX	5	3468	7/7	0.97	0.10	63,63,63,63	0
93	MG	5	4141	1/1	0.97	0.09	38,38,38,38	0
92	OHX	5	3471	7/7	0.97	0.11	66,66,66,66	0
93	MG	5	4143	1/1	0.97	0.26	32,32,32,32	0
92	OHX	5	3474	7/7	0.97	0.16	47,47,47,47	0
92	OHX	1	3432	7/7	0.97	0.11	55,55,55,55	0
92	OHX	O7	102	7/7	0.97	0.21	52,52,52,52	0
92	OHX	5	3477	7/7	0.97	0.11	56,56,56,56	0
92	OHX	1	3441	7/7	0.97	0.10	55,55,55,55	0
92	OHX	5	3494	7/7	0.97	0.17	57,57,57,57	0
92	OHX	6	1902	7/7	0.97	0.12	91,91,91,91	0
92	OHX	m0	301	7/7	0.97	0.17	68,68,68,68	0
92	OHX	5	3498	7/7	0.97	0.18	50,50,50,50	0
92	OHX	5	3499	7/7	0.97	0.11	72,72,72,72	0
92	OHX	6	1905	7/7	0.97	0.10	73,73,73,73	0
92	OHX	6	1919	7/7	0.97	0.14	74,74,74,74	0
92	OHX	5	3507	7/7	0.97	0.23	61,61,61,61	0
92	OHX	5	3508	7/7	0.97	0.19	63,63,63,63	0
92	OHX	5	3514	7/7	0.97	0.11	85,85,85,85	0
92	OHX	6	1920	7/7	0.97	0.09	95,95,95,95	0
92	OHX	6	1925	7/7	0.97	0.11	76,76,76,76	0
92	OHX	5	3525	7/7	0.97	0.17	58,58,58,58	0
92	OHX	1	3655	7/7	0.97	0.21	74,74,74,74	0
92	OHX	6	1928	7/7	0.97	0.12	105,105,105,105	0
92	OHX	5	3529	7/7	0.97	0.25	42,42,42,42	0
92	OHX	1	3656	7/7	0.97	0.25	50,50,50,50	0
92	OHX	5	3531	7/7	0.97	0.14	84,84,84,84	0
93	MG	1	4059	1/1	0.97	0.06	46,46,46,46	0
92	OHX	1	3553	7/7	0.97	0.23	63,63,63,63	0
92	OHX	6	1933	7/7	0.97	0.11	98,98,98,98	0
92	OHX	6	1935	7/7	0.97	0.15	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	5	3537	7/7	0.97	0.14	73,73,73,73	0
93	MG	5	3927	1/1	0.97	0.43	34,34,34,34	0
93	MG	5	3928	1/1	0.97	0.52	29,29,29,29	0
92	OHX	5	3538	7/7	0.97	0.28	47,47,47,47	0
92	OHX	1	3555	7/7	0.97	0.16	81,81,81,81	0
92	OHX	1	3558	7/7	0.97	0.15	69,69,69,69	0
92	OHX	6	1942	7/7	0.97	0.12	73,73,73,73	0
92	OHX	6	1943	7/7	0.97	0.10	102,102,102,102	0
92	OHX	5	3548	7/7	0.97	0.24	49,49,49,49	0
92	OHX	6	1946	7/7	0.97	0.14	79,79,79,79	0
92	OHX	5	3551	7/7	0.97	0.19	46,46,46,46	0
92	OHX	6	1947	7/7	0.97	0.16	71,71,71,71	0
92	OHX	6	1948	7/7	0.97	0.18	82,82,82,82	0
93	MG	6	2158	1/1	0.97	0.06	54,54,54,54	0
92	OHX	5	3556	7/7	0.97	0.17	83,83,83,83	0
92	OHX	5	3557	7/7	0.97	0.16	78,78,78,78	0
92	OHX	5	3558	7/7	0.97	0.25	59,59,59,59	0
92	OHX	2	1967	7/7	0.97	0.15	85,85,85,85	0
92	OHX	5	3561	7/7	0.97	0.28	60,60,60,60	0
92	OHX	1	3661	7/7	0.97	0.30	50,50,50,50	0
92	OHX	6	1952	7/7	0.97	0.16	80,80,80,80	0
93	MG	1	4081	1/1	0.97	0.06	38,38,38,38	0
92	OHX	1	3662	7/7	0.97	0.22	71,71,71,71	0
92	OHX	1	3453	7/7	0.97	0.11	59,59,59,59	0
92	OHX	5	3572	7/7	0.97	0.21	54,54,54,54	0
93	MG	8	221	1/1	0.97	0.07	47,47,47,47	0
92	OHX	6	1955	7/7	0.97	0.09	108,108,108,108	0
92	OHX	6	1956	7/7	0.97	0.13	79,79,79,79	0
92	OHX	6	1957	7/7	0.97	0.17	72,72,72,72	0
92	OHX	5	3582	7/7	0.97	0.15	71,71,71,71	0
92	OHX	5	3584	7/7	0.97	0.24	58,58,58,58	0
93	MG	5	3958	1/1	0.97	0.10	39,39,39,39	0
93	MG	1	4090	1/1	0.97	0.16	42,42,42,42	0
93	MG	12	301	1/1	0.97	0.35	42,42,42,42	0
93	MG	1	4091	1/1	0.97	0.13	33,33,33,33	0
93	MG	6	2177	1/1	0.97	0.08	94,94,94,94	0
92	OHX	5	3586	7/7	0.97	0.28	47,47,47,47	0
92	OHX	1	3561	7/7	0.97	0.21	64,64,64,64	0
92	OHX	5	3589	7/7	0.97	0.31	47,47,47,47	0
92	OHX	5	3591	7/7	0.97	0.21	62,62,62,62	0
