wwPDB X-ray Structure Validation Summary Report (i)

Sep 16, 2026 – 11:53 am BST

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 (i) symbol.

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

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

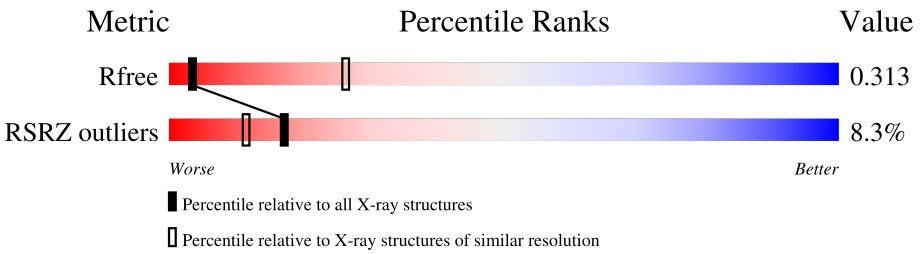
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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
97	SPS	p	101	-	X	-	-

2 Entry composition (i)

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
			Total	C	N	O	P			
1	2	1781	37970	16975	6720	12493	1782	0	1	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	S8	188	1489	925	298	264	2	0	0	0
10	s8	188	1489	925	298	264	2	0	0	0

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

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

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

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

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

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

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
			Total	C	N	O	S			
14	C2	124	890	560	156	172	2	0	0	0
14	c2	124	890	560	156	172	2	0	0	0

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

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

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

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

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
			Total	C	N	O	S			
17	C5	124	977	622	182	166	7	0	0	0
17	c5	135	1039	658	196	178	7	0	0	0

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

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

- Molecule 19 is a protein called ES17.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O			
35	SM	159	1105	655	221	229	0	0	0

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
			Total	C	N	O	P			
36	1	3149	67355	30086	12142	21978	3149	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	L9	191	1518	963	274	277	4	0	0	0
46	l9	191	1518	963	274	277	4	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 82 is a protein called ES17.

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

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
			Total	C	N	O	S			
83	sR	318	2442	1544	418	472	8	0	0	0

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

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

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
			Total	C	N	O	P			
85	5	3150	67376	30095	12145	21987	3149	0	0	0

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

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

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

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

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

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

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

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

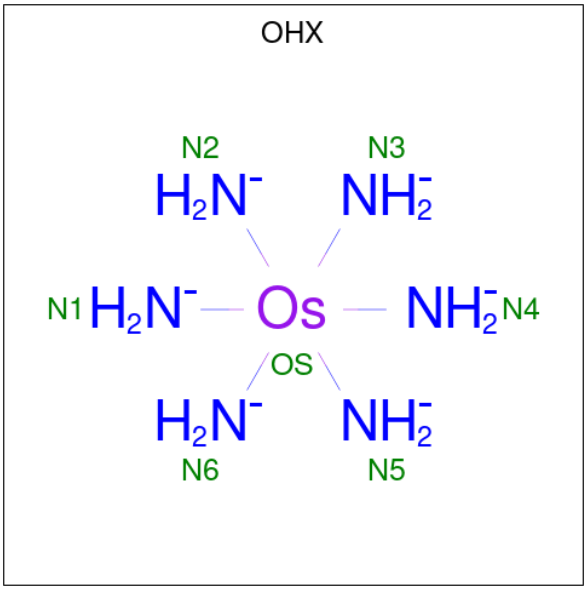
- Molecule 90 is a protein called 60S Ribosomal Protein P1/2.

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

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

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

- Molecule 92 is osmium (III) hexammine (CCD ID: OHX) (formula: $H_{12}N_6Os$).



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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
92	2	1	7	6	1	0	0
			Total	N	Os		
92	2	1	7	6	1	0	0
			Total	N	Os		
92	S8	1	7	6	1	0	0
			Total	N	Os		
92	S9	1	7	6	1	0	0
			Total	N	Os		
92	C3	1	7	6	1	0	0
			Total	N	Os		
92	C5	1	7	6	1	0	0
			Total	N	Os		
92	C7	1	7	6	1	0	0
			Total	N	Os		
92	C8	1	7	6	1	0	0
			Total	N	Os		
92	D9	1	7	6	1	0	0
			Total	N	Os		
92	SR	1	7	6	1	0	0
			Total	N	Os		
92	1	1	7	6	1	0	0
			Total	N	Os		
92	1	1	7	6	1	0	0
			Total	N	Os		
92	1	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
92	1	1	7	6	1	0	0
			Total	N	Os		
92	1	1	7	6	1	0	0
			Total	N	Os		
92	1	1	7	6	1	0	0
			Total	N	Os		
92	1	1	7	6	1	0	0
			Total	N	Os		
92	1	1	7	6	1	0	0
			Total	N	Os		
92	1	1	7	6	1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
92	M7	1	7	6	1	0	0
92	M8	1	7	6	1	0	0
92	M9	1	7	6	1	0	0
92	N9	1	7	6	1	0	0
92	O3	1	7	6	1	0	0
92	O4	1	7	6	1	0	0
92	O7	1	7	6	1	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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92	s8	1	7	6	1	0	0
92	s9	1	7	6	1	0	0
92	c3	1	7	6	1	0	0
92	c5	1	7	6	1	0	0
92	c8	1	7	6	1	0	0
92	d4	1	7	6	1	0	0
92	sR	1	7	6	1	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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			Total	N	Os		
92	5	1	7	6	1	0	0
			Total	N	Os		
92	5	1	7	6	1	0	0
			Total	N	Os		
92	5	1	7	6	1	0	0
			Total	N	Os		
92	5	1	7	6	1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
93	l9	1	1	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
			Total	Zn		
94	D6	1	1	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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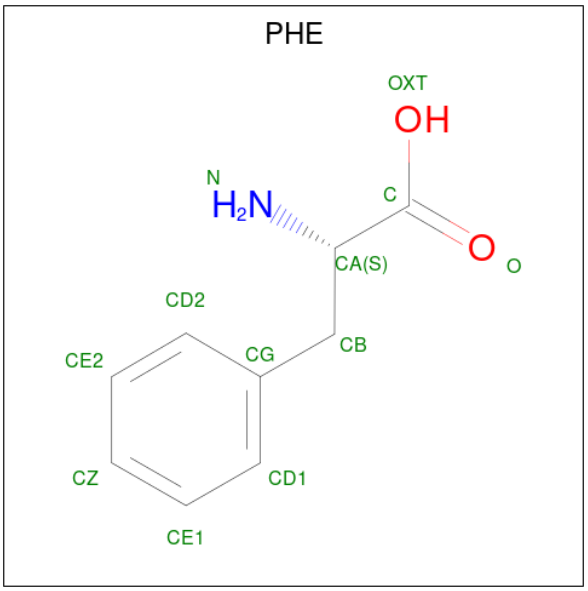
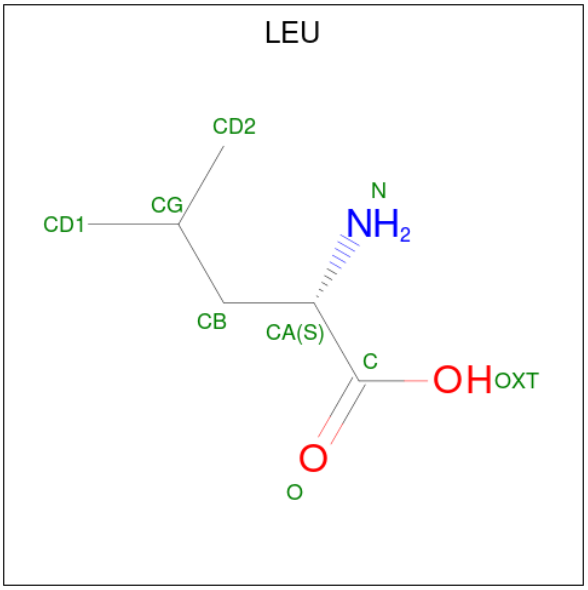
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
94	E1	1	1	1	0	0
94	O7	1	1	1	0	0
94	Q0	1	1	1	0	0
94	Q2	1	1	1	0	0
94	Q3	1	1	1	0	0
94	d6	1	1	1	0	0
94	d7	1	1	1	0	0
94	d9	1	1	1	0	0
94	e1	1	1	1	0	0
94	o7	1	1	1	0	0
94	q0	1	1	1	0	0
94	q2	1	1	1	0	0
94	q3	1	1	1	0	0

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



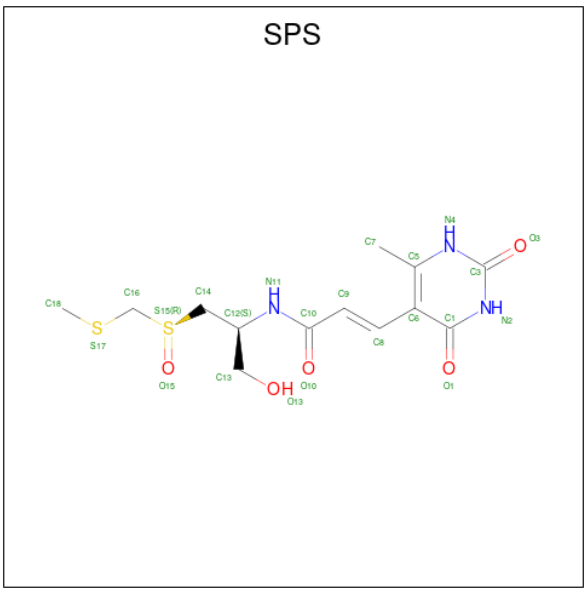
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
95	1	1	11	9	1	1	0	0
			Total	C	N	O		
95	5	1	11	9	1	1	0	0

- Molecule 96 is LEUCINE (CCD ID: LEU) (formula: $C_6H_{13}NO_2$).



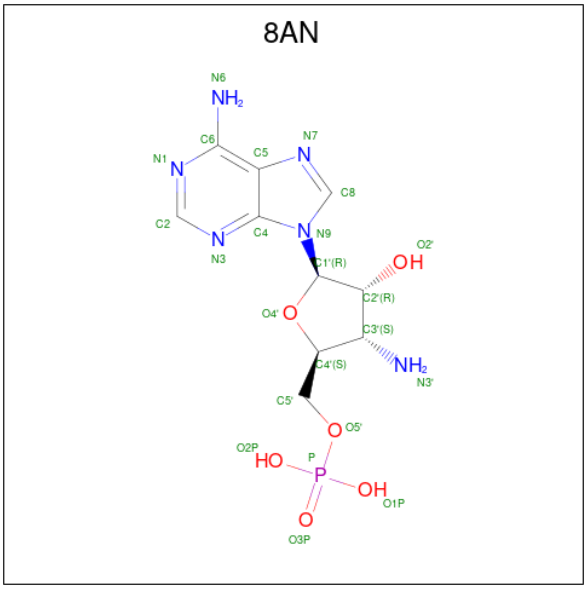
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
96	1	1	8	6	1	1	0	0
			Total	C	N	O		
96	5	1	8	6	1	1	0	0

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



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

- 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
			Total	C	N	O	P		
98	P	1	22	10	6	5	1	0	0
			Total	C	N	O	P		
98	p	1	22	10	6	5	1	0	0

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

3 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	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.*

[1]Intensities estimated from amplitudes.

