



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2026 – 11:49 am BST

PDB ID : 5DGE / pdb_00005dge
Title : Coping with proline stalling: structural basis of hypusine-induced protein synthesis by the eukaryotic ribosome
Authors : Melnikov, S.; Mailliot, J.; Shin, B.-S.; Rigger, L.; Yusupova, G.; Micura, R.; Dever, T.E.; Yusupov, M.
Deposited on : 2015-08-27
Resolution : 3.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	FAILED
Mogul	:	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

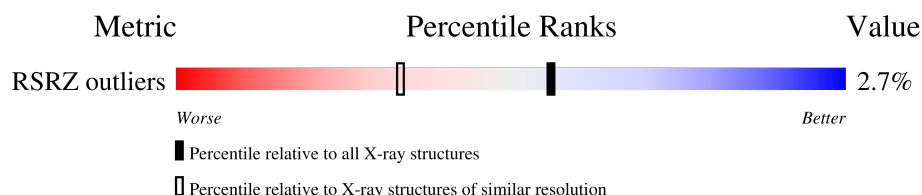
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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))
RSRZ outliers	180081	1070 (3.50-3.42)

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
83	5CT	f	51	-	-	-	X
85	MG	1	3560	-	-	-	X
85	MG	1	3595	-	-	-	X
85	MG	1	3635	-	-	-	X
85	MG	2	1907	-	-	-	X
85	MG	2	1911	-	-	-	X
85	MG	2	1912	-	-	-	X
85	MG	2	1922	-	-	-	X
85	MG	2	1928	-	-	-	X
85	MG	2	1932	-	-	-	X
85	MG	2	1933	-	-	-	X
85	MG	2	1949	-	-	-	X
85	MG	2	1951	-	-	-	X
85	MG	2	1974	-	-	-	X
85	MG	5	3628	-	-	-	X
85	MG	6	1901	-	-	-	X
85	MG	6	1937	-	-	-	X
85	MG	6	1943	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	6	1974	-	-	-	X
85	MG	M7	201	-	-	-	X
88	SPS	5	3403	-	X	-	-

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 413121 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	1781	Total	C	N	O	P	0	1	0
			37970	16975	6720	12493	1782			
1	6	1795	Total	C	N	O	P	0	1	0
			38260	17105	6763	12596	1796			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	S3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			
5	s3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	C0	96	Total	C	N	O	S	0	0	0
			773	500	126	145	2			
12	c0	96	Total	C	N	O	S	0	0	0
			762	491	125	144	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C0	89	ALA	GLY	conflict	UNP Q08745
c0	89	ALA	GLY	conflict	UNP Q08745

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	C2	124	Total	C	N	O	S	0	0	0
			892	562	156	172	2			
14	c2	124	Total	C	N	O	S	0	0	0
			892	562	156	172	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C2	104	ALA	GLY	conflict	UNP P48589
C2	110	ALA	GLY	conflict	UNP P48589
c2	104	ALA	GLY	conflict	UNP P48589
c2	110	ALA	GLY	conflict	UNP P48589

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	C6	141	Total	C	N	O	0	0	0
			1105	708	203	194			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	c6	142	Total	C	N	O	0	0	0
			1111	711	204	196			

- Molecule 19 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	C7	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			
19	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	SR	318	Total	C	N	O	S	0	0	0
			2436	1541	418	469	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	sR	318	Total	C	N	O	S	0	0	0
			2441	1544	418	471	8			

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O		0	0	0
			1104	652	221	231				
35	sM	104	Total	C	N	O		0	0	0
			680	403	140	137				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			
36	5	3150	Total	C	N	O	P	0	0	0
			67376	30095	12145	21987	3149			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	l2	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	l8	231	Total	C	N	O	S	0	0	0
			1764	1131	316	314	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L8	119	ALA	GLY	conflict	UNP P17076
l8	119	ALA	GLY	conflict	UNP P17076

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M1	3	THR	ALA	conflict	UNP P0C0W9
m1	3	THR	ALA	conflict	UNP P0C0W9

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	M4	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			
50	m4	137	Total	C	N	O	S	0	0	0
			1059	678	200	179	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	N4	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			
60	n4	135	Total	C	N	O	S	0	0	0
			1038	651	206	180	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	N5	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			
61	n5	120	Total	C	N	O	S	0	0	0
			959	617	168	172	2			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	O0	97	Total	C	N	O	S	0	0	0
			742	479	124	138	1			
66	o0	100	Total	C	N	O	S	0	0	0
			766	492	128	145	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	Q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			
77	q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

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

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

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

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

- Molecule 80 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
80	m2	150	Total	C	N	O	0	0	0
			739	439	150	150			

- Molecule 81 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 82 is a protein called 60S acidic ribosomal protein P1-alpha.

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

- Molecule 83 is a protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
83	f	148	Total	C	N	O	S	0	0	0
			1122	696	189	228	9			

- Molecule 84 is a RNA chain called DNA (5'-R(*CP*CP*(NA))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
84	B	3	Total	C	N	O	P	0	0	0
			59	28	12	17	2			
84	C	3	Total	C	N	O	P	0	0	0
			62	28	12	19	3			

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	2	90	Total	Mg	0	0
			90	90		
85	S2	1	Total	Mg	0	0
			1	1		
85	D3	1	Total	Mg	0	0
			1	1		
85	SM	1	Total	Mg	0	0
			1	1		
85	1	361	Total	Mg	0	0
			361	361		
85	3	8	Total	Mg	0	0
			8	8		
85	4	15	Total	Mg	0	0
			15	15		
85	L2	2	Total	Mg	0	0
			2	2		
85	L3	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L6	1	Total 1	Mg 1	0	0
85	L7	3	Total 3	Mg 3	0	0
85	M0	2	Total 2	Mg 2	0	0
85	M5	2	Total 2	Mg 2	0	0
85	M6	3	Total 3	Mg 3	0	0
85	M7	4	Total 4	Mg 4	0	0
85	M9	1	Total 1	Mg 1	0	0
85	N3	1	Total 1	Mg 1	0	0
85	N6	1	Total 1	Mg 1	0	0
85	N8	3	Total 3	Mg 3	0	0
85	O4	1	Total 1	Mg 1	0	0
85	O7	2	Total 2	Mg 2	0	0
85	Q2	1	Total 1	Mg 1	0	0
85	6	111	Total 111	Mg 111	0	0
85	s4	1	Total 1	Mg 1	0	0
85	s8	2	Total 2	Mg 2	0	0
85	c8	2	Total 2	Mg 2	0	0
85	c9	1	Total 1	Mg 1	0	0
85	d2	1	Total 1	Mg 1	0	0
85	d3	1	Total 1	Mg 1	0	0
85	d6	1	Total 1	Mg 1	0	0

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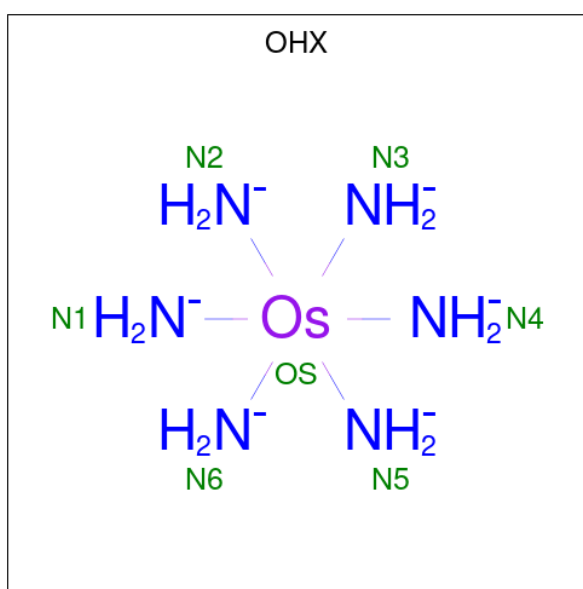
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	5	415	Total 415	Mg 415	0	0
85	7	13	Total 13	Mg 13	0	0
85	8	10	Total 10	Mg 10	0	0
85	l2	2	Total 2	Mg 2	0	0
85	l3	2	Total 2	Mg 2	0	0
85	l4	1	Total 1	Mg 1	0	0
85	l5	1	Total 1	Mg 1	0	0
85	l7	2	Total 2	Mg 2	0	0
85	m0	1	Total 1	Mg 1	0	0
85	m3	1	Total 1	Mg 1	0	0
85	m5	3	Total 3	Mg 3	0	0
85	m7	3	Total 3	Mg 3	0	0
85	n0	1	Total 1	Mg 1	0	0
85	n3	1	Total 1	Mg 1	0	0
85	n6	1	Total 1	Mg 1	0	0
85	n8	2	Total 2	Mg 2	0	0
85	o2	1	Total 1	Mg 1	0	0
85	o3	1	Total 1	Mg 1	0	0
85	o4	1	Total 1	Mg 1	0	0
85	q1	1	Total 1	Mg 1	0	0
85	q2	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	q3	1	Total	Mg	0	0
			1	1		
85	f	1	Total	Mg	0	0
			1	1		
85	B	1	Total	Mg	0	0
			1	1		
85	C	1	Total	Mg	0	0
			1	1		

- Molecule 86 is osmium (III) hexammine (CCD ID: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	1	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	1	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	1	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	1	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	1	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	1	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	S1	1	Total 7	N 6	Os 1	0	0
86	S6	1	Total 7	N 6	Os 1	0	0
86	S8	1	Total 7	N 6	Os 1	0	0
86	S9	1	Total 7	N 6	Os 1	0	0
86	C3	1	Total 7	N 6	Os 1	0	0
86	C5	1	Total 7	N 6	Os 1	0	0
86	C8	1	Total 7	N 6	Os 1	0	0
86	D9	1	Total 7	N 6	Os 1	0	0
86	SR	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	1	0
86	1	1	Total 7	N 6	Os 1	1	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	1	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	1	0
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			7	6	1		
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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			7	6	1		
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			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	2	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	1	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	2	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
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			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	3	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
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86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
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86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
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86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	L3	1	Total 7	N 6	Os 1	0	0
86	L3	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	L3	1	Total 7	N 6	Os 1	0	0
86	L4	1	Total 7	N 6	Os 1	0	0
86	L5	1	Total 7	N 6	Os 1	0	0
86	M0	1	Total 7	N 6	Os 1	0	0
86	M0	1	Total 7	N 6	Os 1	0	0
86	M5	1	Total 7	N 6	Os 1	0	0
86	M5	1	Total 7	N 6	Os 1	0	0
86	M6	1	Total 7	N 6	Os 1	0	0
86	M7	1	Total 7	N 6	Os 1	0	0
86	M8	1	Total 7	N 6	Os 1	0	0
86	M9	1	Total 7	N 6	Os 1	0	0
86	N8	1	Total 7	N 6	Os 1	0	0
86	N9	1	Total 7	N 6	Os 1	0	0
86	O1	1	Total 7	N 6	Os 1	0	0
86	O3	1	Total 7	N 6	Os 1	0	0
86	O4	1	Total 7	N 6	Os 1	0	0
86	O7	1	Total 7	N 6	Os 1	0	0
86	O9	1	Total 7	N 6	Os 1	0	0
86	Q2	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	2	0
86	6	1	Total 7	N 6	Os 1	1	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
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86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	1	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
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86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
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86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	1	0
			7	6	1		
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			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	1	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	s1	1	Total 7	N 6	Os 1	0	0
86	s1	1	Total 7	N 6	Os 1	0	0
86	s4	1	Total 7	N 6	Os 1	0	0
86	s8	1	Total 7	N 6	Os 1	0	0
86	s9	1	Total 7	N 6	Os 1	0	0
86	c3	1	Total 7	N 6	Os 1	0	0
86	c5	1	Total 7	N 6	Os 1	0	0
86	c5	1	Total 7	N 6	Os 1	0	0
86	c8	1	Total 7	N 6	Os 1	0	0
86	d4	1	Total 7	N 6	Os 1	0	0
86	d9	1	Total 7	N 6	Os 1	0	0
86	sR	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	1	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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			7	6	1		
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	5	1	Total	N	Os	0	0
			7	6	1		
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
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86	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	7	1	Total	N	Os	0	0
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86	7	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	8	1	Total	N	Os	1	0
			7	6	1		
86	8	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	l3	1	Total 7	N 6	Os 1	0	0
86	l3	1	Total 7	N 6	Os 1	0	0
86	l4	1	Total 7	N 6	Os 1	0	0
86	l4	1	Total 7	N 6	Os 1	0	0
86	l5	1	Total 7	N 6	Os 1	0	0
86	l5	1	Total 7	N 6	Os 1	1	0
86	l9	1	Total 7	N 6	Os 1	0	0
86	m0	1	Total 7	N 6	Os 1	0	0
86	m0	1	Total 7	N 6	Os 1	0	0
86	m1	1	Total 7	N 6	Os 1	0	0
86	m4	1	Total 7	N 6	Os 1	0	0
86	m5	1	Total 7	N 6	Os 1	0	0
86	m5	1	Total 7	N 6	Os 1	0	0
86	m5	1	Total 7	N 6	Os 1	0	0
86	m6	1	Total 7	N 6	Os 1	0	0
86	m7	1	Total 7	N 6	Os 1	0	0
86	m8	1	Total 7	N 6	Os 1	0	0
86	m9	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	o6	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

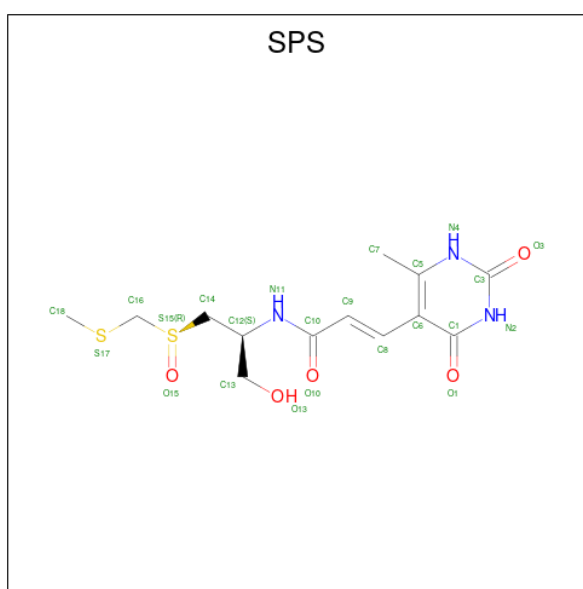
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87	D7	1	Total	Zn	0	0
			1	1		
87	D9	1	Total	Zn	0	0
			1	1		
87	E1	1	Total	Zn	0	0
			1	1		
87	O7	1	Total	Zn	0	0
			1	1		
87	Q0	1	Total	Zn	0	0
			1	1		
87	Q2	1	Total	Zn	0	0
			1	1		
87	Q3	1	Total	Zn	0	0
			1	1		
87	d6	1	Total	Zn	0	0
			1	1		
87	d7	1	Total	Zn	0	0
			1	1		
87	d9	1	Total	Zn	0	0
			1	1		
87	e1	1	Total	Zn	0	0
			1	1		

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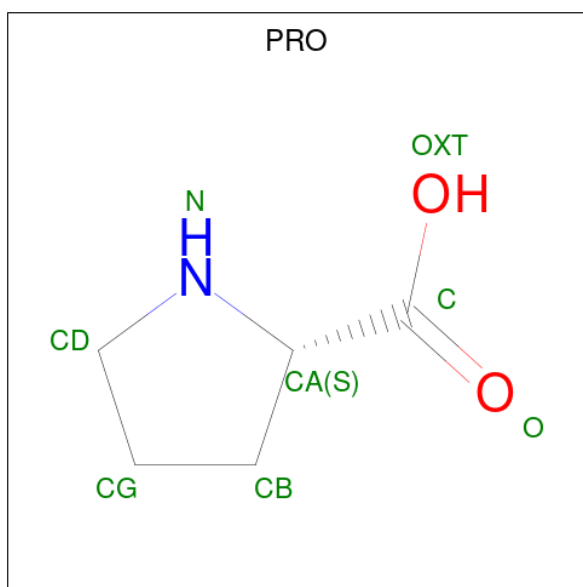
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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			1	1		
87	q0	1	Total	Zn	0	0
			1	1		
87	q2	1	Total	Zn	0	0
			1	1		
87	q3	1	Total	Zn	0	0
			1	1		

- Molecule 88 is SPARSOMYCIN (CCD ID: SPS) (formula: $C_{13}H_{19}N_3O_5S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
88	1	1	Total	C	N	O	S	0	0
			23	13	3	5	2		
88	5	1	Total	C	N	O	S	0	0
			23	13	3	5	2		

- Molecule 89 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
89	1	1	Total	C	N	O	0	0
			7	5	1	1		
89	5	1	Total	C	N	O	0	0
			7	5	1	1		
89	B	1	Total	C	N	O	0	0
			7	5	1	1		
89	C	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 90 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
90	5	6	Total	O	0	0
			6	6		
90	f	6	Total	O	0	0
			6	6		

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

3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	438.00Å 289.05Å 305.26Å 90.00° 98.95° 90.00°	Depositor
Resolution (Å)	122.88 – 3.45 122.88 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (122.88-3.45) 99.9 (122.88-3.45)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.49Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.207 , 0.263 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	90.1	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 97.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	413121	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
84	8AN	B	76	84,89,85	22,24,25	1.43	3 (13%)	26,35,38	2.24	9 (34%)
83	5CT	f	51	83	13,14,15	2.47	3 (23%)	9,15,17	2.36	4 (44%)
84	8AN	C	76	84,89,85	22,24,25	1.44	3 (13%)	26,35,38	2.43	9 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	8AN	B	76	84,89,85	-	2/7/25/26	0/3/3/3
83	5CT	f	51	83	1/1/2/4	6/13/14/16	-
84	8AN	C	76	84,89,85	-	3/7/25/26	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	f	51	5CT	O1-C2	-6.86	1.22	1.43
84	C	76	8AN	C5-C4	4.49	1.47	1.39
84	B	76	8AN	C5-C4	4.22	1.46	1.39
83	f	51	5CT	CB-CA	3.74	1.58	1.53
83	f	51	5CT	C1-NZ	-3.36	1.41	1.47
84	B	76	8AN	C5-C6	2.76	1.48	1.41
84	B	76	8AN	C8-N7	2.65	1.36	1.31
84	C	76	8AN	C5-C6	2.50	1.48	1.41
84	C	76	8AN	C8-N7	2.49	1.36	1.31

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	C	76	8AN	C5-C4-N3	-6.84	117.83	126.75
84	B	76	8AN	C5-C4-N3	-6.05	118.86	126.75
84	C	76	8AN	N3-C4-N9	5.65	136.39	127.08
83	f	51	5CT	C3-C2-C1	5.22	124.06	112.16
84	B	76	8AN	N3-C4-N9	4.21	134.02	127.08
84	C	76	8AN	C2-N3-C4	4.02	121.24	111.75
84	B	76	8AN	C2-N3-C4	3.92	121.01	111.75
84	B	76	8AN	C4-C5-N7	-3.65	106.17	110.62
83	f	51	5CT	O1-C2-C1	3.20	120.25	109.32
84	C	76	8AN	C4-C5-N7	-3.05	106.90	110.62
84	C	76	8AN	N1-C2-N3	-2.98	123.94	128.60
84	B	76	8AN	C5-N7-C8	2.91	107.65	103.51
84	B	76	8AN	N1-C2-N3	-2.89	124.09	128.60
84	C	76	8AN	C5-N7-C8	2.83	107.52	103.51
84	C	76	8AN	C4-N9-C8	2.82	108.79	105.73
84	B	76	8AN	C6-C5-N7	2.80	137.25	132.02
83	f	51	5CT	O1-C2-C3	2.27	115.69	109.21
84	B	76	8AN	C4-N9-C8	2.26	108.18	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	f	51	5CT	C1-NZ-CE	-2.24	108.41	113.42
84	B	76	8AN	N9-C8-N7	-2.22	110.87	113.91
84	C	76	8AN	N9-C8-N7	-2.13	111.01	113.91
84	C	76	8AN	C2'-C3'-C4'	2.12	105.64	102.68