92	OHX	1	3563	7/7	0.97	0.20	70,70,70,70	0
92	OHX	1	3565	7/7	0.97	0.27	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	5	3595	7/7	0.97	0.29	48,48,48,48	0
92	OHX	1	3668	7/7	0.97	0.26	63,63,63,63	0
92	OHX	6	1964	7/7	0.97	0.23	62,62,62,62	0
92	OHX	6	1965	7/7	0.97	0.22	77,77,77,77	0
92	OHX	1	3669	7/7	0.97	0.27	60,60,60,60	0
92	OHX	1	3454	7/7	0.97	0.11	65,65,65,65	0
92	OHX	1	3671	7/7	0.97	0.15	60,60,60,60	0
92	OHX	5	3602	7/7	0.97	0.19	64,64,64,64	0
92	OHX	6	1969	7/7	0.97	0.15	99,99,99,99	0
92	OHX	1	3569	7/7	0.97	0.17	75,75,75,75	0
92	OHX	5	3612	7/7	0.97	0.27	54,54,54,54	0
92	OHX	1	3570	7/7	0.97	0.26	58,58,58,58	0
92	OHX	5	3615	7/7	0.97	0.23	54,54,54,54	0
93	MG	sM	202	1/1	0.97	0.10	45,45,45,45	0
92	OHX	1	3572	7/7	0.97	0.23	60,60,60,60	0
92	OHX	1	3456	7/7	0.97	0.11	73,73,73,73	0
92	OHX	1	3676	7/7	0.97	0.24	67,67,67,67	0
92	OHX	1	3677	7/7	0.97	0.33	54,54,54,54	0
92	OHX	5	3620	7/7	0.97	0.18	76,76,76,76	0
93	MG	n9	102	1/1	0.97	0.49	29,29,29,29	0
93	MG	n9	103	1/1	0.97	0.10	34,34,34,34	0
92	OHX	6	1979	7/7	0.97	0.23	62,62,62,62	0
93	MG	5	3755	1/1	0.97	0.07	34,34,34,34	0
92	OHX	1	3462	7/7	0.97	0.10	80,80,80,80	0
92	OHX	5	3624	7/7	0.97	0.33	53,53,53,53	0
92	OHX	6	1981	7/7	0.97	0.16	87,87,87,87	0
92	OHX	6	1982	7/7	0.97	0.16	96,96,96,96	0
92	OHX	6	1983	7/7	0.97	0.16	89,89,89,89	0
92	OHX	1	3580	7/7	0.97	0.15	79,79,79,79	0
92	OHX	5	3629	7/7	0.97	0.29	53,53,53,53	0
92	OHX	1	3581	7/7	0.97	0.21	53,53,53,53	0
92	OHX	6	1986	7/7	0.97	0.21	77,77,77,77	0
92	OHX	1	3582	7/7	0.97	0.23	53,53,53,53	0
93	MG	1	3916	1/1	0.97	0.34	35,35,35,35	0
92	OHX	5	3635	7/7	0.97	0.32	46,46,46,46	0
92	OHX	2	1988	7/7	0.97	0.23	87,87,87,87	0
93	MG	5	4002	1/1	0.97	0.19	43,43,43,43	0
92	OHX	1	3585	7/7	0.97	0.18	74,74,74,74	0
92	OHX	6	1990	7/7	0.97	0.19	79,79,79,79	0
93	MG	5	4005	1/1	0.97	0.23	37,37,37,37	0
92	OHX	5	3642	7/7	0.97	0.33	49,49,49,49	0
92	OHX	1	3685	7/7	0.97	0.23	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	5	3690	7/7	0.98	0.29	49,49,49,49	0
92	OHX	5	3691	7/7	0.98	0.24	64,64,64,64	0
92	OHX	1	3433	7/7	0.98	0.09	52,52,52,52	0
92	OHX	5	3461	7/7	0.98	0.10	44,44,44,44	0
92	OHX	1	3435	7/7	0.98	0.08	63,63,63,63	0
92	OHX	5	3465	7/7	0.98	0.10	56,56,56,56	0
92	OHX	5	3467	7/7	0.98	0.08	70,70,70,70	0
92	OHX	1	3439	7/7	0.98	0.09	59,59,59,59	0
92	OHX	5	3469	7/7	0.98	0.15	48,48,48,48	0
92	OHX	5	3470	7/7	0.98	0.10	53,53,53,53	0
92	OHX	1	3502	7/7	0.98	0.20	46,46,46,46	0
92	OHX	5	3701	7/7	0.98	0.18	50,50,50,50	0
92	OHX	5	3472	7/7	0.98	0.09	63,63,63,63	0
92	OHX	5	3473	7/7	0.98	0.18	46,46,46,46	0
92	OHX	1	3440	7/7	0.98	0.20	44,44,44,44	0
92	OHX	1	3504	7/7	0.98	0.12	64,64,64,64	0
92	OHX	1	3689	7/7	0.98	0.21	57,57,57,57	0
92	OHX	1	3505	7/7	0.98	0.21	66,66,66,66	0
92	OHX	5	3480	7/7	0.98	0.10	49,49,49,49	0
92	OHX	5	3482	7/7	0.98	0.13	57,57,57,57	0
92	OHX	5	3489	7/7	0.98	0.12	53,53,53,53	0
92	OHX	1	3692	7/7	0.98	0.24	69,69,69,69	0
92	OHX	1	3506	7/7	0.98	0.22	50,50,50,50	0
92	OHX	5	3495	7/7	0.98	0.26	47,47,47,47	0
92	OHX	5	3496	7/7	0.98	0.18	71,71,71,71	0
92	OHX	2	1938	7/7	0.98	0.18	79,79,79,79	0
92	OHX	6	1963	7/7	0.98	0.15	78,78,78,78	0