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

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	5	3515	-	0,6,6	-	-	-		
92	OHX	5	3685	-	0,6,6	-	-	-		
92	OHX	2	1944	-	0,6,6	-	-	-		
92	OHX	5	3724	85	0,6,6	-	-	-		
92	OHX	1	3709	-	0,6,6	-	-	-		
92	OHX	6	1941	80	0,6,6	-	-	-		
92	OHX	5	3505	-	0,6,6	-	-	-		
92	OHX	8	215	38	0,6,6	-	-	-		
92	OHX	5	3509	85	0,6,6	-	-	-		
92	OHX	2	1974	-	0,6,6	-	-	-		
92	OHX	5	3484	85	0,6,6	-	-	-		
92	OHX	5	3709	-	0,6,6	-	-	-		
92	OHX	1	3434	-	0,6,6	-	-	-		
92	OHX	5	3508	-	0,6,6	-	-	-		
92	OHX	5	3720	85	0,6,6	-	-	-		
92	OHX	5	3475	85	0,6,6	-	-	-		
92	OHX	1	3572	36	0,6,6	-	-	-		
92	OHX	6	1959	-	0,6,6	-	-	-		
92	OHX	5	3626	85	0,6,6	-	-	-		
92	OHX	7	205	-	0,6,6	-	-	-		
92	OHX	8	213	-	0,6,6	-	-	-		
92	OHX	6	1929	80	0,6,6	-	-	-		
92	OHX	c8	201	-	0,6,6	-	-	-		
92	OHX	5	3677	85,93	0,6,6	-	-	-		
92	OHX	1	3405	-	0,6,6	-	-	-		
92	OHX	5	3738	85	0,6,6	-	-	-		
92	OHX	s8	301	-	0,6,6	-	-	-		
92	OHX	2	1955	-	0,6,6	-	-	-		
92	OHX	6	1961	-	0,6,6	-	-	-		
92	OHX	2	2029	-	0,6,6	-	-	-		
92	OHX	2	1930	-	0,6,6	-	-	-		
92	OHX	6	1939	80	0,6,6	-	-	-		
92	OHX	5	3405	85	0,6,6	-	-	-		
92	OHX	5	3473	85	0,6,6	-	-	-		
92	OHX	2	1924	-	0,6,6	-	-	-		
92	OHX	1	3719	93	0,6,6	-	-	-		
92	OHX	5	3444	93	0,6,6	-	-	-		
92	OHX	5	3503	-	0,6,6	-	-	-		
92	OHX	5	3517	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	5	3422	85	0,6,6	-	-	-		
92	OHX	1	3473	-	0,6,6	-	-	-		
92	OHX	1	3654	-	0,6,6	-	-	-		
92	OHX	5	3613	-	0,6,6	-	-	-		
92	OHX	5	3418	-	0,6,6	-	-	-		
92	OHX	1	3656	93	0,6,6	-	-	-		
92	OHX	6	1927	80	0,6,6	-	-	-		
92	OHX	6	1903	-	0,6,6	-	-	-		
92	OHX	5	3450	85	0,6,6	-	-	-		
92	OHX	2	2025	-	0,6,6	-	-	-		
92	OHX	5	3671	85,93	0,6,6	-	-	-		
92	OHX	7	207	37	0,6,6	-	-	-		
92	OHX	5	3428	85	0,6,6	-	-	-		
92	OHX	1	3453	-	0,6,6	-	-	-		
92	OHX	6	1975	-	0,6,6	-	-	-		
92	OHX	6	2030	80	0,6,6	-	-	-		
92	OHX	5	3415	-	0,6,6	-	-	-		
92	OHX	l9	201	-	0,6,6	-	-	-		
92	OHX	1	3425	-	0,6,6	-	-	-		
92	OHX	5	3453	85	0,6,6	-	-	-		
92	OHX	6	2015	-	0,6,6	-	-	-		
92	OHX	5	3412	-	0,6,6	-	-	-		
92	OHX	2	1903	-	0,6,6	-	-	-		
92	OHX	1	3456	-	0,6,6	-	-	-		
92	OHX	6	1998	80	0,6,6	-	-	-		
92	OHX	5	3587	-	0,6,6	-	-	-		
92	OHX	5	3476	-	0,6,6	-	-	-		
92	OHX	5	3591	-	0,6,6	-	-	-		
92	OHX	8	202	38	0,6,6	-	-	-		
92	OHX	6	2045	-	0,6,6	-	-	-		
95	PHE	5	3401	96	10,11,12	1.23	1 (10%)	10,13,15	0.62	0
92	OHX	1	3519	-	0,6,6	-	-	-		
92	OHX	5	3711	93	0,6,6	-	-	-		
92	OHX	1	3424	-	0,6,6	-	-	-		
92	OHX	5	3447	85	0,6,6	-	-	-		
92	OHX	5	3521	85	0,6,6	-	-	-		
92	OHX	l3	402	-	0,6,6	-	-	-		
92	OHX	1	3430	93	0,6,6	-	-	-		
92	OHX	1	3505	-	0,6,6	-	-	-		
92	OHX	2	2030	1	0,6,6	-	-	-		
92	OHX	2	1996	-	0,6,6	-	-	-		
92	OHX	2	2035	1	0,6,6	-	-	-		
92	OHX	1	3522	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	2	2038	-	0,6,6	-	-	-		
92	OHX	1	3555	-	0,6,6	-	-	-		
92	OHX	1	3641	-	0,6,6	-	-	-		
92	OHX	6	2019	80,93	0,6,6	-	-	-		
92	OHX	6	2052	80	0,6,6	-	-	-		
92	OHX	2	1902	-	0,6,6	-	-	-		
92	OHX	s1	301	-	0,6,6	-	-	-		
92	OHX	5	3522	-	0,6,6	-	-	-		
92	OHX	7	208	37	0,6,6	-	-	-		
92	OHX	7	204	37	0,6,6	-	-	-		
92	OHX	8	212	38	0,6,6	-	-	-		
92	OHX	5	3665	85	0,6,6	-	-	-		
92	OHX	1	3558	-	0,6,6	-	-	-		
92	OHX	6	2020	-	0,6,6	-	-	-		
92	OHX	L6	202	-	0,6,6	-	-	-		
92	OHX	2	1991	-	0,6,6	-	-	-		
92	OHX	1	3423	-	0,6,6	-	-	-		
92	OHX	5	3706	-	0,6,6	-	-	-		
92	OHX	1	3626	-	0,6,6	-	-	-		
92	OHX	1	3717	-	0,6,6	-	-	-		
92	OHX	1	3451	-	0,6,6	-	-	-		
92	OHX	5	3693	-	0,6,6	-	-	-		
92	OHX	2	1975	-	0,6,6	-	-	-		
92	OHX	6	1917	80	0,6,6	-	-	-		
92	OHX	6	2027	-	0,6,6	-	-	-		
92	OHX	1	3675	-	0,6,6	-	-	-		
92	OHX	7	209	-	0,6,6	-	-	-		
92	OHX	2	2020	-	0,6,6	-	-	-		
92	OHX	1	3541	-	0,6,6	-	-	-		
92	OHX	6	2042	80	0,6,6	-	-	-		
92	OHX	4	211	-	0,6,6	-	-	-		
92	OHX	2	1906	-	0,6,6	-	-	-		
92	OHX	6	2054	-	0,6,6	-	-	-		
92	OHX	6	2007	80	0,6,6	-	-	-		
92	OHX	1	3472	-	0,6,6	-	-	-		
92	OHX	1	3566	36	0,6,6	-	-	-		
92	OHX	1	3409	-	0,6,6	-	-	-		
92	OHX	5	3545	-	0,6,6	-	-	-		
92	OHX	5	3637	85	0,6,6	-	-	-		
92	OHX	1	3668	-	0,6,6	-	-	-		
92	OHX	2	2012	1	0,6,6	-	-	-		
92	OHX	5	3747	85	0,6,6	-	-	-		
92	OHX	3	206	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	5	3485	85	0,6,6	-	-	-		
92	OHX	5	3502	-	0,6,6	-	-	-		
92	OHX	1	3459	-	0,6,6	-	-	-		
92	OHX	1	3702	-	0,6,6	-	-	-		
92	OHX	1	3581	93	0,6,6	-	-	-		
92	OHX	5	3721	85	0,6,6	-	-	-		
92	OHX	2	1985	-	0,6,6	-	-	-		
92	OHX	2	1997	-	0,6,6	-	-	-		
92	OHX	5	3535	85	0,6,6	-	-	-		
92	OHX	5	3655	-	0,6,6	-	-	-		
92	OHX	5	3740	-	0,6,6	-	-	-		
92	OHX	1	3622	-	0,6,6	-	-	-		
92	OHX	M5	301	-	0,6,6	-	-	-		
92	OHX	1	3646	-	0,6,6	-	-	-		
92	OHX	5	3739	-	0,6,6	-	-	-		
92	OHX	1	3593	-	0,6,6	-	-	-		
92	OHX	5	3617	-	0,6,6	-	-	-		
92	OHX	2	1935	-	0,6,6	-	-	-		
92	OHX	1	3437	-	0,6,6	-	-	-		
92	OHX	1	3454	-	0,6,6	-	-	-		
92	OHX	1	3575	-	0,6,6	-	-	-		
92	OHX	5	3487	-	0,6,6	-	-	-		
92	OHX	1	3647	-	0,6,6	-	-	-		
92	OHX	1	3535	-	0,6,6	-	-	-		
92	OHX	5	3437	85	0,6,6	-	-	-		
92	OHX	2	1999	-	0,6,6	-	-	-		
92	OHX	1	3462	-	0,6,6	-	-	-		
92	OHX	6	2048	80	0,6,6	-	-	-		
92	OHX	5	3678	85	0,6,6	-	-	-		
92	OHX	6	1916	-	0,6,6	-	-	-		
96	LEU	1	3402	95	5,7,8	0.43	0	5,8,10	0.61	0
92	OHX	5	3531	85	0,6,6	-	-	-		
92	OHX	sR	401	-	0,6,6	-	-	-		
92	OHX	5	3498	85	0,6,6	-	-	-		
92	OHX	1	3494	36	0,6,6	-	-	-		
92	OHX	2	1907	-	0,6,6	-	-	-		
92	OHX	1	3512	36	0,6,6	-	-	-		
92	OHX	1	3680	-	0,6,6	-	-	-		
92	OHX	6	1952	80	0,6,6	-	-	-		
92	OHX	5	3527	85	0,6,6	-	-	-		
92	OHX	5	3549	-	0,6,6	-	-	-		
92	OHX	5	3632	-	0,6,6	-	-	-		
92	OHX	5	3633	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	5	3687	-	0,6,6	-	-	-		
92	OHX	1	3549	-	0,6,6	-	-	-		
92	OHX	5	3565	85	0,6,6	-	-	-		
92	OHX	1	3531	-	0,6,6	-	-	-		
92	OHX	6	1921	80	0,6,6	-	-	-		
92	OHX	1	3508	-	0,6,6	-	-	-		
92	OHX	5	3514	85	0,6,6	-	-	-		
92	OHX	1	3705	-	0,6,6	-	-	-		
92	OHX	5	3576	-	0,6,6	-	-	-		
92	OHX	1	3685	-	0,6,6	-	-	-		
92	OHX	5	3729	85	0,6,6	-	-	-		
92	OHX	5	3596	85	0,6,6	-	-	-		
92	OHX	1	3727	36	0,6,6	-	-	-		
92	OHX	5	3407	-	0,6,6	-	-	-		
92	OHX	5	3499	85	0,6,6	-	-	-		
92	OHX	5	3425	-	0,6,6	-	-	-		
92	OHX	5	3566	-	0,6,6	-	-	-		
92	OHX	5	3583	-	0,6,6	-	-	-		
92	OHX	6	1934	-	0,6,6	-	-	-		
92	OHX	6	2057	80	0,6,6	-	-	-		
92	OHX	5	3615	85	0,6,6	-	-	-		
92	OHX	2	1979	-	0,6,6	-	-	-		
92	OHX	5	3560	93	0,6,6	-	-	-		
92	OHX	m0	302	-	0,6,6	-	-	-		
92	OHX	SR	401	-	0,6,6	-	-	-		
92	OHX	2	2007	-	0,6,6	-	-	-		
92	OHX	1	3669	-	0,6,6	-	-	-		
92	OHX	2	2017	-	0,6,6	-	-	-		
92	OHX	1	3416	-	0,6,6	-	-	-		
92	OHX	1	3488	-	0,6,6	-	-	-		
92	OHX	2	1919	-	0,6,6	-	-	-		
92	OHX	5	3742	-	0,6,6	-	-	-		
92	OHX	2	1952	1	0,6,6	-	-	-		
92	OHX	1	3659	-	0,6,6	-	-	-		
92	OHX	4	203	-	0,6,6	-	-	-		
92	OHX	1	3523	-	0,6,6	-	-	-		
92	OHX	6	1970	80	0,6,6	-	-	-		
92	OHX	5	3533	85	0,6,6	-	-	-		
92	OHX	5	3653	85	0,6,6	-	-	-		
92	OHX	2	1946	-	0,6,6	-	-	-		
92	OHX	1	3613	-	0,6,6	-	-	-		
92	OHX	1	3469	-	0,6,6	-	-	-		
92	OHX	6	1981	80	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	6	1974	80	0,6,6	-	-	-		
92	OHX	5	3594	-	0,6,6	-	-	-		
92	OHX	6	2004	-	0,6,6	-	-	-		
92	OHX	1	3419	36	0,6,6	-	-	-		
92	OHX	1	3556	-	0,6,6	-	-	-		
92	OHX	5	3715	85	0,6,6	-	-	-		
92	OHX	1	3561	-	0,6,6	-	-	-		
92	OHX	5	3539	85	0,6,6	-	-	-		
92	OHX	5	3474	85	0,6,6	-	-	-		
92	OHX	1	3428	-	0,6,6	-	-	-		
92	OHX	6	2023	80	0,6,6	-	-	-		
92	OHX	5	3472	85	0,6,6	-	-	-		
92	OHX	5	3564	85	0,6,6	-	-	-		
92	OHX	2	2024	-	0,6,6	-	-	-		
92	OHX	2	1911	-	0,6,6	-	-	-		
92	OHX	5	3682	85	0,6,6	-	-	-		
92	OHX	5	3598	85	0,6,6	-	-	-		
92	OHX	2	2010	-	0,6,6	-	-	-		
92	OHX	5	3696	85	0,6,6	-	-	-		
92	OHX	6	2056	80	0,6,6	-	-	-		
92	OHX	5	3649	-	0,6,6	-	-	-		
92	OHX	5	3414	93	0,6,6	-	-	-		
92	OHX	1	3704	93	0,6,6	-	-	-		
92	OHX	2	1932	-	0,6,6	-	-	-		
92	OHX	5	3600	85	0,6,6	-	-	-		
92	OHX	1	3632	-	0,6,6	-	-	-		
92	OHX	1	3578	-	0,6,6	-	-	-		
92	OHX	6	1969	93	0,6,6	-	-	-		
92	OHX	5	3460	85	0,6,6	-	-	-		
92	OHX	1	3415	-	0,6,6	-	-	-		
92	OHX	1	3546	-	0,6,6	-	-	-		
92	OHX	1	3465	-	0,6,6	-	-	-		
92	OHX	5	3529	85	0,6,6	-	-	-		
92	OHX	2	1918	-	0,6,6	-	-	-		
92	OHX	2	1953	-	0,6,6	-	-	-		
92	OHX	1	3484	-	0,6,6	-	-	-		
92	OHX	2	1959	-	0,6,6	-	-	-		
92	OHX	1	3591	-	0,6,6	-	-	-		
92	OHX	5	3602	-	0,6,6	-	-	-		
92	OHX	2	2032	-	0,6,6	-	-	-		
92	OHX	m0	303	-	0,6,6	-	-	-		
92	OHX	1	3475	-	0,6,6	-	-	-		
92	OHX	2	1917	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	5	3519	-	0,6,6	-	-	-		
92	OHX	6	1968	80	0,6,6	-	-	-		
92	OHX	5	3624	-	0,6,6	-	-	-		
92	OHX	1	3560	-	0,6,6	-	-	-		
92	OHX	1	3714	-	0,6,6	-	-	-		
92	OHX	1	3633	-	0,6,6	-	-	-		
92	OHX	1	3584	-	0,6,6	-	-	-		
92	OHX	6	1963	-	0,6,6	-	-	-		
92	OHX	5	3490	85	0,6,6	-	-	-		
92	OHX	1	3569	-	0,6,6	-	-	-		
92	OHX	6	1984	-	0,6,6	-	-	-		
92	OHX	5	3532	85	0,6,6	-	-	-		
92	OHX	5	3593	-	0,6,6	-	-	-		
92	OHX	6	1950	-	0,6,6	-	-	-		
92	OHX	2	2027	-	0,6,6	-	-	-		
92	OHX	1	3570	-	0,6,6	-	-	-		
92	OHX	6	2002	80	0,6,6	-	-	-		
92	OHX	5	3657	85	0,6,6	-	-	-		
92	OHX	5	3714	85	0,6,6	-	-	-		
92	OHX	1	3500	-	0,6,6	-	-	-		
92	OHX	6	2058	-	0,6,6	-	-	-		
92	OHX	5	3650	-	0,6,6	-	-	-		
92	OHX	5	3603	-	0,6,6	-	-	-		