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
83	f	51	5CT	C2

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	f	51	5CT	CD-CE-NZ-C1
83	f	51	5CT	O1-C2-C3-C4
83	f	51	5CT	C2-C3-C4-N1
83	f	51	5CT	CG-CD-CE-NZ
83	f	51	5CT	NZ-C1-C2-O1
84	C	76	8AN	C4'-C5'-O5'-P
84	B	76	8AN	C4'-C5'-O5'-P
84	C	76	8AN	C3'-C4'-C5'-O5'
84	C	76	8AN	O4'-C4'-C5'-O5'
83	f	51	5CT	C2-C1-NZ-CE
84	B	76	8AN	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 2284 ligands modelled in this entry, 1109 are monoatomic - leaving 1175 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	$\# Z > 2$
86	OHX	6	2129	-	0,6,6	-	-	-		
86	OHX	2	2090	-	0,6,6	-	-	-		
86	OHX	2	2036	-	0,6,6	-	-	-		
86	OHX	2	2072	-	0,6,6	-	-	-		
86	OHX	5	4115	85	0,6,6	-	-	-		
86	OHX	6	2026	-	0,6,6	-	-	-		
86	OHX	5	4145	85	0,6,6	-	-	-		
86	OHX	1	4088	-	0,6,6	-	-	-		
86	OHX	m5	304	-	0,6,6	-	-	-		
86	OHX	2	2137	-	0,6,6	-	-	-		
86	OHX	5	3909	-	0,6,6	-	-	-		
86	OHX	2	1999	-	0,6,6	-	-	-		
86	OHX	6	2061	-	0,6,6	-	-	-		
86	OHX	6	2149	-	0,6,6	-	-	-		
86	OHX	5	4151	85	0,6,6	-	-	-		
86	OHX	2	2040	-	0,6,6	-	-	-		
86	OHX	6	2048	-	0,6,6	-	-	-		
86	OHX	6	2070	-	0,6,6	-	-	-		
86	OHX	6	2151	-	0,6,6	-	-	-		
86	OHX	5	4065	-	0,6,6	-	-	-		
86	OHX	6	2015	-	0,6,6	-	-	-		
86	OHX	4	229	-	0,6,6	-	-	-		
86	OHX	2	2026	-	0,6,6	-	-	-		
86	OHX	2	2111	-	0,6,6	-	-	-		
86	OHX	2	2138	-	0,6,6	-	-	-		
86	OHX	6	2157	-	0,6,6	-	-	-		
86	OHX	6	2099	-	0,6,6	-	-	-		
86	OHX	2	2145	-	0,6,6	-	-	-		
86	OHX	5	4116	-	0,6,6	-	-	-		
86	OHX	4	219	-	0,6,6	-	-	-		
86	OHX	1	3983	-	0,6,6	-	-	-		
86	OHX	1	3802	-	0,6,6	-	-	-		
86	OHX	5	3970	-	0,6,6	-	-	-		
86	OHX	5	4073	85	0,6,6	-	-	-		
86	OHX	1	3771	-	0,6,6	-	-	-		
86	OHX	5	4102	-	0,6,6	-	-	-		
86	OHX	1	4048	85	0,6,6	-	-	-		
86	OHX	5	4057	-	0,6,6	-	-	-		
86	OHX	2	2015	-	0,6,6	-	-	-		
86	OHX	2	2113	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2053	-	0,6,6	-	-	-		
86	OHX	2	2095	-	0,6,6	-	-	-		
86	OHX	2	2144	-	0,6,6	-	-	-		
86	OHX	1	4096	-	0,6,6	-	-	-		
86	OHX	1	3895	-	0,6,6	-	-	-		
86	OHX	5	4097	-	0,6,6	-	-	-		
86	OHX	2	2059	-	0,6,6	-	-	-		
86	OHX	2	2086	-	0,6,6	-	-	-		
86	OHX	6	2100	-	0,6,6	-	-	-		
86	OHX	5	4086	-	0,6,6	-	-	-		
86	OHX	6	2170	-	0,6,6	-	-	-		
86	OHX	5	4072	-	0,6,6	-	-	-		
86	OHX	6	2069	-	0,6,6	-	-	-		
86	OHX	5	4042	-	0,6,6	-	-	-		
86	OHX	5	4062	-	0,6,6	-	-	-		
86	OHX	1	3905	-	0,6,6	-	-	-		
86	OHX	6	2050	-	0,6,6	-	-	-		
86	OHX	8	216	-	0,6,6	-	-	-		
86	OHX	m8	201	-	0,6,6	-	-	-		
86	OHX	5	4136	-	0,6,6	-	-	-		
86	OHX	6	2107	-	0,6,6	-	-	-		
86	OHX	5	4125	-	0,6,6	-	-	-		
86	OHX	1	3829	-	0,6,6	-	-	-		
86	OHX	1	3805	-	0,6,6	-	-	-		
86	OHX	1	3825	-	0,6,6	-	-	-		
86	OHX	1	3907	-	0,6,6	-	-	-		
86	OHX	1	3932	-	0,6,6	-	-	-		
86	OHX	6	2180	-	0,6,6	-	-	-		
86	OHX	2	2039	-	0,6,6	-	-	-		
86	OHX	5	4120	-	0,6,6	-	-	-		
86	OHX	1	3884	-	0,6,6	-	-	-		
86	OHX	5	4079	-	0,6,6	-	-	-		
86	OHX	m0	303	-	0,6,6	-	-	-		
86	OHX	2	2079	-	0,6,6	-	-	-		
86	OHX	5	4015	-	0,6,6	-	-	-		
86	OHX	2	2088	-	0,6,6	-	-	-		
86	OHX	1	3831	-	0,6,6	-	-	-		
86	OHX	1	3939	-	0,6,6	-	-	-		
86	OHX	O7	104	73	0,6,6	-	-	-		
86	OHX	1	3886	-	0,6,6	-	-	-		
86	OHX	3	218	-	0,6,6	-	-	-		
86	OHX	2	2046	-	0,6,6	-	-	-		
86	OHX	2	2152	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3858	-	0,6,6	-	-	-		
86	OHX	1	3914	-	0,6,6	-	-	-		
86	OHX	5	3867	-	0,6,6	-	-	-		
86	OHX	5	3897	-	0,6,6	-	-	-		
86	OHX	5	3998	-	0,6,6	-	-	-		
86	OHX	5	4083	-	0,6,6	-	-	-		
86	OHX	s1	301	-	0,6,6	-	-	-		
86	OHX	5	4089	-	0,6,6	-	-	-		
86	OHX	1	3892	-	0,6,6	-	-	-		
86	OHX	5	3910	-	0,6,6	-	-	-		
86	OHX	2	2024	-	0,6,6	-	-	-		
86	OHX	1	3978	-	0,6,6	-	-	-		
86	OHX	2	2109	-	0,6,6	-	-	-		
86	OHX	n3	202	-	0,6,6	-	-	-		
86	OHX	5	3875	-	0,6,6	-	-	-		
86	OHX	1	3972	-	0,6,6	-	-	-		
86	OHX	1	3872	85	0,6,6	-	-	-		
86	OHX	5	4020	-	0,6,6	-	-	-		
86	OHX	6	2024	-	0,6,6	-	-	-		
86	OHX	3	216	-	0,6,6	-	-	-		
86	OHX	5	3837	-	0,6,6	-	-	-		
86	OHX	2	2051	-	0,6,6	-	-	-		
86	OHX	5	3919	-	0,6,6	-	-	-		
86	OHX	1	3868	-	0,6,6	-	-	-		
86	OHX	5	4035	-	0,6,6	-	-	-		
86	OHX	5	4050	-	0,6,6	-	-	-		
86	OHX	5	4038	-	0,6,6	-	-	-		
86	OHX	6	2037	-	0,6,6	-	-	-		
86	OHX	1	4078	-	0,6,6	-	-	-		
86	OHX	5	4170	-	0,6,6	-	-	-		
86	OHX	3	213	-	0,6,6	-	-	-		
86	OHX	2	1998	-	0,6,6	-	-	-		
86	OHX	5	4142	-	0,6,6	-	-	-		
86	OHX	8	224	-	0,6,6	-	-	-		
86	OHX	5	3904	-	0,6,6	-	-	-		
86	OHX	6	2102	-	0,6,6	-	-	-		
86	OHX	5	3899	-	0,6,6	-	-	-		
86	OHX	6	2035	-	0,6,6	-	-	-		
86	OHX	5	4130	-	0,6,6	-	-	-		
86	OHX	1	3851	-	0,6,6	-	-	-		
86	OHX	4	225	-	0,6,6	-	-	-		
86	OHX	2	2106	-	0,6,6	-	-	-		
86	OHX	5	3900	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4101	-	0,6,6	-	-	-		
86	OHX	5	4140	-	0,6,6	-	-	-		
86	OHX	1	3952	-	0,6,6	-	-	-		
86	OHX	6	2091	-	0,6,6	-	-	-		
86	OHX	S8	301	-	0,6,6	-	-	-		
86	OHX	2	2102	-	0,6,6	-	-	-		
86	OHX	2	2005	-	0,6,6	-	-	-		
86	OHX	4	221	-	0,6,6	-	-	-		
86	OHX	5	3880	-	0,6,6	-	-	-		
86	OHX	6	2098	85	0,6,6	-	-	-		
86	OHX	1	3804	-	0,6,6	-	-	-		
86	OHX	5	4004	-	0,6,6	-	-	-		
86	OHX	5	4113	85	0,6,6	-	-	-		
86	OHX	1	3993	-	0,6,6	-	-	-		
86	OHX	1	4000	-	0,6,6	-	-	-		
86	OHX	5	4064	-	0,6,6	-	-	-		
86	OHX	1	3781	-	0,6,6	-	-	-		
89	PRO	1	4114	89	5,7,8	0.57	0	7,8,10	1.06	0
86	OHX	1	3917	-	0,6,6	-	-	-		
86	OHX	M9	202	-	0,6,6	-	-	-		
86	OHX	1	3988	-	0,6,6	-	-	-		
86	OHX	5	4018	-	0,6,6	-	-	-		
86	OHX	5	3881	-	0,6,6	-	-	-		
86	OHX	6	2105	-	0,6,6	-	-	-		
86	OHX	5	4069	-	0,6,6	-	-	-		
86	OHX	2	2001	-	0,6,6	-	-	-		
86	OHX	2	2000	-	0,6,6	-	-	-		
86	OHX	o7	502	-	0,6,6	-	-	-		
86	OHX	5	4164	-	0,6,6	-	-	-		
86	OHX	5	3978	-	0,6,6	-	-	-		
86	OHX	6	2171	-	0,6,6	-	-	-		
86	OHX	1	4076	-	0,6,6	-	-	-		
86	OHX	L3	403	-	0,6,6	-	-	-		
86	OHX	N9	101	-	0,6,6	-	-	-		
86	OHX	5	3821	-	0,6,6	-	-	-		
86	OHX	5	4000	-	0,6,6	-	-	-		
86	OHX	6	2155	-	0,6,6	-	-	-		
86	OHX	5	3886	-	0,6,6	-	-	-		
86	OHX	1	4039	-	0,6,6	-	-	-		
86	OHX	2	2105	-	0,6,6	-	-	-		
86	OHX	1	3797	-	0,6,6	-	-	-		
86	OHX	1	3853	85	0,6,6	-	-	-		
86	OHX	1	4006	85	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2108	-	0,6,6	-	-	-		
86	OHX	6	2052	-	0,6,6	-	-	-		
86	OHX	1	4107	-	0,6,6	-	-	-		
86	OHX	6	2144	-	0,6,6	-	-	-		
86	OHX	2	2013	-	0,6,6	-	-	-		
86	OHX	5	4045	-	0,6,6	-	-	-		
86	OHX	5	3985	-	0,6,6	-	-	-		
86	OHX	4	230	-	0,6,6	-	-	-		
86	OHX	1	4072	-	0,6,6	-	-	-		
86	OHX	5	4043	-	0,6,6	-	-	-		
86	OHX	5	4098	-	0,6,6	-	-	-		
86	OHX	2	2025	-	0,6,6	-	-	-		
86	OHX	6	2145	-	0,6,6	-	-	-		
86	OHX	1	3979	-	0,6,6	-	-	-		
86	OHX	1	3789	-	0,6,6	-	-	-		
86	OHX	1	3786	-	0,6,6	-	-	-		
86	OHX	6	2085	-	0,6,6	-	-	-		
86	OHX	1	4093	-	0,6,6	-	-	-		
86	OHX	1	3799	-	0,6,6	-	-	-		
86	OHX	6	2092	-	0,6,6	-	-	-		
86	OHX	5	3949	-	0,6,6	-	-	-		
86	OHX	1	3772	-	0,6,6	-	-	-		
86	OHX	1	3828	-	0,6,6	-	-	-		
86	OHX	5	4053	85	0,6,6	-	-	-		
86	OHX	1	3964	-	0,6,6	-	-	-		
86	OHX	5	4106	-	0,6,6	-	-	-		
86	OHX	2	2101	-	0,6,6	-	-	-		
86	OHX	1	3987	-	0,6,6	-	-	-		
86	OHX	6	2059	-	0,6,6	-	-	-		
86	OHX	1	3933	-	0,6,6	-	-	-		
86	OHX	5	4001	-	0,6,6	-	-	-		
86	OHX	1	4030	-	0,6,6	-	-	-		
86	OHX	1	4104	-	0,6,6	-	-	-		
86	OHX	5	4005	-	0,6,6	-	-	-		
86	OHX	5	4152	-	0,6,6	-	-	-		
86	OHX	1	4075	-	0,6,6	-	-	-		
86	OHX	6	2134	-	0,6,6	-	-	-		
86	OHX	2	2037	-	0,6,6	-	-	-		
86	OHX	1	3777	-	0,6,6	-	-	-		
86	OHX	1	3778	-	0,6,6	-	-	-		
86	OHX	6	2160	-	0,6,6	-	-	-		
86	OHX	5	4108	-	0,6,6	-	-	-		
86	OHX	5	3911	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	o7	503	-	0,6,6	-	-	-		
86	OHX	1	3776	-	0,6,6	-	-	-		
86	OHX	1	3980	-	0,6,6	-	-	-		
86	OHX	5	3981	-	0,6,6	-	-	-		
86	OHX	2	2053	-	0,6,6	-	-	-		
86	OHX	5	4123	-	0,6,6	-	-	-		
86	OHX	5	3828	-	0,6,6	-	-	-		
86	OHX	4	224	-	0,6,6	-	-	-		
86	OHX	1	4017	-	0,6,6	-	-	-		
86	OHX	5	3866	-	0,6,6	-	-	-		
86	OHX	1	3920	-	0,6,6	-	-	-		
86	OHX	1	4007	-	0,6,6	-	-	-		
86	OHX	5	4051	-	0,6,6	-	-	-		
86	OHX	1	3800	85	0,6,6	-	-	-		
86	OHX	5	3960	-	0,6,6	-	-	-		
86	OHX	5	4061	-	0,6,6	-	-	-		
86	OHX	2	2096	-	0,6,6	-	-	-		
86	OHX	2	2126	-	0,6,6	-	-	-		
86	OHX	1	3847	-	0,6,6	-	-	-		
86	OHX	1	3969	-	0,6,6	-	-	-		
86	OHX	5	3938	-	0,6,6	-	-	-		
86	OHX	1	4031	-	0,6,6	-	-	-		
86	OHX	5	4071	-	0,6,6	-	-	-		
86	OHX	5	4077	-	0,6,6	-	-	-		
86	OHX	5	4082	-	0,6,6	-	-	-		
86	OHX	1	3762	-	0,6,6	-	-	-		
86	OHX	2	2011	-	0,6,6	-	-	-		
86	OHX	5	4036	-	0,6,6	-	-	-		
86	OHX	2	2103	-	0,6,6	-	-	-		
86	OHX	6	2115	-	0,6,6	-	-	-		
86	OHX	5	3849	-	0,6,6	-	-	-		
86	OHX	2	2048	-	0,6,6	-	-	-		
86	OHX	4	220	-	0,6,6	-	-	-		
86	OHX	5	3887	-	0,6,6	-	-	-		
86	OHX	5	4014	-	0,6,6	-	-	-		
86	OHX	5	4068	-	0,6,6	-	-	-		
86	OHX	8	225	-	0,6,6	-	-	-		
86	OHX	5	4066	-	0,6,6	-	-	-		
86	OHX	5	3951	-	0,6,6	-	-	-		
86	OHX	1	3958	-	0,6,6	-	-	-		
86	OHX	2	2099	-	0,6,6	-	-	-		
86	OHX	1	3883	-	0,6,6	-	-	-		
86	OHX	1	3809	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	m5	306	-	0,6,6	-	-	-		
86	OHX	6	2131	-	0,6,6	-	-	-		
86	OHX	5	3864	-	0,6,6	-	-	-		
86	OHX	1	3869	-	0,6,6	-	-	-		
86	OHX	2	2007	-	0,6,6	-	-	-		
86	OHX	2	2130	-	0,6,6	-	-	-		
86	OHX	3	211	-	0,6,6	-	-	-		
86	OHX	3	210	-	0,6,6	-	-	-		
86	OHX	5	4119	-	0,6,6	-	-	-		
86	OHX	2	2114	-	0,6,6	-	-	-		
86	OHX	5	4032	-	0,6,6	-	-	-		
86	OHX	1	3819	-	0,6,6	-	-	-		
86	OHX	1	3888	-	0,6,6	-	-	-		
86	OHX	1	3922	-	0,6,6	-	-	-		
86	OHX	m7	204	-	0,6,6	-	-	-		
86	OHX	5	4169	-	0,6,6	-	-	-		
86	OHX	1	4060	-	0,6,6	-	-	-		
86	OHX	5	4150	-	0,6,6	-	-	-		
86	OHX	5	4044	-	0,6,6	-	-	-		
86	OHX	7	223	-	0,6,6	-	-	-		
86	OHX	5	3878	-	0,6,6	-	-	-		
86	OHX	5	4039	-	0,6,6	-	-	-		
86	OHX	1	3873	-	0,6,6	-	-	-		
86	OHX	5	3957	-	0,6,6	-	-	-		
86	OHX	6	2124	-	0,6,6	-	-	-		
86	OHX	1	3791	-	0,6,6	-	-	-		
86	OHX	1	3842	-	0,6,6	-	-	-		
86	OHX	2	2122	-	0,6,6	-	-	-		
86	OHX	1	3906	-	0,6,6	-	-	-		
86	OHX	5	3928	-	0,6,6	-	-	-		
86	OHX	5	3941	-	0,6,6	-	-	-		
86	OHX	5	4129	-	0,6,6	-	-	-		
86	OHX	5	3918	-	0,6,6	-	-	-		
86	OHX	5	4021	-	0,6,6	-	-	-		
86	OHX	8	219	-	0,6,6	-	-	-		
86	OHX	5	4127	85	0,6,6	-	-	-		
86	OHX	5	4034	-	0,6,6	-	-	-		
86	OHX	5	3877	-	0,6,6	-	-	-		
86	OHX	8	214	-	0,6,6	-	-	-		
86	OHX	5	3861	-	0,6,6	-	-	-		
86	OHX	c5	202	17	0,6,6	-	-	-		
86	OHX	5	3822	-	0,6,6	-	-	-		
86	OHX	D9	102	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2086	-	0,6,6	-	-	-		
86	OHX	5	4012	-	0,6,6	-	-	-		
86	OHX	5	4131	-	0,6,6	-	-	-		
86	OHX	5	3891	-	0,6,6	-	-	-		
86	OHX	5	3940	-	0,6,6	-	-	-		
86	OHX	2	2125	85	0,6,6	-	-	-		
86	OHX	5	4009	-	0,6,6	-	-	-		
86	OHX	1	3806	-	0,6,6	-	-	-		
86	OHX	2	2035	-	0,6,6	-	-	-		
86	OHX	6	2182	-	0,6,6	-	-	-		
86	OHX	5	4024	-	0,6,6	-	-	-		
86	OHX	1	3961	-	0,6,6	-	-	-		
86	OHX	14	403	-	0,6,6	-	-	-		
86	OHX	5	4096	-	0,6,6	-	-	-		
86	OHX	5	3879	-	0,6,6	-	-	-		
86	OHX	1	3855	-	0,6,6	-	-	-		
86	OHX	2	2087	-	0,6,6	-	-	-		
86	OHX	1	3763	-	0,6,6	-	-	-		
86	OHX	6	2030	-	0,6,6	-	-	-		
86	OHX	5	4063	-	0,6,6	-	-	-		
86	OHX	5	4138	-	0,6,6	-	-	-		
86	OHX	4	217	-	0,6,6	-	-	-		
86	OHX	5	4054	-	0,6,6	-	-	-		
86	OHX	1	4010	-	0,6,6	-	-	-		
86	OHX	1	4008	85	0,6,6	-	-	-		
86	OHX	1	3970	-	0,6,6	-	-	-		
86	OHX	6	2118	-	0,6,6	-	-	-		
86	OHX	5	3846	-	0,6,6	-	-	-		
86	OHX	5	3956	-	0,6,6	-	-	-		
86	OHX	5	4055	-	0,6,6	-	-	-		
86	OHX	1	3779	-	0,6,6	-	-	-		
86	OHX	6	2027	-	0,6,6	-	-	-		
86	OHX	6	2146	-	0,6,6	-	-	-		
86	OHX	1	4047	-	0,6,6	-	-	-		
86	OHX	1	4099	-	0,6,6	-	-	-		
86	OHX	O9	101	-	0,6,6	-	-	-		
86	OHX	1	3936	-	0,6,6	-	-	-		
86	OHX	1	3947	-	0,6,6	-	-	-		
86	OHX	2	2016	85	0,6,6	-	-	-		
86	OHX	1	3966	85	0,6,6	-	-	-		
86	OHX	1	4097	-	0,6,6	-	-	-		
86	OHX	5	3830	-	0,6,6	-	-	-		
86	OHX	6	2013	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3954	-	0,6,6	-	-	-		
86	OHX	1	3997	-	0,6,6	-	-	-		
86	OHX	1	4062	-	0,6,6	-	-	-		
86	OHX	6	2014	-	0,6,6	-	-	-		
86	OHX	1	3784	-	0,6,6	-	-	-		
86	OHX	2	2146	-	0,6,6	-	-	-		
86	OHX	1	3820	-	0,6,6	-	-	-		
86	OHX	2	2133	-	0,6,6	-	-	-		
86	OHX	M0	303	-	0,6,6	-	-	-		
86	OHX	6	2025	-	0,6,6	-	-	-		
86	OHX	5	3995	-	0,6,6	-	-	-		
86	OHX	1	3848	-	0,6,6	-	-	-		
86	OHX	O1	201	-	0,6,6	-	-	-		
86	OHX	c5	201	-	0,6,6	-	-	-		
86	OHX	8	217	-	0,6,6	-	-	-		
86	OHX	o6	201	-	0,6,6	-	-	-		
86	OHX	1	3790	85	0,6,6	-	-	-		
86	OHX	5	4058	-	0,6,6	-	-	-		
86	OHX	1	4066	-	0,6,6	-	-	-		
86	OHX	5	4028	-	0,6,6	-	-	-		
86	OHX	1	3808	-	0,6,6	-	-	-		
86	OHX	5	3968	-	0,6,6	-	-	-		
86	OHX	5	3996	-	0,6,6	-	-	-		
86	OHX	5	4095	-	0,6,6	-	-	-		
86	OHX	6	2136	-	0,6,6	-	-	-		
86	OHX	1	3908	-	0,6,6	-	-	-		
86	OHX	1	4079	-	0,6,6	-	-	-		
86	OHX	6	2064	-	0,6,6	-	-	-		
86	OHX	1	3915	-	0,6,6	-	-	-		
86	OHX	1	3816	-	0,6,6	-	-	-		
86	OHX	5	3916	-	0,6,6	-	-	-		
86	OHX	5	4025	-	0,6,6	-	-	-		
86	OHX	2	2080	-	0,6,6	-	-	-		
86	OHX	6	2168	-	0,6,6	-	-	-		
86	OHX	1	3934	-	0,6,6	-	-	-		
86	OHX	6	2103	-	0,6,6	-	-	-		
86	OHX	1	3862	-	0,6,6	-	-	-		
86	OHX	5	3841	-	0,6,6	-	-	-		
86	OHX	1	3852	-	0,6,6	-	-	-		
86	OHX	2	2083	-	0,6,6	-	-	-		
86	OHX	2	2107	-	0,6,6	-	-	-		
86	OHX	6	2078	-	0,6,6	-	-	-		
86	OHX	5	3842	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2098	-	0,6,6	-	-	-		
86	OHX	6	2071	-	0,6,6	-	-	-		
86	OHX	1	3935	-	0,6,6	-	-	-		
86	OHX	6	2032	-	0,6,6	-	-	-		
86	OHX	1	4105	-	0,6,6	-	-	-		
86	OHX	1	3931	-	0,6,6	-	-	-		
86	OHX	5	4155	-	0,6,6	-	-	-		
86	OHX	6	2172	-	0,6,6	-	-	-		
86	OHX	5	3915	-	0,6,6	-	-	-		
86	OHX	6	2034	-	0,6,6	-	-	-		
86	OHX	6	2104	-	0,6,6	-	-	-		
86	OHX	L4	401	-	0,6,6	-	-	-		
86	OHX	M0	304	-	0,6,6	-	-	-		
86	OHX	6	2012	-	0,6,6	-	-	-		
86	OHX	6	2119	-	0,6,6	-	-	-		
86	OHX	1	4080	-	0,6,6	-	-	-		
86	OHX	1	4090	-	0,6,6	-	-	-		
86	OHX	6	2084	-	0,6,6	-	-	-		
86	OHX	1	3845	-	0,6,6	-	-	-		
86	OHX	5	3826	-	0,6,6	-	-	-		
86	OHX	2	2071	-	0,6,6	-	-	-		
86	OHX	5	4067	-	0,6,6	-	-	-		
86	OHX	c3	201	-	0,6,6	-	-	-		
86	OHX	6	2113	-	0,6,6	-	-	-		
86	OHX	6	2114	-	0,6,6	-	-	-		
86	OHX	6	2175	-	0,6,6	-	-	-		
86	OHX	6	2040	-	0,6,6	-	-	-		
86	OHX	5	3818	-	0,6,6	-	-	-		
86	OHX	1	3881	-	0,6,6	-	-	-		
86	OHX	5	4103	-	0,6,6	-	-	-		
86	OHX	5	4110	-	0,6,6	-	-	-		
86	OHX	1	3963	-	0,6,6	-	-	-		
86	OHX	5	3961	-	0,6,6	-	-	-		
86	OHX	1	3840	-	0,6,6	-	-	-		
86	OHX	2	2084	-	0,6,6	-	-	-		
86	OHX	1	3769	-	0,6,6	-	-	-		
86	OHX	8	227	-	0,6,6	-	-	-		
86	OHX	6	2112	-	0,6,6	-	-	-		
86	OHX	1	3913	-	0,6,6	-	-	-		
86	OHX	1	4091	-	0,6,6	-	-	-		
86	OHX	1	3924	-	0,6,6	-	-	-		
86	OHX	5	3942	-	0,6,6	-	-	-		
86	OHX	6	2150	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3948	-	0,6,6	-	-	-		
86	OHX	5	3959	-	0,6,6	-	-	-		
86	OHX	8	221	-	0,6,6	-	-	-		
86	OHX	5	4010	-	0,6,6	-	-	-		
86	OHX	2	2081	-	0,6,6	-	-	-		
86	OHX	1	3971	-	0,6,6	-	-	-		
86	OHX	1	3990	-	0,6,6	-	-	-		
86	OHX	1	3965	-	0,6,6	-	-	-		
86	OHX	1	3999	-	0,6,6	-	-	-		
86	OHX	1	3897	-	0,6,6	-	-	-		
86	OHX	5	4121	-	0,6,6	-	-	-		
86	OHX	6	2143	-	0,6,6	-	-	-		
86	OHX	5	4033	-	0,6,6	-	-	-		
86	OHX	5	4047	-	0,6,6	-	-	-		
86	OHX	1	4040	-	0,6,6	-	-	-		
86	OHX	2	1996	-	0,6,6	-	-	-		
86	OHX	2	2050	-	0,6,6	-	-	-		
86	OHX	6	2046	-	0,6,6	-	-	-		
86	OHX	6	2028	-	0,6,6	-	-	-		
86	OHX	5	4046	-	0,6,6	-	-	-		
86	OHX	l3	403	-	0,6,6	-	-	-		
86	OHX	1	3962	-	0,6,6	-	-	-		
86	OHX	1	4037	-	0,6,6	-	-	-		
86	OHX	1	4084	85	0,6,6	-	-	-		
86	OHX	1	3890	-	0,6,6	-	-	-		
86	OHX	8	230	-	0,6,6	-	-	-		
86	OHX	6	2169	-	0,6,6	-	-	-		
86	OHX	s8	303	-	0,6,6	-	-	-		
86	OHX	2	2129	-	0,6,6	-	-	-		
86	OHX	o3	202	-	0,6,6	-	-	-		
86	OHX	5	3903	-	0,6,6	-	-	-		
86	OHX	1	3823	-	0,6,6	-	-	-		
86	OHX	1	3856	-	0,6,6	-	-	-		
86	OHX	1	3994	-	0,6,6	-	-	-		
86	OHX	1	4056	-	0,6,6	-	-	-		
86	OHX	5	4011	-	0,6,6	-	-	-		
86	OHX	2	2121	-	0,6,6	-	-	-		
86	OHX	1	3817	-	0,6,6	-	-	-		
86	OHX	5	4166	-	0,6,6	-	-	-		
86	OHX	6	2130	-	0,6,6	-	-	-		
86	OHX	1	3912	-	0,6,6	-	-	-		
86	OHX	c8	203	-	0,6,6	-	-	-		
86	OHX	1	3839	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	sR	401	-	0,6,6	-	-	-		
86	OHX	1	3953	-	0,6,6	-	-	-		
86	OHX	5	4163	-	0,6,6	-	-	-		
86	OHX	6	2082	-	0,6,6	-	-	-		
86	OHX	1	3871	-	0,6,6	-	-	-		
86	OHX	4	231	-	0,6,6	-	-	-		
86	OHX	2	2066	-	0,6,6	-	-	-		
86	OHX	2	2027	-	0,6,6	-	-	-		
86	OHX	6	2166	-	0,6,6	-	-	-		
86	OHX	1	3787	-	0,6,6	-	-	-		
86	OHX	5	3902	-	0,6,6	-	-	-		
86	OHX	2	1997	-	0,6,6	-	-	-		
86	OHX	1	4111	-	0,6,6	-	-	-		
86	OHX	1	3812	-	0,6,6	-	-	-		
86	OHX	1	4087	-	0,6,6	-	-	-		
86	OHX	5	3829	-	0,6,6	-	-	-		
86	OHX	5	3992	-	0,6,6	-	-	-		
86	OHX	6	2049	-	0,6,6	-	-	-		
86	OHX	6	2056	-	0,6,6	-	-	-		
86	OHX	5	4154	-	0,6,6	-	-	-		
86	OHX	1	3863	-	0,6,6	-	-	-		
86	OHX	1	3843	-	0,6,6	-	-	-		
86	OHX	2	2108	-	0,6,6	-	-	-		
86	OHX	5	4088	-	0,6,6	-	-	-		
86	OHX	1	3896	-	0,6,6	-	-	-		
86	OHX	5	4143	-	0,6,6	-	-	-		
86	OHX	1	4108	-	0,6,6	-	-	-		
86	OHX	6	2156	-	0,6,6	-	-	-		
86	OHX	7	222	-	0,6,6	-	-	-		
86	OHX	5	3845	-	0,6,6	-	-	-		
86	OHX	5	4144	-	0,6,6	-	-	-		
86	OHX	1	3926	-	0,6,6	-	-	-		
86	OHX	5	3937	-	0,6,6	-	-	-		
86	OHX	5	3930	-	0,6,6	-	-	-		
86	OHX	1	3960	-	0,6,6	-	-	-		
86	OHX	1	4064	-	0,6,6	-	-	-		
86	OHX	5	3990	-	0,6,6	-	-	-		
86	OHX	5	3983	-	0,6,6	-	-	-		
86	OHX	1	4018	-	0,6,6	-	-	-		
86	OHX	1	4019	-	0,6,6	-	-	-		
86	OHX	6	2045	-	0,6,6	-	-	-		
86	OHX	1	4036	-	0,6,6	-	-	-		
86	OHX	5	3984	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4069	-	0,6,6	-	-	-		
86	OHX	4	226	-	0,6,6	-	-	-		
86	OHX	5	4048	-	0,6,6	-	-	-		
86	OHX	5	4084	36	0,6,6	-	-	-		
86	OHX	4	232	-	0,6,6	-	-	-		
86	OHX	5	3895	-	0,6,6	-	-	-		
86	OHX	1	3768	-	0,6,6	-	-	-		
86	OHX	15	303	-	0,6,6	-	-	-		
86	OHX	1	3821	-	0,6,6	-	-	-		
86	OHX	1	4100	-	0,6,6	-	-	-		
86	OHX	2	2142	85	0,6,6	-	-	-		
86	OHX	5	3905	-	0,6,6	-	-	-		
86	OHX	6	2033	-	0,6,6	-	-	-		
86	OHX	6	2067	1	0,6,6	-	-	-		
86	OHX	5	4076	-	0,6,6	-	-	-		
86	OHX	1	3827	-	0,6,6	-	-	-		
86	OHX	C8	201	-	0,6,6	-	-	-		
86	OHX	2	2033	-	0,6,6	-	-	-		
86	OHX	1	3854	-	0,6,6	-	-	-		
86	OHX	1	3893	-	0,6,6	-	-	-		
86	OHX	2	2002	-	0,6,6	-	-	-		
86	OHX	2	2135	-	0,6,6	-	-	-		
86	OHX	1	3918	-	0,6,6	-	-	-		
86	OHX	4	218	-	0,6,6	-	-	-		
86	OHX	6	2076	-	0,6,6	-	-	-		
86	OHX	6	2148	-	0,6,6	-	-	-		
86	OHX	5	3825	-	0,6,6	-	-	-		
86	OHX	5	3907	-	0,6,6	-	-	-		
86	OHX	5	3932	-	0,6,6	-	-	-		
86	OHX	5	4002	-	0,6,6	-	-	-		
86	OHX	2	2038	-	0,6,6	-	-	-		
86	OHX	2	2019	-	0,6,6	-	-	-		
86	OHX	1	3861	-	0,6,6	-	-	-		
86	OHX	8	223	-	0,6,6	-	-	-		
86	OHX	1	3929	-	0,6,6	-	-	-		
86	OHX	5	4100	-	0,6,6	-	-	-		
86	OHX	6	2057	-	0,6,6	-	-	-		
86	OHX	5	3831	-	0,6,6	-	-	-		
86	OHX	5	3939	-	0,6,6	-	-	-		
86	OHX	1	3782	-	0,6,6	-	-	-		
86	OHX	5	3950	-	0,6,6	-	-	-		
86	OHX	O4	202	-	0,6,6	-	-	-		
86	OHX	1	4003	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2021	-	0,6,6	-	-	-		
86	OHX	5	3893	85	0,6,6	-	-	-		
86	OHX	5	3914	-	0,6,6	-	-	-		
86	OHX	1	3796	-	0,6,6	-	-	-		
86	OHX	6	2077	-	0,6,6	-	-	-		
86	OHX	6	2031	-	0,6,6	-	-	-		
86	OHX	1	3879	-	0,6,6	-	-	-		
86	OHX	5	4141	-	0,6,6	-	-	-		
86	OHX	1	3885	-	0,6,6	-	-	-		
86	OHX	6	2135	-	0,6,6	-	-	-		
86	OHX	2	2141	-	0,6,6	-	-	-		
86	OHX	6	2081	-	0,6,6	-	-	-		
86	OHX	5	3868	-	0,6,6	-	-	-		
86	OHX	5	3977	-	0,6,6	-	-	-		
86	OHX	5	4147	-	0,6,6	-	-	-		
89	PRO	B	101	84,89	5,7,8	0.51	0	7,8,10	1.30	1 (14%)
86	OHX	1	3882	-	0,6,6	-	-	-		
86	OHX	2	2147	-	0,6,6	-	-	-		
86	OHX	6	2023	-	0,6,6	-	-	-		
86	OHX	1	4034	-	0,6,6	-	-	-		
86	OHX	s9	201	-	0,6,6	-	-	-		
86	OHX	2	2020	-	0,6,6	-	-	-		
86	OHX	C5	201	17	0,6,6	-	-	-		
86	OHX	6	2083	-	0,6,6	-	-	-		
86	OHX	1	3946	-	0,6,6	-	-	-		
86	OHX	1	3973	-	0,6,6	-	-	-		
86	OHX	5	4078	-	0,6,6	-	-	-		
86	OHX	1	4082	-	0,6,6	-	-	-		
86	OHX	5	3945	-	0,6,6	-	-	-		
86	OHX	5	4156	-	0,6,6	-	-	-		
86	OHX	2	2123	-	0,6,6	-	-	-		
86	OHX	7	215	-	0,6,6	-	-	-		
86	OHX	m1	201	-	0,6,6	-	-	-		
86	OHX	m5	305	-	0,6,6	-	-	-		
86	OHX	4	222	-	0,6,6	-	-	-		
86	OHX	2	2031	-	0,6,6	-	-	-		
86	OHX	5	3993	-	0,6,6	-	-	-		
86	OHX	2	2150	-	0,6,6	-	-	-		
86	OHX	2	2128	-	0,6,6	-	-	-		
86	OHX	C3	201	-	0,6,6	-	-	-		
86	OHX	2	2034	-	0,6,6	-	-	-		
86	OHX	1	3982	-	0,6,6	-	-	-		
86	OHX	5	3989	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4162	-	0,6,6	-	-	-		
86	OHX	2	2012	-	0,6,6	-	-	-		