92	OHX	1	3442	7/7	0.98	0.11	58,58,58,58	0
92	OHX	5	3500	7/7	0.98	0.16	63,63,63,63	0
92	OHX	1	3510	7/7	0.98	0.22	58,58,58,58	0
92	OHX	1	3512	7/7	0.98	0.23	48,48,48,48	0
92	OHX	5	3504	7/7	0.98	0.10	52,52,52,52	0
92	OHX	5	3505	7/7	0.98	0.25	39,39,39,39	0
92	OHX	1	3600	7/7	0.98	0.24	63,63,63,63	0
92	OHX	1	3513	7/7	0.98	0.18	52,52,52,52	0
92	OHX	5	3509	7/7	0.98	0.09	90,90,90,90	0
92	OHX	5	3511	7/7	0.98	0.18	42,42,42,42	0
92	OHX	5	3513	7/7	0.98	0.19	52,52,52,52	0
92	OHX	1	3514	7/7	0.98	0.15	56,56,56,56	0
92	OHX	5	3515	7/7	0.98	0.19	47,47,47,47	0
92	OHX	5	3517	7/7	0.98	0.16	55,55,55,55	0
92	OHX	1	3516	7/7	0.98	0.12	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	5	3519	7/7	0.98	0.21	48,48,48,48	0
92	OHX	5	3523	7/7	0.98	0.19	50,50,50,50	0
92	OHX	1	3445	7/7	0.98	0.08	47,47,47,47	0
92	OHX	1	3605	7/7	0.98	0.13	63,63,63,63	0
92	OHX	1	3606	7/7	0.98	0.20	62,62,62,62	0
92	OHX	6	1976	7/7	0.98	0.22	58,58,58,58	0
92	OHX	1	3520	7/7	0.98	0.16	64,64,64,64	0
92	OHX	1	3521	7/7	0.98	0.16	62,62,62,62	0
92	OHX	2	1904	7/7	0.98	0.08	83,83,83,83	0
92	OHX	5	3532	7/7	0.98	0.21	45,45,45,45	0
92	OHX	5	3533	7/7	0.98	0.24	51,51,51,51	0
92	OHX	1	3708	7/7	0.98	0.28	60,60,60,60	0
92	OHX	5	3745	7/7	0.98	0.10	70,70,70,70	0
92	OHX	1	3447	7/7	0.98	0.09	54,54,54,54	0
92	OHX	1	3611	7/7	0.98	0.25	57,57,57,57	0
93	MG	5	3873	1/1	0.98	0.18	51,51,51,51	0
92	OHX	1	3449	7/7	0.98	0.09	56,56,56,56	0
92	OHX	7	203	7/7	0.98	0.13	52,52,52,52	0
92	OHX	1	3525	7/7	0.98	0.17	77,77,77,77	0
93	MG	1	3812	1/1	0.98	0.09	47,47,47,47	0
92	OHX	7	205	7/7	0.98	0.17	45,45,45,45	0
92	OHX	7	207	7/7	0.98	0.15	56,56,56,56	0
92	OHX	5	3539	7/7	0.98	0.22	55,55,55,55	0
93	MG	1	4030	1/1	0.98	0.08	40,40,40,40	0
92	OHX	1	3526	7/7	0.98	0.15	69,69,69,69	0
92	OHX	7	210	7/7	0.98	0.30	46,46,46,46	0
92	OHX	1	3450	7/7	0.98	0.10	62,62,62,62	0
92	OHX	1	3616	7/7	0.98	0.09	131,131,131,131	0
92	OHX	5	3543	7/7	0.98	0.24	45,45,45,45	0
92	OHX	8	204	7/7	0.98	0.19	58,58,58,58	0
92	OHX	5	3544	7/7	0.98	0.20	66,66,66,66	0
92	OHX	5	3546	7/7	0.98	0.18	68,68,68,68	0
92	OHX	8	207	7/7	0.98	0.28	56,56,56,56	0
92	OHX	1	3528	7/7	0.98	0.13	79,79,79,79	0
92	OHX	1	3529	7/7	0.98	0.20	60,60,60,60	0
92	OHX	1	3619	7/7	0.98	0.27	41,41,41,41	0
92	OHX	5	3550	7/7	0.98	0.25	49,49,49,49	0
93	MG	1	3829	1/1	0.98	0.42	38,38,38,38	0
92	OHX	6	1991	7/7	0.98	0.17	81,81,81,81	0
92	OHX	5	3552	7/7	0.98	0.21	54,54,54,54	0
92	OHX	1	3530	7/7	0.98	0.13	89,89,89,89	0
92	OHX	1	3621	7/7	0.98	0.20	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	1	3622	7/7	0.98	0.27	54,54,54,54	0
92	OHX	l3	401	7/7	0.98	0.12	52,52,52,52	0
92	OHX	1	3531	7/7	0.98	0.21	55,55,55,55	0
93	MG	5	4123	1/1	0.98	0.07	39,39,39,39	0
92	OHX	1	3451	7/7	0.98	0.09	65,65,65,65	0
92	OHX	1	3452	7/7	0.98	0.14	46,46,46,46	0
92	OHX	2	1928	7/7	0.98	0.16	79,79,79,79	0
92	OHX	1	3627	7/7	0.98	0.20	62,62,62,62	0
92	OHX	5	3563	7/7	0.98	0.17	72,72,72,72	0
92	OHX	m6	201	7/7	0.98	0.14	48,48,48,48	0
92	OHX	5	3564	7/7	0.98	0.25	59,59,59,59	0
92	OHX	5	3566	7/7	0.98	0.15	58,58,58,58	0
92	OHX	o3	201	7/7	0.98	0.20	54,54,54,54	0