92	OHX	2	1969	1	0,6,6	-	-	-		
92	OHX	5	3599	85	0,6,6	-	-	-		
92	OHX	O4	201	-	0,6,6	-	-	-		
92	OHX	2	1928	-	0,6,6	-	-	-		
92	OHX	1	3533	-	0,6,6	-	-	-		
92	OHX	2	1945	-	0,6,6	-	-	-		
92	OHX	1	3574	-	0,6,6	-	-	-		
92	OHX	5	3618	-	0,6,6	-	-	-		
92	OHX	5	3702	-	0,6,6	-	-	-		
96	LEU	5	3402	95	5,7,8	0.44	0	5,8,10	0.60	0
92	OHX	5	3666	85	0,6,6	-	-	-		
92	OHX	1	3517	-	0,6,6	-	-	-		
92	OHX	5	3489	-	0,6,6	-	-	-		
92	OHX	6	1925	-	0,6,6	-	-	-		
92	OHX	2	1931	-	0,6,6	-	-	-		
92	OHX	1	3450	-	0,6,6	-	-	-		
92	OHX	5	3621	-	0,6,6	-	-	-		
92	OHX	6	1937	-	0,6,6	-	-	-		
92	OHX	1	3671	-	0,6,6	-	-	-		
92	OHX	1	3724	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	5	3562	-	0,6,6	-	-	-		
92	OHX	1	3520	-	0,6,6	-	-	-		
92	OHX	1	3525	-	0,6,6	-	-	-		
92	OHX	2	1998	-	0,6,6	-	-	-		
92	OHX	4	207	-	0,6,6	-	-	-		
92	OHX	1	3653	93	0,6,6	-	-	-		
92	OHX	1	3412	-	0,6,6	-	-	-		
92	OHX	6	1904	-	0,6,6	-	-	-		
92	OHX	5	3578	85	0,6,6	-	-	-		
92	OHX	1	3440	93	0,6,6	-	-	-		
92	OHX	5	3403	85	0,6,6	-	-	-		
92	OHX	S8	301	-	0,6,6	-	-	-		
92	OHX	6	2031	80	0,6,6	-	-	-		
92	OHX	5	3610	-	0,6,6	-	-	-		
95	PHE	1	3401	96	10,11,12	1.23	1 (10%)	10,13,15	0.62	0
92	OHX	5	3416	85	0,6,6	-	-	-		
92	OHX	5	3457	-	0,6,6	-	-	-		
92	OHX	5	3463	-	0,6,6	-	-	-		
92	OHX	5	3652	93	0,6,6	-	-	-		
92	OHX	1	3526	-	0,6,6	-	-	-		
92	OHX	6	1956	-	0,6,6	-	-	-		
92	OHX	6	1919	80	0,6,6	-	-	-		
92	OHX	3	203	-	0,6,6	-	-	-		
92	OHX	1	3667	-	0,6,6	-	-	-		
92	OHX	2	1956	-	0,6,6	-	-	-		
92	OHX	2	2006	-	0,6,6	-	-	-		
92	OHX	2	1951	-	0,6,6	-	-	-		
92	OHX	1	3597	-	0,6,6	-	-	-		
92	OHX	1	3697	36	0,6,6	-	-	-		
92	OHX	5	3471	85	0,6,6	-	-	-		
92	OHX	1	3503	-	0,6,6	-	-	-		
92	OHX	6	1948	80	0,6,6	-	-	-		
92	OHX	m8	201	-	0,6,6	-	-	-		
92	OHX	5	3732	-	0,6,6	-	-	-		
92	OHX	4	204	-	0,6,6	-	-	-		
92	OHX	1	3426	-	0,6,6	-	-	-		
92	OHX	6	1979	-	0,6,6	-	-	-		
92	OHX	5	3540	85	0,6,6	-	-	-		
92	OHX	5	3703	-	0,6,6	-	-	-		
92	OHX	2	1988	-	0,6,6	-	-	-		
92	OHX	M7	201	-	0,6,6	-	-	-		
92	OHX	5	3588	85	0,6,6	-	-	-		
92	OHX	6	2033	80	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	1	3651	-	0,6,6	-	-	-		
92	OHX	2	1933	-	0,6,6	-	-	-		
92	OHX	6	1911	-	0,6,6	-	-	-		
92	OHX	2	1992	-	0,6,6	-	-	-		
92	OHX	1	3612	-	0,6,6	-	-	-		
92	OHX	1	3643	-	0,6,6	-	-	-		
92	OHX	1	3707	-	0,6,6	-	-	-		
92	OHX	5	3431	85	0,6,6	-	-	-		
92	OHX	2	1948	-	0,6,6	-	-	-		
92	OHX	5	3674	85	0,6,6	-	-	-		
92	OHX	6	2010	80	0,6,6	-	-	-		
92	OHX	5	3686	-	0,6,6	-	-	-		
92	OHX	5	3651	-	0,6,6	-	-	-		
92	OHX	1	3547	-	0,6,6	-	-	-		
92	OHX	1	3672	-	0,6,6	-	-	-		
92	OHX	6	2049	-	0,6,6	-	-	-		
92	OHX	M5	302	-	0,6,6	-	-	-		
92	OHX	6	2053	80	0,6,6	-	-	-		
92	OHX	5	3477	85	0,6,6	-	-	-		
92	OHX	5	3731	93	0,6,6	-	-	-		
92	OHX	5	3421	-	0,6,6	-	-	-		
92	OHX	5	3547	-	0,6,6	-	-	-		
92	OHX	1	3545	-	0,6,6	-	-	-		
92	OHX	1	3637	36	0,6,6	-	-	-		
92	OHX	1	3476	-	0,6,6	-	-	-		
92	OHX	6	2001	-	0,6,6	-	-	-		
92	OHX	1	3553	-	0,6,6	-	-	-		
92	OHX	1	3614	-	0,6,6	-	-	-		
92	OHX	5	3608	-	0,6,6	-	-	-		
92	OHX	5	3713	85	0,6,6	-	-	-		
92	OHX	1	3502	-	0,6,6	-	-	-		
92	OHX	5	3567	-	0,6,6	-	-	-		
92	OHX	2	2039	1	0,6,6	-	-	-		
92	OHX	3	201	-	0,6,6	-	-	-		
92	OHX	2	1908	-	0,6,6	-	-	-		
92	OHX	5	3614	-	0,6,6	-	-	-		
92	OHX	2	1960	-	0,6,6	-	-	-		
92	OHX	1	3664	-	0,6,6	-	-	-		
92	OHX	6	2046	-	0,6,6	-	-	-		
92	OHX	M0	301	-	0,6,6	-	-	-		
92	OHX	6	2059	-	0,6,6	-	-	-		
92	OHX	5	3669	85	0,6,6	-	-	-		
92	OHX	5	3664	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	5	3620	-	0,6,6	-	-	-		
92	OHX	1	3708	-	0,6,6	-	-	-		
92	OHX	1	3617	-	0,6,6	-	-	-		
92	OHX	5	3442	-	0,6,6	-	-	-		
92	OHX	5	3695	-	0,6,6	-	-	-		
92	OHX	8	204	-	0,6,6	-	-	-		
92	OHX	1	3551	-	0,6,6	-	-	-		
92	OHX	6	2039	80	0,6,6	-	-	-		
92	OHX	l3	401	-	0,6,6	-	-	-		
92	OHX	5	3524	85	0,6,6	-	-	-		
92	OHX	6	2006	80	0,6,6	-	-	-		
92	OHX	5	3681	85	0,6,6	-	-	-		
92	OHX	5	3478	-	0,6,6	-	-	-		
92	OHX	5	3718	85	0,6,6	-	-	-		
92	OHX	3	202	-	0,6,6	-	-	-		
92	OHX	2	1947	-	0,6,6	-	-	-		
92	OHX	2	1943	-	0,6,6	-	-	-		
92	OHX	C7	201	-	0,6,6	-	-	-		
92	OHX	1	3583	-	0,6,6	-	-	-		
92	OHX	1	3590	-	0,6,6	-	-	-		
92	OHX	1	3552	-	0,6,6	-	-	-		
92	OHX	5	3528	-	0,6,6	-	-	-		
92	OHX	8	206	38	0,6,6	-	-	-		
92	OHX	6	2009	-	0,6,6	-	-	-		
92	OHX	1	3482	93	0,6,6	-	-	-		
92	OHX	1	3687	-	0,6,6	-	-	-		
92	OHX	1	3527	-	0,6,6	-	-	-		
92	OHX	1	3679	-	0,6,6	-	-	-		
92	OHX	1	3478	-	0,6,6	-	-	-		
92	OHX	5	3590	85	0,6,6	-	-	-		
92	OHX	5	3592	85	0,6,6	-	-	-		
92	OHX	7	202	-	0,6,6	-	-	-		
92	OHX	1	3403	-	0,6,6	-	-	-		
92	OHX	1	3470	-	0,6,6	-	-	-		
92	OHX	1	3684	93	0,6,6	-	-	-		
92	OHX	1	3447	-	0,6,6	-	-	-		
92	OHX	7	212	-	0,6,6	-	-	-		
92	OHX	M6	201	-	0,6,6	-	-	-		
92	OHX	1	3466	-	0,6,6	-	-	-		
92	OHX	5	3684	85	0,6,6	-	-	-		
92	OHX	1	3596	-	0,6,6	-	-	-		
92	OHX	6	2043	-	0,6,6	-	-	-		
92	OHX	1	3407	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	5	3534	85	0,6,6	-	-	-		
92	OHX	1	3499	-	0,6,6	-	-	-		
92	OHX	5	3556	85	0,6,6	-	-	-		
92	OHX	3	207	-	0,6,6	-	-	-		
92	OHX	1	3532	-	0,6,6	-	-	-		
92	OHX	5	3538	-	0,6,6	-	-	-		
92	OHX	5	3660	85,93	0,6,6	-	-	-		
92	OHX	1	3471	-	0,6,6	-	-	-		
92	OHX	5	3455	93	0,6,6	-	-	-		
92	OHX	1	3510	-	0,6,6	-	-	-		
92	OHX	2	2023	93	0,6,6	-	-	-		
92	OHX	2	1977	-	0,6,6	-	-	-		
92	OHX	6	1993	80	0,6,6	-	-	-		
92	OHX	6	2024	-	0,6,6	-	-	-		
92	OHX	5	3555	-	0,6,6	-	-	-		
92	OHX	5	3735	-	0,6,6	-	-	-		
92	OHX	1	3642	93	0,6,6	-	-	-		
92	OHX	1	3511	-	0,6,6	-	-	-		
92	OHX	4	213	-	0,6,6	-	-	-		
92	OHX	6	2000	80	0,6,6	-	-	-		
92	OHX	6	2055	80,93	0,6,6	-	-	-		
92	OHX	5	3433	-	0,6,6	-	-	-		
92	OHX	1	3507	-	0,6,6	-	-	-		
92	OHX	1	3631	-	0,6,6	-	-	-		
92	OHX	1	3644	93	0,6,6	-	-	-		
92	OHX	5	3496	-	0,6,6	-	-	-		
92	OHX	6	2034	-	0,6,6	-	-	-		
92	OHX	5	3558	-	0,6,6	-	-	-		
92	OHX	6	1915	80	0,6,6	-	-	-		
92	OHX	1	3406	-	0,6,6	-	-	-		
92	OHX	5	3480	85	0,6,6	-	-	-		
92	OHX	8	211	-	0,6,6	-	-	-		
92	OHX	2	1983	-	0,6,6	-	-	-		
92	OHX	5	3542	85	0,6,6	-	-	-		
92	OHX	2	1958	-	0,6,6	-	-	-		
92	OHX	1	3594	-	0,6,6	-	-	-		
92	OHX	5	3694	-	0,6,6	-	-	-		
92	OHX	5	3406	-	0,6,6	-	-	-		
92	OHX	5	3585	85	0,6,6	-	-	-		
92	OHX	2	2047	1	0,6,6	-	-	-		
92	OHX	1	3539	-	0,6,6	-	-	-		
92	OHX	5	3500	-	0,6,6	-	-	-		
92	OHX	2	1967	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	5	3536	-	0,6,6	-	-	-		
92	OHX	1	3438	-	0,6,6	-	-	-		
92	OHX	3	204	-	0,6,6	-	-	-		
92	OHX	1	3629	36	0,6,6	-	-	-		
92	OHX	1	3630	-	0,6,6	-	-	-		
92	OHX	6	1989	80	0,6,6	-	-	-		
92	OHX	1	3564	36	0,6,6	-	-	-		
92	OHX	L4	401	-	0,6,6	-	-	-		
92	OHX	1	3598	93	0,6,6	-	-	-		
92	OHX	1	3718	-	0,6,6	-	-	-		
92	OHX	5	3727	-	0,6,6	-	-	-		
92	OHX	1	3696	-	0,6,6	-	-	-		
92	OHX	5	3625	85	0,6,6	-	-	-		
92	OHX	1	3420	-	0,6,6	-	-	-		
92	OHX	2	1909	-	0,6,6	-	-	-		
92	OHX	1	3600	-	0,6,6	-	-	-		
92	OHX	5	3704	85	0,6,6	-	-	-		
92	OHX	5	3420	-	0,6,6	-	-	-		
92	OHX	6	1944	80	0,6,6	-	-	-		
92	OHX	1	3720	-	0,6,6	-	-	-		
92	OHX	2	2026	-	0,6,6	-	-	-		
92	OHX	2	1940	-	0,6,6	-	-	-		
92	OHX	2	2013	-	0,6,6	-	-	-		
92	OHX	6	2003	-	0,6,6	-	-	-		
92	OHX	5	3725	-	0,6,6	-	-	-		
92	OHX	1	3529	36	0,6,6	-	-	-		
92	OHX	6	1945	80	0,6,6	-	-	-		
92	OHX	5	3443	37	0,6,6	-	-	-		
92	OHX	1	3706	-	0,6,6	-	-	-		
92	OHX	5	3492	-	0,6,6	-	-	-		
92	OHX	4	205	38	0,6,6	-	-	-		
92	OHX	1	3602	-	0,6,6	-	-	-		
92	OHX	6	1986	-	0,6,6	-	-	-		
92	OHX	1	3577	-	0,6,6	-	-	-		
92	OHX	5	3611	-	0,6,6	-	-	-		
92	OHX	L6	201	93	0,6,6	-	-	-		
92	OHX	2	1963	1	0,6,6	-	-	-		
92	OHX	5	3513	85	0,6,6	-	-	-		
92	OHX	5	3543	85	0,6,6	-	-	-		
92	OHX	5	3642	85	0,6,6	-	-	-		
92	OHX	1	3548	-	0,6,6	-	-	-		
92	OHX	1	3624	-	0,6,6	-	-	-		
92	OHX	1	3606	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	1	3550	-	0,6,6	-	-	-		
92	OHX	5	3495	85,93	0,6,6	-	-	-		
92	OHX	5	3746	85,93	0,6,6	-	-	-		
92	OHX	1	3490	-	0,6,6	-	-	-		
92	OHX	2	1993	-	0,6,6	-	-	-		
92	OHX	5	3734	-	0,6,6	-	-	-		
92	OHX	5	3544	85	0,6,6	-	-	-		
92	OHX	C8	201	36,93	0,6,6	-	-	-		
92	OHX	6	1972	80	0,6,6	-	-	-		
92	OHX	1	3657	-	0,6,6	-	-	-		
92	OHX	8	209	38	0,6,6	-	-	-		
92	OHX	2	2018	-	0,6,6	-	-	-		
92	OHX	6	1955	80	0,6,6	-	-	-		
92	OHX	1	3477	-	0,6,6	-	-	-		
92	OHX	6	1977	80	0,6,6	-	-	-		
92	OHX	1	3411	-	0,6,6	-	-	-		
92	OHX	1	3603	-	0,6,6	-	-	-		
92	OHX	1	3700	-	0,6,6	-	-	-		
92	OHX	6	1943	-	0,6,6	-	-	-		
92	OHX	2	2034	-	0,6,6	-	-	-		
92	OHX	2	2044	-	0,6,6	-	-	-		
92	OHX	1	3628	-	0,6,6	-	-	-		
92	OHX	1	3645	93	0,6,6	-	-	-		
92	OHX	6	1965	-	0,6,6	-	-	-		
92	OHX	o7	503	-	0,6,6	-	-	-		
92	OHX	1	3530	36	0,6,6	-	-	-		
92	OHX	1	3666	-	0,6,6	-	-	-		
92	OHX	6	1999	80	0,6,6	-	-	-		
92	OHX	3	209	-	0,6,6	-	-	-		
92	OHX	1	3713	-	0,6,6	-	-	-		
92	OHX	1	3585	-	0,6,6	-	-	-		
92	OHX	5	3441	85	0,6,6	-	-	-		
92	OHX	1	3498	36	0,6,6	-	-	-		
92	OHX	1	3621	36	0,6,6	-	-	-		
92	OHX	5	3465	-	0,6,6	-	-	-		
92	OHX	1	3562	-	0,6,6	-	-	-		
92	OHX	s4	301	-	0,6,6	-	-	-		
92	OHX	5	3662	-	0,6,6	-	-	-		
92	OHX	2	1942	-	0,6,6	-	-	-		
92	OHX	2	2028	-	0,6,6	-	-	-		
92	OHX	1	3563	-	0,6,6	-	-	-		
92	OHX	5	3581	93	0,6,6	-	-	-		
92	OHX	1	3489	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	1	3711	-	0,6,6	-	-	-		