86	OHX	1	4074	-	0,6,6	-	-	-		
86	OHX	5	3952	-	0,6,6	-	-	-		
86	OHX	1	3951	-	0,6,6	-	-	-		
86	OHX	1	3865	-	0,6,6	-	-	-		
86	OHX	1	4038	-	0,6,6	-	-	-		
86	OHX	M7	205	-	0,6,6	-	-	-		
86	OHX	1	3967	-	0,6,6	-	-	-		
86	OHX	1	4085	-	0,6,6	-	-	-		
86	OHX	1	3807	-	0,6,6	-	-	-		
86	OHX	6	2132	-	0,6,6	-	-	-		
86	OHX	6	2120	-	0,6,6	-	-	-		
86	OHX	5	3820	-	0,6,6	-	-	-		
86	OHX	5	3834	-	0,6,6	-	-	-		
86	OHX	5	3832	-	0,6,6	-	-	-		
86	OHX	1	3976	-	0,6,6	-	-	-		
86	OHX	1	3996	-	0,6,6	-	-	-		
86	OHX	1	3894	-	0,6,6	-	-	-		
86	OHX	5	3850	-	0,6,6	-	-	-		
86	OHX	5	3827	-	0,6,6	-	-	-		
86	OHX	1	4049	-	0,6,6	-	-	-		
86	OHX	1	4023	-	0,6,6	-	-	-		
86	OHX	6	2063	-	0,6,6	-	-	-		
86	OHX	6	2097	-	0,6,6	-	-	-		
86	OHX	5	3853	-	0,6,6	-	-	-		
86	OHX	5	3931	-	0,6,6	-	-	-		
86	OHX	5	3988	-	0,6,6	-	-	-		
86	OHX	5	3994	-	0,6,6	-	-	-		
86	OHX	1	3835	-	0,6,6	-	-	-		
88	SPS	5	3403	-	20,23,23	3.55	14 (70%)	24,30,30	2.69	14 (58%)
86	OHX	8	215	-	0,6,6	-	-	-		
86	OHX	8	226	-	0,6,6	-	-	-		
86	OHX	1	3878	-	0,6,6	-	-	-		
86	OHX	2	2067	-	0,6,6	-	-	-		
86	OHX	1	3943	-	0,6,6	-	-	-		
86	OHX	5	3953	-	0,6,6	-	-	-		
86	OHX	5	4056	-	0,6,6	-	-	-		
86	OHX	5	4124	-	0,6,6	-	-	-		
86	OHX	6	2044	-	0,6,6	-	-	-		
86	OHX	1	4109	-	0,6,6	-	-	-		
86	OHX	1	3975	-	0,6,6	-	-	-		
86	OHX	1	4016	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	1994	-	0,6,6	-	-	-		
86	OHX	5	4006	-	0,6,6	-	-	-		
86	OHX	6	2177	-	0,6,6	-	-	-		
86	OHX	6	2039	-	0,6,6	-	-	-		
86	OHX	19	201	-	0,6,6	-	-	-		
86	OHX	2	2116	-	0,6,6	-	-	-		
86	OHX	1	4027	-	0,6,6	-	-	-		
86	OHX	5	3925	-	0,6,6	-	-	-		
86	OHX	5	3933	-	0,6,6	-	-	-		
86	OHX	m6	201	-	0,6,6	-	-	-		
86	OHX	5	3927	-	0,6,6	-	-	-		
86	OHX	1	3916	-	0,6,6	-	-	-		
86	OHX	2	2029	-	0,6,6	-	-	-		
86	OHX	2	2054	-	0,6,6	-	-	-		
86	OHX	M5	303	-	0,6,6	-	-	-		
86	OHX	6	2051	-	0,6,6	-	-	-		
86	OHX	5	4087	85	0,6,6	-	-	-		
86	OHX	5	4157	-	0,6,6	-	-	-		
86	OHX	1	3833	-	0,6,6	-	-	-		
86	OHX	2	2093	-	0,6,6	-	-	-		
86	OHX	5	3944	-	0,6,6	-	-	-		
86	OHX	5	3979	-	0,6,6	-	-	-		
86	OHX	5	4099	-	0,6,6	-	-	-		
86	OHX	1	3795	-	0,6,6	-	-	-		
86	OHX	5	4013	-	0,6,6	-	-	-		
86	OHX	5	3926	-	0,6,6	-	-	-		
86	OHX	N8	204	-	0,6,6	-	-	-		
86	OHX	2	2143	-	0,6,6	-	-	-		
86	OHX	2	2049	-	0,6,6	-	-	-		
86	OHX	5	4027	-	0,6,6	-	-	-		
86	OHX	5	4030	85	0,6,6	-	-	-		
86	OHX	5	3922	-	0,6,6	-	-	-		
86	OHX	5	4104	-	0,6,6	-	-	-		
86	OHX	5	4160	-	0,6,6	-	-	-		
86	OHX	5	4060	-	0,6,6	-	-	-		
86	OHX	5	4075	-	0,6,6	-	-	-		
86	OHX	7	219	-	0,6,6	-	-	-		
88	SPS	1	4113	85	20,23,23	3.65	13 (65%)	24,30,30	2.58	11 (45%)
86	OHX	5	4126	-	0,6,6	-	-	-		
86	OHX	1	4102	-	0,6,6	-	-	-		
86	OHX	5	3833	85	0,6,6	-	-	-		
86	OHX	2	2082	-	0,6,6	-	-	-		
86	OHX	m9	201	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	S9	201	-	0,6,6	-	-	-		
86	OHX	1	4057	-	0,6,6	-	-	-		
86	OHX	2	2018	-	0,6,6	-	-	-		
86	OHX	2	2022	-	0,6,6	-	-	-		
86	OHX	6	2174	-	0,6,6	-	-	-		
86	OHX	5	3873	-	0,6,6	-	-	-		
86	OHX	2	2047	-	0,6,6	-	-	-		
86	OHX	1	4065	-	0,6,6	-	-	-		
86	OHX	2	2148	-	0,6,6	-	-	-		
86	OHX	5	3876	-	0,6,6	-	-	-		
86	OHX	5	3908	-	0,6,6	-	-	-		
86	OHX	6	2058	-	0,6,6	-	-	-		
86	OHX	5	3920	-	0,6,6	-	-	-		
86	OHX	5	4007	-	0,6,6	-	-	-		
86	OHX	7	214	-	0,6,6	-	-	-		
86	OHX	1	3923	-	0,6,6	-	-	-		
86	OHX	6	2068	-	0,6,6	-	-	-		
86	OHX	5	3847	-	0,6,6	-	-	-		
86	OHX	1	4086	-	0,6,6	-	-	-		
86	OHX	2	2078	-	0,6,6	-	-	-		
86	OHX	M5	304	-	0,6,6	-	-	-		
86	OHX	2	2030	-	0,6,6	-	-	-		
86	OHX	2	2057	-	0,6,6	-	-	-		
86	OHX	1	3937	-	0,6,6	-	-	-		
86	OHX	2	1992	-	0,6,6	-	-	-		
86	OHX	1	4042	-	0,6,6	-	-	-		
86	OHX	1	3977	-	0,6,6	-	-	-		
86	OHX	5	3862	-	0,6,6	-	-	-		
86	OHX	5	3890	85	0,6,6	-	-	-		
86	OHX	2	2118	-	0,6,6	-	-	-		
86	OHX	5	3986	-	0,6,6	-	-	-		
86	OHX	5	3967	-	0,6,6	-	-	-		
86	OHX	2	2021	-	0,6,6	-	-	-		
86	OHX	1	3788	-	0,6,6	-	-	-		
86	OHX	1	3945	-	0,6,6	-	-	-		
86	OHX	1	3844	-	0,6,6	-	-	-		
86	OHX	4	223	-	0,6,6	-	-	-		
86	OHX	5	3964	-	0,6,6	-	-	-		
86	OHX	1	3959	-	0,6,6	-	-	-		
86	OHX	1	3857	-	0,6,6	-	-	-		
86	OHX	2	2077	-	0,6,6	-	-	-		
86	OHX	5	4109	-	0,6,6	-	-	-		
86	OHX	5	3859	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3958	-	0,6,6	-	-	-		
86	OHX	6	2126	-	0,6,6	-	-	-		
86	OHX	6	2153	-	0,6,6	-	-	-		
86	OHX	6	2176	-	0,6,6	-	-	-		
86	OHX	5	3883	-	0,6,6	-	-	-		
86	OHX	5	4137	-	0,6,6	-	-	-		
86	OHX	2	2008	-	0,6,6	-	-	-		
86	OHX	1	4015	-	0,6,6	-	-	-		
86	OHX	1	3858	-	0,6,6	-	-	-		
86	OHX	2	2014	-	0,6,6	-	-	-		
86	OHX	3	215	-	0,6,6	-	-	-		
86	OHX	1	3998	-	0,6,6	-	-	-		
86	OHX	5	3848	-	0,6,6	-	-	-		
86	OHX	8	220	-	0,6,6	-	-	-		
86	OHX	1	3867	-	0,6,6	-	-	-		
86	OHX	8	231	-	0,6,6	-	-	-		
86	OHX	1	4083	-	0,6,6	-	-	-		
86	OHX	2	2092	-	0,6,6	-	-	-		
86	OHX	6	2065	-	0,6,6	-	-	-		
86	OHX	1	4089	-	0,6,6	-	-	-		
86	OHX	1	3910	-	0,6,6	-	-	-		
86	OHX	O3	201	-	0,6,6	-	-	-		
86	OHX	6	2022	-	0,6,6	-	-	-		
86	OHX	5	3819	-	0,6,6	-	-	-		
86	OHX	5	3888	-	0,6,6	-	-	-		
86	OHX	6	2060	-	0,6,6	-	-	-		
86	OHX	1	4020	-	0,6,6	-	-	-		
86	OHX	8	211	-	0,6,6	-	-	-		
86	OHX	1	3919	-	0,6,6	-	-	-		
86	OHX	5	4128	-	0,6,6	-	-	-		
86	OHX	1	4035	-	0,6,6	-	-	-		
86	OHX	1	4073	85	0,6,6	-	-	-		
86	OHX	5	4153	-	0,6,6	-	-	-		
86	OHX	5	4026	-	0,6,6	-	-	-		
86	OHX	1	4050	85	0,6,6	-	-	-		
86	OHX	2	2064	-	0,6,6	-	-	-		
86	OHX	5	3898	-	0,6,6	-	-	-		
86	OHX	2	2065	-	0,6,6	-	-	-		
86	OHX	s4	602	-	0,6,6	-	-	-		
86	OHX	1	3921	-	0,6,6	-	-	-		
86	OHX	5	4168	-	0,6,6	-	-	-		
86	OHX	6	2138	-	0,6,6	-	-	-		
86	OHX	6	2163	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3904	-	0,6,6	-	-	-		
86	OHX	6	2159	-	0,6,6	-	-	-		
86	OHX	5	3906	-	0,6,6	-	-	-		
86	OHX	1	3974	-	0,6,6	-	-	-		
86	OHX	1	3785	-	0,6,6	-	-	-		
86	OHX	5	4159	-	0,6,6	-	-	-		
86	OHX	6	2074	-	0,6,6	-	-	-		
86	OHX	5	4029	-	0,6,6	-	-	-		
86	OHX	1	3900	-	0,6,6	-	-	-		
86	OHX	1	4101	-	0,6,6	-	-	-		
86	OHX	2	2052	-	0,6,6	-	-	-		
86	OHX	2	1995	-	0,6,6	-	-	-		
86	OHX	5	3874	-	0,6,6	-	-	-		
86	OHX	M6	203	-	0,6,6	-	-	-		
86	OHX	2	2140	-	0,6,6	-	-	-		
86	OHX	1	3765	-	0,6,6	-	-	-		
86	OHX	6	2043	-	0,6,6	-	-	-		
86	OHX	2	2089	-	0,6,6	-	-	-		
86	OHX	5	4085	85	0,6,6	-	-	-		
86	OHX	1	3925	-	0,6,6	-	-	-		
86	OHX	1	3859	-	0,6,6	-	-	-		
86	OHX	5	4149	-	0,6,6	-	-	-		
86	OHX	1	3955	-	0,6,6	-	-	-		
86	OHX	6	2075	-	0,6,6	-	-	-		
86	OHX	5	3974	-	0,6,6	-	-	-		
86	OHX	1	4004	-	0,6,6	-	-	-		
86	OHX	5	4070	-	0,6,6	-	-	-		
86	OHX	1	3834	-	0,6,6	-	-	-		
86	OHX	1	3901	-	0,6,6	-	-	-		
86	OHX	2	2003	-	0,6,6	-	-	-		
86	OHX	5	4139	-	0,6,6	-	-	-		
86	OHX	2	2043	-	0,6,6	-	-	-		
86	OHX	5	3855	-	0,6,6	-	-	-		
86	OHX	5	4117	-	0,6,6	-	-	-		
86	OHX	1	3773	-	0,6,6	-	-	-		
86	OHX	6	2139	-	0,6,6	-	-	-		
86	OHX	1	3766	-	0,6,6	-	-	-		
86	OHX	5	3824	-	0,6,6	-	-	-		
86	OHX	1	3930	-	0,6,6	-	-	-		
86	OHX	5	3852	-	0,6,6	-	-	-		
86	OHX	5	3860	-	0,6,6	-	-	-		
86	OHX	1	3836	-	0,6,6	-	-	-		
86	OHX	1	3875	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3954	-	0,6,6	-	-	-		
86	OHX	5	4146	85	0,6,6	-	-	-		
86	OHX	1	3838	-	0,6,6	-	-	-		
86	OHX	1	3984	-	0,6,6	-	-	-		
86	OHX	5	4008	-	0,6,6	-	-	-		
86	OHX	6	2054	-	0,6,6	-	-	-		
86	OHX	6	2041	-	0,6,6	-	-	-		
86	OHX	6	2128	-	0,6,6	-	-	-		
86	OHX	6	2093	-	0,6,6	-	-	-		
86	OHX	5	4111	-	0,6,6	-	-	-		
86	OHX	6	2036	-	0,6,6	-	-	-		
86	OHX	d9	102	-	0,6,6	-	-	-		
86	OHX	1	3761	-	0,6,6	-	-	-		
86	OHX	6	2072	-	0,6,6	-	-	-		
86	OHX	5	3966	-	0,6,6	-	-	-		
86	OHX	1	4045	-	0,6,6	-	-	-		
86	OHX	6	2183	-	0,6,6	-	-	-		
86	OHX	8	218	-	0,6,6	-	-	-		
86	OHX	5	3896	-	0,6,6	-	-	-		
86	OHX	1	3832	-	0,6,6	-	-	-		
86	OHX	2	2120	-	0,6,6	-	-	-		
86	OHX	2	2124	-	0,6,6	-	-	-		
86	OHX	6	2079	-	0,6,6	-	-	-		
86	OHX	1	4059	-	0,6,6	-	-	-		
86	OHX	5	4132	-	0,6,6	-	-	-		
86	OHX	1	3775	-	0,6,6	-	-	-		
86	OHX	1	4098	-	0,6,6	-	-	-		
86	OHX	l4	402	-	0,6,6	-	-	-		
86	OHX	m4	201	-	0,6,6	-	-	-		
86	OHX	6	2164	-	0,6,6	-	-	-		
86	OHX	1	3870	85	0,6,6	-	-	-		
86	OHX	5	4161	-	0,6,6	-	-	-		
86	OHX	1	3902	-	0,6,6	-	-	-		
86	OHX	1	4012	-	0,6,6	-	-	-		
86	OHX	6	2018	-	0,6,6	-	-	-		
86	OHX	5	4037	-	0,6,6	-	-	-		
86	OHX	1	3767	-	0,6,6	-	-	-		
86	OHX	1	4053	-	0,6,6	-	-	-		
86	OHX	1	3880	-	0,6,6	-	-	-		
86	OHX	1	3783	-	0,6,6	-	-	-		
86	OHX	1	4106	-	0,6,6	-	-	-		
86	OHX	7	216	-	0,6,6	-	-	-		
86	OHX	S6	301	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4122	-	0,6,6	-	-	-		
86	OHX	1	4001	-	0,6,6	-	-	-		
86	OHX	1	4005	-	0,6,6	-	-	-		
86	OHX	5	4059	-	0,6,6	-	-	-		
86	OHX	Q2	503	85	0,6,6	-	-	-		
86	OHX	2	2073	-	0,6,6	-	-	-		
86	OHX	1	3950	-	0,6,6	-	-	-		
86	OHX	5	3870	-	0,6,6	-	-	-		
86	OHX	5	3972	-	0,6,6	-	-	-		
86	OHX	2	2061	-	0,6,6	-	-	-		
86	OHX	6	2154	-	0,6,6	-	-	-		
86	OHX	5	3934	-	0,6,6	-	-	-		
86	OHX	1	3981	-	0,6,6	-	-	-		
86	OHX	1	3811	-	0,6,6	-	-	-		
86	OHX	L5	301	-	0,6,6	-	-	-		
86	OHX	n9	101	-	0,6,6	-	-	-		
86	OHX	1	4051	-	0,6,6	-	-	-		
86	OHX	5	3935	-	0,6,6	-	-	-		
86	OHX	1	4052	-	0,6,6	-	-	-		
86	OHX	1	4077	-	0,6,6	-	-	-		
86	OHX	5	4105	-	0,6,6	-	-	-		
86	OHX	2	2076	-	0,6,6	-	-	-		
86	OHX	1	3938	-	0,6,6	-	-	-		
86	OHX	8	228	-	0,6,6	-	-	-		
86	OHX	2	2151	-	0,6,6	-	-	-		
86	OHX	1	3803	85	0,6,6	-	-	-		
86	OHX	5	3901	-	0,6,6	-	-	-		
86	OHX	2	2131	-	0,6,6	-	-	-		
86	OHX	2	2044	-	0,6,6	-	-	-		
86	OHX	7	221	-	0,6,6	-	-	-		
86	OHX	5	3844	-	0,6,6	-	-	-		
86	OHX	1	3849	-	0,6,6	-	-	-		
86	OHX	1	4014	-	0,6,6	-	-	-		
86	OHX	1	4094	-	0,6,6	-	-	-		
86	OHX	1	3887	-	0,6,6	-	-	-		
86	OHX	1	4068	-	0,6,6	-	-	-		
86	OHX	5	3823	-	0,6,6	-	-	-		
86	OHX	5	3851	-	0,6,6	-	-	-		
86	OHX	5	4090	-	0,6,6	-	-	-		
86	OHX	2	2091	-	0,6,6	-	-	-		
86	OHX	L3	404	-	0,6,6	-	-	-		
86	OHX	m0	302	-	0,6,6	-	-	-		
86	OHX	5	4052	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2017	-	0,6,6	-	-	-		
86	OHX	1	4043	85	0,6,6	-	-	-		
86	OHX	1	4071	36	0,6,6	-	-	-		
86	OHX	6	2123	-	0,6,6	-	-	-		
86	OHX	1	3989	-	0,6,6	-	-	-		
86	OHX	5	3963	-	0,6,6	-	-	-		
86	OHX	7	224	85	0,6,6	-	-	-		
86	OHX	5	3840	-	0,6,6	-	-	-		
86	OHX	4	228	-	0,6,6	-	-	-		
86	OHX	1	3864	-	0,6,6	-	-	-		
86	OHX	6	2042	-	0,6,6	-	-	-		
86	OHX	6	2087	-	0,6,6	-	-	-		
86	OHX	8	213	-	0,6,6	-	-	-		
86	OHX	1	4002	85	0,6,6	-	-	-		
86	OHX	5	3913	-	0,6,6	-	-	-		
86	OHX	5	3924	-	0,6,6	-	-	-		
86	OHX	5	4091	-	0,6,6	-	-	-		
86	OHX	6	2047	-	0,6,6	-	-	-		
86	OHX	1	4092	-	0,6,6	-	-	-		
86	OHX	5	4112	-	0,6,6	-	-	-		
86	OHX	6	2116	-	0,6,6	-	-	-		
86	OHX	1	4032	-	0,6,6	-	-	-		
86	OHX	5	3917	-	0,6,6	-	-	-		
86	OHX	5	3971	-	0,6,6	-	-	-		
86	OHX	5	3999	85	0,6,6	-	-	-		
86	OHX	1	3794	-	0,6,6	-	-	-		
86	OHX	1	4044	-	0,6,6	-	-	-		
86	OHX	6	2152	-	0,6,6	-	-	-		
86	OHX	5	3965	-	0,6,6	-	-	-		
86	OHX	1	3850	-	0,6,6	-	-	-		
86	OHX	1	4041	-	0,6,6	-	-	-		
86	OHX	6	2055	-	0,6,6	-	-	-		
86	OHX	L3	402	-	0,6,6	-	-	-		
86	OHX	5	4040	-	0,6,6	-	-	-		
86	OHX	5	3889	-	0,6,6	-	-	-		
86	OHX	2	2069	-	0,6,6	-	-	-		
86	OHX	3	219	-	0,6,6	-	-	-		
86	OHX	1	3985	-	0,6,6	-	-	-		
86	OHX	6	2140	-	0,6,6	-	-	-		
86	OHX	5	4167	-	0,6,6	-	-	-		
86	OHX	5	4092	-	0,6,6	-	-	-		
86	OHX	1	3810	-	0,6,6	-	-	-		
86	OHX	1	4061	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2165	-	0,6,6	-	-	-		
86	OHX	1	3780	-	0,6,6	-	-	-		
86	OHX	5	3892	-	0,6,6	-	-	-		
86	OHX	2	2085	-	0,6,6	-	-	-		
86	OHX	1	3928	-	0,6,6	-	-	-		
86	OHX	5	3872	-	0,6,6	-	-	-		
86	OHX	5	3962	-	0,6,6	-	-	-		
86	OHX	1	3941	-	0,6,6	-	-	-		
86	OHX	2	2132	-	0,6,6	-	-	-		
86	OHX	1	4021	-	0,6,6	-	-	-		
86	OHX	s1	302	-	0,6,6	-	-	-		
86	OHX	3	214	-	0,6,6	-	-	-		
86	OHX	q2	203	-	0,6,6	-	-	-		
86	OHX	2	2127	-	0,6,6	-	-	-		
86	OHX	1	3877	-	0,6,6	-	-	-		
86	OHX	5	3856	-	0,6,6	-	-	-		
86	OHX	1	4081	-	0,6,6	-	-	-		
86	OHX	5	3991	-	0,6,6	-	-	-		
86	OHX	2	2119	-	0,6,6	-	-	-		
86	OHX	1	3822	-	0,6,6	-	-	-		
86	OHX	1	4029	-	0,6,6	-	-	-		
86	OHX	2	2062	-	0,6,6	-	-	-		
86	OHX	5	3817	-	0,6,6	-	-	-		
86	OHX	1	3889	-	0,6,6	-	-	-		
86	OHX	2	2097	-	0,6,6	-	-	-		
86	OHX	5	3884	-	0,6,6	-	-	-		
86	OHX	8	212	-	0,6,6	-	-	-		
86	OHX	1	3927	-	0,6,6	-	-	-		
86	OHX	1	3940	-	0,6,6	-	-	-		
86	OHX	1	4009	-	0,6,6	-	-	-		
86	OHX	1	3991	-	0,6,6	-	-	-		
86	OHX	5	3839	-	0,6,6	-	-	-		
86	OHX	1	4024	-	0,6,6	-	-	-		
86	OHX	2	2074	-	0,6,6	-	-	-		
86	OHX	1	4013	-	0,6,6	-	-	-		
86	OHX	6	2117	-	0,6,6	-	-	-		
86	OHX	5	3871	-	0,6,6	-	-	-		
86	OHX	7	217	-	0,6,6	-	-	-		
86	OHX	S1	301	-	0,6,6	-	-	-		
86	OHX	3	209	-	0,6,6	-	-	-		
86	OHX	d4	201	-	0,6,6	-	-	-		
86	OHX	6	2095	-	0,6,6	-	-	-		
86	OHX	5	4081	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2023	-	0,6,6	-	-	-		
86	OHX	5	4118	-	0,6,6	-	-	-		
86	OHX	1	4063	-	0,6,6	-	-	-		
86	OHX	5	3863	-	0,6,6	-	-	-		
86	OHX	5	3843	-	0,6,6	-	-	-		
86	OHX	7	218	-	0,6,6	-	-	-		
86	OHX	7	220	-	0,6,6	-	-	-		
86	OHX	8	229	-	0,6,6	-	-	-		
86	OHX	2	2117	-	0,6,6	-	-	-		
86	OHX	6	2094	-	0,6,6	-	-	-		
86	OHX	2	2149	-	0,6,6	-	-	-		
86	OHX	2	2004	-	0,6,6	-	-	-		
86	OHX	1	3846	-	0,6,6	-	-	-		
86	OHX	1	3956	-	0,6,6	-	-	-		
86	OHX	1	4055	-	0,6,6	-	-	-		
86	OHX	6	2106	-	0,6,6	-	-	-		
86	OHX	6	2161	-	0,6,6	-	-	-		
86	OHX	5	3982	-	0,6,6	-	-	-		
86	OHX	1	3909	-	0,6,6	-	-	-		
86	OHX	6	2181	-	0,6,6	-	-	-		
86	OHX	6	2066	-	0,6,6	-	-	-		
86	OHX	5	4094	-	0,6,6	-	-	-		
89	PRO	5	4173	89	5,7,8	0.41	0	7,8,10	1.30	1 (14%)
86	OHX	6	2167	-	0,6,6	-	-	-		
86	OHX	5	4114	-	0,6,6	-	-	-		
86	OHX	2	2032	-	0,6,6	-	-	-		
86	OHX	1	3957	-	0,6,6	-	-	-		
86	OHX	1	3876	-	0,6,6	-	-	-		
86	OHX	6	2096	-	0,6,6	-	-	-		
86	OHX	5	4133	-	0,6,6	-	-	-		
86	OHX	3	217	-	0,6,6	-	-	-		
86	OHX	1	3949	-	0,6,6	-	-	-		
86	OHX	5	4172	85	0,6,6	-	-	-		
86	OHX	2	2094	-	0,6,6	-	-	-		
86	OHX	2	2104	-	0,6,6	-	-	-		
86	OHX	2	2075	-	0,6,6	-	-	-		
86	OHX	2	2136	-	0,6,6	-	-	-		
86	OHX	2	2028	-	0,6,6	-	-	-		
86	OHX	1	3995	-	0,6,6	-	-	-		
86	OHX	6	2089	-	0,6,6	-	-	-		
86	OHX	1	3793	-	0,6,6	-	-	-		
86	OHX	5	4041	-	0,6,6	-	-	-		
86	OHX	5	4019	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	8	222	-	0,6,6	-	-	-		
86	OHX	6	2101	-	0,6,6	-	-	-		
86	OHX	2	2070	-	0,6,6	-	-	-		
86	OHX	6	2178	-	0,6,6	-	-	-		
86	OHX	1	4058	-	0,6,6	-	-	-		
86	OHX	6	2158	-	0,6,6	-	-	-		
86	OHX	1	3764	85	0,6,6	-	-	-		
86	OHX	M8	201	-	0,6,6	-	-	-		
86	OHX	6	2111	-	0,6,6	-	-	-		
86	OHX	5	3936	-	0,6,6	-	-	-		
86	OHX	1	4028	-	0,6,6	-	-	-		
86	OHX	1	3815	-	0,6,6	-	-	-		
86	OHX	6	2109	-	0,6,6	-	-	-		
86	OHX	1	3770	-	0,6,6	-	-	-		
86	OHX	5	4134	-	0,6,6	-	-	-		
86	OHX	1	4095	-	0,6,6	-	-	-		
86	OHX	6	2133	-	0,6,6	-	-	-		
86	OHX	2	2058	-	0,6,6	-	-	-		
86	OHX	2	2134	-	0,6,6	-	-	-		
86	OHX	1	4025	-	0,6,6	-	-	-		
86	OHX	6	2029	-	0,6,6	-	-	-		
86	OHX	5	3921	-	0,6,6	-	-	-		
86	OHX	5	3854	-	0,6,6	-	-	-		
86	OHX	5	4093	-	0,6,6	-	-	-		
86	OHX	2	1991	-	0,6,6	-	-	-		
86	OHX	1	3774	-	0,6,6	-	-	-		
86	OHX	2	1993	-	0,6,6	-	-	-		
86	OHX	6	2122	-	0,6,6	-	-	-		
86	OHX	1	3874	-	0,6,6	-	-	-		
86	OHX	15	302	-	0,6,6	-	-	-		
86	OHX	1	3944	-	0,6,6	-	-	-		
86	OHX	1	3968	-	0,6,6	-	-	-		
86	OHX	2	2063	-	0,6,6	-	-	-		
86	OHX	1	3792	-	0,6,6	-	-	-		
86	OHX	6	2088	-	0,6,6	-	-	-		
86	OHX	5	4158	-	0,6,6	-	-	-		
86	OHX	6	2142	-	0,6,6	-	-	-		
86	OHX	6	2020	-	0,6,6	-	-	-		
86	OHX	5	3836	-	0,6,6	-	-	-		
86	OHX	5	3929	85	0,6,6	-	-	-		
86	OHX	2	2110	-	0,6,6	-	-	-		
86	OHX	1	3814	-	0,6,6	-	-	-		
86	OHX	5	3955	36	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4107	-	0,6,6	-	-	-		
86	OHX	1	3826	-	0,6,6	-	-	-		
86	OHX	4	227	-	0,6,6	-	-	-		
86	OHX	5	4148	-	0,6,6	-	-	-		
86	OHX	5	4003	-	0,6,6	-	-	-		
86	OHX	2	2112	-	0,6,6	-	-	-		
86	OHX	5	3946	-	0,6,6	-	-	-		
86	OHX	5	3980	-	0,6,6	-	-	-		
86	OHX	1	4067	-	0,6,6	-	-	-		
86	OHX	2	2009	-	0,6,6	-	-	-		
86	OHX	1	3830	-	0,6,6	-	-	-		
86	OHX	1	4022	-	0,6,6	-	-	-		
86	OHX	2	2056	-	0,6,6	-	-	-		
86	OHX	5	3885	-	0,6,6	-	-	-		
86	OHX	5	3969	-	0,6,6	-	-	-		
86	OHX	1	3818	-	0,6,6	-	-	-		
86	OHX	1	4103	-	0,6,6	-	-	-		
86	OHX	2	2100	-	0,6,6	-	-	-		
86	OHX	1	4110	85	0,6,6	-	-	-		
86	OHX	6	2073	-	0,6,6	-	-	-		
86	OHX	5	3882	-	0,6,6	-	-	-		
86	OHX	5	4031	-	0,6,6	-	-	-		
86	OHX	1	3899	-	0,6,6	-	-	-		
86	OHX	6	2162	-	0,6,6	-	-	-		
86	OHX	2	2042	-	0,6,6	-	-	-		
86	OHX	3	212	-	0,6,6	-	-	-		
86	OHX	6	2016	-	0,6,6	-	-	-		
86	OHX	5	4171	-	0,6,6	-	-	-		
86	OHX	1	3942	-	0,6,6	-	-	-		
86	OHX	5	3973	-	0,6,6	-	-	-		
86	OHX	5	3987	-	0,6,6	-	-	-		
86	OHX	1	3948	-	0,6,6	-	-	-		
86	OHX	1	4070	-	0,6,6	-	-	-		
86	OHX	6	2173	-	0,6,6	-	-	-		
86	OHX	5	3838	-	0,6,6	-	-	-		
86	OHX	5	4022	85	0,6,6	-	-	-		
86	OHX	1	3866	-	0,6,6	-	-	-		
86	OHX	5	4135	-	0,6,6	-	-	-		
86	OHX	5	4165	-	0,6,6	-	-	-		
86	OHX	1	3986	-	0,6,6	-	-	-		
86	OHX	4	216	-	0,6,6	-	-	-		
86	OHX	6	2141	-	0,6,6	-	-	-		
86	OHX	13	404	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2041	-	0,6,6	-	-	-		
86	OHX	5	3976	-	0,6,6	-	-	-		
86	OHX	5	3894	-	0,6,6	-	-	-		
86	OHX	2	2068	-	0,6,6	-	-	-		
86	OHX	6	2110	-	0,6,6	-	-	-		
86	OHX	1	4033	-	0,6,6	-	-	-		
86	OHX	6	2147	-	0,6,6	-	-	-		
86	OHX	5	4017	-	0,6,6	-	-	-		
86	OHX	5	4074	-	0,6,6	-	-	-		
86	OHX	1	3841	-	0,6,6	-	-	-		
86	OHX	5	3865	-	0,6,6	-	-	-		
86	OHX	1	3911	-	0,6,6	-	-	-		
86	OHX	1	3824	-	0,6,6	-	-	-		
86	OHX	6	2127	-	0,6,6	-	-	-		
86	OHX	6	2062	-	0,6,6	-	-	-		
86	OHX	5	3857	-	0,6,6	-	-	-		
86	OHX	5	3912	-	0,6,6	-	-	-		
86	OHX	1	4046	-	0,6,6	-	-	-		
86	OHX	6	2017	-	0,6,6	-	-	-		
86	OHX	5	4080	-	0,6,6	-	-	-		
86	OHX	5	4016	85	0,6,6	-	-	-		
86	OHX	1	3903	-	0,6,6	-	-	-		
86	OHX	1	3860	-	0,6,6	-	-	-		
86	OHX	5	4023	-	0,6,6	-	-	-		
86	OHX	SR	401	-	0,6,6	-	-	-		
86	OHX	5	4049	-	0,6,6	-	-	-		
86	OHX	6	2179	-	0,6,6	-	-	-		
86	OHX	1	4011	-	0,6,6	-	-	-		
86	OHX	6	2125	-	0,6,6	-	-	-		
86	OHX	5	3835	-	0,6,6	-	-	-		
86	OHX	5	3947	-	0,6,6	-	-	-		
86	OHX	6	2038	-	0,6,6	-	-	-		
86	OHX	1	3798	-	0,6,6	-	-	-		
86	OHX	1	3891	-	0,6,6	-	-	-		
86	OHX	1	4026	-	0,6,6	-	-	-		
86	OHX	6	2019	-	0,6,6	-	-	-		
86	OHX	6	2090	-	0,6,6	-	-	-		
86	OHX	2	2045	-	0,6,6	-	-	-		
86	OHX	2	2139	-	0,6,6	-	-	-		
86	OHX	1	3898	-	0,6,6	-	-	-		
86	OHX	6	2080	-	0,6,6	-	-	-		
86	OHX	5	3869	85	0,6,6	-	-	-		
86	OHX	5	3923	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2010	-	0,6,6	-	-	-		
86	OHX	5	3943	-	0,6,6	-	-	-		
86	OHX	1	3837	-	0,6,6	-	-	-		
86	OHX	2	2060	-	0,6,6	-	-	-		
86	OHX	2	2055	-	0,6,6	-	-	-		
86	OHX	4	233	-	0,6,6	-	-	-		
86	OHX	5	3997	-	0,6,6	-	-	-		
86	OHX	2	2006	-	0,6,6	-	-	-		
86	OHX	1	3813	-	0,6,6	-	-	-		
86	OHX	5	3975	-	0,6,6	-	-	-		
86	OHX	6	2137	-	0,6,6	-	-	-		
89	PRO	C	101	84,89	5,7,8	0.48	0	7,8,10	1.39	1 (14%)
86	OHX	1	4054	-	0,6,6	-	-	-		
86	OHX	1	3992	-	0,6,6	-	-	-		
86	OHX	2	2115	-	0,6,6	-	-	-		
86	OHX	1	3801	85	0,6,6	-	-	-		
86	OHX	6	2121	-	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
89	PRO	C	101	84,89	-	0/0/9/11	0/1/1/1
88	SPS	5	3403	-	-	2/15/18/18	0/1/1/1
88	SPS	1	4113	85	-	4/15/18/18	0/1/1/1
89	PRO	5	4173	89	-	0/0/9/11	0/1/1/1
89	PRO	B	101	84,89	-	0/0/9/11	0/1/1/1
89	PRO	1	4114	89	-	0/0/9/11	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4113	SPS	C9-C10	-8.24	1.31	1.48
88	5	3403	SPS	C9-C10	-8.07	1.31	1.48
88	5	3403	SPS	C9-C8	6.35	1.52	1.33
88	1	4113	SPS	C9-C8	6.21	1.51	1.33
88	5	3403	SPS	O13-C13	-5.41	1.19	1.42
88	1	4113	SPS	O13-C13	-5.33	1.19	1.42
88	1	4113	SPS	C5-N4	-5.17	1.31	1.38
88	5	3403	SPS	C5-N4	-4.66	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4113	SPS	O15-S15	4.33	1.65	1.50
88	1	4113	SPS	C10-N11	4.29	1.44	1.34
88	5	3403	SPS	C10-N11	4.08	1.44	1.34
88	5	3403	SPS	O15-S15	4.00	1.64	1.50
88	1	4113	SPS	C6-C1	-3.91	1.37	1.45
88	5	3403	SPS	C1-N2	-3.48	1.32	1.38
88	1	4113	SPS	C1-N2	-3.44	1.32	1.38
88	5	3403	SPS	C6-C1	-3.07	1.39	1.45
88	1	4113	SPS	C3-N4	-3.05	1.32	1.37
88	5	3403	SPS	O10-C10	-2.85	1.19	1.24
88	1	4113	SPS	O10-C10	-2.73	1.19	1.24
88	5	3403	SPS	C3-N4	-2.46	1.33	1.37
88	5	3403	SPS	O1-C1	-2.46	1.18	1.23
88	1	4113	SPS	O1-C1	-2.44	1.18	1.23
88	5	3403	SPS	C8-C6	2.20	1.53	1.46
88	1	4113	SPS	C8-C6	2.19	1.53	1.46
88	5	3403	SPS	C7-C5	2.19	1.53	1.49
88	1	4113	SPS	O3-C3	-2.06	1.19	1.23
88	5	3403	SPS	C3-N2	-2.04	1.34	1.37