92	OHX	5	3567	7/7	0.98	0.21	53,53,53,53	0
92	OHX	1	3628	7/7	0.98	0.19	79,79,79,79	0
92	OHX	2	1929	7/7	0.98	0.12	83,83,83,83	0
92	OHX	2	1916	7/7	0.98	0.09	84,84,84,84	0
92	OHX	5	3571	7/7	0.98	0.23	61,61,61,61	0
92	OHX	1	3458	7/7	0.98	0.09	72,72,72,72	0
92	OHX	5	3573	7/7	0.98	0.18	60,60,60,60	0
92	OHX	5	3574	7/7	0.98	0.17	55,55,55,55	0
92	OHX	5	3575	7/7	0.98	0.26	65,65,65,65	0
92	OHX	3	202	7/7	0.98	0.21	54,54,54,54	0
92	OHX	5	3578	7/7	0.98	0.15	63,63,63,63	0
92	OHX	1	3459	7/7	0.98	0.12	44,44,44,44	0
92	OHX	3	204	7/7	0.98	0.21	49,49,49,49	0
92	OHX	5	3581	7/7	0.98	0.25	56,56,56,56	0
92	OHX	1	3634	7/7	0.98	0.21	57,57,57,57	0
93	MG	1	3861	1/1	0.98	0.52	38,38,38,38	0
92	OHX	5	3583	7/7	0.98	0.18	52,52,52,52	0
92	OHX	1	3460	7/7	0.98	0.10	58,58,58,58	0
92	OHX	5	3585	7/7	0.98	0.23	51,51,51,51	0
92	OHX	1	3543	7/7	0.98	0.13	72,72,72,72	0
92	OHX	1	3544	7/7	0.98	0.13	77,77,77,77	0
92	OHX	2	1901	7/7	0.98	0.14	78,78,78,78	0
92	OHX	5	3590	7/7	0.98	0.28	60,60,60,60	0
93	MG	5	4157	1/1	0.98	0.19	33,33,33,33	0
92	OHX	1	3546	7/7	0.98	0.20	65,65,65,65	0
92	OHX	5	3592	7/7	0.98	0.18	54,54,54,54	0
92	OHX	4	204	7/7	0.98	0.16	51,51,51,51	0
93	MG	5	3938	1/1	0.98	0.36	34,34,34,34	0
92	OHX	4	205	7/7	0.98	0.21	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	4	207	7/7	0.98	0.14	55,55,55,55	0
92	OHX	2	1910	7/7	0.98	0.08	89,89,89,89	0
92	OHX	1	3549	7/7	0.98	0.20	63,63,63,63	0
92	OHX	4	210	7/7	0.98	0.24	53,53,53,53	0
92	OHX	1	3642	7/7	0.98	0.24	77,77,77,77	0
92	OHX	4	212	7/7	0.98	0.28	50,50,50,50	0
92	OHX	1	3465	7/7	0.98	0.09	70,70,70,70	0
92	OHX	4	214	7/7	0.98	0.20	70,70,70,70	0
92	OHX	5	3603	7/7	0.98	0.27	57,57,57,57	0
92	OHX	2	1907	7/7	0.98	0.10	93,93,93,93	0
92	OHX	5	3605	7/7	0.98	0.24	61,61,61,61	0
92	OHX	2	1923	7/7	0.98	0.12	84,84,84,84	0
93	MG	5	4175	1/1	0.98	0.08	39,39,39,39	0
92	OHX	5	3608	7/7	0.98	0.28	67,67,67,67	0
93	MG	5	3953	1/1	0.98	0.06	41,41,41,41	0
92	OHX	5	3610	7/7	0.98	0.28	45,45,45,45	0
92	OHX	5	3611	7/7	0.98	0.22	49,49,49,49	0
92	OHX	2	1962	7/7	0.98	0.15	86,86,86,86	0
92	OHX	1	3554	7/7	0.98	0.13	70,70,70,70	0
92	OHX	1	3472	7/7	0.98	0.11	62,62,62,62	0
92	OHX	1	3649	7/7	0.98	0.18	64,64,64,64	0
92	OHX	1	3556	7/7	0.98	0.20	56,56,56,56	0
92	OHX	1	3651	7/7	0.98	0.25	64,64,64,64	0
92	OHX	1	3557	7/7	0.98	0.17	74,74,74,74	0
92	OHX	1	3473	7/7	0.98	0.10	55,55,55,55	0
92	OHX	1	3474	7/7	0.98	0.13	51,51,51,51	0
92	OHX	2	1912	7/7	0.98	0.07	93,93,93,93	0
92	OHX	2	1949	7/7	0.98	0.10	94,94,94,94	0
92	OHX	1	3562	7/7	0.98	0.20	58,58,58,58	0
92	OHX	1	3477	7/7	0.98	0.18	51,51,51,51	0
92	OHX	2	1913	7/7	0.98	0.09	84,84,84,84	0
92	OHX	1	3567	7/7	0.98	0.20	45,45,45,45	0
92	OHX	1	3480	7/7	0.98	0.10	48,48,48,48	0
92	OHX	5	3630	7/7	0.98	0.19	65,65,65,65	0
92	OHX	2	1966	7/7	0.98	0.17	65,65,65,65	0
92	OHX	1	3482	7/7	0.98	0.12	57,57,57,57	0
92	OHX	6	1904	7/7	0.98	0.08	68,68,68,68	0
92	OHX	5	3634	7/7	0.98	0.24	57,57,57,57	0
92	OHX	1	3664	7/7	0.98	0.24	66,66,66,66	0
92	OHX	6	1907	7/7	0.98	0.10	77,77,77,77	0
92	OHX	5	3637	7/7	0.98	0.30	41,41,41,41	0
92	OHX	1	3571	7/7	0.98	0.19	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	5	3639	7/7	0.98	0.26	58,58,58,58	0