92	OHX	4	216	-	0,6,6	-	-	-		
92	OHX	5	3563	85	0,6,6	-	-	-		
92	OHX	5	3719	93	0,6,6	-	-	-		
92	OHX	6	1926	80	0,6,6	-	-	-		
92	OHX	5	3537	93	0,6,6	-	-	-		
92	OHX	2	1937	-	0,6,6	-	-	-		
92	OHX	1	3463	-	0,6,6	-	-	-		
92	OHX	6	1906	-	0,6,6	-	-	-		
92	OHX	6	2051	80	0,6,6	-	-	-		
92	OHX	5	3726	85	0,6,6	-	-	-		
92	OHX	5	3748	93	0,6,6	-	-	-		
92	OHX	5	3553	85	0,6,6	-	-	-		
92	OHX	5	3698	-	0,6,6	-	-	-		
92	OHX	1	3588	36	0,6,6	-	-	-		
92	OHX	1	3610	-	0,6,6	-	-	-		
92	OHX	1	3528	-	0,6,6	-	-	-		
92	OHX	1	3701	36	0,6,6	-	-	-		
92	OHX	5	3636	-	0,6,6	-	-	-		
92	OHX	2	1901	-	0,6,6	-	-	-		
92	OHX	5	3631	85	0,6,6	-	-	-		
92	OHX	5	3570	-	0,6,6	-	-	-		
92	OHX	6	2025	80	0,6,6	-	-	-		
92	OHX	6	1922	80	0,6,6	-	-	-		
92	OHX	8	210	38	0,6,6	-	-	-		
92	OHX	5	3728	85	0,6,6	-	-	-		
92	OHX	6	1996	80	0,6,6	-	-	-		
92	OHX	6	2038	-	0,6,6	-	-	-		
92	OHX	o3	201	-	0,6,6	-	-	-		
92	OHX	1	3673	-	0,6,6	-	-	-		
92	OHX	5	3619	-	0,6,6	-	-	-		
92	OHX	5	3730	-	0,6,6	-	-	-		
92	OHX	5	3584	85	0,6,6	-	-	-		
92	OHX	4	221	-	0,6,6	-	-	-		
92	OHX	5	3629	85	0,6,6	-	-	-		
92	OHX	1	3703	-	0,6,6	-	-	-		
92	OHX	5	3430	-	0,6,6	-	-	-		
92	OHX	5	3582	-	0,6,6	-	-	-		
92	OHX	2	1938	-	0,6,6	-	-	-		
92	OHX	1	3427	36	0,6,6	-	-	-		
92	OHX	1	3431	93	0,6,6	-	-	-		
92	OHX	1	3674	-	0,6,6	-	-	-		
92	OHX	6	1936	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	2	2042	-	0,6,6	-	-	-		
92	OHX	L3	401	-	0,6,6	-	-	-		
92	OHX	1	3513	-	0,6,6	-	-	-		
92	OHX	1	3479	-	0,6,6	-	-	-		
92	OHX	1	3640	93	0,6,6	-	-	-		
92	OHX	6	1902	80	0,6,6	-	-	-		
92	OHX	5	3440	-	0,6,6	-	-	-		
92	OHX	5	3451	-	0,6,6	-	-	-		
92	OHX	1	3649	-	0,6,6	-	-	-		
92	OHX	5	3733	-	0,6,6	-	-	-		
92	OHX	2	1981	-	0,6,6	-	-	-		
92	OHX	6	1940	80	0,6,6	-	-	-		
92	OHX	1	3567	-	0,6,6	-	-	-		
92	OHX	5	3577	85	0,6,6	-	-	-		
92	OHX	1	3627	36	0,6,6	-	-	-		
92	OHX	2	1923	1	0,6,6	-	-	-		
92	OHX	1	3417	-	0,6,6	-	-	-		
92	OHX	1	3618	93	0,6,6	-	-	-		
92	OHX	2	1982	-	0,6,6	-	-	-		
92	OHX	5	3736	85	0,6,6	-	-	-		
92	OHX	1	3663	-	0,6,6	-	-	-		
92	OHX	1	3726	-	0,6,6	-	-	-		
92	OHX	6	1985	-	0,6,6	-	-	-		
92	OHX	6	1920	80	0,6,6	-	-	-		
92	OHX	2	1973	-	0,6,6	-	-	-		
92	OHX	6	1990	-	0,6,6	-	-	-		
92	OHX	5	3417	-	0,6,6	-	-	-		
92	OHX	5	3550	85	0,6,6	-	-	-		
92	OHX	1	3445	-	0,6,6	-	-	-		
92	OHX	5	3481	-	0,6,6	-	-	-		
92	OHX	o7	502	-	0,6,6	-	-	-		
92	OHX	6	2050	80	0,6,6	-	-	-		
92	OHX	1	3695	36	0,6,6	-	-	-		
92	OHX	5	3464	85	0,6,6	-	-	-		
92	OHX	1	3586	-	0,6,6	-	-	-		
92	OHX	6	1935	80	0,6,6	-	-	-		
92	OHX	6	2032	-	0,6,6	-	-	-		
92	OHX	1	3661	-	0,6,6	-	-	-		
92	OHX	1	3524	-	0,6,6	-	-	-		
92	OHX	1	3681	-	0,6,6	-	-	-		
92	OHX	5	3526	93	0,6,6	-	-	-		
92	OHX	2	1941	-	0,6,6	-	-	-		
92	OHX	4	201	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	S9	201	-	0,6,6	-	-	-		
92	OHX	5	3605	-	0,6,6	-	-	-		
92	OHX	m9	201	-	0,6,6	-	-	-		
92	OHX	1	3514	-	0,6,6	-	-	-		
92	OHX	5	3683	85	0,6,6	-	-	-		
92	OHX	1	3408	-	0,6,6	-	-	-		
92	OHX	5	3646	-	0,6,6	-	-	-		
92	OHX	1	3592	-	0,6,6	-	-	-		
92	OHX	1	3421	-	0,6,6	-	-	-		
92	OHX	C3	201	-	0,6,6	-	-	-		
92	OHX	5	3616	-	0,6,6	-	-	-		
92	OHX	5	3408	85	0,6,6	-	-	-		
92	OHX	6	1987	80	0,6,6	-	-	-		
92	OHX	1	3636	-	0,6,6	-	-	-		
92	OHX	5	3647	-	0,6,6	-	-	-		
92	OHX	2	2019	-	0,6,6	-	-	-		
92	OHX	5	3712	85	0,6,6	-	-	-		
92	OHX	5	3716	-	0,6,6	-	-	-		
92	OHX	1	3689	-	0,6,6	-	-	-		
92	OHX	4	202	-	0,6,6	-	-	-		
92	OHX	6	1967	80	0,6,6	-	-	-		
92	OHX	2	1990	-	0,6,6	-	-	-		
92	OHX	2	2031	-	0,6,6	-	-	-		
92	OHX	1	3534	-	0,6,6	-	-	-		
92	OHX	1	3660	-	0,6,6	-	-	-		
92	OHX	6	1995	-	0,6,6	-	-	-		
92	OHX	2	1934	-	0,6,6	-	-	-		
92	OHX	1	3504	-	0,6,6	-	-	-		
92	OHX	4	212	-	0,6,6	-	-	-		
92	OHX	5	3689	-	0,6,6	-	-	-		
92	OHX	1	3455	-	0,6,6	-	-	-		
92	OHX	1	3587	-	0,6,6	-	-	-		
92	OHX	5	3501	85	0,6,6	-	-	-		
92	OHX	5	3690	93	0,6,6	-	-	-		
92	OHX	8	207	38	0,6,6	-	-	-		
92	OHX	5	3449	-	0,6,6	-	-	-		
92	OHX	1	3616	36	0,6,6	-	-	-		
92	OHX	5	3607	-	0,6,6	-	-	-		
92	OHX	2	2041	-	0,6,6	-	-	-		
92	OHX	1	3650	-	0,6,6	-	-	-		
92	OHX	3	208	-	0,6,6	-	-	-		
92	OHX	5	3504	-	0,6,6	-	-	-		
92	OHX	1	3444	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	2	1962	-	0,6,6	-	-	-		
92	OHX	m0	301	-	0,6,6	-	-	-		
92	OHX	5	3705	-	0,6,6	-	-	-		
92	OHX	6	1997	-	0,6,6	-	-	-		
92	OHX	1	3487	-	0,6,6	-	-	-		
92	OHX	1	3495	-	0,6,6	-	-	-		
92	OHX	5	3627	-	0,6,6	-	-	-		
92	OHX	5	3548	85,93	0,6,6	-	-	-		
92	OHX	1	3418	-	0,6,6	-	-	-		
92	OHX	2	1978	-	0,6,6	-	-	-		
92	OHX	5	3427	-	0,6,6	-	-	-		
92	OHX	2	1989	-	0,6,6	-	-	-		
92	OHX	1	3542	-	0,6,6	-	-	-		
92	OHX	O7	102	93	0,6,6	-	-	-		
92	OHX	1	3694	-	0,6,6	-	-	-		
92	OHX	6	2012	-	0,6,6	-	-	-		
92	OHX	5	3432	-	0,6,6	-	-	-		
92	OHX	m5	302	-	0,6,6	-	-	-		
92	OHX	5	3634	-	0,6,6	-	-	-		
92	OHX	1	3536	-	0,6,6	-	-	-		
92	OHX	2	2045	-	0,6,6	-	-	-		
92	OHX	6	1914	80	0,6,6	-	-	-		
92	OHX	2	1920	-	0,6,6	-	-	-		
92	OHX	6	1966	80	0,6,6	-	-	-		
92	OHX	5	3488	85	0,6,6	-	-	-		
92	OHX	5	3448	-	0,6,6	-	-	-		
92	OHX	5	3604	85	0,6,6	-	-	-		
92	OHX	1	3537	-	0,6,6	-	-	-		
92	OHX	1	3480	-	0,6,6	-	-	-		
92	OHX	1	3699	-	0,6,6	-	-	-		
92	OHX	4	209	-	0,6,6	-	-	-		
92	OHX	6	1938	-	0,6,6	-	-	-		
92	OHX	6	1954	-	0,6,6	-	-	-		
92	OHX	5	3439	-	0,6,6	-	-	-		
92	OHX	2	1926	-	0,6,6	-	-	-		
92	OHX	c5	201	-	0,6,6	-	-	-		
92	OHX	5	3409	-	0,6,6	-	-	-		
92	OHX	5	3572	85	0,6,6	-	-	-		
92	OHX	1	3688	36	0,6,6	-	-	-		
92	OHX	6	1931	80	0,6,6	-	-	-		
92	OHX	2	1954	-	0,6,6	-	-	-		
92	OHX	1	3492	93	0,6,6	-	-	-		
92	OHX	1	3568	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	5	3579	-	0,6,6	-	-	-		
92	OHX	l5	301	-	0,6,6	-	-	-		
92	OHX	2	2005	-	0,6,6	-	-	-		
92	OHX	5	3589	85	0,6,6	-	-	-		
92	OHX	7	206	37	0,6,6	-	-	-		
92	OHX	1	3538	-	0,6,6	-	-	-		
92	OHX	6	1994	-	0,6,6	-	-	-		
92	OHX	6	1928	80	0,6,6	-	-	-		
92	OHX	1	3486	-	0,6,6	-	-	-		
92	OHX	6	1982	80	0,6,6	-	-	-		
92	OHX	6	2040	80	0,6,6	-	-	-		
92	OHX	5	3491	-	0,6,6	-	-	-		
92	OHX	c3	201	-	0,6,6	-	-	-		
92	OHX	5	3546	-	0,6,6	-	-	-		
92	OHX	2	2011	1	0,6,6	-	-	-		
92	OHX	5	3507	-	0,6,6	-	-	-		
92	OHX	4	206	38	0,6,6	-	-	-		
92	OHX	1	3544	-	0,6,6	-	-	-		
92	OHX	1	3433	-	0,6,6	-	-	-		
92	OHX	5	3741	-	0,6,6	-	-	-		
92	OHX	5	3609	-	0,6,6	-	-	-		
92	OHX	O3	201	-	0,6,6	-	-	-		
92	OHX	5	3410	-	0,6,6	-	-	-		
92	OHX	1	3620	-	0,6,6	-	-	-		
92	OHX	4	210	93	0,6,6	-	-	-		
92	OHX	4	219	-	0,6,6	-	-	-		
92	OHX	1	3580	-	0,6,6	-	-	-		
92	OHX	5	3435	-	0,6,6	-	-	-		
92	OHX	6	2008	-	0,6,6	-	-	-		
92	OHX	5	3691	-	0,6,6	-	-	-		
92	OHX	1	3655	-	0,6,6	-	-	-		
92	OHX	6	1930	80	0,6,6	-	-	-		
92	OHX	5	3429	85	0,6,6	-	-	-		
92	OHX	5	3468	-	0,6,6	-	-	-		
92	OHX	2	1914	-	0,6,6	-	-	-		
92	OHX	2	1994	-	0,6,6	-	-	-		
92	OHX	1	3662	-	0,6,6	-	-	-		
97	SPS	P	101	93	20,23,23	3.42	11 (55%)	24,30,30	4.20	12 (50%)
92	OHX	5	3482	85	0,6,6	-	-	-		
92	OHX	1	3604	-	0,6,6	-	-	-		
92	OHX	6	1957	80	0,6,6	-	-	-		
92	OHX	5	3511	85	0,6,6	-	-	-		
92	OHX	7	211	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	5	3574	-	0,6,6	-	-	-		
92	OHX	M8	201	-	0,6,6	-	-	-		
92	OHX	5	3557	-	0,6,6	-	-	-		
92	OHX	N9	101	-	0,6,6	-	-	-		
92	OHX	5	3483	-	0,6,6	-	-	-		
92	OHX	2	1913	-	0,6,6	-	-	-		
92	OHX	5	3658	85,93	0,6,6	-	-	-		
92	OHX	5	3452	-	0,6,6	-	-	-		
92	OHX	1	3509	36,93	0,6,6	-	-	-		
92	OHX	6	1918	80	0,6,6	-	-	-		
92	OHX	5	3493	85	0,6,6	-	-	-		
92	OHX	5	3423	85	0,6,6	-	-	-		
92	OHX	5	3510	85	0,6,6	-	-	-		
92	OHX	5	3559	-	0,6,6	-	-	-		
92	OHX	1	3565	-	0,6,6	-	-	-		
92	OHX	1	3448	36	0,6,6	-	-	-		
92	OHX	1	3728	-	0,6,6	-	-	-		
92	OHX	d4	201	-	0,6,6	-	-	-		
92	OHX	6	2036	80	0,6,6	-	-	-		
92	OHX	1	3485	-	0,6,6	-	-	-		
92	OHX	1	3639	-	0,6,6	-	-	-		
92	OHX	1	3619	93	0,6,6	-	-	-		
92	OHX	2	2048	-	0,6,6	-	-	-		
92	OHX	5	3486	-	0,6,6	-	-	-		
92	OHX	1	3730	36	0,6,6	-	-	-		
92	OHX	6	1953	80	0,6,6	-	-	-		
92	OHX	2	2016	-	0,6,6	-	-	-		
92	OHX	5	3458	85	0,6,6	-	-	-		
92	OHX	5	3676	-	0,6,6	-	-	-		
92	OHX	5	3723	85	0,6,6	-	-	-		
92	OHX	1	3497	-	0,6,6	-	-	-		
92	OHX	1	3635	-	0,6,6	-	-	-		
92	OHX	2	2043	1	0,6,6	-	-	-		
92	OHX	2	1984	-	0,6,6	-	-	-		
92	OHX	6	1946	-	0,6,6	-	-	-		
92	OHX	5	3466	-	0,6,6	-	-	-		
92	OHX	2	1995	-	0,6,6	-	-	-		
92	OHX	5	3456	85	0,6,6	-	-	-		
92	OHX	1	3601	-	0,6,6	-	-	-		
92	OHX	2	1936	1	0,6,6	-	-	-		
92	OHX	8	205	-	0,6,6	-	-	-		
92	OHX	1	3582	36	0,6,6	-	-	-		
92	OHX	2	2033	1,93	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	1	3683	36	0,6,6	-	-	-		
92	OHX	6	1973	80	0,6,6	-	-	-		
92	OHX	2	2014	-	0,6,6	-	-	-		
92	OHX	5	3744	-	0,6,6	-	-	-		
92	OHX	1	3609	-	0,6,6	-	-	-		
92	OHX	1	3410	-	0,6,6	-	-	-		
92	OHX	5	3628	-	0,6,6	-	-	-		
92	OHX	1	3686	-	0,6,6	-	-	-		
92	OHX	6	1951	80	0,6,6	-	-	-		
92	OHX	1	3712	36	0,6,6	-	-	-		
92	OHX	5	3413	-	0,6,6	-	-	-		
92	OHX	5	3552	85	0,6,6	-	-	-		
92	OHX	5	3426	-	0,6,6	-	-	-		
92	OHX	6	1905	-	0,6,6	-	-	-		
92	OHX	1	3501	-	0,6,6	-	-	-		
92	OHX	8	203	-	0,6,6	-	-	-		
92	OHX	1	3715	36	0,6,6	-	-	-		
92	OHX	5	3638	85	0,6,6	-	-	-		
92	OHX	1	3429	-	0,6,6	-	-	-		
92	OHX	1	3474	-	0,6,6	-	-	-		
98	8AN	p	102	91,93	22,24,25	1.49	4 (18%)	26,35,38	2.36	11 (42%)
92	OHX	5	3643	85	0,6,6	-	-	-		
92	OHX	4	208	-	0,6,6	-	-	-		