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	5	3403	SPS	C7-C5-N4	5.32	119.78	113.45
88	1	4113	SPS	C7-C5-C6	-5.08	119.27	126.69
88	1	4113	SPS	C7-C5-N4	4.85	119.22	113.45
88	5	3403	SPS	C12-N11-C10	-4.66	116.01	122.57
88	5	3403	SPS	C7-C5-C6	-4.56	120.02	126.69
88	1	4113	SPS	C5-N4-C3	-4.45	120.24	123.71
88	1	4113	SPS	C18-S17-C16	3.76	110.52	100.10
88	5	3403	SPS	C1-N2-C3	-3.62	121.12	126.34
88	1	4113	SPS	O13-C13-C12	3.40	120.73	111.95
88	5	3403	SPS	C6-C1-N2	3.25	119.98	114.35
88	5	3403	SPS	C9-C10-N11	3.25	120.80	114.56
88	5	3403	SPS	C18-S17-C16	3.20	108.95	100.10
88	1	4113	SPS	C1-N2-C3	-3.08	121.90	126.34
88	5	3403	SPS	O13-C13-C12	3.00	119.70	111.95
88	5	3403	SPS	C5-N4-C3	-2.78	121.54	123.71
89	5	4173	PRO	O-C-CA	-2.66	117.80	124.78
89	C	101	PRO	O-C-CA	-2.62	117.92	124.78
88	1	4113	SPS	C6-C1-N2	2.61	118.86	114.35
88	5	3403	SPS	O10-C10-N11	-2.57	118.95	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4113	SPS	N4-C3-N2	2.54	119.88	115.80
88	1	4113	SPS	O15-S15-C16	2.52	109.47	106.47
88	5	3403	SPS	N4-C3-N2	2.46	119.76	115.80
88	5	3403	SPS	O15-S15-C16	2.46	109.39	106.47
89	B	101	PRO	O-C-CA	-2.34	118.65	124.78
88	1	4113	SPS	C12-N11-C10	-2.33	119.29	122.57
88	5	3403	SPS	C9-C8-C6	-2.27	116.62	125.27
88	1	4113	SPS	C6-C5-N4	2.23	121.50	118.39
88	5	3403	SPS	C8-C9-C10	-2.08	117.25	125.72

There are no chirality outliers.

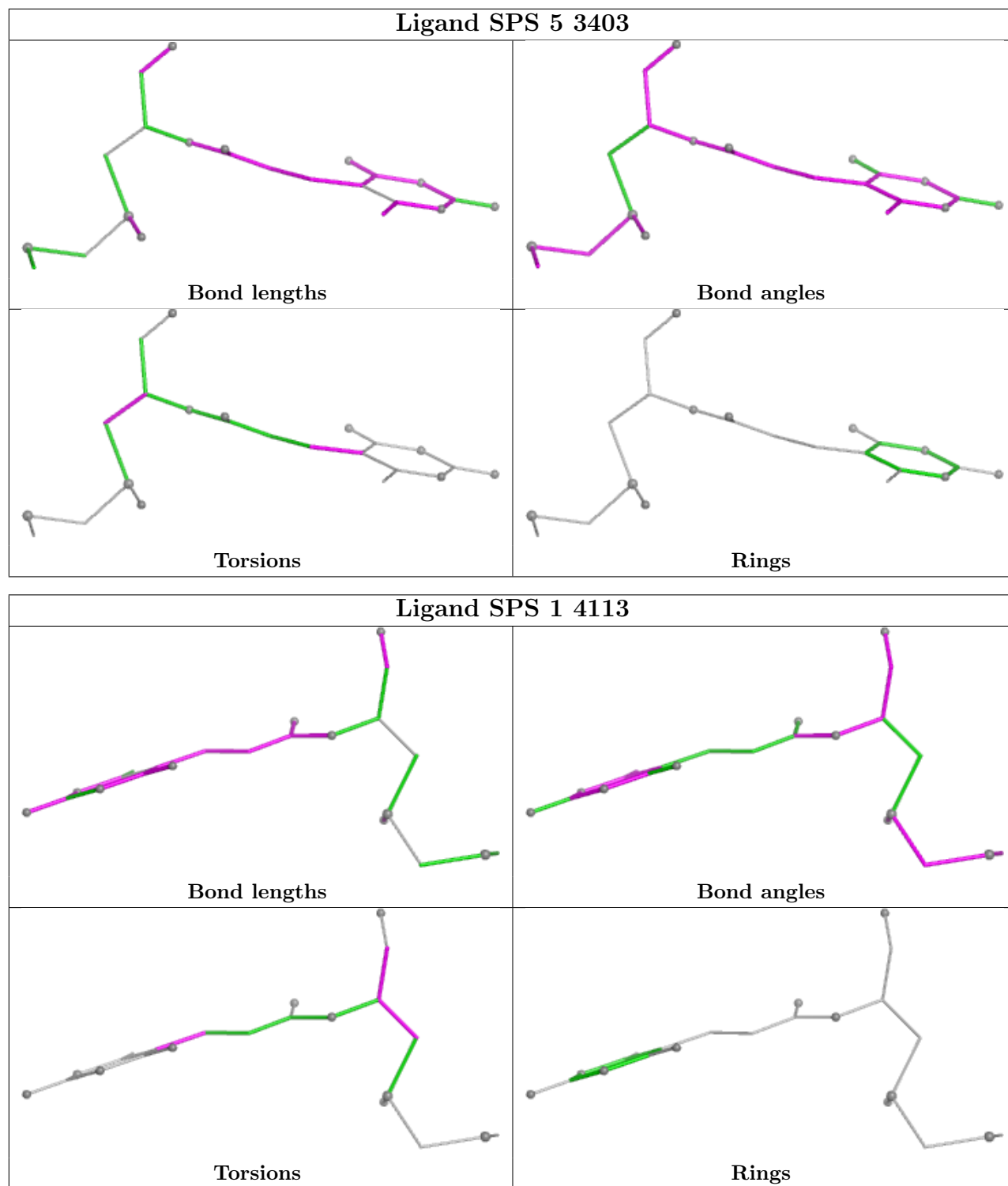
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	1	4113	SPS	N11-C12-C13-O13
88	1	4113	SPS	C14-C12-C13-O13
88	1	4113	SPS	N11-C12-C14-S15
88	5	3403	SPS	N11-C12-C14-S15
88	1	4113	SPS	C5-C6-C8-C9
88	5	3403	SPS	C5-C6-C8-C9

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	2
80	m2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1716:C	O3'	1717:G	P	5.10
1	m2	23:LEU	C	28:ARG	N	3.71
1	m2	52:LYS	C	54:LYS	N	3.25
1	2	1685:G	O3'	1686:C	P	2.98

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	2	1781/1800 (98%)	0.08	29 (1%) 70 46	42, 100, 190, 245	1 (0%)
1	6	1795/1800 (99%)	-0.12	23 (1%) 75 51	33, 84, 172, 231	1 (0%)
2	S0	206/251 (82%)	0.73	9 (4%) 39 23	99, 112, 122, 125	0
2	s0	206/251 (82%)	0.50	7 (3%) 48 29	78, 93, 107, 115	0
3	S1	214/254 (84%)	0.92	22 (10%) 12 9	114, 152, 175, 179	0
3	s1	216/254 (85%)	0.26	4 (1%) 66 42	80, 93, 110, 126	0
4	S2	217/253 (85%)	0.55	9 (4%) 41 24	79, 95, 109, 118	0
4	s2	217/253 (85%)	0.38	10 (4%) 37 21	63, 79, 90, 99	0
5	S3	223/239 (93%)	0.45	7 (3%) 51 31	90, 103, 122, 135	0
5	s3	223/239 (93%)	0.36	6 (2%) 56 33	83, 108, 131, 139	0
6	S4	260/260 (100%)	0.51	8 (3%) 51 31	78, 101, 111, 133	0
6	s4	260/260 (100%)	0.23	3 (1%) 76 53	56, 79, 94, 113	0
7	S5	206/224 (91%)	0.61	13 (6%) 26 17	107, 122, 134, 144	0
7	s5	206/224 (91%)	0.51	6 (2%) 53 32	88, 106, 123, 134	0
8	S6	226/236 (95%)	0.79	22 (9%) 13 10	77, 113, 131, 142	0
8	s6	218/236 (92%)	0.35	10 (4%) 37 21	56, 85, 110, 123	0
9	S7	184/189 (97%)	0.68	6 (3%) 49 29	96, 127, 147, 152	0
9	s7	186/189 (98%)	0.30	3 (1%) 70 46	70, 103, 132, 139	0
10	S8	188/200 (94%)	0.49	2 (1%) 78 54	68, 88, 122, 139	0
10	s8	188/200 (94%)	0.35	8 (4%) 40 23	52, 69, 110, 129	0
11	S9	185/196 (94%)	0.61	7 (3%) 44 26	91, 107, 137, 157	0
11	s9	185/196 (94%)	0.65	11 (5%) 28 18	68, 87, 125, 146	0
12	C0	96/105 (91%)	0.64	5 (5%) 33 20	96, 121, 141, 151	0
12	c0	96/105 (91%)	0.91	14 (14%) 6 5	105, 136, 149, 150	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	C1	155/155 (100%)	0.58	9 (5%) 29 18	71, 84, 118, 130	0
13	c1	146/155 (94%)	0.50	8 (5%) 30 19	54, 66, 94, 115	0
14	C2	124/142 (87%)	0.95	14 (11%) 10 8	149, 161, 174, 180	0
14	c2	124/142 (87%)	0.97	16 (12%) 7 6	180, 196, 211, 215	0
15	C3	150/150 (100%)	0.38	4 (2%) 56 33	79, 94, 109, 115	0
15	c3	150/150 (100%)	0.14	2 (1%) 75 51	62, 76, 93, 96	0
16	C4	127/136 (93%)	1.15	15 (11%) 9 7	83, 146, 158, 162	0
16	c4	128/136 (94%)	0.34	0 100 100	64, 96, 104, 109	0
17	C5	124/141 (87%)	0.44	3 (2%) 59 37	87, 103, 120, 130	0
17	c5	135/141 (95%)	0.53	8 (5%) 28 18	72, 107, 122, 123	0
18	C6	141/142 (99%)	0.80	10 (7%) 22 15	92, 110, 116, 118	0
18	c6	142/142 (100%)	0.83	14 (9%) 13 9	82, 104, 118, 136	0
19	C7	120/136 (88%)	0.61	7 (5%) 29 18	95, 110, 129, 131	0
19	c7	117/136 (86%)	0.54	5 (4%) 40 23	85, 102, 114, 122	0
20	C8	145/145 (100%)	0.58	4 (2%) 55 33	85, 109, 135, 142	0
20	c8	145/145 (100%)	0.61	9 (6%) 26 17	83, 101, 117, 124	0
21	C9	143/143 (100%)	0.86	8 (5%) 30 19	95, 110, 125, 133	0
21	c9	143/143 (100%)	0.61	8 (5%) 30 19	82, 98, 115, 123	0
22	D0	107/120 (89%)	0.68	5 (4%) 36 21	86, 114, 136, 138	0
22	d0	110/120 (91%)	0.56	6 (5%) 30 19	85, 115, 144, 149	0
23	D1	87/87 (100%)	0.46	3 (3%) 48 29	96, 103, 117, 122	0
23	d1	87/87 (100%)	0.21	0 100 100	71, 82, 104, 111	0
24	D2	129/129 (100%)	0.65	2 (1%) 70 46	80, 92, 101, 111	0
24	d2	129/129 (100%)	0.05	0 100 100	59, 68, 75, 84	0
25	D3	144/144 (100%)	0.34	2 (1%) 73 49	70, 78, 90, 102	0
25	d3	144/144 (100%)	0.17	3 (2%) 63 39	52, 57, 70, 81	0
26	D4	134/134 (100%)	0.58	7 (5%) 33 20	89, 111, 123, 127	0
26	d4	134/134 (100%)	0.41	4 (2%) 52 31	65, 88, 100, 105	0
27	D5	70/107 (65%)	0.57	3 (4%) 40 23	118, 134, 141, 146	0
27	d5	69/107 (64%)	0.60	4 (5%) 29 18	98, 112, 124, 126	0
28	D6	97/97 (100%)	1.00	15 (15%) 5 5	86, 108, 160, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	d6	97/97 (100%)	0.60	3 (3%) 51 31	67, 84, 111, 116	0
29	D7	81/81 (100%)	0.74	4 (4%) 35 21	95, 113, 139, 143	0
29	d7	81/81 (100%)	0.49	4 (4%) 35 21	72, 90, 127, 128	0
30	D8	63/66 (95%)	0.62	4 (6%) 26 17	114, 131, 139, 144	0
30	d8	63/66 (95%)	0.51	3 (4%) 35 21	105, 118, 125, 128	0
31	D9	53/55 (96%)	0.76	4 (7%) 20 14	85, 90, 108, 114	0
31	d9	53/55 (96%)	0.67	3 (5%) 29 18	82, 92, 128, 145	0
32	E0	60/63 (95%)	0.37	1 (1%) 69 44	80, 110, 134, 137	0
32	e0	62/63 (98%)	0.62	7 (11%) 10 8	60, 88, 117, 120	0
33	E1	71/76 (93%)	0.89	8 (11%) 10 8	115, 142, 155, 157	0
33	e1	76/76 (100%)	1.07	14 (18%) 3 4	117, 168, 186, 187	0
34	SR	318/318 (100%)	0.69	27 (8%) 16 12	109, 122, 138, 156	0
34	sR	318/318 (100%)	0.59	12 (3%) 44 26	112, 127, 141, 153	0
35	SM	159/273 (58%)	0.57	11 (6%) 23 15	58, 100, 159, 163	0
35	sM	104/273 (38%)	0.61	5 (4%) 35 21	51, 115, 188, 197	0
36	1	3149/3396 (92%)	-0.32	28 (0%) 81 58	33, 58, 136, 238	0
36	5	3150/3396 (92%)	-0.43	22 (0%) 84 64	28, 52, 127, 213	0
37	3	121/121 (100%)	-0.31	0 100 100	42, 77, 90, 98	0
37	7	121/121 (100%)	-0.48	1 (0%) 82 61	33, 55, 66, 75	0
38	4	158/158 (100%)	-0.46	1 (0%) 85 66	42, 63, 102, 146	0
38	8	158/158 (100%)	-0.50	1 (0%) 85 66	42, 63, 101, 131	0
39	L2	252/253 (99%)	0.22	3 (1%) 76 53	40, 60, 78, 84	0
39	l2	252/253 (99%)	0.16	2 (0%) 82 61	36, 55, 73, 80	0
40	L3	386/386 (100%)	0.06	4 (1%) 79 56	37, 62, 77, 88	0
40	l3	386/386 (100%)	-0.16	7 (1%) 67 43	28, 45, 60, 81	0
41	L4	361/361 (100%)	0.06	8 (2%) 62 39	38, 54, 69, 74	0
41	l4	361/361 (100%)	0.02	5 (1%) 73 49	37, 56, 74, 82	0
42	L5	296/296 (100%)	0.32	3 (1%) 79 56	58, 80, 98, 119	0
42	l5	294/296 (99%)	0.04	6 (2%) 65 41	42, 56, 82, 97	0
43	L6	156/175 (89%)	0.04	2 (1%) 75 51	46, 56, 72, 87	0
43	l6	157/175 (89%)	-0.00	1 (0%) 85 66	48, 57, 78, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	L7	222/243 (91%)	-0.13	1 (0%) 87 70	38, 47, 77, 104	0
44	l7	223/243 (91%)	-0.22	1 (0%) 88 73	33, 45, 82, 112	0
45	L8	233/255 (91%)	0.43	8 (3%) 48 29	68, 84, 110, 120	0
45	l8	231/255 (90%)	0.41	6 (2%) 57 34	69, 82, 107, 117	0
46	L9	191/191 (100%)	0.15	2 (1%) 79 56	59, 71, 82, 94	0
46	l9	191/191 (100%)	-0.16	1 (0%) 87 70	41, 51, 68, 78	0
47	M0	211/220 (95%)	0.16	7 (3%) 49 29	44, 63, 94, 105	0
47	m0	213/220 (96%)	0.09	5 (2%) 61 38	39, 54, 78, 94	0
48	M1	169/173 (97%)	0.31	3 (1%) 67 43	68, 85, 97, 103	0
48	m1	169/173 (97%)	-0.04	1 (0%) 85 66	47, 66, 77, 81	0
49	M3	193/198 (97%)	-0.02	0 100 100	36, 63, 101, 122	0
49	m3	194/198 (97%)	0.08	4 (2%) 63 39	38, 67, 104, 119	0
50	M4	136/137 (99%)	-0.09	0 100 100	50, 59, 72, 83	0
50	m4	137/137 (100%)	-0.20	3 (2%) 62 39	43, 50, 66, 84	0
51	M5	203/203 (100%)	0.36	2 (0%) 79 56	39, 56, 67, 71	0
51	m5	203/203 (100%)	0.28	2 (0%) 79 56	40, 58, 68, 73	0
52	M6	197/198 (99%)	0.08	2 (1%) 79 56	25, 32, 46, 49	0
52	m6	197/198 (99%)	0.03	2 (1%) 79 56	18, 24, 45, 52	0
53	M7	183/183 (100%)	0.12	10 (5%) 30 19	44, 52, 105, 133	0
53	m7	155/183 (84%)	-0.17	0 100 100	36, 45, 55, 77	0
54	M8	185/185 (100%)	0.03	3 (1%) 70 46	42, 51, 68, 88	0
54	m8	185/185 (100%)	-0.04	0 100 100	39, 53, 64, 72	0
55	M9	188/188 (100%)	0.37	8 (4%) 40 23	64, 78, 147, 156	0
55	m9	188/188 (100%)	0.03	0 100 100	50, 62, 123, 138	0
56	N0	172/172 (100%)	-0.03	3 (1%) 69 44	37, 56, 70, 75	0
56	n0	172/172 (100%)	-0.29	2 (1%) 76 53	32, 45, 57, 67	0
57	N1	159/159 (100%)	0.03	1 (0%) 85 66	41, 56, 99, 105	0
57	n1	159/159 (100%)	-0.08	2 (1%) 75 51	37, 45, 82, 88	0
58	N2	100/120 (83%)	0.53	4 (4%) 42 25	94, 106, 112, 117	0
58	n2	98/120 (81%)	0.32	2 (2%) 65 41	74, 85, 93, 95	0
59	N3	136/136 (100%)	0.14	1 (0%) 84 64	49, 59, 73, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
59	n3	136/136 (100%)	-0.27	0 100 100	31, 41, 52, 57	0
60	N4	98/155 (63%)	0.72	14 (14%) 6 6	59, 74, 147, 155	0
60	n4	135/155 (87%)	0.50	15 (11%) 10 8	41, 93, 124, 142	0
61	N5	121/141 (85%)	0.15	0 100 100	59, 71, 86, 103	0
61	n5	120/141 (85%)	-0.01	3 (2%) 58 35	55, 68, 82, 97	0
62	N6	126/126 (100%)	0.22	3 (2%) 59 37	48, 64, 77, 85	0
62	n6	126/126 (100%)	0.13	0 100 100	50, 66, 82, 85	0
63	N7	135/135 (100%)	0.50	2 (1%) 72 48	83, 96, 107, 111	0
63	n7	135/135 (100%)	0.35	1 (0%) 84 64	78, 89, 101, 109	0
64	N8	148/148 (100%)	-0.15	0 100 100	32, 54, 76, 82	0
64	n8	148/148 (100%)	0.03	3 (2%) 65 41	34, 55, 72, 75	0
65	N9	58/58 (100%)	0.05	1 (1%) 69 44	36, 59, 97, 113	0
65	n9	58/58 (100%)	0.19	1 (1%) 69 44	36, 55, 76, 82	0
66	O0	97/104 (93%)	0.13	2 (2%) 63 39	83, 90, 106, 111	0
66	o0	100/104 (96%)	0.09	1 (1%) 79 56	69, 79, 98, 105	0
67	O1	109/112 (97%)	0.25	0 100 100	60, 73, 94, 101	0
67	o1	109/112 (97%)	-0.02	0 100 100	44, 56, 89, 97	0
68	O2	127/129 (98%)	-0.04	2 (1%) 70 46	34, 48, 63, 79	0
68	o2	127/129 (98%)	-0.04	1 (0%) 82 61	32, 52, 67, 78	0
69	O3	106/106 (100%)	0.05	1 (0%) 81 58	39, 46, 70, 82	0
69	o3	106/106 (100%)	-0.10	0 100 100	36, 44, 71, 82	0
70	O4	112/121 (92%)	0.62	4 (3%) 46 27	57, 74, 110, 117	0
70	o4	112/121 (92%)	0.60	10 (8%) 15 11	50, 66, 101, 108	0
71	O5	119/119 (100%)	0.22	1 (0%) 82 61	56, 73, 80, 83	0
71	o5	119/119 (100%)	0.14	1 (0%) 82 61	58, 71, 86, 96	0
72	O6	99/99 (100%)	0.18	0 100 100	59, 70, 100, 111	0
72	o6	99/99 (100%)	0.19	1 (1%) 79 56	62, 72, 91, 110	0
73	O7	87/87 (100%)	0.22	1 (1%) 78 54	41, 49, 70, 80	0
73	o7	87/87 (100%)	-0.03	1 (1%) 78 54	37, 48, 79, 85	0
74	O8	77/77 (100%)	0.35	2 (2%) 57 34	85, 97, 107, 108	0
74	o8	77/77 (100%)	0.11	1 (1%) 75 51	75, 85, 94, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	O9	50/50 (100%)	0.25	0 100 100	51, 57, 61, 62	0
75	o9	50/50 (100%)	0.02	1 (2%) 65 41	49, 54, 63, 64	0
76	Q0	52/52 (100%)	0.21	0 100 100	53, 59, 74, 82	0
76	q0	52/52 (100%)	-0.31	1 (1%) 66 42	38, 42, 52, 57	0
77	Q1	25/25 (100%)	0.53	1 (4%) 42 25	62, 66, 72, 74	0
77	q1	25/25 (100%)	0.01	0 100 100	49, 53, 54, 55	0
78	Q2	105/105 (100%)	-0.10	0 100 100	41, 55, 76, 97	0
78	q2	105/105 (100%)	-0.14	1 (0%) 79 56	40, 53, 69, 96	0
79	Q3	91/91 (100%)	0.16	1 (1%) 78 54	49, 65, 79, 85	0
79	q3	91/91 (100%)	0.03	2 (2%) 62 39	40, 55, 71, 81	0
80	m2	150/165 (90%)	1.13	20 (13%) 7 6	102, 138, 156, 161	0
81	p0	143/311 (45%)	0.81	13 (9%) 15 11	100, 125, 220, 229	0
82	p1	47/106 (44%)	1.32	7 (14%) 5 5	179, 224, 242, 245	0
82	p2	46/106 (43%)	1.55	12 (26%) 1 2	275, 283, 288, 289	0
83	f	147/157 (93%)	1.94	51 (34%) 1 1	23, 77, 157, 159	74 (50%)
84	B	2/3 (66%)	0.00	0 100 100	45, 45, 45, 48	0
84	C	2/3 (66%)	-0.11	0 100 100	40, 40, 40, 45	0
All	All	33488/35639 (93%)	0.14	914 (2%) 56 33	18, 74, 141, 289	76 (0%)