92	OHX	5	3640	7/7	0.98	0.25	59,59,59,59	0
92	OHX	2	1951	7/7	0.98	0.12	82,82,82,82	0
92	OHX	6	1921	7/7	0.98	0.18	64,64,64,64	0
92	OHX	6	1923	7/7	0.98	0.09	81,81,81,81	0
92	OHX	1	3573	7/7	0.98	0.17	73,73,73,73	0
92	OHX	1	3574	7/7	0.98	0.22	57,57,57,57	0
92	OHX	C8	201	7/7	0.98	0.10	80,80,80,80	0
92	OHX	1	3576	7/7	0.98	0.15	60,60,60,60	0
92	OHX	1	3577	7/7	0.98	0.24	51,51,51,51	0
92	OHX	5	3649	7/7	0.98	0.25	71,71,71,71	0
92	OHX	5	3650	7/7	0.98	0.26	50,50,50,50	0
92	OHX	2	1937	7/7	0.98	0.12	84,84,84,84	0
92	OHX	5	3652	7/7	0.98	0.27	59,59,59,59	0
92	OHX	5	3653	7/7	0.98	0.26	54,54,54,54	0
92	OHX	6	1934	7/7	0.98	0.14	68,68,68,68	0
92	OHX	1	3579	7/7	0.98	0.15	67,67,67,67	0
92	OHX	2	1969	7/7	0.98	0.11	87,87,87,87	0
92	OHX	s1	301	7/7	0.98	0.10	77,77,77,77	0
92	OHX	6	1938	7/7	0.98	0.12	76,76,76,76	0
92	OHX	1	3490	7/7	0.98	0.22	53,53,53,53	0
92	OHX	6	1940	7/7	0.98	0.14	59,59,59,59	0
92	OHX	6	1941	7/7	0.98	0.16	96,96,96,96	0
93	MG	5	3786	1/1	0.98	0.11	33,33,33,33	0
92	OHX	5	3662	7/7	0.98	0.27	47,47,47,47	0
92	OHX	1	3415	7/7	0.98	0.09	53,53,53,53	0
92	OHX	1	3418	7/7	0.98	0.08	52,52,52,52	0
92	OHX	6	1944	7/7	0.98	0.18	71,71,71,71	0
92	OHX	6	1945	7/7	0.98	0.14	72,72,72,72	0
93	MG	n8	202	1/1	0.98	0.06	34,34,34,34	0
92	OHX	5	3405	7/7	0.98	0.09	36,36,36,36	0
92	OHX	5	3407	7/7	0.98	0.14	44,44,44,44	0
92	OHX	5	3429	7/7	0.98	0.08	47,47,47,47	0
92	OHX	5	3434	7/7	0.98	0.10	46,46,46,46	0
92	OHX	5	3435	7/7	0.98	0.09	64,64,64,64	0
92	OHX	5	3437	7/7	0.98	0.09	46,46,46,46	0
92	OHX	5	3442	7/7	0.98	0.10	59,59,59,59	0
92	OHX	5	3674	7/7	0.98	0.24	43,43,43,43	0
92	OHX	1	3584	7/7	0.98	0.18	80,80,80,80	0
92	OHX	5	3676	7/7	0.98	0.25	66,66,66,66	0
92	OHX	5	3445	7/7	0.98	0.10	45,45,45,45	0
93	MG	1	3739	1/1	0.98	0.34	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	5	3446	7/7	0.98	0.09	56,56,56,56	0
92	OHX	5	3448	7/7	0.98	0.11	48,48,48,48	0
92	OHX	5	3449	7/7	0.98	0.08	58,58,58,58	0
92	OHX	5	3450	7/7	0.98	0.07	65,65,65,65	0
92	OHX	5	3682	7/7	0.98	0.22	83,83,83,83	0
92	OHX	1	3431	7/7	0.98	0.21	46,46,46,46	0
92	OHX	5	3684	7/7	0.98	0.20	73,73,73,73	0
92	OHX	1	3586	7/7	0.98	0.23	46,46,46,46	0
92	OHX	5	3455	7/7	0.98	0.24	41,41,41,41	0
92	OHX	5	3456	7/7	0.98	0.11	58,58,58,58	0
92	OHX	2	1987	7/7	0.98	0.18	94,94,94,94	0
92	OHX	6	1950	7/7	0.98	0.12	90,90,90,90	0
92	OHX	2	1922	7/7	0.99	0.09	83,83,83,83	0
92	OHX	1	3434	7/7	0.99	0.06	58,58,58,58	0
92	OHX	6	2000	7/7	0.99	0.18	69,69,69,69	0
92	OHX	6	1906	7/7	0.99	0.07	60,60,60,60	0
92	OHX	2	1914	7/7	0.99	0.11	78,78,78,78	0
92	OHX	6	1908	7/7	0.99	0.08	65,65,65,65	0
93	MG	5	4091	1/1	0.99	0.05	32,32,32,32	0
92	OHX	6	1909	7/7	0.99	0.06	91,91,91,91	0
92	OHX	6	1910	7/7	0.99	0.07	62,62,62,62	0
92	OHX	6	1911	7/7	0.99	0.05	57,57,57,57	0
92	OHX	6	1912	7/7	0.99	0.10	74,74,74,74	0
92	OHX	5	3478	7/7	0.99	0.12	58,58,58,58	0
92	OHX	5	3479	7/7	0.99	0.09	52,52,52,52	0
92	OHX	6	1913	7/7	0.99	0.07	80,80,80,80	0
92	OHX	5	3481	7/7	0.99	0.10	49,49,49,49	0
92	OHX	6	1914	7/7	0.99	0.12	61,61,61,61	0
92	OHX	5	3483	7/7	0.99	0.14	43,43,43,43	0