92	OHX	1	3442	-	0,6,6	-	-	-		
92	OHX	2	1966	1	0,6,6	-	-	-		
92	OHX	2	2050	1	0,6,6	-	-	-		
92	OHX	5	3672	-	0,6,6	-	-	-		
92	OHX	5	3462	-	0,6,6	-	-	-		
92	OHX	2	1905	-	0,6,6	-	-	-		
92	OHX	2	2002	-	0,6,6	-	-	-		
92	OHX	6	1992	-	0,6,6	-	-	-		
92	OHX	2	2004	-	0,6,6	-	-	-		
92	OHX	1	3658	-	0,6,6	-	-	-		
92	OHX	5	3411	-	0,6,6	-	-	-		
92	OHX	5	3445	-	0,6,6	-	-	-		
92	OHX	1	3414	-	0,6,6	-	-	-		
92	OHX	1	3464	-	0,6,6	-	-	-		
92	OHX	1	3432	-	0,6,6	-	-	-		
92	OHX	6	1976	80	0,6,6	-	-	-		
92	OHX	1	3677	93	0,6,6	-	-	-		
92	OHX	8	216	38	0,6,6	-	-	-		
92	OHX	1	3665	-	0,6,6	-	-	-		
92	OHX	1	3692	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	6	1910	-	0,6,6	-	-	-		
92	OHX	2	1904	1	0,6,6	-	-	-		
92	OHX	5	3438	-	0,6,6	-	-	-		
92	OHX	5	3469	85	0,6,6	-	-	-		
92	OHX	8	208	-	0,6,6	-	-	-		
92	OHX	5	3692	-	0,6,6	-	-	-		
92	OHX	2	1986	1	0,6,6	-	-	-		
92	OHX	6	1949	-	0,6,6	-	-	-		
92	OHX	1	3676	-	0,6,6	-	-	-		
92	OHX	6	2047	93	0,6,6	-	-	-		
92	OHX	5	3612	-	0,6,6	-	-	-		
92	OHX	5	3699	-	0,6,6	-	-	-		
92	OHX	8	201	-	0,6,6	-	-	-		
92	OHX	2	1910	-	0,6,6	-	-	-		
92	OHX	6	1991	80	0,6,6	-	-	-		
92	OHX	1	3571	-	0,6,6	-	-	-		
92	OHX	2	1927	-	0,6,6	-	-	-		
92	OHX	1	3605	93	0,6,6	-	-	-		
92	OHX	5	3745	-	0,6,6	-	-	-		
92	OHX	6	1912	-	0,6,6	-	-	-		
92	OHX	5	3630	-	0,6,6	-	-	-		
92	OHX	2	1949	-	0,6,6	-	-	-		
92	OHX	5	3461	85	0,6,6	-	-	-		
92	OHX	2	2049	-	0,6,6	-	-	-		
92	OHX	1	3404	-	0,6,6	-	-	-		
92	OHX	1	3722	-	0,6,6	-	-	-		
92	OHX	1	3690	-	0,6,6	-	-	-		
92	OHX	4	214	-	0,6,6	-	-	-		
92	OHX	1	3449	36	0,6,6	-	-	-		
92	OHX	1	3607	-	0,6,6	-	-	-		
92	OHX	2	1970	-	0,6,6	-	-	-		
92	OHX	6	2028	80	0,6,6	-	-	-		
92	OHX	2	1976	-	0,6,6	-	-	-		
92	OHX	5	3434	-	0,6,6	-	-	-		
92	OHX	5	3645	93	0,6,6	-	-	-		
92	OHX	5	3663	-	0,6,6	-	-	-		
92	OHX	5	3404	-	0,6,6	-	-	-		
92	OHX	2	1968	-	0,6,6	-	-	-		
92	OHX	5	3419	85,93	0,6,6	-	-	-		
92	OHX	5	3673	85	0,6,6	-	-	-		
92	OHX	6	1980	-	0,6,6	-	-	-		
92	OHX	O9	101	-	0,6,6	-	-	-		
92	OHX	5	3436	85	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	5	3688	-	0,6,6	-	-	-		
92	OHX	2	1915	-	0,6,6	-	-	-		
92	OHX	6	2022	-	0,6,6	-	-	-		
92	OHX	5	3639	-	0,6,6	-	-	-		
92	OHX	1	3648	-	0,6,6	-	-	-		
92	OHX	2	2008	-	0,6,6	-	-	-		
92	OHX	6	1901	-	0,6,6	-	-	-		
92	OHX	6	2021	-	0,6,6	-	-	-		
92	OHX	5	3551	85	0,6,6	-	-	-		
92	OHX	5	3701	-	0,6,6	-	-	-		
92	OHX	1	3543	-	0,6,6	-	-	-		
92	OHX	2	2046	-	0,6,6	-	-	-		
92	OHX	6	1909	80	0,6,6	-	-	-		
92	OHX	5	3648	-	0,6,6	-	-	-		
92	OHX	m5	301	-	0,6,6	-	-	-		
92	OHX	1	3481	-	0,6,6	-	-	-		
92	OHX	1	3576	36	0,6,6	-	-	-		
92	OHX	1	3506	-	0,6,6	-	-	-		
92	OHX	2	1971	-	0,6,6	-	-	-		
92	OHX	5	3446	-	0,6,6	-	-	-		
92	OHX	5	3601	-	0,6,6	-	-	-		
92	OHX	8	214	38	0,6,6	-	-	-		
92	OHX	L3	402	-	0,6,6	-	-	-		
92	OHX	2	2051	-	0,6,6	-	-	-		
92	OHX	2	2037	1	0,6,6	-	-	-		
92	OHX	1	3698	36	0,6,6	-	-	-		
92	OHX	5	3506	-	0,6,6	-	-	-		
92	OHX	1	3693	-	0,6,6	-	-	-		
92	OHX	6	1924	80,93	0,6,6	-	-	-		
92	OHX	6	2035	-	0,6,6	-	-	-		
92	OHX	5	3623	-	0,6,6	-	-	-		
92	OHX	1	3435	-	0,6,6	-	-	-		
92	OHX	5	3644	93	0,6,6	-	-	-		
92	OHX	5	3654	-	0,6,6	-	-	-		
92	OHX	1	3515	-	0,6,6	-	-	-		
92	OHX	l5	302	-	0,6,6	-	-	-		
92	OHX	1	3452	-	0,6,6	-	-	-		
92	OHX	1	3652	-	0,6,6	-	-	-		
92	OHX	1	3439	-	0,6,6	-	-	-		
92	OHX	1	3725	93	0,6,6	-	-	-		
92	OHX	4	217	-	0,6,6	-	-	-		
92	OHX	5	3523	-	0,6,6	-	-	-		
92	OHX	1	3623	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	1	3611	-	0,6,6	-	-	-		
92	OHX	1	3608	-	0,6,6	-	-	-		
92	OHX	5	3622	85	0,6,6	-	-	-		
92	OHX	5	3635	85	0,6,6	-	-	-		
92	OHX	6	1962	80	0,6,6	-	-	-		
92	OHX	5	3520	-	0,6,6	-	-	-		
92	OHX	6	1988	-	0,6,6	-	-	-		
92	OHX	1	3579	-	0,6,6	-	-	-		
92	OHX	5	3710	-	0,6,6	-	-	-		
97	SPS	p	101	93	20,23,23	3.51	11 (55%)	24,30,30	4.12	14 (58%)
92	OHX	1	3540	-	0,6,6	-	-	-		
92	OHX	2	2040	-	0,6,6	-	-	-		
92	OHX	5	3424	-	0,6,6	-	-	-		
92	OHX	1	3518	-	0,6,6	-	-	-		
92	OHX	1	3589	-	0,6,6	-	-	-		
92	OHX	5	3641	-	0,6,6	-	-	-		
92	OHX	6	1932	80	0,6,6	-	-	-		
92	OHX	6	2029	80	0,6,6	-	-	-		
92	OHX	1	3491	-	0,6,6	-	-	-		
92	OHX	1	3422	-	0,6,6	-	-	-		
92	OHX	1	3468	-	0,6,6	-	-	-		
92	OHX	1	3721	-	0,6,6	-	-	-		
92	OHX	n9	101	-	0,6,6	-	-	-		
92	OHX	2	1972	1	0,6,6	-	-	-		
92	OHX	5	3717	85	0,6,6	-	-	-		
92	OHX	2	1925	-	0,6,6	-	-	-		
92	OHX	5	3743	-	0,6,6	-	-	-		
92	OHX	6	1907	80	0,6,6	-	-	-		
92	OHX	q2	502	93	0,6,6	-	-	-		
92	OHX	5	3675	-	0,6,6	-	-	-		
92	OHX	1	3441	-	0,6,6	-	-	-		
92	OHX	6	2005	-	0,6,6	-	-	-		
92	OHX	2	2022	-	0,6,6	-	-	-		
92	OHX	5	3525	85	0,6,6	-	-	-		
92	OHX	2	1916	-	0,6,6	-	-	-		
92	OHX	1	3460	-	0,6,6	-	-	-		
92	OHX	5	3541	-	0,6,6	-	-	-		
92	OHX	4	218	-	0,6,6	-	-	-		
92	OHX	5	3680	93	0,6,6	-	-	-		
92	OHX	1	3691	-	0,6,6	-	-	-		
92	OHX	2	1957	-	0,6,6	-	-	-		
92	OHX	1	3554	-	0,6,6	-	-	-		
92	OHX	6	1983	93	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	6	1958	80	0,6,6	-	-	-		
92	OHX	2	2001	-	0,6,6	-	-	-		
92	OHX	5	3554	-	0,6,6	-	-	-		
92	OHX	6	1913	80	0,6,6	-	-	-		
92	OHX	5	3661	-	0,6,6	-	-	-		
92	OHX	5	3700	85	0,6,6	-	-	-		
92	OHX	1	3729	-	0,6,6	-	-	-		
92	OHX	1	3557	-	0,6,6	-	-	-		
92	OHX	2	1987	1	0,6,6	-	-	-		
92	OHX	5	3459	85	0,6,6	-	-	-		
92	OHX	5	3530	-	0,6,6	-	-	-		
92	OHX	5	3656	-	0,6,6	-	-	-		
92	OHX	5	3670	85	0,6,6	-	-	-		
92	OHX	5	3569	93	0,6,6	-	-	-		
92	OHX	s9	201	-	0,6,6	-	-	-		
92	OHX	2	2009	1	0,6,6	-	-	-		
92	OHX	1	3467	-	0,6,6	-	-	-		
92	OHX	2	1950	1	0,6,6	-	-	-		
92	OHX	2	2036	-	0,6,6	-	-	-		
92	OHX	2	1929	-	0,6,6	-	-	-		
92	OHX	Q2	502	93	0,6,6	-	-	-		
92	OHX	1	3493	36	0,6,6	-	-	-		
92	OHX	6	2018	80	0,6,6	-	-	-		
92	OHX	5	3568	-	0,6,6	-	-	-		
92	OHX	2	1922	-	0,6,6	-	-	-		
92	OHX	5	3467	-	0,6,6	-	-	-		
92	OHX	6	1942	80	0,6,6	-	-	-		
92	OHX	6	2041	-	0,6,6	-	-	-		
92	OHX	5	3518	-	0,6,6	-	-	-		
92	OHX	2	1921	-	0,6,6	-	-	-		
92	OHX	2	1961	-	0,6,6	-	-	-		
92	OHX	5	3454	-	0,6,6	-	-	-		
92	OHX	2	1939	-	0,6,6	-	-	-		
92	OHX	m6	201	-	0,6,6	-	-	-		
92	OHX	1	3573	36	0,6,6	-	-	-		
92	OHX	M9	201	-	0,6,6	-	-	-		
92	OHX	1	3458	-	0,6,6	-	-	-		
92	OHX	1	3723	-	0,6,6	-	-	-		
92	OHX	6	1947	-	0,6,6	-	-	-		
92	OHX	6	1964	80	0,6,6	-	-	-		
92	OHX	5	3479	-	0,6,6	-	-	-		
92	OHX	5	3573	-	0,6,6	-	-	-		
92	OHX	2	2003	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	OHX	5	3494	-	0,6,6	-	-	-		
92	OHX	5	3470	-	0,6,6	-	-	-		
92	OHX	5	3512	-	0,6,6	-	-	-		
92	OHX	6	1978	-	0,6,6	-	-	-		
92	OHX	5	3497	85	0,6,6	-	-	-		
92	OHX	6	1971	80	0,6,6	-	-	-		
92	OHX	5	3708	-	0,6,6	-	-	-		
92	OHX	1	3599	93	0,6,6	-	-	-		
92	OHX	6	2037	80	0,6,6	-	-	-		
92	OHX	6	2013	80	0,6,6	-	-	-		
92	OHX	2	1964	-	0,6,6	-	-	-		
92	OHX	5	3586	85,93	0,6,6	-	-	-		
92	OHX	1	3682	-	0,6,6	-	-	-		
92	OHX	5	3679	-	0,6,6	-	-	-		
92	OHX	2	1980	-	0,6,6	-	-	-		
92	OHX	1	3496	-	0,6,6	-	-	-		
92	OHX	5	3580	-	0,6,6	-	-	-		
92	OHX	5	3595	85	0,6,6	-	-	-		
92	OHX	D9	102	-	0,6,6	-	-	-		
92	OHX	5	3597	85	0,6,6	-	-	-		
92	OHX	2	2015	-	0,6,6	-	-	-		
92	OHX	1	3457	-	0,6,6	-	-	-		
92	OHX	1	3443	-	0,6,6	-	-	-		
92	OHX	1	3483	-	0,6,6	-	-	-		
92	OHX	1	3615	-	0,6,6	-	-	-		
92	OHX	4	220	-	0,6,6	-	-	-		
92	OHX	1	3461	93	0,6,6	-	-	-		
92	OHX	5	3668	85	0,6,6	-	-	-		
92	OHX	C5	201	-	0,6,6	-	-	-		
92	OHX	3	205	-	0,6,6	-	-	-		
92	OHX	6	2044	-	0,6,6	-	-	-		
92	OHX	2	2000	-	0,6,6	-	-	-		
92	OHX	2	2021	-	0,6,6	-	-	-		
92	OHX	5	3737	85	0,6,6	-	-	-		
92	OHX	1	3716	-	0,6,6	-	-	-		
92	OHX	1	3595	-	0,6,6	-	-	-		
92	OHX	1	3559	-	0,6,6	-	-	-		
92	OHX	1	3521	93	0,6,6	-	-	-		
92	OHX	4	215	38	0,6,6	-	-	-		
92	OHX	2	1912	-	0,6,6	-	-	-		
92	OHX	5	3667	-	0,6,6	-	-	-		
92	OHX	2	1965	-	0,6,6	-	-	-		
92	OHX	5	3697	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
98	8AN	P	102	91,93	22,24,25	1.50	4 (18%)	26,35,38	2.36	11 (42%)
92	OHX	6	1923	80	0,6,6	-	-	-		
92	OHX	1	3413	-	0,6,6	-	-	-		
92	OHX	5	3571	-	0,6,6	-	-	-		
92	OHX	1	3436	-	0,6,6	-	-	-		
92	OHX	1	3638	-	0,6,6	-	-	-		
92	OHX	1	3634	-	0,6,6	-	-	-		
92	OHX	5	3640	85,93	0,6,6	-	-	-		
92	OHX	5	3659	-	0,6,6	-	-	-		
92	OHX	5	3707	-	0,6,6	-	-	-		
92	OHX	6	2016	80	0,6,6	-	-	-		
92	OHX	1	3670	-	0,6,6	-	-	-		
92	OHX	6	2017	80	0,6,6	-	-	-		
92	OHX	5	3575	-	0,6,6	-	-	-		
92	OHX	3	210	-	0,6,6	-	-	-		
92	OHX	1	3625	-	0,6,6	-	-	-		
92	OHX	6	2026	80	0,6,6	-	-	-		
92	OHX	5	3606	85	0,6,6	-	-	-		
92	OHX	5	3722	85	0,6,6	-	-	-		
92	OHX	6	1933	-	0,6,6	-	-	-		
92	OHX	1	3678	36	0,6,6	-	-	-		
92	OHX	5	3561	85	0,6,6	-	-	-		
92	OHX	6	1908	80	0,6,6	-	-	-		
92	OHX	1	3446	-	0,6,6	-	-	-		
92	OHX	6	2014	80,93	0,6,6	-	-	-		
92	OHX	6	2011	-	0,6,6	-	-	-		
92	OHX	1	3516	93	0,6,6	-	-	-		
92	OHX	7	203	37	0,6,6	-	-	-		
92	OHX	7	210	37	0,6,6	-	-	-		
92	OHX	5	3516	85	0,6,6	-	-	-		
92	OHX	6	1960	80	0,6,6	-	-	-		
92	OHX	1	3710	36	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
97	SPS	P	101	93	-	3/15/18/18	0/1/1/1
95	PHE	1	3401	96	-	3/5/6/8	0/1/1/1
96	LEU	5	3402	95	-	4/5/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
96	LEU	1	3402	95	-	4/5/6/8	-
98	8AN	p	102	91,93	-	1/7/25/26	0/3/3/3
95	PHE	5	3401	96	-	3/5/6/8	0/1/1/1
98	8AN	P	102	91,93	-	1/7/25/26	0/3/3/3
97	SPS	p	101	93	-	4/15/18/18	0/1/1/1