All (914) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
83	f	52	HIS	15.6
83	f	50	GLY	15.0
83	f	53	GLY	11.6
83	f	49	THR	10.0
13	c1	3	THR	8.3
8	S6	78	THR	7.0
1	2	1756[A]	A	6.0
60	N4	88	ASP	5.8
10	S8	152	ILE	5.7
1	2	913	G	5.7
73	O7	88	ALA	5.6
60	N4	86	SER	5.6
7	s5	37	GLN	5.5
8	S6	77	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
22	d0	64	LYS	5.5
13	c1	4	GLU	5.3
56	N0	1	MET	5.2
36	1	3275	U	5.2
37	7	73	C	5.1
8	S6	80	ASN	5.1
83	f	54	HIS	5.1
80	m2	18	VAL	5.0
36	1	2205	U	5.0
1	6	794	U	4.9
60	N4	85	ALA	4.8
83	f	24	SER	4.8
12	c0	2	LEU	4.7
83	f	149	SER	4.7
60	N4	84	GLY	4.6
11	s9	148	VAL	4.5
16	C4	39	ILE	4.4
83	f	69	LYS	4.4
6	s4	39	ARG	4.4
16	C4	75	GLY	4.4
8	S6	79	LYS	4.4
21	c9	18	TYR	4.4
3	S1	91	VAL	4.3
22	D0	81	THR	4.3
82	p2	8	SER	4.3
20	c8	18	LEU	4.3
53	M7	161	ALA	4.3
82	p2	31	ASN	4.3
21	C9	36	ILE	4.2
34	SR	79	TYR	4.2
83	f	14	GLY	4.2
60	n4	95	SER	4.2
7	S5	152	GLY	4.2
11	S9	4	ALA	4.1
83	f	62	ILE	4.1
16	C4	15	GLY	4.1
18	c6	2	SER	4.1
83	f	157	ASP	4.1
13	c1	117	VAL	4.0
4	s2	181	SER	4.0
28	d6	16	GLY	4.0
21	c9	55	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
22	D0	82	TYR	4.0
45	l8	124	ASP	4.0
8	S6	74	LYS	4.0
80	m2	19	LYS	4.0
60	n4	88	ASP	4.0
60	N4	76	VAL	3.9
7	S5	37	GLN	3.9
1	2	1702	A	3.9
12	c0	22	VAL	3.9
36	5	3275	U	3.9
18	C6	20	ALA	3.9
1	2	1694	A	3.9
7	S5	71	ALA	3.9
40	l3	363	SER	3.9
3	S1	47	LEU	3.9
59	N3	2	SER	3.9
18	c6	49	TYR	3.8
13	C1	68	GLY	3.8
30	d8	24	GLY	3.8
36	1	2401	A	3.8
1	2	1699	G	3.8
53	M7	165	VAL	3.8
41	L4	63	GLU	3.8
18	c6	46	PHE	3.8
2	s0	170	ILE	3.8
15	C3	11	ILE	3.8
41	L4	69	ARG	3.8
80	m2	121	GLU	3.8
8	s6	76	LEU	3.8
29	d7	24	LEU	3.8
80	m2	58	ASP	3.7
48	M1	127	PHE	3.7
17	c5	134	THR	3.7
33	e1	77	GLY	3.7
53	M7	160	ALA	3.7
20	C8	146	ALA	3.7
53	M7	162	GLU	3.7
14	c2	126	TRP	3.7
32	e0	53	LYS	3.7
60	n4	97	LYS	3.7
80	m2	91	SER	3.6
1	6	1695	G	3.6

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Mol	Chain	Res	Type	RSRZ
13	c1	5	LEU	3.6
5	S3	25	PHE	3.6
35	SM	89	ARG	3.6
60	N4	83	THR	3.6
13	C1	145	ALA	3.6
1	2	1698	G	3.6
58	N2	89	LEU	3.6
43	L6	130	ILE	3.6
14	C2	41	LEU	3.5
9	S7	98	ILE	3.5
83	f	47	SER	3.5
3	S1	55	LYS	3.5
33	e1	78	LYS	3.5
41	L4	65	TRP	3.5
19	c7	96	SER	3.5
34	sR	32	LEU	3.5
33	E1	145	HIS	3.5
4	s2	92	ALA	3.5
28	D6	83	ILE	3.5
14	c2	123	VAL	3.5
1	2	1692	G	3.5
1	2	1695	G	3.5
33	e1	79	LYS	3.4
3	S1	110	LEU	3.4
8	S6	75	LEU	3.4
35	sM	83	LYS	3.4
1	6	678	A	3.4
32	e0	51	ASN	3.4
60	n4	83	THR	3.4
82	p2	30	THR	3.4
70	O4	21	LYS	3.4
26	D4	70	VAL	3.4
18	C6	130	GLY	3.4
83	f	142	MET	3.4
34	SR	44	SER	3.4
19	C7	110	VAL	3.4
83	f	71	GLU	3.4
81	p0	107	ALA	3.4
27	D5	41	ILE	3.4
3	S1	92	GLN	3.4
1	2	1709	C	3.3
21	c9	40	SER	3.3

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Mol	Chain	Res	Type	RSRZ
36	1	3079	U	3.3
36	5	250	U	3.3
18	c6	124	PRO	3.3
26	D4	31	ASN	3.3
60	N4	87	LEU	3.3
2	S0	99	ALA	3.3
28	D6	16	GLY	3.3
41	L4	74	ILE	3.3
1	6	663	U	3.3
12	C0	4	PRO	3.3
28	D6	20	PRO	3.3
3	S1	95	ASN	3.3
14	C2	103	LEU	3.3
70	o4	57	LEU	3.3
82	p1	37	VAL	3.3
10	s8	61	GLU	3.3
10	s8	40	ALA	3.3
60	n4	85	ALA	3.3
80	m2	157	ASP	3.3
1	2	1693	A	3.3
13	c1	116	ARG	3.3
83	f	43	ASP	3.3
82	p1	12	LEU	3.3
4	S2	144	TRP	3.3
31	d9	7	TRP	3.3
36	1	1563	C	3.3
73	o7	88	ALA	3.3
18	c6	142	TYR	3.2
34	SR	33	LEU	3.2
19	c7	25	THR	3.2
27	d5	62	VAL	3.2
35	SM	87	THR	3.2
8	S6	91	GLU	3.2
60	n4	84	GLY	3.2
80	m2	57	GLU	3.2
83	f	87	ARG	3.2
36	5	2505	U	3.2
21	C9	85	SER	3.2
21	c9	41	SER	3.2
13	C1	147	ALA	3.2
35	sM	35	ALA	3.2
6	S4	44	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
16	C4	102	LEU	3.2
8	S6	179	VAL	3.2
43	L6	135	VAL	3.2
1	2	261	U	3.2
18	c6	139	GLN	3.2
34	SR	102	ARG	3.2
1	2	1337	A	3.2
34	SR	289	ALA	3.2
70	o4	38	LEU	3.2
4	S2	63	VAL	3.2
41	l4	26	PHE	3.2
8	S6	101	ILE	3.2
42	l5	235	SER	3.2
13	C1	146	ALA	3.2
17	c5	133	ALA	3.2
70	O4	2	ALA	3.2
79	Q3	92	ALA	3.2
60	N4	89	LEU	3.1
55	M9	181	ARG	3.1
7	s5	187	ILE	3.1
83	f	46	THR	3.1
53	M7	157	VAL	3.1
34	sR	244	ALA	3.1
12	c0	98	THR	3.1
20	C8	2	SER	3.1
1	2	1696	G	3.1
36	5	2503	G	3.1
11	S9	2	PRO	3.1
16	C4	83	ILE	3.1
18	c6	132	LYS	3.1
33	e1	82	LYS	3.1
16	C4	33	LEU	3.1
36	1	3170	A	3.1
1	6	659	C	3.1
8	S6	73	ILE	3.1
14	c2	71	ILE	3.1
36	1	2507	C	3.0
36	1	1349	G	3.0
11	s9	127	VAL	3.0
36	5	620	U	3.0
83	f	68	LYS	3.0
10	s8	58	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
14	c2	59	LEU	3.0
83	f	22	GLN	3.0
83	f	60	VAL	3.0
57	n1	79	MET	3.0
12	c0	64	TYR	3.0
60	n4	68	ALA	3.0
28	D6	14	GLY	3.0
83	f	85	VAL	3.0
49	m3	145	PHE	3.0
12	c0	23	ALA	3.0
15	c3	40	TYR	3.0
33	e1	80	ARG	3.0
60	n4	122	ALA	3.0
5	s3	151	LYS	3.0
83	f	35	LYS	3.0
47	m0	124	GLY	3.0
45	L8	58	VAL	3.0
34	SR	115	ILE	3.0
33	E1	150	VAL	3.0
36	1	2506	U	3.0
8	s6	88	ARG	2.9
21	C9	92	LYS	2.9
74	O8	2	ALA	2.9
10	s8	45	SER	2.9
1	2	1708	U	2.9
1	6	662	U	2.9
45	l8	25	PRO	2.9
28	d6	86	VAL	2.9
54	M8	167	SER	2.9
19	c7	95	ARG	2.9
45	l8	238	LEU	2.9
46	l9	191	LEU	2.9
80	m2	155	ARG	2.9
65	n9	25	LYS	2.9
43	l6	129	GLU	2.9
20	c8	22	VAL	2.9
32	e0	62	VAL	2.9
10	s8	176	SER	2.9
14	C2	117	GLY	2.9
30	D8	53	ILE	2.9
82	p1	16	ASP	2.9
22	d0	67	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	6	660	G	2.9
8	s6	80	ASN	2.9
35	SM	167	PRO	2.9
7	S5	70	VAL	2.9
1	6	679	U	2.9
8	S6	68	LEU	2.9
9	S7	91	ILE	2.9
16	C4	34	SER	2.9
20	c8	17	LEU	2.9
47	m0	112	GLN	2.9
16	C4	119	THR	2.9
11	S9	148	VAL	2.9
70	o4	16	ARG	2.9
27	d5	50	ILE	2.9
83	f	18	THR	2.8
12	c0	21	VAL	2.8
39	l2	164	GLY	2.8
12	c0	65	TYR	2.8
16	C4	40	ALA	2.8
4	s2	208	GLU	2.8
63	n7	96	VAL	2.8
26	d4	102	LYS	2.8
3	s1	110	LEU	2.8
23	D1	23	ILE	2.8
18	c6	141	SER	2.8
3	S1	66	VAL	2.8
5	S3	75	LYS	2.8
1	2	1710	U	2.8
15	C3	53	LEU	2.8
3	S1	53	GLY	2.8
15	c3	16	ILE	2.8
16	C4	76	ILE	2.8
60	N4	90	ILE	2.8
8	s6	169	TYR	2.8
29	D7	51	GLN	2.8
34	SR	83	ALA	2.8
35	SM	90	ALA	2.8
70	o4	58	ARG	2.8
14	C2	82	PRO	2.8
35	SM	106	VAL	2.8
7	S5	91	GLU	2.8
34	SR	141	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
60	N4	75	THR	2.8
36	1	2872	A	2.8
34	sR	24	ALA	2.8
28	D6	32	LYS	2.8
83	f	56	LYS	2.8
10	s8	46	VAL	2.8
21	c9	22	LEU	2.8
83	f	45	SER	2.8
11	s9	140	ILE	2.8
33	e1	85	TYR	2.7
79	q3	2	ALA	2.7
83	f	42	VAL	2.7
83	f	84	VAL	2.7
2	S0	98	ILE	2.7
9	S7	33	GLU	2.7
34	SR	186	PHE	2.7
48	M1	96	PHE	2.7
64	n8	16	SER	2.7
13	C1	3	THR	2.7
33	e1	87	THR	2.7
45	L8	158	ASP	2.7
19	C7	60	ARG	2.7
33	e1	83	LYS	2.7
41	l4	62	ALA	2.7
56	N0	2	ALA	2.7
82	p2	11	ALA	2.7
16	C4	28	VAL	2.7
3	S1	184	LEU	2.7
14	C2	59	LEU	2.7
28	D6	44	ILE	2.7
62	N6	127	GLU	2.7
35	sM	82	THR	2.7
83	f	15	SER	2.7
14	c2	101	ALA	2.7
19	c7	97	ASN	2.7
20	c8	146	ALA	2.7
24	D2	92	ASN	2.7
5	S3	24	PHE	2.7
11	s9	104	PHE	2.7
34	sR	136	ILE	2.7
3	S1	46	THR	2.7
33	e1	86	THR	2.7

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Mol	Chain	Res	Type	RSRZ
7	S5	96	SER	2.7
69	O3	56	SER	2.7
1	6	1491	U	2.7
36	1	1351	U	2.7
34	sR	303	ALA	2.7
64	n8	149	ALA	2.7
4	S2	121	VAL	2.7
42	L5	277	LEU	2.7
47	m0	103	LEU	2.7
13	C1	152	GLN	2.7
66	O0	12	GLN	2.7
51	m5	147	ARG	2.7
34	SR	137	LYS	2.7
45	l8	121	SER	2.7
71	o5	120	ALA	2.7
83	f	25	ALA	2.7
29	d7	33	LEU	2.7
61	n5	24	LEU	2.7
82	p2	29	LEU	2.7
83	f	33	VAL	2.7
45	L8	25	PRO	2.6
3	S1	176	VAL	2.6
5	s3	3	ALA	2.6
34	SR	27	ALA	2.6
60	n4	86	SER	2.6
25	D3	48	HIS	2.6
1	2	1697	G	2.6
34	SR	43	ILE	2.6
4	s2	84	LYS	2.6
34	SR	259	GLY	2.6
22	D0	27	THR	2.6
31	D9	6	VAL	2.6
33	e1	84	VAL	2.6
47	M0	221	ALA	2.6
82	p2	9	TYR	2.6
16	C4	14	PHE	2.6
48	M1	104	PHE	2.6
80	m2	110	ASN	2.6
12	c0	84	GLU	2.6
26	d4	18	LEU	2.6
81	p0	93	LEU	2.6
14	C2	104	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
68	o2	127	ALA	2.6
1	2	506	A	2.6
11	s9	152	SER	2.6
81	p0	211	SER	2.6
82	p1	23	SER	2.6
56	N0	4	PHE	2.6
35	sM	124	GLN	2.6
62	N6	120	GLN	2.6
3	S1	98	THR	2.6
58	n2	14	THR	2.6
70	o4	39	ALA	2.6
22	d0	77	LYS	2.6
80	m2	127	ARG	2.6
83	f	86	LYS	2.6
35	SM	85	SER	2.6
7	S5	75	GLY	2.6
17	c5	129	GLY	2.6
20	C8	124	GLY	2.6
32	e0	49	LEU	2.6
2	S0	189	VAL	2.6
26	D4	5	VAL	2.6
36	1	1802	C	2.6
41	l4	71	VAL	2.6
34	SR	46	LYS	2.6
83	f	61	ALA	2.6
17	C5	84	ILE	2.5
72	o6	93	ILE	2.5
5	s3	150	MET	2.5
52	M6	80	PHE	2.5
33	e1	145	HIS	2.5
54	M8	156	GLY	2.5
12	c0	25	LYS	2.5
1	6	754	A	2.5
1	6	1694	A	2.5
13	c1	144	ALA	2.5
36	5	1350	A	2.5
3	s1	84	ILE	2.5
4	s2	90	THR	2.5
9	s7	91	ILE	2.5
34	SR	136	ILE	2.5
83	f	148	ILE	2.5
1	6	658	C	2.5

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Mol	Chain	Res	Type	RSRZ
2	S0	7	PHE	2.5
28	D6	62	TYR	2.5
5	s3	176	LEU	2.5
18	c6	44	LEU	2.5
40	l3	178	LEU	2.5
83	f	76	SER	2.5
25	d3	60	GLU	2.5
52	M6	40	GLU	2.5
4	s2	85	PRO	2.5
32	e0	40	TYR	2.5
20	C8	142	GLY	2.5
70	o4	19	LYS	2.5
31	d9	20	GLN	2.5
14	C2	115	VAL	2.5
16	C4	16	VAL	2.5
47	M0	218	ALA	2.5
13	C1	4	GLU	2.5
53	M7	182	ILE	2.5
76	q0	77	ILE	2.5
2	S0	97	PRO	2.5
5	s3	148	LYS	2.5
14	c2	62	LEU	2.5
30	d8	9	LEU	2.5
42	L5	146	LEU	2.5
36	1	1103	A	2.5
14	c2	75	VAL	2.5
34	SR	78	ALA	2.5
39	l2	59	ALA	2.5
45	L8	66	SER	2.5
36	1	1216	C	2.5
33	E1	86	THR	2.5
36	1	3175	U	2.5
60	N4	64	THR	2.5
74	O8	6	THR	2.5
60	N4	77	LYS	2.5
11	s9	76	LEU	2.5
14	C2	52	LEU	2.5
18	C6	35	PRO	2.5
30	D8	16	LEU	2.5
33	E1	103	LEU	2.5
32	e0	52	GLY	2.5
70	o4	48	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
14	C2	37	VAL	2.5
34	SR	6	VAL	2.5
34	SR	58	VAL	2.5
35	sM	119	ALA	2.4
45	l8	196	ALA	2.4
83	f	41	ILE	2.4
3	S1	103	MET	2.4
2	S0	203	PHE	2.4
70	O4	7	PHE	2.4
4	s2	88	LYS	2.4
25	d3	110	LYS	2.4
35	SM	11	ASP	2.4
5	S3	21	LEU	2.4
42	l5	236	LEU	2.4
66	o0	104	LEU	2.4
80	m2	101	PRO	2.4
6	S4	167	GLY	2.4
6	s4	208	VAL	2.4
13	c1	145	ALA	2.4
40	l3	179	ALA	2.4
17	c5	136	SER	2.4
29	d7	57	GLU	2.4
58	N2	28	PHE	2.4
83	f	23	CYS	2.4
25	D3	3	LYS	2.4
11	s9	80	LEU	2.4
35	SM	117	LEU	2.4
19	C7	6	THR	2.4
34	SR	45	TRP	2.4
12	c0	97	PRO	2.4
6	s4	183	VAL	2.4
12	C0	66	TYR	2.4
15	C3	2	GLY	2.4
25	d3	2	GLY	2.4
30	D8	7	VAL	2.4
36	1	1581	C	2.4
74	o8	2	ALA	2.4
81	p0	106	ALA	2.4
12	C0	93	GLN	2.4
36	1	2954	U	2.4
51	M5	15	GLN	2.4
83	f	44	MET	2.4

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Mol	Chain	Res	Type	RSRZ
31	D9	11	PRO	2.4
33	E1	87	THR	2.4
3	S1	212	VAL	2.4
21	C9	37	VAL	2.4
83	f	72	ASP	2.4
20	c8	135	GLY	2.4
80	m2	149	ALA	2.4
83	f	11	ALA	2.4
1	2	1410	A	2.4
1	6	755	A	2.4
11	s9	48	GLN	2.4
18	C6	123	ARG	2.4
27	D5	97	LYS	2.4
27	d5	97	LYS	2.4
8	s6	166	GLU	2.4
14	c2	32	LEU	2.4
20	c8	3	LEU	2.4
40	L3	387	LEU	2.4
8	S6	67	VAL	2.4
20	c8	140	THR	2.4
30	d8	7	VAL	2.4
2	s0	164	ASN	2.4
52	m6	183	ALA	2.4
83	f	17	ALA	2.4
4	s2	87	GLN	2.4
8	s6	176	GLN	2.4
80	m2	74	GLN	2.4
3	S1	61	LEU	2.4
83	f	81	GLU	2.4
5	S3	181	VAL	2.4
8	S6	86	PRO	2.4
36	5	1567	U	2.4
1	2	1686	C	2.3
3	S1	60	ALA	2.3
28	D6	63	ALA	2.3
39	L2	189	TYR	2.3
40	l3	146	ARG	2.3
3	S1	54	LEU	2.3
4	S2	134	LEU	2.3
30	D8	9	LEU	2.3
47	M0	112	GLN	2.3
83	f	150	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
21	C9	41	SER	2.3
29	D7	58	SER	2.3
34	sR	313	TRP	2.3
48	m1	8	PRO	2.3
36	1	1217	A	2.3
36	5	1580	A	2.3
36	5	2404	A	2.3
81	p0	215	SER	2.3
8	S6	24	ILE	2.3
12	c0	67	THR	2.3
77	Q1	17	ARG	2.3
47	M0	219	ALA	2.3
81	p0	216	ALA	2.3
82	p1	15	ALA	2.3
1	6	1285	U	2.3
36	5	1351	U	2.3
62	N6	7	ASP	2.3
83	f	124	LEU	2.3
39	L2	253	GLN	2.3
70	O4	52	GLN	2.3
21	C9	104	VAL	2.3
24	D2	121	VAL	2.3
45	L8	116	VAL	2.3
52	m6	3	VAL	2.3
2	s0	173	ILE	2.3
47	m0	166	ILE	2.3
18	c6	79	TYR	2.3
6	S4	180	LEU	2.3
34	SR	42	LEU	2.3
60	n4	109	LEU	2.3
12	c0	27	PHE	2.3
36	5	3167	A	2.3
36	1	1570	U	2.3
36	1	2514	U	2.3
60	N4	66	GLU	2.3
1	2	1703	C	2.3
4	s2	64	LYS	2.3
18	C6	39	VAL	2.3
18	c6	90	VAL	2.3
36	5	1582	C	2.3
36	5	2098	C	2.3
55	M9	52	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
16	C4	18	ARG	2.3
21	c9	24	ARG	2.3
6	S4	29	PRO	2.3
7	S5	130	ILE	2.3
8	S6	226	ILE	2.3
34	sR	27	ALA	2.3
19	C7	125	SER	2.3
31	D9	9	SER	2.3
60	n4	72	SER	2.3
81	p0	219	THR	2.3
63	N7	42	LEU	2.3
2	S0	110	TYR	2.3
28	D6	12	LYS	2.3
23	D1	10	GLU	2.3
34	sR	167	VAL	2.3
36	5	2401	A	2.3
3	S1	84	ILE	2.3
14	c2	102	GLY	2.3
19	c7	90	ALA	2.3
29	D7	50	ALA	2.3
60	n4	121	ALA	2.3
68	O2	127	ALA	2.3
3	s1	217	LEU	2.3
7	s5	174	LEU	2.3
9	S7	41	LEU	2.3
34	sR	72	THR	2.3
41	L4	324	LEU	2.3
42	l5	18	THR	2.3
55	M9	184	LEU	2.3
82	p2	28	THR	2.3
55	M9	85	ARG	2.3
36	5	1576	G	2.2
36	5	3276	G	2.2
8	S6	99	GLY	2.2
27	d5	99	ALA	2.2
40	L3	245	GLY	2.2
80	m2	60	ALA	2.2
1	2	1704	U	2.2
1	6	261	U	2.2
1	6	1719	A	2.2
3	S1	181	LEU	2.2
14	C2	97	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
81	p0	70	LEU	2.2
34	SR	12	THR	2.2
34	SR	74	THR	2.2
81	p0	88	PHE	2.2
2	s0	2	SER	2.2
8	S6	96	SER	2.2
33	e1	105	TYR	2.2
58	N2	33	TYR	2.2
1	2	1711	C	2.2
12	C0	39	ASN	2.2
14	c2	116	VAL	2.2
17	C5	76	VAL	2.2
3	S1	89	ASP	2.2
42	l5	263	GLU	2.2
55	M9	116	ASP	2.2
55	M9	182	ASP	2.2
60	n4	66	GLU	2.2
81	p0	20	GLU	2.2
8	S6	100	ALA	2.2
18	c6	24	ALA	2.2
26	D4	125	LEU	2.2
41	l4	242	ALA	2.2
50	m4	88	ALA	2.2
54	M8	166	LEU	2.2
61	n5	23	ALA	2.2
80	m2	32	GLY	2.2
6	S4	22	LYS	2.2
10	s8	44	HIS	2.2
18	c6	115	THR	2.2
61	n5	28	THR	2.2
1	2	715	U	2.2
36	1	3156	U	2.2
36	5	1764	U	2.2
70	o4	41	ARG	2.2
13	C1	2	SER	2.2
33	E1	146	SER	2.2
36	1	2207	A	2.2
36	1	2404	A	2.2
80	m2	133	SER	2.2
28	D6	86	VAL	2.2
58	N2	27	VAL	2.2
21	C9	116	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
55	M9	72	GLU	2.2
36	1	131	C	2.2
14	C2	101	ALA	2.2
80	m2	23	LEU	2.2
17	c5	9	LYS	2.2
26	d4	99	LYS	2.2
60	n4	69	LYS	2.2
10	S8	21	PHE	2.2
41	l4	65	TRP	2.2
82	p2	45	PHE	2.2
53	M7	167	ARG	2.2
18	C6	21	HIS	2.2
14	C2	116	VAL	2.2
55	M9	51	VAL	2.2
11	S9	87	SER	2.2
1	2	1385	G	2.2
12	c0	94	GLU	2.2
14	c2	133	LEU	2.2
36	1	1605	A	2.2
36	1	1800	A	2.2
45	L8	202	GLU	2.2
5	S3	149	ALA	2.2
10	s8	177	GLY	2.2
11	S9	18	PRO	2.2
14	c2	127	GLY	2.2
16	C4	98	GLY	2.2
32	e0	32	GLY	2.2
81	p0	69	ASP	2.2
26	d4	72	PHE	2.2
31	D9	52	PHE	2.2
46	L9	31	ARG	2.2
22	d0	78	THR	2.2
17	C5	126	VAL	2.2
14	c2	119	SER	2.2
18	C6	36	ILE	2.2
39	L2	150	LEU	2.2
2	s0	136	ALA	2.2
64	n8	120	ASN	2.2
82	p2	4	GLU	2.2
2	s0	82	GLY	2.2
65	N9	59	LYS	2.2
38	4	82	U	2.2