92	OHX	5	3484	7/7	0.99	0.15	48,48,48,48	0
92	OHX	5	3485	7/7	0.99	0.18	52,52,52,52	0
92	OHX	5	3486	7/7	0.99	0.14	53,53,53,53	0
92	OHX	5	3487	7/7	0.99	0.13	47,47,47,47	0
92	OHX	5	3488	7/7	0.99	0.14	41,41,41,41	0
92	OHX	6	1915	7/7	0.99	0.06	62,62,62,62	0
92	OHX	6	1916	7/7	0.99	0.08	70,70,70,70	0
92	OHX	5	3492	7/7	0.99	0.12	48,48,48,48	0
92	OHX	5	3493	7/7	0.99	0.15	51,51,51,51	0
92	OHX	6	1917	7/7	0.99	0.10	55,55,55,55	0
92	OHX	6	1918	7/7	0.99	0.10	49,49,49,49	0
92	OHX	1	3436	7/7	0.99	0.10	52,52,52,52	0
92	OHX	1	3478	7/7	0.99	0.16	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	1	3532	7/7	0.99	0.15	48,48,48,48	0
92	OHX	6	1922	7/7	0.99	0.13	60,60,60,60	0
92	OHX	1	3437	7/7	0.99	0.07	47,47,47,47	0
92	OHX	6	1924	7/7	0.99	0.10	63,63,63,63	0
92	OHX	5	3502	7/7	0.99	0.18	44,44,44,44	0
92	OHX	1	3438	7/7	0.99	0.07	56,56,56,56	0
92	OHX	6	1926	7/7	0.99	0.18	67,67,67,67	0
92	OHX	2	1924	7/7	0.99	0.07	103,103,103,103	0
92	OHX	5	3506	7/7	0.99	0.23	52,52,52,52	0
92	OHX	2	1902	7/7	0.99	0.06	81,81,81,81	0
92	OHX	6	1929	7/7	0.99	0.12	63,63,63,63	0
92	OHX	6	1930	7/7	0.99	0.14	64,64,64,64	0
92	OHX	5	3510	7/7	0.99	0.08	35,35,35,35	0
92	OHX	1	3483	7/7	0.99	0.14	72,72,72,72	0
92	OHX	5	3512	7/7	0.99	0.14	60,60,60,60	0
92	OHX	1	3538	7/7	0.99	0.15	54,54,54,54	0
92	OHX	1	3539	7/7	0.99	0.16	52,52,52,52	0
92	OHX	1	3404	7/7	0.99	0.11	43,43,43,43	0
92	OHX	5	3516	7/7	0.99	0.21	51,51,51,51	0
92	OHX	1	3405	7/7	0.99	0.07	43,43,43,43	0
92	OHX	6	1936	7/7	0.99	0.12	74,74,74,74	0
92	OHX	1	3486	7/7	0.99	0.09	57,57,57,57	0
92	OHX	5	3520	7/7	0.99	0.17	60,60,60,60	0
92	OHX	5	3521	7/7	0.99	0.16	47,47,47,47	0
92	OHX	5	3522	7/7	0.99	0.14	61,61,61,61	0
92	OHX	1	3443	7/7	0.99	0.07	53,53,53,53	0
92	OHX	1	3444	7/7	0.99	0.07	66,66,66,66	0
92	OHX	1	3489	7/7	0.99	0.16	51,51,51,51	0
92	OHX	1	3406	7/7	0.99	0.12	52,52,52,52	0
92	OHX	1	3547	7/7	0.99	0.17	58,58,58,58	0
92	OHX	5	3528	7/7	0.99	0.15	42,42,42,42	0
92	OHX	1	3407	7/7	0.99	0.06	41,41,41,41	0
92	OHX	1	3408	7/7	0.99	0.07	41,41,41,41	0
92	OHX	3	201	7/7	0.99	0.10	60,60,60,60	0
92	OHX	1	3493	7/7	0.99	0.17	42,42,42,42	0
92	OHX	1	3494	7/7	0.99	0.12	67,67,67,67	0
92	OHX	1	3410	7/7	0.99	0.08	48,48,48,48	0
92	OHX	1	3496	7/7	0.99	0.14	53,53,53,53	0
92	OHX	1	3411	7/7	0.99	0.05	43,43,43,43	0
92	OHX	1	3412	7/7	0.99	0.06	51,51,51,51	0
92	OHX	1	3499	7/7	0.99	0.11	40,40,40,40	0
92	OHX	2	1940	7/7	0.99	0.10	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	1	3416	7/7	0.99	0.07	38,38,38,38	0
92	OHX	4	201	7/7	0.99	0.08	41,41,41,41	0
92	OHX	4	202	7/7	0.99	0.06	47,47,47,47	0
92	OHX	4	203	7/7	0.99	0.11	49,49,49,49	0
92	OHX	1	3417	7/7	0.99	0.10	52,52,52,52	0
92	OHX	5	3545	7/7	0.99	0.21	49,49,49,49	0
92	OHX	1	3455	7/7	0.99	0.10	50,50,50,50	0
92	OHX	4	206	7/7	0.99	0.14	49,49,49,49	0
92	OHX	2	1919	7/7	0.99	0.07	73,73,73,73	0
92	OHX	6	1962	7/7	0.99	0.18	69,69,69,69	0
92	OHX	1	3457	7/7	0.99	0.11	53,53,53,53	0
92	OHX	1	3421	7/7	0.99	0.07	57,57,57,57	0
92	OHX	1	3683	7/7	0.99	0.26	56,56,56,56	0
92	OHX	1	3564	7/7	0.99	0.18	50,50,50,50	0
92	OHX	5	3554	7/7	0.99	0.18	52,52,52,52	0