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
97	p	101	SPS	C9-C10	-7.39	1.32	1.48
97	P	101	SPS	C9-C8	7.10	1.54	1.33
97	p	101	SPS	C9-C8	6.60	1.53	1.33
97	P	101	SPS	C9-C10	-5.96	1.35	1.48
97	P	101	SPS	C10-N11	5.15	1.46	1.34

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
97	P	101	SPS	O15-S15-C16	-11.93	92.28	106.47
97	p	101	SPS	C7-C5-C6	-9.46	112.86	126.69
97	p	101	SPS	C7-C5-N4	8.58	123.64	113.45
97	P	101	SPS	C7-C5-C6	-7.49	115.75	126.69
97	P	101	SPS	O13-C13-C12	7.47	131.24	111.95

There are no chirality outliers.

5 of 23 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 then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

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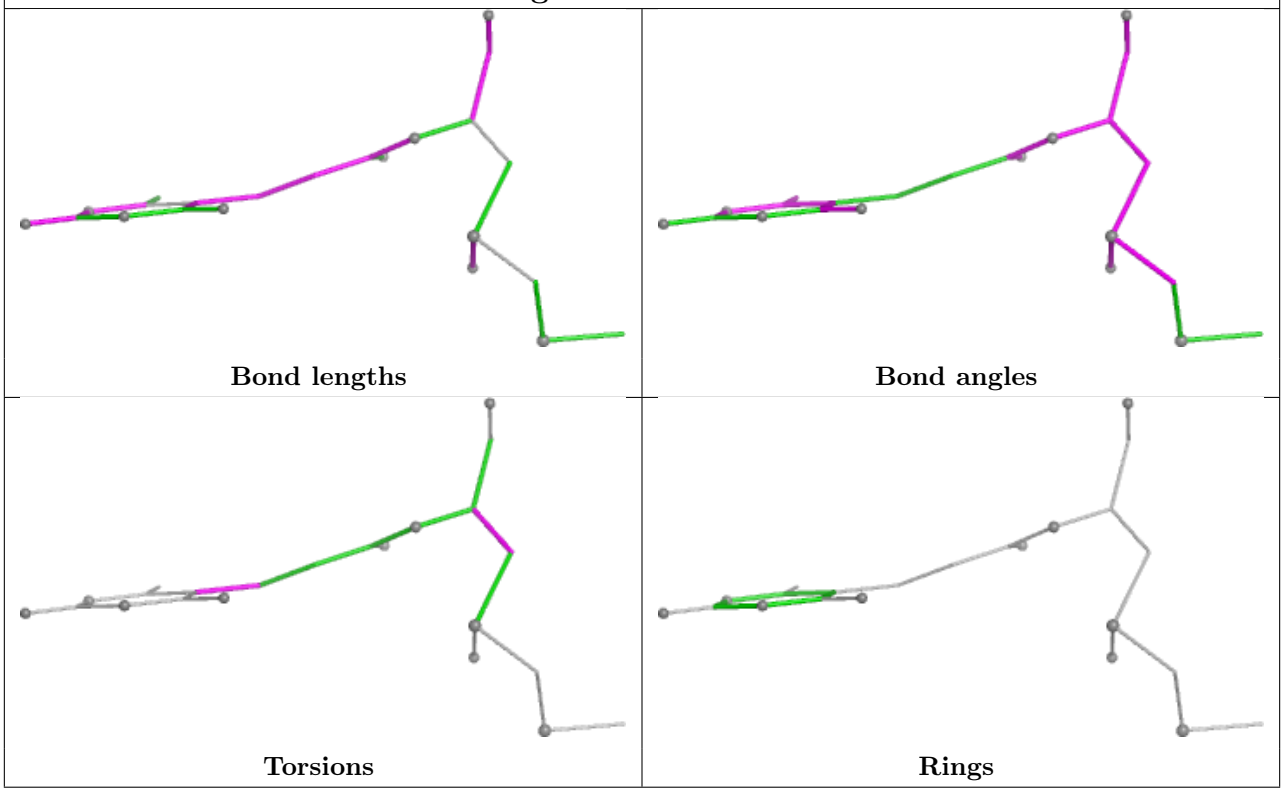