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Mol	Chain	Res	Type	RSRZ
2	S0	107	PHE	2.2
81	p0	206	ASP	2.2
1	6	793	A	2.2
1	6	1199	G	2.2
82	p2	41	TRP	2.2
20	c8	20	THR	2.1
29	d7	67	THR	2.1
35	SM	166	VAL	2.1
47	M0	149	VAL	2.1
71	O5	46	THR	2.1
8	s6	208	TYR	2.1
18	C6	96	TYR	2.1
1	2	716	C	2.1
36	1	1556	C	2.1
9	s7	58	LEU	2.1
14	c2	97	LEU	2.1
34	SR	81	LEU	2.1
45	l8	65	LEU	2.1
35	SM	84	LYS	2.1
46	L9	14	GLU	2.1
47	m0	68	ALA	2.1
83	f	123	SER	2.1
26	D4	30	PRO	2.1
26	D4	67	GLY	2.1
83	f	67	GLY	2.1
1	6	1473	U	2.1
36	5	2504	U	2.1
36	5	2506	U	2.1
12	C0	22	VAL	2.1
40	l3	106	TRP	2.1
8	S6	170	THR	2.1
1	6	1469	A	2.1
11	s9	19	TYR	2.1
23	D1	34	ILE	2.1
4	S2	64	LYS	2.1
6	S4	23	LEU	2.1
13	C1	148	LYS	2.1
44	l7	202	LEU	2.1
47	M0	36	LEU	2.1
34	SR	121	MET	2.1
83	f	80	MET	2.1
5	S3	171	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
18	C6	66	ARG	2.1
45	L8	154	ALA	2.1
49	m3	195	ALA	2.1
51	m5	26	ARG	2.1
70	o4	2	ALA	2.1
79	q3	92	ALA	2.1
2	s0	97	PRO	2.1
11	s9	20	GLU	2.1
20	c8	124	GLY	2.1
57	n1	86	GLU	2.1
80	m2	46	PRO	2.1
82	p1	22	SER	2.1
44	L7	231	ASN	2.1
14	c2	63	VAL	2.1
6	S4	52	LEU	2.1
8	s6	78	THR	2.1
8	s6	163	THR	2.1
9	s7	153	LEU	2.1
11	S9	29	LYS	2.1
34	SR	161	LYS	2.1
34	sR	168	THR	2.1
40	l3	137	TYR	2.1
47	M0	152	LEU	2.1
82	p2	25	LYS	2.1
22	D0	84	MET	2.1
42	L5	273	ARG	2.1
56	n0	1	MET	2.1
70	o4	31	ARG	2.1
80	m2	28	ARG	2.1
75	o9	11	GLN	2.1
38	8	80	A	2.1
50	m4	92	GLU	2.1
60	N4	81	PRO	2.1
4	S2	66	PHE	2.1
28	D6	76	SER	2.1
83	f	74	SER	2.1
7	s5	44	ASN	2.1
5	s3	85	VAL	2.1
3	S1	32	ILE	2.1
7	S5	199	ILE	2.1
28	D6	72	HIS	2.1
50	m4	101	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
34	SR	34	LEU	2.1
42	l5	293	LEU	2.1
49	m3	147	ILE	2.1
78	q2	90	HIS	2.1
12	c0	95	ARG	2.1
22	d0	81	THR	2.1
11	s9	147	MET	2.1
7	S5	154	ALA	2.1
7	S5	155	ALA	2.1
28	D6	35	ALA	2.1
56	n0	2	ALA	2.1
58	n2	46	ALA	2.1
36	5	124	U	2.1
9	S7	66	SER	2.1
2	S0	50	VAL	2.1
22	d0	100	VAL	2.1
1	6	1756[A]	A	2.1
18	C6	132	LYS	2.1
26	D4	128	LYS	2.1
36	5	1797	A	2.1
18	c6	118	ILE	2.1
49	m3	54	LEU	2.1
53	M7	176	ILE	2.1
31	d9	27	HIS	2.1
33	E1	148	TYR	2.1
40	L3	49	TYR	2.1
41	L4	60	THR	2.1
1	2	658	C	2.1
1	6	1720	G	2.1
3	s1	141	ALA	2.1
9	S7	12	ALA	2.1
40	l3	362	ALA	2.1
82	p2	46	ALA	2.1
17	c5	55	GLY	2.1
19	C7	62	GLN	2.1
21	C9	87	GLY	2.1
42	l5	200	PHE	2.1
13	c1	32	LYS	2.0
14	c2	105	LYS	2.0
17	c5	126	VAL	2.0
28	D6	24	VAL	2.0
80	m2	156	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
83	f	40	LYS	2.0
7	s5	90	ILE	2.0
45	L8	67	ILE	2.0
66	O0	100	ILE	2.0
83	f	26	LEU	2.0
4	s2	96	THR	2.0
6	S4	110	ALA	2.0
27	D5	67	ASP	2.0
29	D7	13	ALA	2.0
32	E0	48	THR	2.0
36	1	621	A	2.0
40	L3	31	ALA	2.0
53	M7	156	ALA	2.0
53	M7	184	ALA	2.0
4	S2	57	PHE	2.0
8	S6	123	GLY	2.0
8	S6	176	GLN	2.0
34	sR	298	GLY	2.0
51	M5	2	GLY	2.0
83	f	75	PRO	2.0
7	s5	31	GLU	2.0
1	2	1705	C	2.0
33	e1	81	LYS	2.0
8	s6	162	VAL	2.0
63	N7	26	VAL	2.0
4	S2	207	LEU	2.0
8	S6	76	LEU	2.0
60	n4	87	LEU	2.0
82	p1	14	LEU	2.0
14	C2	136	ILE	2.0
21	c9	97	SER	2.0
35	SM	25	ILE	2.0
1	2	1362	U	2.0
19	C7	123	ASN	2.0
57	N1	77	ASN	2.0
3	S1	101	HIS	2.0
14	C2	42	ALA	2.0
41	L4	70	ALA	2.0
33	E1	85	TYR	2.0
34	sR	25	THR	2.0
4	S2	78	ASP	2.0
81	p0	192	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
7	S5	151	GLY	2.0
7	S5	212	LYS	2.0
19	C7	63	LYS	2.0
21	c9	25	GLN	2.0
28	d6	65	PRO	2.0
41	L4	4	PRO	2.0
83	f	48	LYS	2.0
1	2	1701	A	2.0
17	c5	137	ARG	2.0
28	D6	58	VAL	2.0
11	S9	28	LEU	2.0
15	C3	54	LEU	2.0
33	e1	117	LEU	2.0
34	SR	32	LEU	2.0
68	O2	128	LEU	2.0
22	D0	103	ILE	2.0
1	6	1709	C	2.0
36	5	1581	C	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
83	5CT	f	51	15/16	0.80	0.54	44,44,44,44	15
84	8AN	C	76	22/23	0.96	0.09	40,42,43,43	0
84	8AN	B	76	22/23	0.97	0.08	44,44,45,45	0