92	OHX	1	3507	7/7	0.99	0.21	51,51,51,51	0
92	OHX	1	3566	7/7	0.99	0.15	71,71,71,71	0
92	OHX	1	3422	7/7	0.99	0.07	55,55,55,55	0
92	OHX	1	3423	7/7	0.99	0.07	61,61,61,61	0
92	OHX	6	1971	7/7	0.99	0.20	55,55,55,55	0
92	OHX	5	3560	7/7	0.99	0.16	41,41,41,41	0
92	OHX	5	3720	7/7	0.99	0.24	49,49,49,49	0
92	OHX	6	1972	7/7	0.99	0.14	67,67,67,67	0
92	OHX	1	3461	7/7	0.99	0.11	43,43,43,43	0
92	OHX	5	3403	7/7	0.99	0.10	43,43,43,43	0
92	OHX	1	3690	7/7	0.99	0.20	52,52,52,52	0
92	OHX	5	3565	7/7	0.99	0.17	55,55,55,55	0
92	OHX	5	3406	7/7	0.99	0.07	38,38,38,38	0
92	OHX	1	3629	7/7	0.99	0.13	50,50,50,50	0
93	MG	1	3909	1/1	0.99	0.36	29,29,29,29	0
92	OHX	5	3408	7/7	0.99	0.11	47,47,47,47	0
92	OHX	5	3409	7/7	0.99	0.07	43,43,43,43	0
92	OHX	5	3410	7/7	0.99	0.09	45,45,45,45	0
92	OHX	5	3411	7/7	0.99	0.08	44,44,44,44	0
92	OHX	5	3413	7/7	0.99	0.09	47,47,47,47	0
92	OHX	5	3414	7/7	0.99	0.07	42,42,42,42	0
92	OHX	5	3415	7/7	0.99	0.06	42,42,42,42	0
92	OHX	5	3416	7/7	0.99	0.09	43,43,43,43	0
92	OHX	5	3576	7/7	0.99	0.16	50,50,50,50	0
92	OHX	5	3418	7/7	0.99	0.07	40,40,40,40	0
92	OHX	5	3419	7/7	0.99	0.06	50,50,50,50	0
92	OHX	5	3420	7/7	0.99	0.07	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	5	3422	7/7	0.99	0.05	51,51,51,51	0
92	OHX	5	3423	7/7	0.99	0.05	54,54,54,54	0
92	OHX	5	3424	7/7	0.99	0.07	41,41,41,41	0
92	OHX	5	3425	7/7	0.99	0.07	52,52,52,52	0
92	OHX	5	3426	7/7	0.99	0.06	51,51,51,51	0
92	OHX	5	3428	7/7	0.99	0.06	37,37,37,37	0
92	OHX	1	3511	7/7	0.99	0.16	45,45,45,45	0
92	OHX	5	3587	7/7	0.99	0.21	44,44,44,44	0
92	OHX	5	3431	7/7	0.99	0.12	46,46,46,46	0
92	OHX	7	202	7/7	0.99	0.07	49,49,49,49	0
92	OHX	5	3432	7/7	0.99	0.19	45,45,45,45	0
92	OHX	1	3424	7/7	0.99	0.07	55,55,55,55	0
92	OHX	1	3463	7/7	0.99	0.11	54,54,54,54	0
92	OHX	7	206	7/7	0.99	0.11	55,55,55,55	0
92	OHX	5	3436	7/7	0.99	0.06	41,41,41,41	0
92	OHX	1	3425	7/7	0.99	0.07	50,50,50,50	0
92	OHX	5	3438	7/7	0.99	0.10	46,46,46,46	0
92	OHX	5	3439	7/7	0.99	0.10	43,43,43,43	0
92	OHX	5	3440	7/7	0.99	0.08	45,45,45,45	0
92	OHX	5	3441	7/7	0.99	0.05	57,57,57,57	0
92	OHX	8	201	7/7	0.99	0.05	41,41,41,41	0
92	OHX	8	202	7/7	0.99	0.09	40,40,40,40	0
92	OHX	1	3515	7/7	0.99	0.16	39,39,39,39	0
92	OHX	1	3426	7/7	0.99	0.07	58,58,58,58	0
92	OHX	5	3444	7/7	0.99	0.10	51,51,51,51	0
92	OHX	L6	201	7/7	0.99	0.09	44,44,44,44	0
92	OHX	1	3466	7/7	0.99	0.14	43,43,43,43	0
92	OHX	5	3447	7/7	0.99	0.10	41,41,41,41	0
92	OHX	1	3518	7/7	0.99	0.22	46,46,46,46	0
92	OHX	M5	301	7/7	0.99	0.06	46,46,46,46	0
92	OHX	1	3519	7/7	0.99	0.22	53,53,53,53	0
92	OHX	5	3607	7/7	0.99	0.20	40,40,40,40	0
92	OHX	M6	201	7/7	0.99	0.15	54,54,54,54	0
92	OHX	5	3609	7/7	0.99	0.15	57,57,57,57	0
92	OHX	5	3452	7/7	0.99	0.08	55,55,55,55	0
92	OHX	5	3453	7/7	0.99	0.08	91,91,91,91	0
92	OHX	1	3467	7/7	0.99	0.11	54,54,54,54	0
92	OHX	1	3427	7/7	0.99	0.07	52,52,52,52	0
92	OHX	5	3614	7/7	0.99	0.13	47,47,47,47	0
92	OHX	1	3429	7/7	0.99	0.05	55,55,55,55	0
92	OHX	N9	101	7/7	0.99	0.07	42,42,42,42	0
92	OHX	O3	201	7/7	0.99	0.21	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	m0	302	7/7	0.99	0.30	49,49,49,49	0
92	OHX	5	3459	7/7	0.99	0.10	46,46,46,46	0