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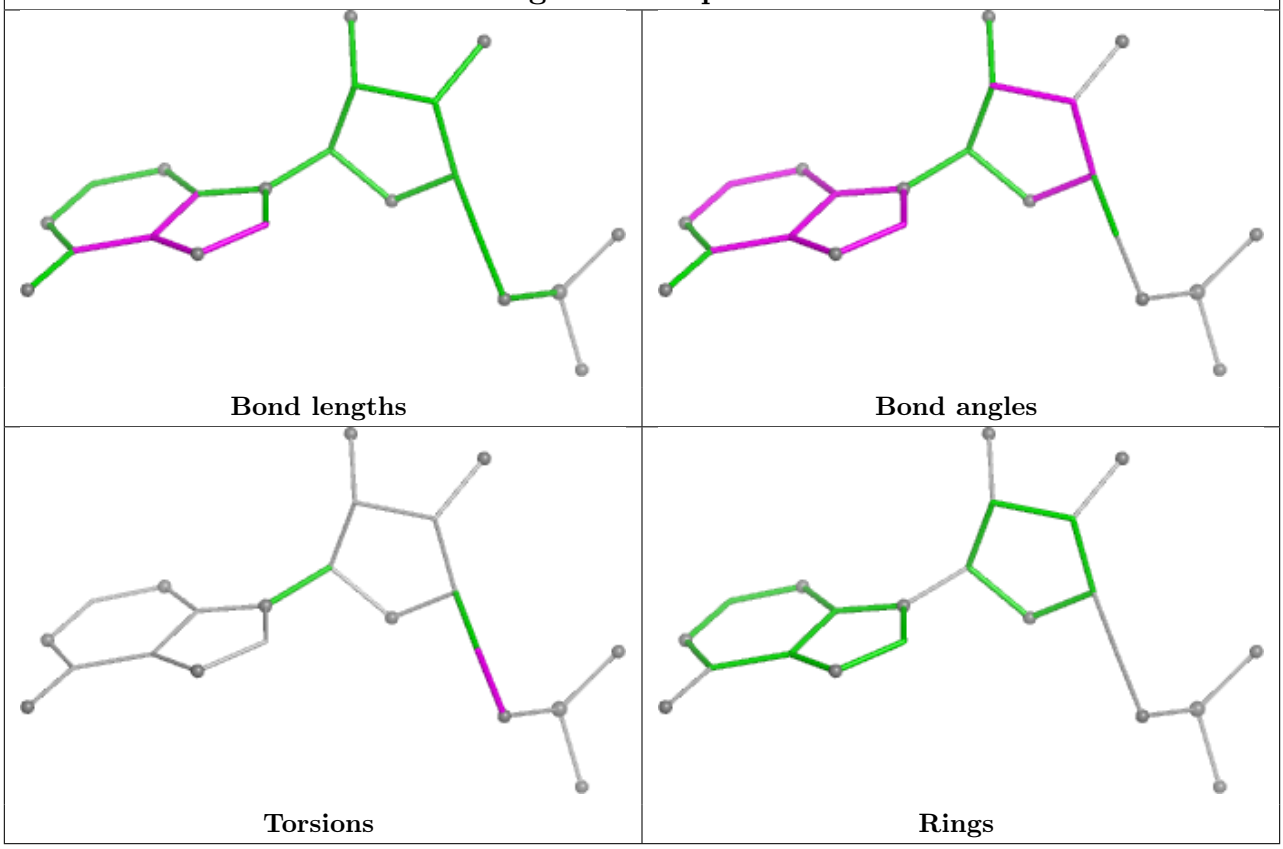
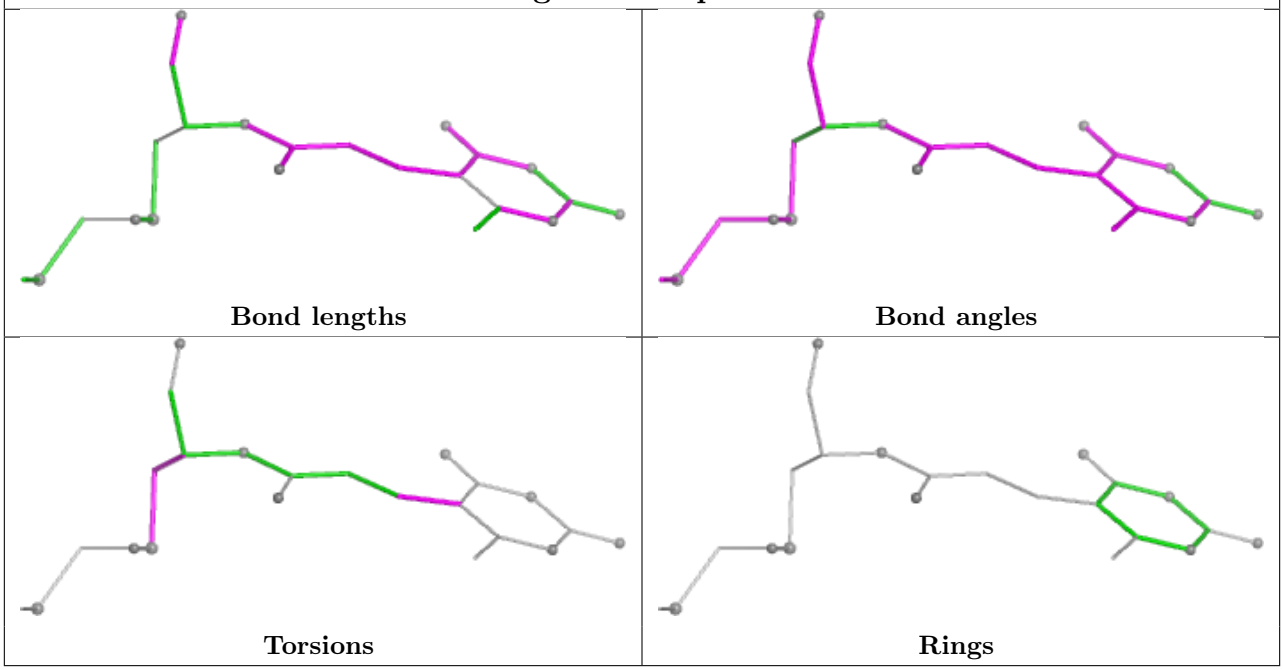
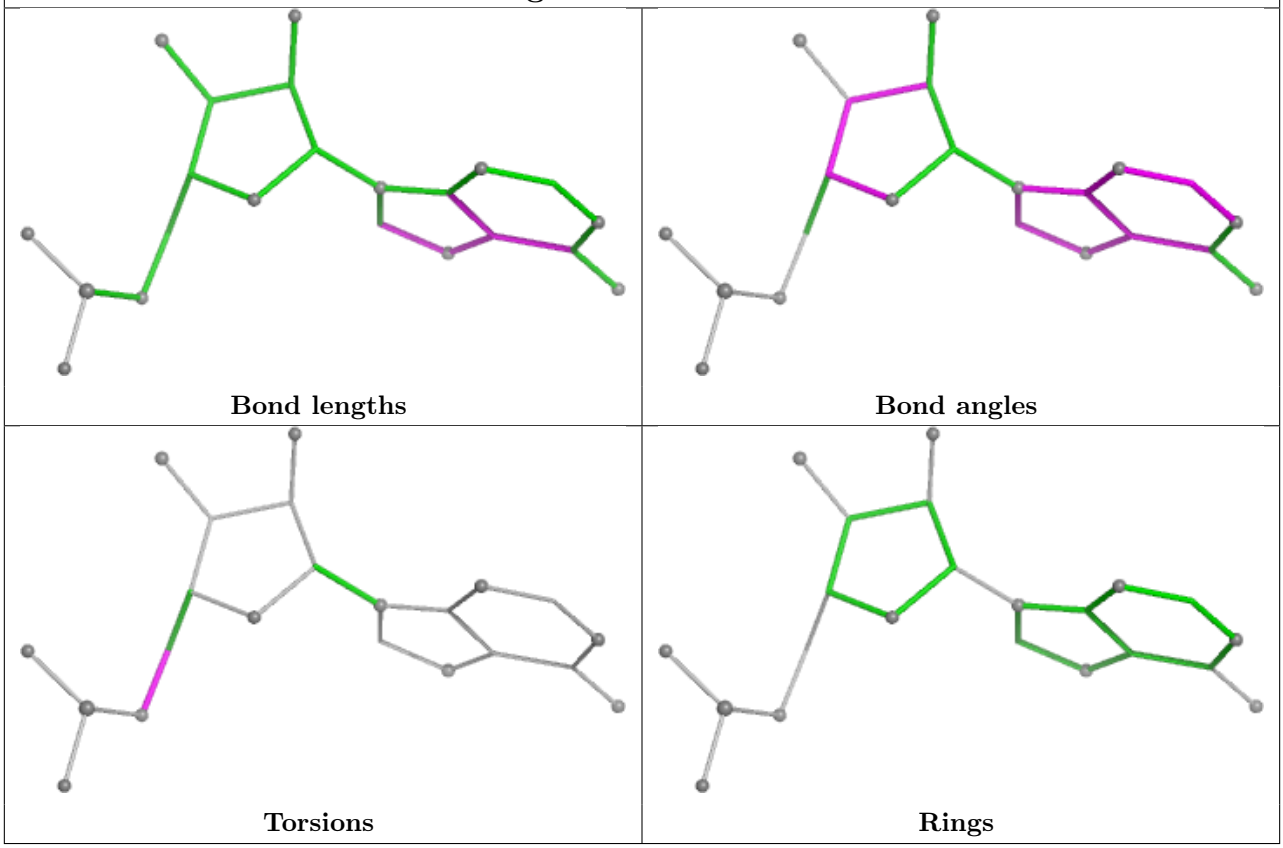


Ligand SPS p 101



Ligand 8AN P 102



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

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Mol	Chain	Number of breaks
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 (i)

5.1 Protein, DNA and RNA chains (i)

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%)	1.33	297 (16%)	4	4	38, 89, 120, 149	1 (0%)
2	S0	206/206 (100%)	1.12	24 (11%)	9	6	93, 99, 105, 107	0
2	s0	206/206 (100%)	0.83	16 (7%)	19	12	77, 83, 89, 90	0
3	S1	214/216 (99%)	1.21	26 (12%)	8	6	95, 106, 113, 113	0
3	s1	216/216 (100%)	0.69	5 (2%)	61	37	70, 75, 81, 84	0
4	S2	217/217 (100%)	1.01	21 (9%)	13	9	81, 88, 96, 99	0
4	s2	217/217 (100%)	0.97	30 (13%)	6	5	67, 73, 79, 81	0
5	S3	223/223 (100%)	0.99	26 (11%)	9	6	85, 96, 110, 115	0
5	s3	223/223 (100%)	0.88	19 (8%)	16	11	91, 102, 113, 114	0
6	S4	260/260 (100%)	1.16	32 (12%)	8	6	75, 88, 91, 93	0
6	s4	260/260 (100%)	0.86	12 (4%)	37	20	59, 73, 78, 80	0
7	S5	206/206 (100%)	1.58	53 (25%)	1	2	97, 105, 111, 113	0
7	s5	206/206 (100%)	1.24	34 (16%)	4	4	90, 95, 101, 103	0
8	S6	226/226 (100%)	1.17	36 (15%)	5	4	62, 76, 96, 101	0
8	s6	218/226 (96%)	0.69	13 (5%)	27	16	55, 63, 82, 86	0
9	S7	184/186 (98%)	1.33	26 (14%)	6	5	92, 102, 108, 109	0
9	s7	186/186 (100%)	1.12	20 (10%)	11	8	75, 90, 101, 104	0
10	S8	188/188 (100%)	1.02	15 (7%)	18	12	72, 78, 92, 95	0
10	s8	188/188 (100%)	1.08	18 (9%)	13	9	57, 68, 89, 95	0
11	S9	185/185 (100%)	1.18	25 (13%)	7	5	81, 89, 99, 103	0
11	s9	185/185 (100%)	0.78	10 (5%)	31	18	63, 74, 82, 84	0
12	C0	83/96 (86%)	0.81	3 (3%)	46	25	94, 100, 105, 107	0
13	C1	146/155 (94%)	1.28	22 (15%)	5	5	75, 79, 85, 89	0
13	c1	146/155 (94%)	1.33	27 (18%)	3	4	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%)	1.25	16 (13%) 7 6	111, 116, 118, 119	0
14	c2	119/124 (95%)	1.66	33 (27%) 1 1	133, 142, 148, 149	0
15	C3	150/150 (100%)	1.11	15 (10%) 12 8	80, 88, 92, 94	0
15	c3	150/150 (100%)	0.97	11 (7%) 21 13	65, 75, 80, 82	0
16	C4	127/128 (99%)	1.65	37 (29%) 1 1	82, 105, 111, 112	0
16	c4	128/128 (100%)	0.91	8 (6%) 26 15	63, 74, 79, 80	0
17	C5	122/135 (90%)	0.98	13 (10%) 11 8	80, 90, 96, 101	0
17	c5	125/135 (92%)	1.38	28 (22%) 2 2	65, 91, 98, 100	0
18	C6	141/142 (99%)	1.60	40 (28%) 1 1	88, 105, 109, 110	0
18	c6	142/142 (100%)	1.45	31 (21%) 2 2	90, 98, 102, 104	0
19	C7	120/120 (100%)	1.02	8 (6%) 24 15	98, 104, 108, 109	0
20	C8	145/145 (100%)	0.77	4 (2%) 55 32	83, 95, 107, 110	0
20	c8	145/145 (100%)	0.85	8 (5%) 30 18	69, 86, 93, 97	0
21	C9	143/143 (100%)	1.25	20 (13%) 6 5	92, 101, 106, 108	0
21	c9	143/143 (100%)	0.99	11 (7%) 19 13	87, 92, 96, 98	0
22	D0	107/110 (97%)	1.24	20 (18%) 3 4	87, 100, 105, 106	0
22	d0	110/110 (100%)	0.91	8 (7%) 21 13	92, 104, 110, 111	0
23	D1	87/87 (100%)	0.85	5 (5%) 29 17	90, 94, 102, 106	0
23	d1	87/87 (100%)	0.73	2 (2%) 61 37	74, 78, 86, 89	0
24	D2	129/129 (100%)	1.40	25 (19%) 3 3	82, 88, 92, 98	0
24	d2	129/129 (100%)	0.94	4 (3%) 51 29	67, 72, 75, 76	0
25	D3	144/144 (100%)	1.49	36 (25%) 2 2	71, 76, 79, 80	0
25	d3	144/144 (100%)	1.06	19 (13%) 7 6	57, 59, 64, 66	0
26	D4	134/134 (100%)	0.90	8 (5%) 27 16	76, 88, 92, 94	0
26	d4	134/134 (100%)	0.82	12 (8%) 15 10	60, 71, 74, 76	0
27	D5	70/70 (100%)	0.99	5 (7%) 22 14	104, 108, 111, 112	0
27	d5	69/70 (98%)	1.05	4 (5%) 29 17	93, 97, 100, 101	0
28	D6	97/97 (100%)	1.48	18 (18%) 3 4	84, 91, 112, 113	0
28	d6	97/97 (100%)	1.08	12 (12%) 8 6	65, 72, 81, 83	0
29	D7	81/81 (100%)	1.02	7 (8%) 16 11	90, 94, 99, 100	0
29	d7	81/81 (100%)	0.94	8 (9%) 13 8	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%)	1.52	13 (20%)	2	3	98, 107, 112, 113	0
30	d8	63/63 (100%)	1.12	6 (9%)	14	9	90, 95, 99, 100	0
31	D9	53/53 (100%)	1.18	12 (22%)	2	2	89, 91, 96, 97	0
31	d9	53/53 (100%)	1.63	17 (32%)	1	1	93, 97, 113, 120	0
32	E0	60/62 (96%)	1.41	13 (21%)	2	3	72, 87, 97, 101	0
32	e0	62/62 (100%)	0.67	4 (6%)	25	15	58, 72, 77, 80	0
33	E1	71/76 (93%)	1.57	17 (23%)	2	2	92, 108, 113, 113	0
33	e1	76/76 (100%)	2.21	40 (52%)	0	0	99, 127, 139, 140	0
34	SR	318/318 (100%)	1.18	46 (14%)	6	5	104, 111, 118, 122	0
35	SM	121/159 (76%)	0.84	10 (8%)	17	11	55, 83, 96, 98	0
36	1	3149/3149 (100%)	0.70	250 (7%)	18	12	31, 49, 82, 154	0
37	3	121/121 (100%)	0.32	1 (0%)	82	60	41, 59, 64, 65	0
37	7	121/121 (100%)	0.44	2 (1%)	69	43	36, 47, 51, 54	0
38	4	158/158 (100%)	0.30	3 (1%)	66	41	33, 45, 63, 84	0
38	8	158/158 (100%)	0.46	10 (6%)	26	15	36, 49, 68, 76	0
39	L2	252/252 (100%)	0.76	15 (5%)	27	16	40, 52, 61, 73	0
39	l2	252/252 (100%)	0.83	23 (9%)	15	10	39, 53, 62, 66	0
40	L3	386/386 (100%)	0.63	20 (5%)	33	19	38, 50, 58, 62	0
40	l3	386/386 (100%)	0.49	13 (3%)	48	27	32, 39, 47, 58	0
41	L4	361/361 (100%)	0.32	10 (2%)	55	32	31, 37, 47, 51	0
41	l4	361/361 (100%)	0.40	18 (4%)	34	19	33, 41, 48, 58	0
42	L5	296/296 (100%)	0.46	8 (2%)	56	33	50, 60, 67, 69	0
42	l5	294/296 (99%)	0.40	8 (2%)	56	33	43, 49, 57, 66	0
43	L6	156/175 (89%)	0.50	8 (5%)	33	19	38, 46, 49, 55	0
43	l6	157/175 (89%)	0.61	10 (6%)	25	15	40, 46, 49, 52	0
44	L7	222/223 (99%)	0.47	5 (2%)	61	37	36, 40, 48, 50	0
44	l7	223/223 (100%)	0.35	5 (2%)	62	37	34, 38, 48, 54	0
45	L8	233/233 (100%)	0.66	5 (2%)	63	38	54, 60, 74, 77	0
46	L9	191/191 (100%)	0.35	2 (1%)	79	56	48, 51, 53, 59	0
46	l9	191/191 (100%)	0.45	7 (3%)	45	25	39, 44, 52, 63	0
47	M0	211/220 (95%)	0.45	3 (1%)	73	48	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%)	0.49	6 (2%) 55 32	36, 42, 57, 67	0
48	M1	169/169 (100%)	0.55	4 (2%) 59 35	57, 67, 73, 76	0
48	m1	169/169 (100%)	0.35	2 (1%) 76 52	44, 54, 59, 63	0
49	M3	193/194 (99%)	0.29	3 (1%) 70 45	33, 46, 59, 74	0
49	m3	194/194 (100%)	0.43	3 (1%) 72 47	35, 50, 61, 70	0
50	M4	136/137 (99%)	0.53	6 (4%) 39 21	45, 49, 54, 56	0
50	m4	137/137 (100%)	0.32	4 (2%) 53 31	39, 43, 52, 60	0
51	M5	203/203 (100%)	0.51	4 (1%) 65 39	35, 46, 54, 56	0
51	m5	203/203 (100%)	0.55	7 (3%) 48 27	38, 50, 57, 59	0
52	M6	197/197 (100%)	0.54	9 (4%) 37 20	39, 42, 50, 52	0
52	m6	197/197 (100%)	0.35	7 (3%) 46 25	32, 36, 49, 50	0
53	M7	183/183 (100%)	0.67	19 (10%) 11 8	38, 43, 58, 62	0
53	m7	155/183 (84%)	0.27	3 (1%) 66 41	34, 37, 40, 43	0
54	M8	185/185 (100%)	0.61	9 (4%) 35 19	36, 44, 54, 61	0
54	m8	185/185 (100%)	0.48	7 (3%) 44 24	35, 44, 48, 50	0
55	M9	188/188 (100%)	0.75	18 (9%) 13 9	49, 61, 103, 111	0
55	m9	188/188 (100%)	0.69	10 (5%) 32 18	43, 55, 98, 106	0
56	N0	172/172 (100%)	0.38	3 (1%) 69 43	42, 46, 51, 53	0
56	n0	172/172 (100%)	0.29	3 (1%) 69 43	36, 39, 44, 48	0
57	N1	159/159 (100%)	0.49	3 (1%) 66 41	40, 47, 56, 57	0
57	n1	159/159 (100%)	0.34	3 (1%) 66 41	36, 42, 53, 55	0
58	N2	100/100 (100%)	0.73	3 (3%) 52 30	65, 69, 72, 73	0
58	n2	98/100 (98%)	0.40	0 100 100	56, 59, 60, 61	0
59	N3	136/136 (100%)	0.74	9 (6%) 24 15	43, 49, 52, 54	0
59	n3	136/136 (100%)	0.44	4 (2%) 53 31	33, 37, 41, 43	0
60	N4	98/98 (100%)	1.46	26 (26%) 1 2	49, 59, 89, 91	0
61	N5	121/121 (100%)	0.30	1 (0%) 82 60	43, 45, 62, 72	0
61	n5	120/121 (99%)	0.46	1 (0%) 82 60	44, 48, 65, 67	0
62	N6	126/126 (100%)	0.28	2 (1%) 70 45	35, 41, 44, 45	0
62	n6	126/126 (100%)	0.27	4 (3%) 50 29	38, 45, 49, 50	0
63	N7	135/135 (100%)	0.54	3 (2%) 62 37	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%)	0.68	2 (1%) 72 47	65, 71, 78, 83	0
64	N8	148/148 (100%)	0.27	0 100 100	31, 43, 50, 57	0
64	n8	148/148 (100%)	0.27	3 (2%) 65 39	31, 45, 48, 50	0
65	N9	58/58 (100%)	0.54	2 (3%) 48 27	36, 49, 66, 71	0
65	n9	58/58 (100%)	0.33	2 (3%) 48 27	34, 45, 52, 53	0
66	O0	97/100 (97%)	0.43	1 (1%) 79 56	60, 64, 70, 71	0
66	o0	100/100 (100%)	0.49	3 (3%) 52 30	61, 66, 73, 75	0
67	O1	109/109 (100%)	0.77	3 (2%) 55 32	51, 55, 59, 67	0
67	o1	109/109 (100%)	0.44	3 (2%) 55 32	41, 43, 47, 49	0
68	O2	127/127 (100%)	0.61	10 (7%) 18 12	32, 39, 41, 43	0
68	o2	127/127 (100%)	0.38	2 (1%) 70 45	31, 40, 43, 44	0
69	O3	106/106 (100%)	0.51	5 (4%) 36 20	37, 42, 50, 52	0
69	o3	106/106 (100%)	0.53	4 (3%) 44 24	34, 40, 50, 51	0
70	O4	112/112 (100%)	0.80	6 (5%) 31 18	47, 60, 70, 73	0
70	o4	112/112 (100%)	0.75	9 (8%) 18 12	46, 62, 70, 72	0
71	O5	119/119 (100%)	0.21	1 (0%) 82 60	42, 44, 56, 58	0
71	o5	119/119 (100%)	0.42	1 (0%) 82 60	46, 48, 60, 64	0
72	O6	99/99 (100%)	0.44	4 (4%) 42 23	44, 54, 62, 66	0
72	o6	99/99 (100%)	0.46	1 (1%) 79 56	48, 57, 62, 66	0
73	O7	87/87 (100%)	0.38	1 (1%) 78 54	35, 41, 46, 49	0
73	o7	87/87 (100%)	0.44	4 (4%) 37 20	37, 42, 51, 58	0
74	O8	77/77 (100%)	0.41	1 (1%) 75 50	57, 60, 66, 66	0
74	o8	77/77 (100%)	0.56	2 (2%) 57 33	59, 63, 66, 68	0
75	O9	50/50 (100%)	0.39	1 (2%) 65 39	40, 42, 44, 45	0
75	o9	50/50 (100%)	0.37	1 (2%) 65 39	40, 44, 46, 49	0
76	Q0	52/52 (100%)	0.20	1 (1%) 66 41	46, 49, 50, 52	0
76	q0	52/52 (100%)	0.11	0 100 100	38, 39, 43, 45	0
77	Q1	25/25 (100%)	1.37	5 (20%) 3 3	60, 70, 78, 78	0
77	q1	25/25 (100%)	0.87	2 (8%) 18 12	49, 56, 59, 60	0
78	Q2	105/105 (100%)	0.29	1 (0%) 79 56	38, 49, 58, 66	0
78	q2	105/105 (100%)	0.37	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%)	0.64	2 (2%) 62 37	49, 53, 57, 58	0
79	q3	91/91 (100%)	0.63	5 (5%) 30 18	45, 53, 60, 64	0
80	6	1795/1800 (99%)	1.15	238 (13%) 7 6	30, 75, 111, 134	1 (0%)
81	c0	79/96 (82%)	1.09	8 (10%) 12 8	105, 116, 121, 122	0
82	c7	117/121 (96%)	0.84	10 (8%) 16 11	86, 94, 99, 100	0
83	sR	318/318 (100%)	1.30	52 (16%) 4 4	90, 107, 111, 114	0
84	sM	63/104 (60%)	0.97	11 (17%) 4 4	45, 78, 89, 91	0
85	5	3150/3150 (100%)	0.62	219 (6%) 22 14	31, 45, 82, 107	0
86	l8	225/231 (97%)	0.82	16 (7%) 22 14	58, 64, 78, 81	0
87	m2	0/150	-	-	-	-
88	n4	135/135 (100%)	0.84	11 (8%) 18 12	37, 62, 81, 82	0
89	p0	120/143 (83%)	0.71	7 (5%) 29 17	78, 91, 98, 104	0
90	p1	0/47	-	-	-	-
90	p2	0/47	-	-	-	-
91	P	2/2 (100%)	0.27	0 100 100	38, 38, 38, 40	0
91	p	2/2 (100%)	2.16	1 (50%) 0 1	34, 34, 34, 38	0
All	All	32929/33519 (98%)	0.79	2737 (8%) 17 11	30, 60, 107, 154	2 (0%)