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($\text{\AA}^2$)	Q<0.9
85	MG	2	1939	1/1	-0.07	0.35	130,130,130,130	0
85	MG	1	3405	1/1	-0.00	0.37	132,132,132,132	0
85	MG	2	1986	1/1	0.01	0.30	118,118,118,118	0
85	MG	2	1943	1/1	0.18	0.40	115,115,115,115	0
85	MG	5	3778	1/1	0.25	0.31	115,115,115,115	0
85	MG	2	1950	1/1	0.26	0.30	108,108,108,108	0
85	MG	6	1937	1/1	0.30	0.45	98,98,98,98	0
85	MG	5	3686	1/1	0.39	0.28	92,92,92,92	0
85	MG	1	3662	1/1	0.45	0.26	101,101,101,101	0
85	MG	1	3753	1/1	0.46	0.28	107,107,107,107	0
85	MG	2	1958	1/1	0.46	0.33	104,104,104,104	0
85	MG	6	1959	1/1	0.47	0.36	98,98,98,98	0
85	MG	5	3748	1/1	0.49	0.12	124,124,124,124	0
85	MG	2	1961	1/1	0.50	0.32	86,86,86,86	0
85	MG	5	3462	1/1	0.51	0.28	109,109,109,109	0
85	MG	2	1922	1/1	0.51	0.47	85,85,85,85	0
85	MG	2	1904	1/1	0.52	0.30	90,90,90,90	0
85	MG	2	1957	1/1	0.52	0.21	99,99,99,99	0
85	MG	O4	201	1/1	0.52	0.37	77,77,77,77	0
85	MG	6	1954	1/1	0.53	0.35	64,64,64,64	0
85	MG	2	1989	1/1	0.53	0.26	65,65,65,65	0
85	MG	6	1908	1/1	0.54	0.29	109,109,109,109	0
85	MG	2	1974	1/1	0.55	0.43	83,83,83,83	0
86	OHX	5	4123	7/7	0.56	0.28	76,76,76,76	5
85	MG	2	1912	1/1	0.57	0.43	88,88,88,88	0
86	OHX	6	2183	7/7	0.58	0.28	76,76,76,76	5
85	MG	5	3757	1/1	0.58	0.27	73,73,73,73	0
85	MG	2	1953	1/1	0.59	0.35	89,89,89,89	0
85	MG	1	3423	1/1	0.59	0.24	46,46,46,46	0
85	MG	2	1936	1/1	0.60	0.30	83,83,83,83	0
85	MG	5	3464	1/1	0.60	0.22	125,125,125,125	0
85	MG	6	1948	1/1	0.60	0.34	85,85,85,85	0
85	MG	6	1971	1/1	0.60	0.35	90,90,90,90	0
85	MG	6	1963	1/1	0.61	0.27	80,80,80,80	0
86	OHX	2	2145	7/7	0.61	0.19	103,103,103,103	4
85	MG	1	3635	1/1	0.62	0.45	88,88,88,88	0
85	MG	2	1955	1/1	0.62	0.36	62,62,62,62	0
85	MG	2	1924	1/1	0.62	0.30	100,100,100,100	0
85	MG	2	1945	1/1	0.62	0.24	107,107,107,107	0
85	MG	2	1969	1/1	0.63	0.36	108,108,108,108	0
85	MG	2	1941	1/1	0.63	0.32	100,100,100,100	0
85	MG	2	1967	1/1	0.63	0.15	93,93,93,93	0
85	MG	1	3560	1/1	0.63	0.48	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	6	1984	1/1	0.64	0.28	109,109,109,109	0
85	MG	5	3667	1/1	0.64	0.33	86,86,86,86	0
85	MG	M7	201	1/1	0.64	0.43	71,71,71,71	0
85	MG	5	3503	1/1	0.65	0.34	57,57,57,57	0
86	OHX	2	2149	7/7	0.65	0.13	137,137,137,137	6
86	OHX	6	2178	7/7	0.65	0.15	145,145,145,145	6
85	MG	2	1909	1/1	0.65	0.39	83,83,83,83	0
86	OHX	2	2104	7/7	0.65	0.22	119,119,119,119	5
85	MG	6	1974	1/1	0.66	0.42	94,94,94,94	0
85	MG	5	3474	1/1	0.66	0.29	63,63,63,63	0
85	MG	17	2200	1/1	0.67	0.18	50,50,50,50	0
85	MG	2	1927	1/1	0.67	0.33	85,85,85,85	0
85	MG	2	1964	1/1	0.67	0.39	92,92,92,92	0
86	OHX	2	2147	7/7	0.67	0.14	116,116,116,116	6
85	MG	1	3729	1/1	0.67	0.15	69,69,69,69	0
86	OHX	3	219	7/7	0.67	0.18	82,82,82,82	5
85	MG	2	1978	1/1	0.67	0.33	74,74,74,74	0
85	MG	1	3537	1/1	0.67	0.27	57,57,57,57	0
85	MG	2	1952	1/1	0.67	0.33	64,64,64,64	0
85	MG	2	1933	1/1	0.68	0.41	70,70,70,70	0
85	MG	2	1968	1/1	0.68	0.30	101,101,101,101	0
85	MG	6	1938	1/1	0.68	0.25	60,60,60,60	0
85	MG	2	1925	1/1	0.68	0.35	67,67,67,67	0
86	OHX	M0	304	7/7	0.68	0.20	101,101,101,101	6
85	MG	5	3628	1/1	0.68	0.40	92,92,92,92	0
85	MG	1	3424	1/1	0.68	0.22	59,59,59,59	0
86	OHX	2	2123	7/7	0.68	0.16	121,121,121,121	5
85	MG	3	205	1/1	0.69	0.37	68,68,68,68	0
85	MG	2	1913	1/1	0.69	0.40	79,79,79,79	0
85	MG	2	1919	1/1	0.69	0.39	62,62,62,62	0
85	MG	6	1972	1/1	0.69	0.26	81,81,81,81	0
85	MG	5	3540	1/1	0.69	0.39	62,62,62,62	0
85	MG	1	3434	1/1	0.69	0.29	62,62,62,62	0
85	MG	6	1957	1/1	0.69	0.34	94,94,94,94	0
86	OHX	2	2141	7/7	0.69	0.19	90,90,90,90	6
85	MG	2	1905	1/1	0.70	0.39	63,63,63,63	0
86	OHX	1	3871	7/7	0.70	0.34	61,61,61,61	2
86	OHX	2	2121	7/7	0.70	0.26	94,94,94,94	4
85	MG	1	3672	1/1	0.70	0.29	76,76,76,76	0
85	MG	s4	601	1/1	0.70	0.29	66,66,66,66	0
85	MG	6	1910	1/1	0.70	0.30	91,91,91,91	0
85	MG	1	3660	1/1	0.70	0.23	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	6	1931	1/1	0.71	0.25	92,92,92,92	0
85	MG	2	1954	1/1	0.71	0.20	105,105,105,105	0
85	MG	2	1951	1/1	0.71	0.43	71,71,71,71	0
85	MG	6	1980	1/1	0.71	0.11	76,76,76,76	0
86	OHX	1	4044	7/7	0.71	0.19	108,108,108,108	4
86	OHX	1	4106	7/7	0.71	0.13	72,72,72,72	4
85	MG	6	1960	1/1	0.71	0.23	65,65,65,65	0
86	OHX	2	2117	7/7	0.71	0.15	93,93,93,93	4
86	OHX	6	2175	7/7	0.71	0.23	100,100,100,100	6
85	MG	2	1988	1/1	0.71	0.28	88,88,88,88	0
85	MG	c9	201	1/1	0.71	0.17	83,83,83,83	0
85	MG	5	3446	1/1	0.71	0.22	64,64,64,64	0
86	OHX	5	4147	7/7	0.71	0.16	89,89,89,89	7
86	OHX	1	4013	7/7	0.72	0.35	54,54,54,54	3
85	MG	3	206	1/1	0.72	0.29	65,65,65,65	0
86	OHX	1	4093	7/7	0.72	0.17	64,64,64,64	4
85	MG	6	1986	1/1	0.72	0.40	93,93,93,93	0
85	MG	2	1973	1/1	0.72	0.33	80,80,80,80	0
85	MG	c8	202	1/1	0.72	0.39	84,84,84,84	0
86	OHX	6	2137	7/7	0.72	0.19	95,95,95,95	4
86	OHX	6	2149	7/7	0.72	0.19	95,95,95,95	6
85	MG	6	1967	1/1	0.72	0.27	76,76,76,76	0
85	MG	2	1911	1/1	0.72	0.55	77,77,77,77	0
85	MG	2	1962	1/1	0.72	0.25	88,88,88,88	0
85	MG	2	1929	1/1	0.72	0.33	83,83,83,83	0
85	MG	2	1987	1/1	0.72	0.31	104,104,104,104	0
86	OHX	5	4150	7/7	0.72	0.24	62,62,62,62	5
86	OHX	5	4165	7/7	0.72	0.32	51,51,51,51	3
85	MG	6	1987	1/1	0.73	0.34	77,77,77,77	0
85	MG	2	1901	1/1	0.73	0.30	87,87,87,87	0
86	OHX	5	4062	7/7	0.73	0.24	56,56,56,56	3
85	MG	1	3566	1/1	0.73	0.40	47,47,47,47	0
85	MG	2	1970	1/1	0.73	0.32	65,65,65,65	0
85	MG	5	3422	1/1	0.73	0.34	44,44,44,44	0
86	OHX	1	4104	7/7	0.73	0.12	73,73,73,73	6
85	MG	6	1929	1/1	0.74	0.25	49,49,49,49	0
85	MG	5	3690	1/1	0.74	0.20	75,75,75,75	0
86	OHX	5	4034	7/7	0.74	0.19	66,66,66,66	4
85	MG	5	3424	1/1	0.74	0.28	56,56,56,56	0
86	OHX	5	4086	7/7	0.74	0.20	70,70,70,70	4
85	MG	1	3472	1/1	0.74	0.27	42,42,42,42	0
85	MG	6	1916	1/1	0.74	0.24	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4067	7/7	0.74	0.16	107,107,107,107	7
85	MG	6	1962	1/1	0.74	0.15	93,93,93,93	0
86	OHX	8	228	7/7	0.74	0.19	73,73,73,73	5
85	MG	1	3700	1/1	0.75	0.23	51,51,51,51	0
85	MG	1	3607	1/1	0.75	0.33	85,85,85,85	0
86	OHX	L3	404	7/7	0.75	0.15	84,84,84,84	6
85	MG	1	3409	1/1	0.75	0.32	52,52,52,52	0
85	MG	6	1927	1/1	0.75	0.31	63,63,63,63	0
86	OHX	2	2151	7/7	0.75	0.16	112,112,112,112	7
86	OHX	2	2152	7/7	0.75	0.11	122,122,122,122	6
85	MG	3	201	1/1	0.75	0.20	80,80,80,80	0
86	OHX	1	3995	7/7	0.75	0.24	50,50,50,50	2
85	MG	2	1944	1/1	0.75	0.22	102,102,102,102	0
86	OHX	1	4021	7/7	0.75	0.22	58,58,58,58	3
86	OHX	1	4039	7/7	0.75	0.10	278,278,278,278	6
86	OHX	5	4119	7/7	0.75	0.29	52,52,52,52	3
85	MG	1	3661	1/1	0.75	0.27	51,51,51,51	0
85	MG	2	1946	1/1	0.75	0.20	108,108,108,108	0
86	OHX	1	4089	7/7	0.75	0.28	55,55,55,55	6
85	MG	2	1959	1/1	0.75	0.26	87,87,87,87	0
86	OHX	5	4172	7/7	0.75	0.26	45,45,45,45	3
85	MG	5	3680	1/1	0.75	0.24	70,70,70,70	0
86	OHX	8	229	7/7	0.75	0.14	101,101,101,101	6
86	OHX	m1	201	7/7	0.75	0.14	78,78,78,78	3
85	MG	1	3407	1/1	0.76	0.36	33,33,33,33	0
85	MG	6	1903	1/1	0.76	0.22	88,88,88,88	0
85	MG	2	1938	1/1	0.76	0.35	72,72,72,72	0
86	OHX	5	3948	7/7	0.76	0.28	49,49,49,49	2
85	MG	5	3739	1/1	0.76	0.13	109,109,109,109	0
85	MG	6	1979	1/1	0.76	0.23	101,101,101,101	0
85	MG	2	1949	1/1	0.76	0.41	86,86,86,86	0
85	MG	5	3547	1/1	0.76	0.39	53,53,53,53	0
85	MG	14	401	1/1	0.76	0.10	42,42,42,42	0
85	MG	5	3567	1/1	0.76	0.23	37,37,37,37	0
86	OHX	1	3965	7/7	0.76	0.27	56,56,56,56	3
86	OHX	1	3983	7/7	0.76	0.14	77,77,77,77	2
86	OHX	6	2131	7/7	0.76	0.18	89,89,89,89	6
85	MG	1	3714	1/1	0.76	0.12	46,46,46,46	0
85	MG	1	3576	1/1	0.76	0.36	46,46,46,46	0
86	OHX	8	230	7/7	0.76	0.20	68,68,68,68	3
86	OHX	19	201	7/7	0.76	0.17	61,61,61,61	2
86	OHX	6	2169	7/7	0.76	0.22	89,89,89,89	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3674	1/1	0.77	0.11	65,65,65,65	0
85	MG	5	3507	1/1	0.77	0.34	38,38,38,38	0
85	MG	5	3685	1/1	0.77	0.28	48,48,48,48	0
85	MG	1	3487	1/1	0.77	0.27	49,49,49,49	0
86	OHX	5	4083	7/7	0.77	0.31	53,53,53,53	3
86	OHX	1	4108	7/7	0.77	0.19	59,59,59,59	5
86	OHX	2	2120	7/7	0.77	0.18	87,87,87,87	3
85	MG	1	3517	1/1	0.77	0.36	46,46,46,46	0
85	MG	5	3712	1/1	0.77	0.21	67,67,67,67	0
86	OHX	6	2114	7/7	0.77	0.20	66,66,66,66	3
85	MG	1	3447	1/1	0.77	0.27	51,51,51,51	0
86	OHX	6	2133	7/7	0.77	0.15	125,125,125,125	6
86	OHX	1	4036	7/7	0.77	0.15	83,83,83,83	6
85	MG	5	3571	1/1	0.77	0.34	34,34,34,34	0
85	MG	6	1947	1/1	0.77	0.30	50,50,50,50	0
85	MG	6	2011	1/1	0.77	0.27	48,48,48,48	0
86	OHX	1	4070	7/7	0.77	0.12	111,111,111,111	6
85	MG	2	1932	1/1	0.78	0.41	64,64,64,64	0
86	OHX	1	3928	7/7	0.78	0.23	49,49,49,49	3
85	MG	5	3684	1/1	0.78	0.11	62,62,62,62	0
85	MG	2	1981	1/1	0.78	0.22	79,79,79,79	0
86	OHX	3	217	7/7	0.78	0.22	78,78,78,78	4
85	MG	5	3518	1/1	0.78	0.39	38,38,38,38	0
85	MG	1	3464	1/1	0.78	0.31	38,38,38,38	0
85	MG	2	1985	1/1	0.78	0.37	86,86,86,86	0
86	OHX	5	4139	7/7	0.78	0.12	108,108,108,108	5
86	OHX	N8	204	7/7	0.78	0.15	90,90,90,90	7
85	MG	5	3722	1/1	0.78	0.30	41,41,41,41	0
85	MG	2	1965	1/1	0.78	0.39	76,76,76,76	0
86	OHX	5	4169	7/7	0.78	0.16	81,81,81,81	7
85	MG	6	1961	1/1	0.78	0.32	95,95,95,95	0
85	MG	6	1909	1/1	0.78	0.26	53,53,53,53	0
85	MG	6	1943	1/1	0.78	0.41	70,70,70,70	0
86	OHX	1	4075	7/7	0.78	0.18	75,75,75,75	5
86	OHX	1	4079	7/7	0.78	0.13	108,108,108,108	6
85	MG	1	3586	1/1	0.78	0.39	45,45,45,45	0
86	OHX	2	2083	7/7	0.79	0.17	87,87,87,87	2
86	OHX	2	2103	7/7	0.79	0.19	118,118,118,118	4
85	MG	2	1937	1/1	0.79	0.22	80,80,80,80	0
85	MG	6	1913	1/1	0.79	0.30	79,79,79,79	0
85	MG	1	3417	1/1	0.79	0.40	78,78,78,78	0
85	MG	6	1919	1/1	0.79	0.35	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4073	7/7	0.79	0.14	71,71,71,71	5
85	MG	1	3739	1/1	0.79	0.25	72,72,72,72	0
85	MG	6	1928	1/1	0.79	0.15	57,57,57,57	0
86	OHX	5	4078	7/7	0.79	0.23	68,68,68,68	3
86	OHX	2	2142	7/7	0.79	0.14	132,132,132,132	7
85	MG	2	1907	1/1	0.79	0.40	62,62,62,62	0
86	OHX	1	4096	7/7	0.79	0.18	80,80,80,80	4
85	MG	6	1906	1/1	0.79	0.26	76,76,76,76	0
85	MG	6	1988	1/1	0.79	0.29	80,80,80,80	0
86	OHX	5	4143	7/7	0.79	0.23	50,50,50,50	4
86	OHX	2	2150	7/7	0.79	0.11	151,151,151,151	7
86	OHX	1	4111	7/7	0.79	0.11	104,104,104,104	7
86	OHX	5	4153	7/7	0.79	0.27	35,35,35,35	4
85	MG	5	3531	1/1	0.79	0.27	55,55,55,55	0
86	OHX	5	4166	7/7	0.79	0.25	49,49,49,49	4
85	MG	6	1996	1/1	0.79	0.23	70,70,70,70	0
85	MG	6	1932	1/1	0.79	0.12	72,72,72,72	0
85	MG	1	3538	1/1	0.79	0.40	39,39,39,39	0
85	MG	8	205	1/1	0.79	0.14	43,43,43,43	0
85	MG	8	210	1/1	0.79	0.09	48,48,48,48	0
85	MG	6	1964	1/1	0.79	0.20	82,82,82,82	0
85	MG	2	1966	1/1	0.79	0.26	74,74,74,74	0
87	ZN	d7	101	1/1	0.79	0.17	147,147,147,147	0
86	OHX	s1	302	7/7	0.80	0.17	99,99,99,99	6
85	MG	1	3401	1/1	0.80	0.32	43,43,43,43	0
85	MG	4	205	1/1	0.80	0.25	58,58,58,58	0
85	MG	1	3694	1/1	0.80	0.19	46,46,46,46	0
85	MG	1	3595	1/1	0.80	0.42	78,78,78,78	0
85	MG	5	3548	1/1	0.80	0.30	25,25,25,25	0
86	OHX	1	4107	7/7	0.80	0.14	91,91,91,91	6
85	MG	6	1901	1/1	0.80	0.41	52,52,52,52	0
85	MG	1	3701	1/1	0.80	0.17	52,52,52,52	0
85	MG	5	3591	1/1	0.80	0.31	42,42,42,42	0
85	MG	2	1928	1/1	0.80	0.41	71,71,71,71	0
85	MG	1	3551	1/1	0.80	0.22	38,38,38,38	0
85	MG	1	3507	1/1	0.80	0.38	30,30,30,30	0
85	MG	6	1946	1/1	0.80	0.31	53,53,53,53	0
86	OHX	5	4159	7/7	0.80	0.26	48,48,48,48	4
86	OHX	1	4032	7/7	0.80	0.20	52,52,52,52	3
85	MG	1	3415	1/1	0.80	0.28	43,43,43,43	0
85	MG	1	3533	1/1	0.80	0.25	49,49,49,49	0
85	MG	6	1981	1/1	0.80	0.35	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	2	2135	7/7	0.80	0.10	188,188,188,188	6
85	MG	5	3481	1/1	0.80	0.37	76,76,76,76	0
85	MG	6	1915	1/1	0.80	0.34	75,75,75,75	0
86	OHX	6	2177	7/7	0.80	0.11	141,141,141,141	7
86	OHX	2	2143	7/7	0.80	0.22	84,84,84,84	5
85	MG	1	3669	1/1	0.80	0.23	59,59,59,59	0
85	MG	5	3715	1/1	0.81	0.33	62,62,62,62	0
85	MG	6	1990	1/1	0.81	0.30	79,79,79,79	0
85	MG	6	1992	1/1	0.81	0.26	61,61,61,61	0
85	MG	2	1916	1/1	0.81	0.33	63,63,63,63	0
86	OHX	5	4054	7/7	0.81	0.16	50,50,50,50	2
85	MG	2	1914	1/1	0.81	0.33	83,83,83,83	0
86	OHX	1	4094	7/7	0.81	0.16	77,77,77,77	4
85	MG	1	3473	1/1	0.81	0.26	56,56,56,56	0
85	MG	1	3760	1/1	0.81	0.15	62,62,62,62	0
86	OHX	5	4091	7/7	0.81	0.14	45,45,45,45	2
86	OHX	5	4108	7/7	0.81	0.24	66,66,66,66	3
85	MG	6	1940	1/1	0.81	0.42	36,36,36,36	0
86	OHX	S6	301	7/7	0.81	0.15	117,117,117,117	7
86	OHX	1	3867	7/7	0.81	0.24	51,51,51,51	4
85	MG	2	1920	1/1	0.81	0.34	76,76,76,76	0
85	MG	5	3600	1/1	0.81	0.12	37,37,37,37	0
86	OHX	5	4149	7/7	0.81	0.09	145,145,145,145	7
85	MG	1	3544	1/1	0.81	0.20	55,55,55,55	0
85	MG	1	3674	1/1	0.81	0.26	68,68,68,68	0
85	MG	2	1960	1/1	0.81	0.19	76,76,76,76	0
86	OHX	2	2112	7/7	0.81	0.16	121,121,121,121	6
85	MG	6	1918	1/1	0.81	0.35	41,41,41,41	0
85	MG	5	3469	1/1	0.81	0.14	38,38,38,38	1
85	MG	1	3609	1/1	0.81	0.22	44,44,44,44	0
85	MG	M9	201	1/1	0.81	0.20	75,75,75,75	0
85	MG	1	3557	1/1	0.81	0.39	55,55,55,55	0
86	OHX	1	4061	7/7	0.81	0.17	72,72,72,72	4
86	OHX	2	2137	7/7	0.81	0.10	219,219,219,219	7
86	OHX	1	4069	7/7	0.81	0.21	58,58,58,58	5
85	MG	1	3652	1/1	0.81	0.18	48,48,48,48	0
86	OHX	5	4061	7/7	0.82	0.21	55,55,55,55	4
85	MG	1	3570	1/1	0.82	0.26	46,46,46,46	0
85	MG	1	3597	1/1	0.82	0.28	47,47,47,47	0
85	MG	1	3602	1/1	0.82	0.32	58,58,58,58	0
85	MG	2	1940	1/1	0.82	0.47	80,80,80,80	0
85	MG	1	3460	1/1	0.82	0.36	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	6	2110	7/7	0.82	0.19	112,112,112,112	6
86	OHX	5	4111	7/7	0.82	0.15	74,74,74,74	7
85	MG	1	3612	1/1	0.82	0.28	55,55,55,55	0
86	OHX	2	2109	7/7	0.82	0.14	105,105,105,105	6
85	MG	1	3751	1/1	0.82	0.28	67,67,67,67	0
86	OHX	5	4140	7/7	0.82	0.18	88,88,88,88	7
86	OHX	6	2135	7/7	0.82	0.28	94,94,94,94	7
85	MG	5	3629	1/1	0.82	0.12	35,35,35,35	0
85	MG	5	3640	1/1	0.82	0.20	50,50,50,50	0
86	OHX	6	2162	7/7	0.82	0.19	114,114,114,114	5
85	MG	1	3587	1/1	0.82	0.33	35,35,35,35	0
86	OHX	6	2174	7/7	0.82	0.11	92,92,92,92	6
86	OHX	5	4161	7/7	0.82	0.13	123,123,123,123	7
86	OHX	2	2122	7/7	0.82	0.20	91,91,91,91	7
85	MG	1	3692	1/1	0.82	0.31	61,61,61,61	0
86	OHX	2	2128	7/7	0.82	0.17	115,115,115,115	7
86	OHX	5	4171	7/7	0.82	0.18	90,90,90,90	5
86	OHX	2	2133	7/7	0.82	0.10	214,214,214,214	6
86	OHX	7	224	7/7	0.82	0.16	54,54,54,54	5
85	MG	5	3790	1/1	0.82	0.25	69,69,69,69	0
85	MG	5	3809	1/1	0.82	0.27	42,42,42,42	0
86	OHX	5	4008	7/7	0.82	0.20	66,66,66,66	3
86	OHX	1	4029	7/7	0.82	0.15	82,82,82,82	3
86	OHX	5	4048	7/7	0.82	0.19	69,69,69,69	3
86	OHX	m4	201	7/7	0.82	0.15	108,108,108,108	7
85	MG	6	1905	1/1	0.82	0.27	51,51,51,51	0
86	OHX	5	4082	7/7	0.83	0.13	92,92,92,92	3
85	MG	5	3514	1/1	0.83	0.28	35,35,35,35	0
86	OHX	6	2097	7/7	0.83	0.23	49,49,49,49	1
85	MG	6	1936	1/1	0.83	0.28	76,76,76,76	0
85	MG	5	3441	1/1	0.83	0.29	30,30,30,30	0
85	MG	2	1931	1/1	0.83	0.41	65,65,65,65	0
85	MG	5	3542	1/1	0.83	0.42	46,46,46,46	0
85	MG	5	3451	1/1	0.83	0.20	40,40,40,40	0
86	OHX	5	4125	7/7	0.83	0.27	48,48,48,48	5
86	OHX	5	4127	7/7	0.83	0.27	44,44,44,44	3
86	OHX	5	4128	7/7	0.83	0.18	47,47,47,47	4
86	OHX	5	4137	7/7	0.83	0.15	50,50,50,50	4
86	OHX	2	2105	7/7	0.83	0.15	87,87,87,87	3
85	MG	5	3695	1/1	0.83	0.23	54,54,54,54	0
86	OHX	6	2161	7/7	0.83	0.21	84,84,84,84	6
86	OHX	1	4078	7/7	0.83	0.10	167,167,167,167	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	6	2165	7/7	0.83	0.18	74,74,74,74	6
86	OHX	6	2167	7/7	0.83	0.20	73,73,73,73	7
85	MG	6	2002	1/1	0.83	0.10	66,66,66,66	0
85	MG	6	2003	1/1	0.83	0.20	96,96,96,96	0
85	MG	1	3690	1/1	0.83	0.29	63,63,63,63	0
86	OHX	5	4164	7/7	0.83	0.19	61,61,61,61	7
86	OHX	1	3915	7/7	0.83	0.18	66,66,66,66	4
85	MG	5	3724	1/1	0.83	0.29	35,35,35,35	0
86	OHX	6	2182	7/7	0.83	0.20	113,113,113,113	7
85	MG	2	1923	1/1	0.83	0.32	45,45,45,45	0
85	MG	1	3433	1/1	0.83	0.30	34,34,34,34	0
86	OHX	2	2124	7/7	0.83	0.12	128,128,128,128	6
85	MG	5	3485	1/1	0.83	0.18	38,38,38,38	0
86	OHX	1	4110	7/7	0.83	0.30	55,55,55,55	5
86	OHX	1	4016	7/7	0.83	0.23	56,56,56,56	3
85	MG	2	1908	1/1	0.83	0.16	90,90,90,90	0
85	MG	1	3532	1/1	0.83	0.35	42,42,42,42	0
85	MG	5	3508	1/1	0.83	0.37	31,31,31,31	0
85	MG	5	3673	1/1	0.83	0.33	78,78,78,78	0
85	MG	6	1933	1/1	0.84	0.33	56,56,56,56	0
85	MG	6	1934	1/1	0.84	0.29	43,43,43,43	0
85	MG	5	3638	1/1	0.84	0.17	50,50,50,50	0
86	OHX	1	4042	7/7	0.84	0.09	70,70,70,70	5
86	OHX	2	2114	7/7	0.84	0.17	103,103,103,103	4
85	MG	1	3523	1/1	0.84	0.33	54,54,54,54	0
86	OHX	1	4065	7/7	0.84	0.19	59,59,59,59	5
85	MG	5	3663	1/1	0.84	0.24	48,48,48,48	0
85	MG	1	3426	1/1	0.84	0.28	52,52,52,52	0
85	MG	1	3465	1/1	0.84	0.29	28,28,28,28	0
85	MG	6	1982	1/1	0.84	0.28	53,53,53,53	0
85	MG	1	3741	1/1	0.84	0.29	46,46,46,46	0
85	MG	5	3479	1/1	0.84	0.28	70,70,70,70	0
85	MG	2	1935	1/1	0.84	0.24	70,70,70,70	0
86	OHX	1	4086	7/7	0.84	0.21	65,65,65,65	4
85	MG	5	3483	1/1	0.84	0.29	52,52,52,52	0
86	OHX	1	4092	7/7	0.84	0.22	47,47,47,47	3
85	MG	2	1942	1/1	0.84	0.22	69,69,69,69	0
85	MG	5	3502	1/1	0.84	0.40	31,31,31,31	0
86	OHX	5	4107	7/7	0.84	0.17	81,81,81,81	5
85	MG	5	3697	1/1	0.84	0.10	61,61,61,61	0
85	MG	1	3758	1/1	0.84	0.28	48,48,48,48	0
85	MG	1	3445	1/1	0.84	0.37	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	4112	1/1	0.84	0.11	44,44,44,44	0
85	MG	5	3510	1/1	0.84	0.22	39,39,39,39	0
85	MG	1	3497	1/1	0.84	0.35	25,25,25,25	0
85	MG	1	3505	1/1	0.84	0.35	38,38,38,38	0
86	OHX	5	4132	7/7	0.84	0.21	45,45,45,45	4
85	MG	2	1948	1/1	0.84	0.30	72,72,72,72	0
85	MG	6	2004	1/1	0.84	0.28	74,74,74,74	0
85	MG	5	3782	1/1	0.84	0.18	48,48,48,48	0
85	MG	6	1921	1/1	0.84	0.33	66,66,66,66	0
85	MG	1	3414	1/1	0.84	0.40	43,43,43,43	0
86	OHX	6	2080	7/7	0.84	0.20	82,82,82,82	1
86	OHX	1	3924	7/7	0.84	0.20	71,71,71,71	4
85	MG	7	212	1/1	0.84	0.27	51,51,51,51	0
86	OHX	5	4158	7/7	0.84	0.18	35,35,35,35	3
86	OHX	1	3955	7/7	0.84	0.21	71,71,71,71	3
86	OHX	6	2118	7/7	0.84	0.22	89,89,89,89	5
86	OHX	1	3963	7/7	0.84	0.27	51,51,51,51	3
85	MG	M6	201	1/1	0.84	0.13	34,34,34,34	0
85	MG	5	3557	1/1	0.84	0.35	29,29,29,29	0
85	MG	1	3630	1/1	0.84	0.24	76,76,76,76	0
86	OHX	6	2148	7/7	0.84	0.21	54,54,54,54	3
85	MG	5	3420	1/1	0.84	0.33	26,26,26,26	0
86	OHX	6	2150	7/7	0.84	0.15	78,78,78,78	6
86	OHX	6	2152	7/7	0.84	0.17	107,107,107,107	5
85	MG	5	3590	1/1	0.84	0.28	35,35,35,35	0
86	OHX	1	4018	7/7	0.84	0.13	69,69,69,69	3
86	OHX	l5	302	7/7	0.84	0.14	105,105,105,105	4
85	MG	1	3567	1/1	0.84	0.20	48,48,48,48	0
86	OHX	m0	302	7/7	0.84	0.24	49,49,49,49	3
86	OHX	1	4028	7/7	0.84	0.15	58,58,58,58	3
85	MG	1	3710	1/1	0.84	0.09	46,46,46,46	0
86	OHX	6	2173	7/7	0.84	0.15	64,64,64,64	5
85	MG	5	3598	1/1	0.85	0.25	48,48,48,48	0
86	OHX	sR	401	7/7	0.85	0.13	129,129,129,129	6
86	OHX	5	3936	7/7	0.85	0.21	49,49,49,49	3
85	MG	5	3800	1/1	0.85	0.11	70,70,70,70	0
85	MG	6	1953	1/1	0.85	0.36	63,63,63,63	0
86	OHX	C3	201	7/7	0.85	0.14	100,100,100,100	5
86	OHX	5	4046	7/7	0.85	0.09	53,53,53,53	5
86	OHX	1	4095	7/7	0.85	0.23	55,55,55,55	5
85	MG	5	3602	1/1	0.85	0.24	30,30,30,30	0
86	OHX	1	4098	7/7	0.85	0.13	61,61,61,61	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4102	7/7	0.85	0.16	65,65,65,65	3
86	OHX	1	4103	7/7	0.85	0.21	53,53,53,53	5
85	MG	5	3619	1/1	0.85	0.25	47,47,47,47	0
85	MG	1	3712	1/1	0.85	0.34	44,44,44,44	0
85	MG	1	3571	1/1	0.85	0.35	53,53,53,53	0
86	OHX	5	4087	7/7	0.85	0.30	39,39,39,39	5
85	MG	5	3632	1/1	0.85	0.11	36,36,36,36	0
86	OHX	2	2065	7/7	0.85	0.19	106,106,106,106	5
85	MG	N3	201	1/1	0.85	0.31	36,36,36,36	0
86	OHX	2	2101	7/7	0.85	0.17	110,110,110,110	5
86	OHX	5	4117	7/7	0.85	0.23	40,40,40,40	5
85	MG	1	3488	1/1	0.85	0.35	37,37,37,37	0
85	MG	5	3659	1/1	0.85	0.28	39,39,39,39	0
86	OHX	1	4000	7/7	0.85	0.22	55,55,55,55	3
86	OHX	1	4009	7/7	0.85	0.09	131,131,131,131	7
85	MG	5	3501	1/1	0.85	0.25	42,42,42,42	0
85	MG	2	1906	1/1	0.85	0.27	68,68,68,68	0
86	OHX	5	4136	7/7	0.85	0.10	180,180,180,180	7
85	MG	1	3542	1/1	0.85	0.35	50,50,50,50	0
86	OHX	1	4019	7/7	0.85	0.20	47,47,47,47	2
85	MG	2	1917	1/1	0.85	0.35	54,54,54,54	0
86	OHX	5	4142	7/7	0.85	0.12	58,58,58,58	4
86	OHX	6	2120	7/7	0.85	0.11	70,70,70,70	3
86	OHX	1	4027	7/7	0.85	0.15	75,75,75,75	3
85	MG	2	1976	1/1	0.85	0.24	77,77,77,77	0
85	MG	1	3555	1/1	0.85	0.33	26,26,26,26	0
85	MG	1	3604	1/1	0.85	0.39	39,39,39,39	0
86	OHX	5	4154	7/7	0.85	0.10	111,111,111,111	6
85	MG	5	3401	1/1	0.85	0.20	53,53,53,53	0
85	MG	1	3512	1/1	0.85	0.31	31,31,31,31	0
85	MG	1	3693	1/1	0.85	0.28	49,49,49,49	0
85	MG	1	3430	1/1	0.85	0.27	57,57,57,57	0
86	OHX	6	2157	7/7	0.85	0.12	90,90,90,90	7
86	OHX	6	2158	7/7	0.85	0.10	131,131,131,131	7
85	MG	6	1945	1/1	0.85	0.33	51,51,51,51	0
86	OHX	1	4063	7/7	0.85	0.10	159,159,159,159	7
85	MG	2	1977	1/1	0.85	0.23	72,72,72,72	0
86	OHX	6	2166	7/7	0.85	0.14	66,66,66,66	4
85	MG	2	1956	1/1	0.85	0.42	70,70,70,70	0
85	MG	5	3564	1/1	0.85	0.40	27,27,27,27	0
85	MG	2	1934	1/1	0.85	0.28	80,80,80,80	0
85	MG	5	3747	1/1	0.85	0.25	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	6	1949	1/1	0.85	0.28	77,77,77,77	0
85	MG	5	3589	1/1	0.85	0.36	28,28,28,28	0
85	MG	6	1950	1/1	0.85	0.43	66,66,66,66	0
86	OHX	1	4085	7/7	0.85	0.10	61,61,61,61	6
87	ZN	D7	101	1/1	0.85	0.16	161,161,161,161	0
85	MG	5	3472	1/1	0.85	0.24	39,39,39,39	0
85	MG	3	208	1/1	0.86	0.19	42,42,42,42	0
86	OHX	1	4077	7/7	0.86	0.12	62,62,62,62	4
86	OHX	6	2181	7/7	0.86	0.15	117,117,117,117	7
85	MG	4	203	1/1	0.86	0.32	57,57,57,57	0
85	MG	1	3534	1/1	0.86	0.29	69,69,69,69	0
85	MG	4	214	1/1	0.86	0.26	41,41,41,41	0
86	OHX	c5	202	7/7	0.86	0.16	109,109,109,109	6
85	MG	4	215	1/1	0.86	0.36	55,55,55,55	0
85	MG	5	3592	1/1	0.86	0.39	35,35,35,35	0
85	MG	5	3596	1/1	0.86	0.18	47,47,47,47	0
86	OHX	5	3970	7/7	0.86	0.21	80,80,80,80	3
85	MG	1	3715	1/1	0.86	0.31	46,46,46,46	0
85	MG	6	1926	1/1	0.86	0.20	65,65,65,65	0
85	MG	1	3561	1/1	0.86	0.24	22,22,22,22	0
85	MG	1	3483	1/1	0.86	0.25	54,54,54,54	0
85	MG	1	3421	1/1	0.86	0.26	58,58,58,58	0
86	OHX	1	4101	7/7	0.86	0.14	66,66,66,66	4
85	MG	SM	301	1/1	0.86	0.28	58,58,58,58	0