92	OHX	m5	301	7/7	0.99	0.06	48,48,48,48	0
92	OHX	m5	302	7/7	0.99	0.18	66,66,66,66	0
92	OHX	1	3470	7/7	0.99	0.12	48,48,48,48	0
94	ZN	D9	101	1/1	0.99	0.03	90,90,90,90	0
92	OHX	1	3430	7/7	0.99	0.11	43,43,43,43	0
92	OHX	2	1920	7/7	0.99	0.06	76,76,76,76	0
94	ZN	d9	101	1/1	0.99	0.04	97,97,97,97	0
92	OHX	n9	101	7/7	0.99	0.06	41,41,41,41	0
94	ZN	q2	501	1/1	0.99	0.11	47,47,47,47	0
92	OHX	5	3463	7/7	0.99	0.10	50,50,50,50	0
92	OHX	o7	502	7/7	0.99	0.15	54,54,54,54	0
92	OHX	5	3623	7/7	0.99	0.21	58,58,58,58	0
92	OHX	q2	502	7/7	0.99	0.09	45,45,45,45	0
92	OHX	5	3464	7/7	0.99	0.06	57,57,57,57	0
92	OHX	2	1905	7/7	0.99	0.07	76,76,76,76	0
92	OHX	5	3466	7/7	0.99	0.13	45,45,45,45	0
92	OHX	6	1903	7/7	0.99	0.07	61,61,61,61	0
92	OHX	5	3491	7/7	1.00	0.10	46,46,46,46	0
92	OHX	1	3414	7/7	1.00	0.04	47,47,47,47	0
92	OHX	1	3419	7/7	1.00	0.04	38,38,38,38	0
92	OHX	1	3420	7/7	1.00	0.04	59,59,59,59	0
92	OHX	5	3412	7/7	1.00	0.06	33,33,33,33	0
94	ZN	D6	500	1/1	1.00	0.05	87,87,87,87	0
92	OHX	5	3427	7/7	1.00	0.07	41,41,41,41	0
92	OHX	1	3448	7/7	1.00	0.07	54,54,54,54	0
92	OHX	1	3409	7/7	1.00	0.04	39,39,39,39	0
94	ZN	O7	101	1/1	1.00	0.02	39,39,39,39	0
94	ZN	Q0	500	1/1	1.00	0.02	47,47,47,47	0
94	ZN	Q2	501	1/1	1.00	0.07	51,51,51,51	0
94	ZN	Q3	501	1/1	1.00	0.03	55,55,55,55	0
94	ZN	d6	101	1/1	1.00	0.03	67,67,67,67	0
93	MG	5	4150	1/1	1.00	0.04	37,37,37,37	0
92	OHX	5	3430	7/7	1.00	0.05	53,53,53,53	0
93	MG	5	4094	1/1	1.00	0.05	32,32,32,32	0
94	ZN	o7	501	1/1	1.00	0.01	41,41,41,41	0
94	ZN	q0	500	1/1	1.00	0.02	37,37,37,37	0
92	OHX	1	3428	7/7	1.00	0.04	47,47,47,47	0
94	ZN	q3	501	1/1	1.00	0.02	55,55,55,55	0
92	OHX	5	3404	7/7	1.00	0.08	36,36,36,36	0
92	OHX	5	3433	7/7	1.00	0.05	39,39,39,39	0

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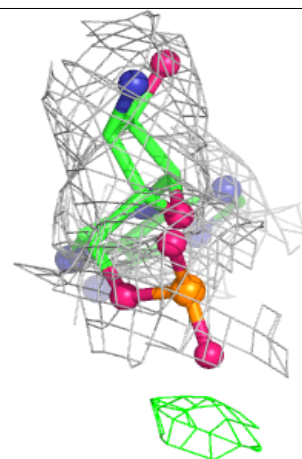
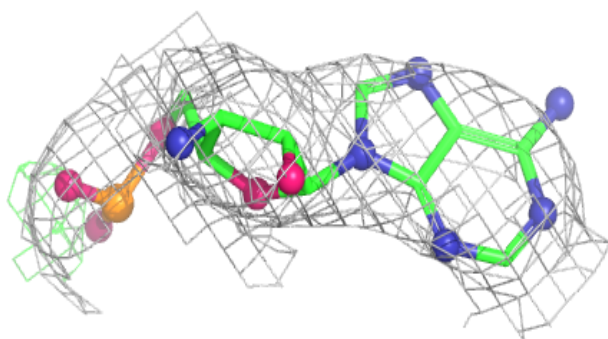
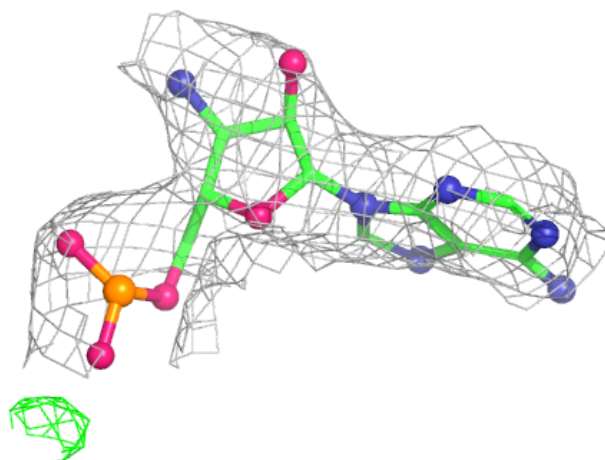
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
92	OHX	5	3417	7/7	1.00	0.07	41,41,41,41	0
92	OHX	Q2	502	7/7	1.00	0.09	41,41,41,41	0
92	OHX	6	1901	7/7	1.00	0.10	59,59,59,59	0
92	OHX	1	3403	7/7	1.00	0.09	37,37,37,37	0
92	OHX	5	3421	7/7	1.00	0.04	44,44,44,44	0
92	OHX	1	3413	7/7	1.00	0.06	45,45,45,45	0

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

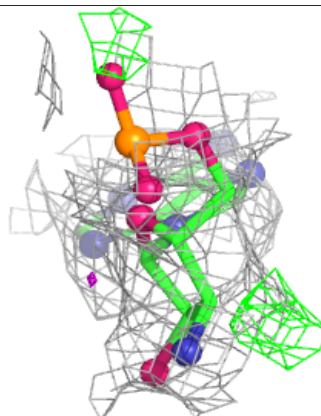
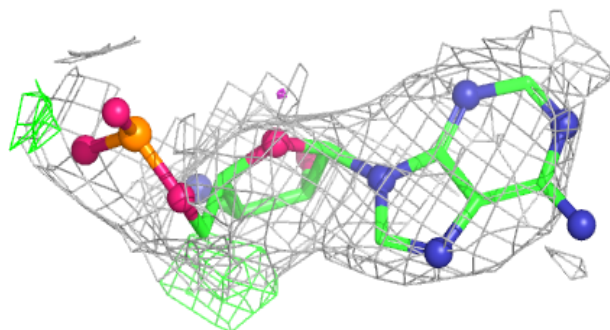
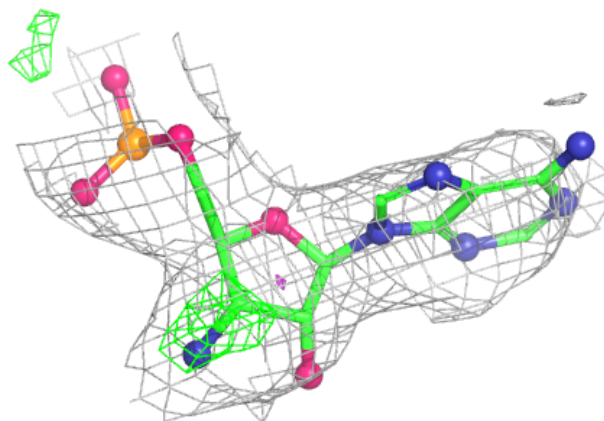
Electron density around 8AN P 102:

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

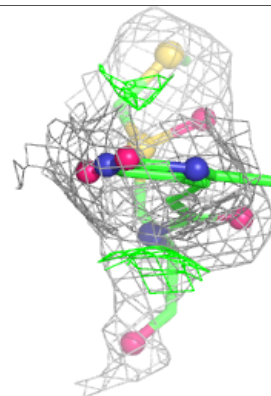
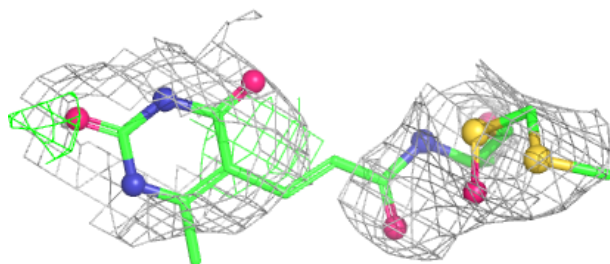
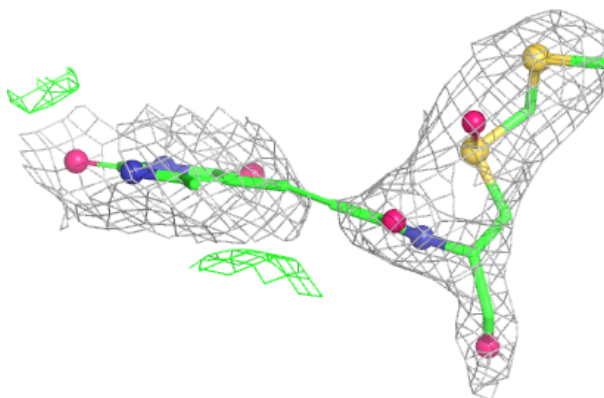


Electron density around 8AN p 102:

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

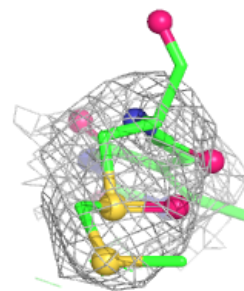
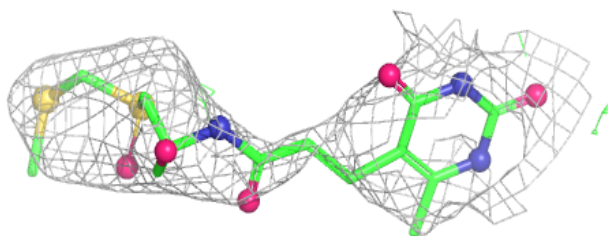
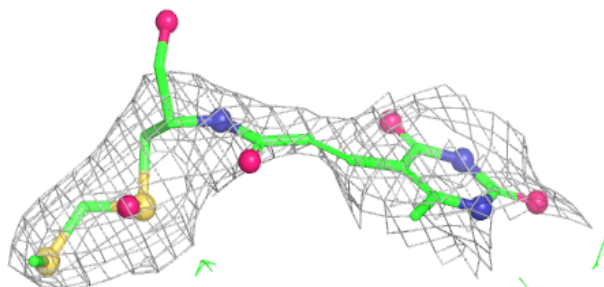
**Electron density around SPS P 101:**

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



Electron density around SPS p 101:

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



5.5 Other polymers [i](#)

There are no such residues in this entry.