The worst 5 of 2737 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	N4	88	ASP	9.4
7	S5	152	GLY	9.1
1	2	1805	C	9.1
1	2	1804	U	8.7
1	2	1789	A	7.9

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

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

5.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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	l2	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	l9	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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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	l3	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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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	l7	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	l5	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	l9	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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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	l2	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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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(Å^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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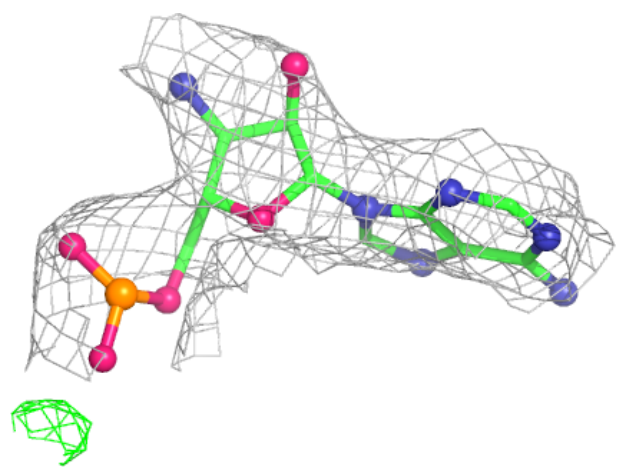
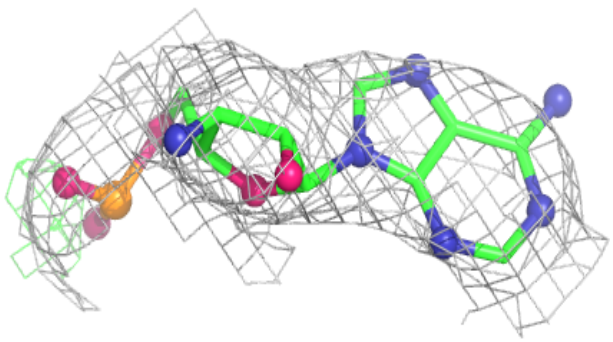
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
92	OHX	5	3417	7/7	1.00	0.07	41,41,41,41	0
92	OHX	Q2	502	7/7	1.00	0.09	41,41,41,41	0
92	OHX	6	1901	7/7	1.00	0.10	59,59,59,59	0
92	OHX	1	3403	7/7	1.00	0.09	37,37,37,37	0
92	OHX	5	3421	7/7	1.00	0.04	44,44,44,44	0
92	OHX	1	3413	7/7	1.00	0.06	45,45,45,45	0

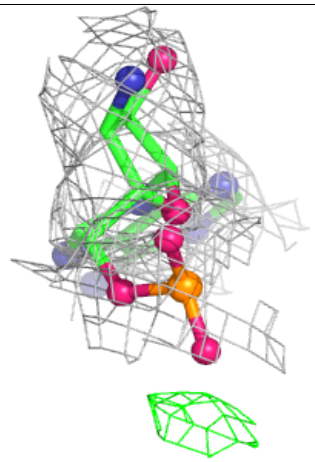
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

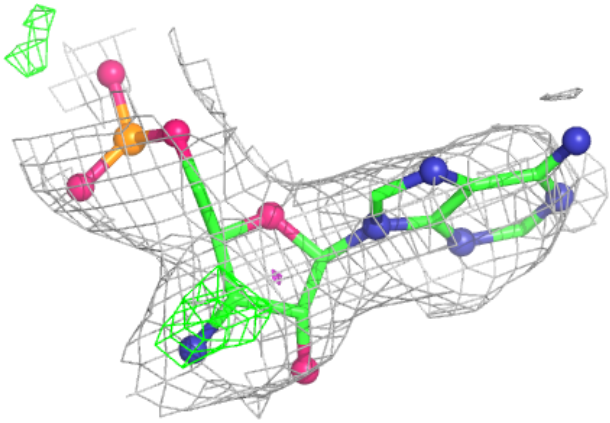


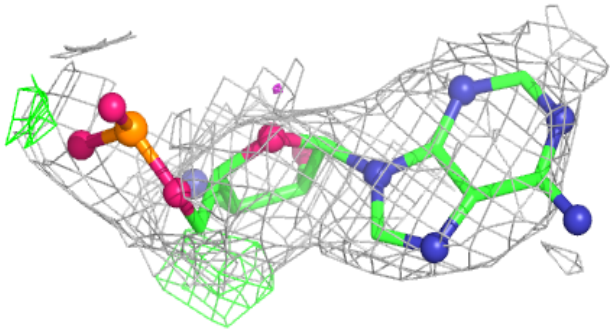




Electron density around 8AN p 102:

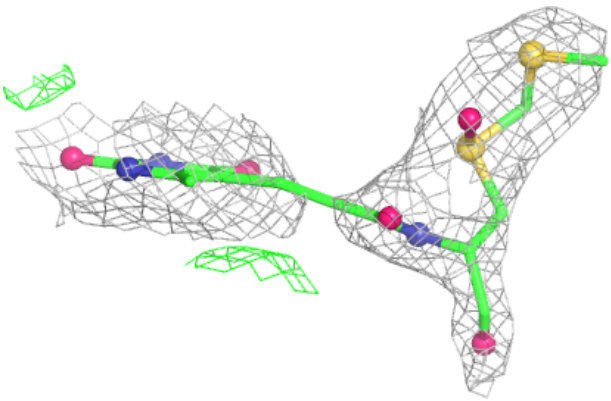
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

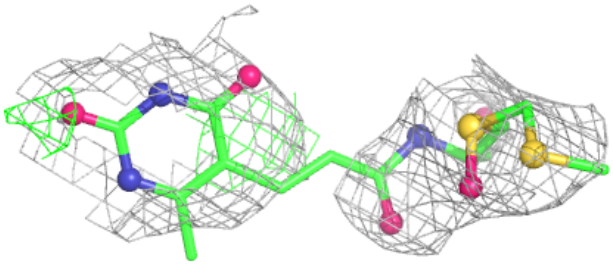


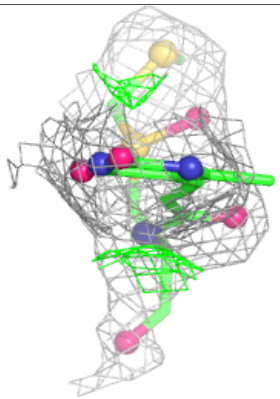


Electron density around SPS P 101:

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

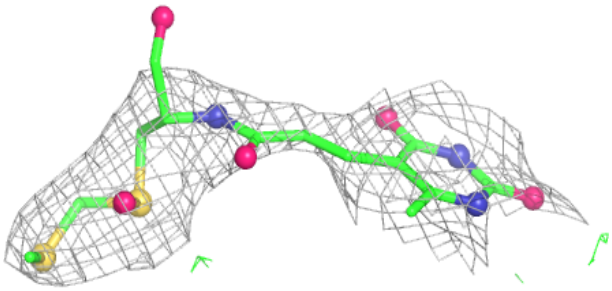


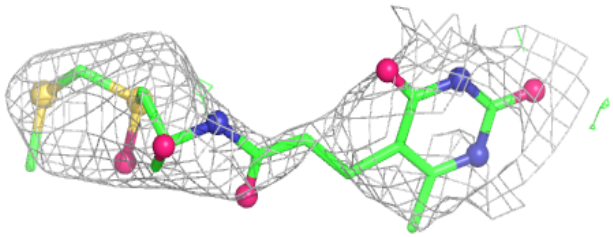


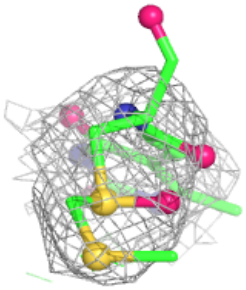


Electron density around SPS p 101:

$2mF_o$-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.