86	OHX	1	3927	7/7	0.86	0.21	51,51,51,51	3
85	MG	1	3491	1/1	0.86	0.35	51,51,51,51	0
86	OHX	2	2049	7/7	0.86	0.15	100,100,100,100	4
85	MG	6	1902	1/1	0.86	0.35	40,40,40,40	0
86	OHX	2	2074	7/7	0.86	0.14	85,85,85,85	3
86	OHX	1	4109	7/7	0.86	0.19	48,48,48,48	4
86	OHX	1	3974	7/7	0.86	0.24	63,63,63,63	5
86	OHX	1	3975	7/7	0.86	0.12	88,88,88,88	3
86	OHX	2	2076	7/7	0.86	0.15	87,87,87,87	5
86	OHX	5	4115	7/7	0.86	0.18	63,63,63,63	6
86	OHX	1	3986	7/7	0.86	0.16	76,76,76,76	3
86	OHX	4	228	7/7	0.86	0.23	51,51,51,51	4
86	OHX	4	232	7/7	0.86	0.15	73,73,73,73	5
86	OHX	1	3989	7/7	0.86	0.18	94,94,94,94	5
86	OHX	2	2081	7/7	0.86	0.17	120,120,120,120	6
86	OHX	M9	202	7/7	0.86	0.12	77,77,77,77	3
85	MG	6	2006	1/1	0.86	0.32	67,67,67,67	0
86	OHX	2	2092	7/7	0.86	0.18	73,73,73,73	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	6	2091	7/7	0.86	0.24	83,83,83,83	3
86	OHX	2	2093	7/7	0.86	0.21	110,110,110,110	5
85	MG	6	2009	1/1	0.86	0.22	64,64,64,64	0
85	MG	1	3546	1/1	0.86	0.34	36,36,36,36	0
85	MG	6	1935	1/1	0.86	0.36	44,44,44,44	0
85	MG	1	3529	1/1	0.86	0.30	34,34,34,34	0
85	MG	5	3513	1/1	0.86	0.23	37,37,37,37	0
85	MG	1	3432	1/1	0.86	0.16	49,49,49,49	0
86	OHX	5	4152	7/7	0.86	0.16	76,76,76,76	5
85	MG	5	3515	1/1	0.86	0.24	42,42,42,42	0
85	MG	d6	102	1/1	0.86	0.21	68,68,68,68	0
85	MG	5	3526	1/1	0.86	0.35	29,29,29,29	0
86	OHX	1	4038	7/7	0.86	0.28	56,56,56,56	4
85	MG	1	3659	1/1	0.86	0.12	78,78,78,78	0
86	OHX	5	4162	7/7	0.86	0.12	100,100,100,100	7
85	MG	5	3406	1/1	0.86	0.09	47,47,47,47	0
85	MG	5	3417	1/1	0.86	0.27	64,64,64,64	0
86	OHX	1	4045	7/7	0.86	0.17	54,54,54,54	1
86	OHX	5	4168	7/7	0.86	0.17	64,64,64,64	5
86	OHX	1	4046	7/7	0.86	0.12	50,50,50,50	2
86	OHX	1	4050	7/7	0.86	0.23	58,58,58,58	5
86	OHX	6	2163	7/7	0.86	0.18	61,61,61,61	4
86	OHX	6	2164	7/7	0.86	0.18	44,44,44,44	5
85	MG	1	3592	1/1	0.86	0.18	61,61,61,61	0
85	MG	5	3714	1/1	0.86	0.14	36,36,36,36	0
85	MG	6	1978	1/1	0.86	0.22	77,77,77,77	0
86	OHX	8	231	7/7	0.86	0.23	62,62,62,62	5
86	OHX	6	2168	7/7	0.86	0.16	76,76,76,76	3
85	MG	5	3719	1/1	0.86	0.27	63,63,63,63	1
86	OHX	6	2171	7/7	0.86	0.22	53,53,53,53	7
85	MG	2	1926	1/1	0.86	0.22	76,76,76,76	0
85	MG	5	3431	1/1	0.86	0.20	41,41,41,41	0
85	MG	5	3733	1/1	0.86	0.19	50,50,50,50	0
86	OHX	6	2176	7/7	0.86	0.16	62,62,62,62	7
86	OHX	2	2079	7/7	0.87	0.23	82,82,82,82	3
86	OHX	5	4026	7/7	0.87	0.21	54,54,54,54	4
86	OHX	5	4033	7/7	0.87	0.16	98,98,98,98	7
85	MG	1	3504	1/1	0.87	0.36	42,42,42,42	0
85	MG	1	3439	1/1	0.87	0.25	60,60,60,60	0
86	OHX	1	3990	7/7	0.87	0.14	92,92,92,92	6
85	MG	6	1917	1/1	0.87	0.33	64,64,64,64	0
86	OHX	5	4055	7/7	0.87	0.19	56,56,56,56	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4059	7/7	0.87	0.20	47,47,47,47	3
85	MG	1	3613	1/1	0.87	0.32	58,58,58,58	0
85	MG	6	2007	1/1	0.87	0.24	51,51,51,51	0
85	MG	1	3619	1/1	0.87	0.22	53,53,53,53	0
86	OHX	5	4081	7/7	0.87	0.19	35,35,35,35	3
85	MG	4	202	1/1	0.87	0.16	64,64,64,64	0
85	MG	6	1922	1/1	0.87	0.14	55,55,55,55	0
85	MG	2	1979	1/1	0.87	0.13	70,70,70,70	0
85	MG	1	3474	1/1	0.87	0.26	48,48,48,48	0
85	MG	5	3523	1/1	0.87	0.35	29,29,29,29	0
86	OHX	5	4105	7/7	0.87	0.12	84,84,84,84	4
86	OHX	6	2083	7/7	0.87	0.21	94,94,94,94	7
85	MG	4	211	1/1	0.87	0.10	54,54,54,54	0
85	MG	1	3641	1/1	0.87	0.24	49,49,49,49	0
85	MG	5	3703	1/1	0.87	0.29	58,58,58,58	0
85	MG	5	3705	1/1	0.87	0.21	66,66,66,66	0
85	MG	5	3535	1/1	0.87	0.31	36,36,36,36	0
85	MG	1	3642	1/1	0.87	0.31	32,32,32,32	0
86	OHX	5	4124	7/7	0.87	0.23	51,51,51,51	6
86	OHX	2	2126	7/7	0.87	0.11	64,64,64,64	4
85	MG	5	3407	1/1	0.87	0.31	35,35,35,35	0
85	MG	5	3413	1/1	0.87	0.31	36,36,36,36	0
85	MG	1	3419	1/1	0.87	0.12	36,36,36,36	0
85	MG	1	3519	1/1	0.87	0.33	49,49,49,49	0
86	OHX	1	4058	7/7	0.87	0.20	100,100,100,100	4
86	OHX	2	2140	7/7	0.87	0.17	85,85,85,85	5
86	OHX	1	4062	7/7	0.87	0.22	51,51,51,51	3
86	OHX	6	2154	7/7	0.87	0.22	49,49,49,49	3
86	OHX	6	2155	7/7	0.87	0.17	71,71,71,71	3
86	OHX	5	4144	7/7	0.87	0.20	65,65,65,65	5
85	MG	5	3421	1/1	0.87	0.28	38,38,38,38	0
85	MG	1	3717	1/1	0.87	0.34	59,59,59,59	0
86	OHX	1	4066	7/7	0.87	0.16	63,63,63,63	6
85	MG	1	3719	1/1	0.87	0.20	65,65,65,65	0
85	MG	5	3585	1/1	0.87	0.38	35,35,35,35	0
86	OHX	2	2146	7/7	0.87	0.17	87,87,87,87	7
86	OHX	5	4155	7/7	0.87	0.09	97,97,97,97	7
85	MG	1	3454	1/1	0.87	0.33	31,31,31,31	0
85	MG	5	3777	1/1	0.87	0.12	41,41,41,41	0
85	MG	1	3413	1/1	0.87	0.31	41,41,41,41	0
85	MG	D3	201	1/1	0.87	0.12	54,54,54,54	0
85	MG	1	3496	1/1	0.87	0.33	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	4080	7/7	0.87	0.21	57,57,57,57	4
85	MG	5	3594	1/1	0.87	0.34	35,35,35,35	0
85	MG	6	1985	1/1	0.87	0.15	55,55,55,55	0
85	MG	7	201	1/1	0.87	0.34	41,41,41,41	0
85	MG	1	3752	1/1	0.87	0.22	64,64,64,64	0
85	MG	1	3564	1/1	0.87	0.24	30,30,30,30	0
86	OHX	7	220	7/7	0.87	0.17	73,73,73,73	1
85	MG	1	3755	1/1	0.87	0.13	45,45,45,45	0
86	OHX	8	218	7/7	0.87	0.20	63,63,63,63	4
85	MG	5	3614	1/1	0.87	0.38	41,41,41,41	0
85	MG	2	1963	1/1	0.87	0.18	83,83,83,83	0
85	MG	1	3676	1/1	0.87	0.21	52,52,52,52	0
85	MG	6	1993	1/1	0.87	0.11	66,66,66,66	0
86	OHX	s8	303	7/7	0.87	0.14	105,105,105,105	3
86	OHX	2	2069	7/7	0.87	0.16	115,115,115,115	4
85	MG	1	3684	1/1	0.87	0.43	52,52,52,52	0
85	MG	6	1997	1/1	0.87	0.24	53,53,53,53	0
86	OHX	1	3978	7/7	0.87	0.19	77,77,77,77	3
86	OHX	1	3980	7/7	0.87	0.16	51,51,51,51	1
86	OHX	5	3975	7/7	0.87	0.22	85,85,85,85	3
85	MG	5	3709	1/1	0.88	0.19	51,51,51,51	0
85	MG	1	3577	1/1	0.88	0.21	39,39,39,39	0
86	OHX	5	4043	7/7	0.88	0.29	38,38,38,38	4
85	MG	5	3494	1/1	0.88	0.30	45,45,45,45	0
85	MG	5	3498	1/1	0.88	0.24	32,32,32,32	0
85	MG	5	3718	1/1	0.88	0.26	26,26,26,26	1
85	MG	6	1912	1/1	0.88	0.30	39,39,39,39	0
85	MG	1	3451	1/1	0.88	0.22	53,53,53,53	0
86	OHX	1	4023	7/7	0.88	0.15	73,73,73,73	3
86	OHX	1	4026	7/7	0.88	0.13	52,52,52,52	5
86	OHX	5	4069	7/7	0.88	0.18	58,58,58,58	5
86	OHX	5	4070	7/7	0.88	0.14	73,73,73,73	3
85	MG	1	3485	1/1	0.88	0.21	58,58,58,58	0
86	OHX	5	4079	7/7	0.88	0.21	54,54,54,54	5
85	MG	6	1944	1/1	0.88	0.30	63,63,63,63	0
86	OHX	6	2088	7/7	0.88	0.16	99,99,99,99	3
85	MG	5	3734	1/1	0.88	0.21	45,45,45,45	0
85	MG	5	3735	1/1	0.88	0.26	37,37,37,37	0
86	OHX	6	2102	7/7	0.88	0.20	97,97,97,97	4
85	MG	1	3721	1/1	0.88	0.28	43,43,43,43	0
86	OHX	5	4095	7/7	0.88	0.10	41,41,41,41	2
86	OHX	5	4104	7/7	0.88	0.18	68,68,68,68	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	2	2134	7/7	0.88	0.13	74,74,74,74	4
85	MG	1	3678	1/1	0.88	0.32	53,53,53,53	0
85	MG	5	3617	1/1	0.88	0.32	35,35,35,35	0
86	OHX	6	2121	7/7	0.88	0.20	86,86,86,86	5
86	OHX	6	2123	7/7	0.88	0.17	70,70,70,70	4
86	OHX	5	4116	7/7	0.88	0.16	52,52,52,52	4
86	OHX	6	2126	7/7	0.88	0.20	53,53,53,53	3
86	OHX	2	2139	7/7	0.88	0.11	114,114,114,114	6
85	MG	6	1983	1/1	0.88	0.38	57,57,57,57	0
85	MG	1	3631	1/1	0.88	0.18	42,42,42,42	0
86	OHX	1	4049	7/7	0.88	0.21	61,61,61,61	5
85	MG	1	3453	1/1	0.88	0.29	39,39,39,39	0
85	MG	5	3630	1/1	0.88	0.28	56,56,56,56	0
86	OHX	1	4059	7/7	0.88	0.17	72,72,72,72	4
86	OHX	5	4133	7/7	0.88	0.23	34,34,34,34	3
86	OHX	5	4134	7/7	0.88	0.09	157,157,157,157	7
85	MG	1	3748	1/1	0.88	0.32	67,67,67,67	0
85	MG	2	1910	1/1	0.88	0.39	69,69,69,69	0
85	MG	5	3802	1/1	0.88	0.19	44,44,44,44	0
86	OHX	6	2156	7/7	0.88	0.08	150,150,150,150	5
85	MG	6	1923	1/1	0.88	0.35	46,46,46,46	0
85	MG	5	3815	1/1	0.88	0.20	44,44,44,44	0
86	OHX	6	2159	7/7	0.88	0.13	93,93,93,93	5
85	MG	5	3643	1/1	0.88	0.20	64,64,64,64	0
86	OHX	5	4148	7/7	0.88	0.14	100,100,100,100	6
85	MG	5	3648	1/1	0.88	0.18	37,37,37,37	0
85	MG	5	3652	1/1	0.88	0.27	35,35,35,35	0
85	MG	1	3458	1/1	0.88	0.31	51,51,51,51	0
86	OHX	1	3856	7/7	0.88	0.19	76,76,76,76	3
85	MG	1	3539	1/1	0.88	0.38	44,44,44,44	0
85	MG	5	3664	1/1	0.88	0.21	62,62,62,62	0
86	OHX	1	3883	7/7	0.88	0.17	71,71,71,71	1
86	OHX	1	3899	7/7	0.88	0.27	52,52,52,52	4
86	OHX	1	4082	7/7	0.88	0.18	63,63,63,63	5
85	MG	o3	201	1/1	0.88	0.45	51,51,51,51	0
85	MG	C	102	1/1	0.88	0.31	39,39,39,39	0
86	OHX	1	4088	7/7	0.88	0.16	92,92,92,92	7
85	MG	1	3696	1/1	0.88	0.27	30,30,30,30	0
85	MG	5	3672	1/1	0.88	0.40	62,62,62,62	0
86	OHX	1	3949	7/7	0.88	0.14	111,111,111,111	7
85	MG	1	3603	1/1	0.88	0.18	63,63,63,63	0
85	MG	1	3492	1/1	0.88	0.28	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3709	1/1	0.88	0.15	48,48,48,48	0
86	OHX	1	3971	7/7	0.88	0.20	47,47,47,47	4
85	MG	1	3449	1/1	0.88	0.31	57,57,57,57	0
86	OHX	c3	201	7/7	0.88	0.12	84,84,84,84	4
85	MG	3	202	1/1	0.88	0.36	56,56,56,56	0
85	MG	5	3566	1/1	0.88	0.30	31,31,31,31	0
85	MG	1	3526	1/1	0.88	0.27	45,45,45,45	0
85	MG	5	3569	1/1	0.88	0.27	38,38,38,38	0
85	MG	6	1969	1/1	0.88	0.31	55,55,55,55	0
85	MG	5	3700	1/1	0.88	0.14	43,43,43,43	0
86	OHX	5	3986	7/7	0.88	0.31	58,58,58,58	5
86	OHX	5	4006	7/7	0.88	0.23	109,109,109,109	5
85	MG	6	1970	1/1	0.88	0.36	64,64,64,64	0
85	MG	1	3476	1/1	0.88	0.38	43,43,43,43	0
86	OHX	2	2107	7/7	0.89	0.15	66,66,66,66	4
86	OHX	5	4040	7/7	0.89	0.10	149,149,149,149	6
85	MG	5	3444	1/1	0.89	0.19	34,34,34,34	0
85	MG	1	3599	1/1	0.89	0.08	32,32,32,32	0
85	MG	5	3448	1/1	0.89	0.23	36,36,36,36	0
85	MG	1	3448	1/1	0.89	0.23	49,49,49,49	0
86	OHX	O9	101	7/7	0.89	0.18	51,51,51,51	6
86	OHX	6	2071	7/7	0.89	0.24	58,58,58,58	4
86	OHX	5	4060	7/7	0.89	0.18	45,45,45,45	5
86	OHX	2	2119	7/7	0.89	0.15	62,62,62,62	3
85	MG	5	3458	1/1	0.89	0.30	28,28,28,28	0
85	MG	5	3584	1/1	0.89	0.23	27,27,27,27	0
85	MG	5	3460	1/1	0.89	0.10	36,36,36,36	0
86	OHX	5	4072	7/7	0.89	0.22	40,40,40,40	4
85	MG	5	3586	1/1	0.89	0.30	29,29,29,29	0
85	MG	1	3531	1/1	0.89	0.28	40,40,40,40	0
86	OHX	2	2125	7/7	0.89	0.11	147,147,147,147	6
86	OHX	6	2111	7/7	0.89	0.12	73,73,73,73	5
85	MG	1	3502	1/1	0.89	0.29	30,30,30,30	0
85	MG	1	3680	1/1	0.89	0.29	45,45,45,45	0
86	OHX	2	2131	7/7	0.89	0.12	109,109,109,109	5
85	MG	1	3681	1/1	0.89	0.35	37,37,37,37	0
86	OHX	5	4092	7/7	0.89	0.19	33,33,33,33	2
85	MG	1	3466	1/1	0.89	0.22	37,37,37,37	0
85	MG	5	3476	1/1	0.89	0.22	42,42,42,42	0
85	MG	1	3689	1/1	0.89	0.08	44,44,44,44	0
85	MG	1	3608	1/1	0.89	0.30	46,46,46,46	0
85	MG	1	3486	1/1	0.89	0.22	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	6	2136	7/7	0.89	0.29	62,62,62,62	4
86	OHX	1	4055	7/7	0.89	0.15	81,81,81,81	5
86	OHX	6	2138	7/7	0.89	0.11	120,120,120,120	7
86	OHX	6	2146	7/7	0.89	0.21	48,48,48,48	4
85	MG	5	3612	1/1	0.89	0.18	40,40,40,40	0
85	MG	1	3535	1/1	0.89	0.27	39,39,39,39	0
85	MG	5	3759	1/1	0.89	0.26	46,46,46,46	0
85	MG	1	3506	1/1	0.89	0.29	32,32,32,32	0
86	OHX	6	2153	7/7	0.89	0.14	67,67,67,67	3
85	MG	1	3618	1/1	0.89	0.20	39,39,39,39	0
86	OHX	5	4130	7/7	0.89	0.09	171,171,171,171	7
85	MG	1	3455	1/1	0.89	0.28	29,29,29,29	0
85	MG	5	3784	1/1	0.89	0.12	35,35,35,35	0
85	MG	5	3789	1/1	0.89	0.16	49,49,49,49	0
85	MG	1	3621	1/1	0.89	0.35	52,52,52,52	0
85	MG	4	208	1/1	0.89	0.29	37,37,37,37	0
85	MG	2	1915	1/1	0.89	0.28	57,57,57,57	0
85	MG	1	3572	1/1	0.89	0.36	57,57,57,57	0
85	MG	1	3575	1/1	0.89	0.31	32,32,32,32	0
85	MG	5	3405	1/1	0.89	0.26	49,49,49,49	0
85	MG	1	3540	1/1	0.89	0.30	41,41,41,41	0
85	MG	5	3649	1/1	0.89	0.22	47,47,47,47	0
85	MG	2	1980	1/1	0.89	0.20	104,104,104,104	0
86	OHX	1	3905	7/7	0.89	0.18	57,57,57,57	1
85	MG	5	3408	1/1	0.89	0.14	40,40,40,40	0
85	MG	15	301	1/1	0.89	0.20	63,63,63,63	0
85	MG	1	3647	1/1	0.89	0.29	64,64,64,64	0
85	MG	1	3580	1/1	0.89	0.32	35,35,35,35	0
85	MG	5	3666	1/1	0.89	0.27	54,54,54,54	0
86	OHX	5	4157	7/7	0.89	0.17	44,44,44,44	5
85	MG	1	3475	1/1	0.89	0.33	44,44,44,44	0
85	MG	1	3545	1/1	0.89	0.27	31,31,31,31	0
85	MG	1	3493	1/1	0.89	0.31	42,42,42,42	0
86	OHX	6	2179	7/7	0.89	0.17	61,61,61,61	7
86	OHX	1	3968	7/7	0.89	0.17	72,72,72,72	3
86	OHX	1	4099	7/7	0.89	0.10	53,53,53,53	3
85	MG	5	3423	1/1	0.89	0.17	43,43,43,43	0
85	MG	5	3543	1/1	0.89	0.31	41,41,41,41	0
85	MG	5	3681	1/1	0.89	0.09	43,43,43,43	0
85	MG	5	3682	1/1	0.89	0.14	45,45,45,45	0
86	OHX	1	4105	7/7	0.89	0.32	46,46,46,46	5
85	MG	5	3683	1/1	0.89	0.15	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3545	1/1	0.89	0.27	57,57,57,57	0
86	OHX	5	3941	7/7	0.89	0.22	34,34,34,34	4
85	MG	1	3549	1/1	0.89	0.23	59,59,59,59	0
86	OHX	1	3988	7/7	0.89	0.16	87,87,87,87	5
85	MG	1	3742	1/1	0.89	0.18	44,44,44,44	0
85	MG	5	3687	1/1	0.89	0.27	37,37,37,37	0
86	OHX	5	3995	7/7	0.89	0.15	88,88,88,88	5
85	MG	5	3555	1/1	0.89	0.22	54,54,54,54	0
85	MG	2	1930	1/1	0.89	0.39	72,72,72,72	0
86	OHX	5	4019	7/7	0.89	0.18	76,76,76,76	6
86	OHX	1	4002	7/7	0.89	0.17	65,65,65,65	7
86	OHX	m9	201	7/7	0.89	0.10	61,61,61,61	6
86	OHX	o6	201	7/7	0.89	0.22	68,68,68,68	4
86	OHX	5	4032	7/7	0.89	0.15	71,71,71,71	4
86	OHX	4	231	7/7	0.89	0.11	75,75,75,75	5
85	MG	5	3625	1/1	0.90	0.22	51,51,51,51	0
85	MG	5	3781	1/1	0.90	0.25	43,43,43,43	0
85	MG	1	3437	1/1	0.90	0.28	44,44,44,44	0
85	MG	2	1921	1/1	0.90	0.22	63,63,63,63	0
85	MG	1	3410	1/1	0.90	0.22	39,39,39,39	0
86	OHX	5	3988	7/7	0.90	0.16	64,64,64,64	5
85	MG	5	3631	1/1	0.90	0.25	52,52,52,52	0
86	OHX	S8	301	7/7	0.90	0.10	115,115,115,115	7
85	MG	5	3791	1/1	0.90	0.17	46,46,46,46	0
86	OHX	5	4011	7/7	0.90	0.13	120,120,120,120	3
85	MG	5	3792	1/1	0.90	0.27	55,55,55,55	0
85	MG	5	3509	1/1	0.90	0.34	25,25,25,25	0
85	MG	5	3633	1/1	0.90	0.22	34,34,34,34	0
85	MG	5	3803	1/1	0.90	0.17	35,35,35,35	0
86	OHX	1	3884	7/7	0.90	0.17	74,74,74,74	4
85	MG	1	3508	1/1	0.90	0.17	38,38,38,38	0
85	MG	1	3671	1/1	0.90	0.26	47,47,47,47	0
86	OHX	1	3908	7/7	0.90	0.16	91,91,91,91	3
85	MG	1	3723	1/1	0.90	0.18	67,67,67,67	0
86	OHX	5	4050	7/7	0.90	0.18	45,45,45,45	3
85	MG	7	210	1/1	0.90	0.26	43,43,43,43	0
86	OHX	3	214	7/7	0.90	0.19	83,83,83,83	4
85	MG	5	3646	1/1	0.90	0.28	56,56,56,56	0
85	MG	8	202	1/1	0.90	0.19	42,42,42,42	0
86	OHX	4	226	7/7	0.90	0.12	106,106,106,106	5
85	MG	1	3726	1/1	0.90	0.23	64,64,64,64	0
85	MG	M6	202	1/1	0.90	0.11	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3581	1/1	0.90	0.38	29,29,29,29	0
86	OHX	1	3964	7/7	0.90	0.16	71,71,71,71	4
86	OHX	5	4075	7/7	0.90	0.14	47,47,47,47	3
86	OHX	L5	301	7/7	0.90	0.17	88,88,88,88	6
85	MG	1	3735	1/1	0.90	0.10	49,49,49,49	0
86	OHX	5	4080	7/7	0.90	0.18	55,55,55,55	3
85	MG	5	3530	1/1	0.90	0.27	31,31,31,31	0
85	MG	l7	2201	1/1	0.90	0.16	46,46,46,46	0
86	OHX	O4	202	7/7	0.90	0.14	82,82,82,82	5
86	OHX	1	3973	7/7	0.90	0.15	63,63,63,63	5
85	MG	m5	302	1/1	0.90	0.15	46,46,46,46	0
85	MG	1	3614	1/1	0.90	0.25	54,54,54,54	0
85	MG	5	3426	1/1	0.90	0.23	45,45,45,45	0
86	OHX	6	2086	7/7	0.90	0.19	70,70,70,70	5
86	OHX	5	4098	7/7	0.90	0.11	106,106,106,106	5
86	OHX	5	4100	7/7	0.90	0.16	46,46,46,46	5
86	OHX	2	2011	7/7	0.90	0.15	83,83,83,83	3
85	MG	5	3539	1/1	0.90	0.30	33,33,33,33	0
86	OHX	6	2095	7/7	0.90	0.16	99,99,99,99	3
86	OHX	2	2064	7/7	0.90	0.15	135,135,135,135	5
85	MG	5	3670	1/1	0.90	0.17	35,35,35,35	0
85	MG	5	3429	1/1	0.90	0.21	31,31,31,31	0
85	MG	N6	201	1/1	0.90	0.29	70,70,70,70	0
85	MG	5	3432	1/1	0.90	0.12	32,32,32,32	0
85	MG	1	3616	1/1	0.90	0.18	58,58,58,58	0
86	OHX	5	4122	7/7	0.90	0.14	52,52,52,52	3
85	MG	5	3546	1/1	0.90	0.37	46,46,46,46	0
85	MG	6	1939	1/1	0.90	0.25	34,34,34,34	0
86	OHX	6	2122	7/7	0.90	0.14	77,77,77,77	4
86	OHX	2	2086	7/7	0.90	0.13	112,112,112,112	5
86	OHX	6	2125	7/7	0.90	0.13	52,52,52,52	5
86	OHX	2	2088	7/7	0.90	0.17	91,91,91,91	6
85	MG	Q2	502	1/1	0.90	0.28	63,63,63,63	0
85	MG	1	3583	1/1	0.90	0.31	31,31,31,31	0
86	OHX	2	2095	7/7	0.90	0.13	75,75,75,75	5
86	OHX	2	2098	7/7	0.90	0.15	111,111,111,111	6
85	MG	1	3743	1/1	0.90	0.15	50,50,50,50	0
85	MG	5	3454	1/1	0.90	0.12	59,59,59,59	0
85	MG	1	3744	1/1	0.90	0.19	44,44,44,44	0
86	OHX	5	4141	7/7	0.90	0.16	49,49,49,49	4
85	MG	6	1904	1/1	0.90	0.29	59,59,59,59	0
86	OHX	1	4030	7/7	0.90	0.10	130,130,130,130	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3481	1/1	0.90	0.21	40,40,40,40	0
86	OHX	1	4033	7/7	0.90	0.17	66,66,66,66	5
85	MG	1	3516	1/1	0.90	0.35	33,33,33,33	0
86	OHX	2	2111	7/7	0.90	0.13	112,112,112,112	5
85	MG	5	3577	1/1	0.90	0.30	31,31,31,31	0
85	MG	5	3466	1/1	0.90	0.20	37,37,37,37	0
86	OHX	2	2115	7/7	0.90	0.18	91,91,91,91	6
86	OHX	2	2116	7/7	0.90	0.10	127,127,127,127	7
85	MG	5	3467	1/1	0.90	0.20	47,47,47,47	0
86	OHX	1	4047	7/7	0.90	0.15	101,101,101,101	5
85	MG	1	3622	1/1	0.90	0.28	44,44,44,44	0
85	MG	5	3588	1/1	0.90	0.26	29,29,29,29	0
86	OHX	5	4160	7/7	0.90	0.21	37,37,37,37	5
86	OHX	1	4052	7/7	0.90	0.16	58,58,58,58	4
85	MG	5	3470	1/1	0.90	0.29	56,56,56,56	0
85	MG	1	3624	1/1	0.90	0.14	33,33,33,33	0
85	MG	1	3446	1/1	0.90	0.20	41,41,41,41	0
85	MG	1	3469	1/1	0.90	0.28	41,41,41,41	0
85	MG	1	3520	1/1	0.90	0.27	35,35,35,35	0
85	MG	1	3501	1/1	0.90	0.28	26,26,26,26	0
85	MG	1	3600	1/1	0.90	0.15	60,60,60,60	0
86	OHX	2	2129	7/7	0.90	0.18	87,87,87,87	5
86	OHX	2	2130	7/7	0.90	0.11	84,84,84,84	4
85	MG	1	3644	1/1	0.90	0.29	52,52,52,52	0
85	MG	1	3543	1/1	0.90	0.10	58,58,58,58	0
86	OHX	8	223	7/7	0.90	0.15	75,75,75,75	5
85	MG	5	3605	1/1	0.90	0.25	33,33,33,33	0
85	MG	5	3495	1/1	0.90	0.17	33,33,33,33	0
85	MG	1	3411	1/1	0.90	0.20	43,43,43,43	0
86	OHX	2	2138	7/7	0.90	0.18	67,67,67,67	5
85	MG	5	3750	1/1	0.90	0.22	37,37,37,37	0
85	MG	5	3753	1/1	0.90	0.23	30,30,30,30	0
85	MG	1	3657	1/1	0.90	0.26	49,49,49,49	0
85	MG	5	3618	1/1	0.90	0.25	34,34,34,34	0
85	MG	5	3769	1/1	0.90	0.16	50,50,50,50	0
86	OHX	m8	201	7/7	0.90	0.19	47,47,47,47	3
86	OHX	d4	201	7/7	0.90	0.11	90,90,90,90	6
85	MG	5	3770	1/1	0.90	0.23	47,47,47,47	0
86	OHX	5	3926	7/7	0.90	0.15	60,60,60,60	4
85	MG	1	3428	1/1	0.90	0.18	52,52,52,52	0
86	OHX	5	3971	7/7	0.91	0.15	41,41,41,41	7
85	MG	1	3598	1/1	0.91	0.25	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3639	1/1	0.91	0.18	36,36,36,36	0
85	MG	5	3807	1/1	0.91	0.18	54,54,54,54	0
85	MG	5	3808	1/1	0.91	0.13	36,36,36,36	0
86	OHX	5	4005	7/7	0.91	0.19	82,82,82,82	3
85	MG	5	3409	1/1	0.91	0.22	45,45,45,45	0
85	MG	1	3450	1/1	0.91	0.16	31,31,31,31	0
86	OHX	1	3891	7/7	0.91	0.10	103,103,103,103	5
86	OHX	5	4016	7/7	0.91	0.16	62,62,62,62	7
86	OHX	5	4017	7/7	0.91	0.18	36,36,36,36	2
85	MG	5	3644	1/1	0.91	0.19	34,34,34,34	0
86	OHX	5	4024	7/7	0.91	0.14	66,66,66,66	5
85	MG	2	1972	1/1	0.91	0.06	57,57,57,57	0
86	OHX	5	4030	7/7	0.91	0.15	70,70,70,70	5
85	MG	1	3452	1/1	0.91	0.30	55,55,55,55	0
86	OHX	1	3914	7/7	0.91	0.14	79,79,79,79	3
85	MG	5	3516	1/1	0.91	0.33	21,21,21,21	0
85	MG	4	204	1/1	0.91	0.32	64,64,64,64	0
85	MG	5	3657	1/1	0.91	0.21	33,33,33,33	0
86	OHX	5	4045	7/7	0.91	0.17	48,48,48,48	2
85	MG	1	3422	1/1	0.91	0.22	32,32,32,32	0
86	OHX	1	3930	7/7	0.91	0.14	118,118,118,118	2
86	OHX	3	215	7/7	0.91	0.13	90,90,90,90	3
86	OHX	1	3947	7/7	0.91	0.14	80,80,80,80	3
85	MG	6	1975	1/1	0.91	0.16	90,90,90,90	0
86	OHX	5	4057	7/7	0.91	0.17	50,50,50,50	2
86	OHX	1	3952	7/7	0.91	0.11	140,140,140,140	5
85	MG	1	3403	1/1	0.91	0.20	42,42,42,42	0
86	OHX	4	230	7/7	0.91	0.11	45,45,45,45	3
85	MG	1	3478	1/1	0.91	0.19	60,60,60,60	0
85	MG	2	1947	1/1	0.91	0.14	76,76,76,76	0
86	OHX	4	233	7/7	0.91	0.15	65,65,65,65	5
85	MG	n6	201	1/1	0.91	0.16	56,56,56,56	0
86	OHX	1	3966	7/7	0.91	0.22	35,35,35,35	3
85	MG	1	3444	1/1	0.91	0.25	35,35,35,35	0
85	MG	L6	201	1/1	0.91	0.18	57,57,57,57	0
85	MG	5	3541	1/1	0.91	0.25	41,41,41,41	0
86	OHX	2	2036	7/7	0.91	0.11	145,145,145,145	5
85	MG	5	3433	1/1	0.91	0.26	37,37,37,37	0
86	OHX	2	2058	7/7	0.91	0.18	67,67,67,67	4
86	OHX	5	4085	7/7	0.91	0.10	143,143,143,143	7
85	MG	5	3676	1/1	0.91	0.18	51,51,51,51	0
86	OHX	1	3981	7/7	0.91	0.21	53,53,53,53	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	4090	7/7	0.91	0.16	51,51,51,51	4
85	MG	5	3434	1/1	0.91	0.25	33,33,33,33	0
86	OHX	6	2087	7/7	0.91	0.11	109,109,109,109	6
85	MG	5	3436	1/1	0.91	0.15	44,44,44,44	0
86	OHX	1	3987	7/7	0.91	0.14	73,73,73,73	5
86	OHX	5	4099	7/7	0.91	0.12	73,73,73,73	5
85	MG	M0	301	1/1	0.91	0.23	41,41,41,41	0
85	MG	5	3442	1/1	0.91	0.18	32,32,32,32	0
85	MG	2	1983	1/1	0.91	0.11	84,84,84,84	0
85	MG	5	3549	1/1	0.91	0.11	43,43,43,43	0
85	MG	5	3551	1/1	0.91	0.27	32,32,32,32	0
86	OHX	6	2112	7/7	0.91	0.21	66,66,66,66	4
85	MG	1	3728	1/1	0.91	0.18	47,47,47,47	0
86	OHX	2	2087	7/7	0.91	0.14	89,89,89,89	5
86	OHX	1	4010	7/7	0.91	0.21	44,44,44,44	5
85	MG	1	3462	1/1	0.91	0.22	44,44,44,44	0
85	MG	5	3693	1/1	0.91	0.25	38,38,38,38	0
85	MG	1	3673	1/1	0.91	0.20	39,39,39,39	0
85	MG	5	3565	1/1	0.91	0.25	32,32,32,32	0
86	OHX	1	4020	7/7	0.91	0.14	47,47,47,47	3
86	OHX	6	2127	7/7	0.91	0.17	58,58,58,58	5
85	MG	1	3736	1/1	0.91	0.09	50,50,50,50	0
86	OHX	6	2132	7/7	0.91	0.13	94,94,94,94	6
86	OHX	5	4131	7/7	0.91	0.10	64,64,64,64	5
85	MG	5	3455	1/1	0.91	0.23	31,31,31,31	0
85	MG	6	1989	1/1	0.91	0.20	57,57,57,57	0
85	MG	1	3513	1/1	0.91	0.28	34,34,34,34	0
85	MG	5	3710	1/1	0.91	0.18	55,55,55,55	0
85	MG	1	3578	1/1	0.91	0.31	60,60,60,60	0
86	OHX	6	2143	7/7	0.91	0.19	51,51,51,51	3
85	MG	5	3463	1/1	0.91	0.12	39,39,39,39	0
86	OHX	2	2110	7/7	0.91	0.15	112,112,112,112	5
85	MG	O7	103	1/1	0.91	0.22	49,49,49,49	0
86	OHX	1	4035	7/7	0.91	0.12	65,65,65,65	4
85	MG	5	3716	1/1	0.91	0.20	34,34,34,34	0
85	MG	1	3515	1/1	0.91	0.24	28,28,28,28	0
85	MG	2	1971	1/1	0.91	0.19	81,81,81,81	0
85	MG	5	3468	1/1	0.91	0.22	47,47,47,47	0
85	MG	1	3429	1/1	0.91	0.21	36,36,36,36	0
85	MG	5	3726	1/1	0.91	0.08	46,46,46,46	0
85	MG	1	3683	1/1	0.91	0.35	39,39,39,39	1
85	MG	1	3585	1/1	0.91	0.41	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3490	1/1	0.91	0.30	34,34,34,34	0
85	MG	1	3627	1/1	0.91	0.26	41,41,41,41	0
85	MG	5	3743	1/1	0.91	0.12	32,32,32,32	0
85	MG	5	3746	1/1	0.91	0.33	76,76,76,76	0
85	MG	6	2008	1/1	0.91	0.39	61,61,61,61	0
85	MG	2	1975	1/1	0.91	0.33	60,60,60,60	0
85	MG	5	3749	1/1	0.91	0.23	30,30,30,30	0
85	MG	1	3588	1/1	0.91	0.22	39,39,39,39	0
85	MG	6	1955	1/1	0.91	0.28	60,60,60,60	0
85	MG	5	3756	1/1	0.91	0.16	42,42,42,42	0
85	MG	5	3608	1/1	0.91	0.34	50,50,50,50	0
85	MG	5	3493	1/1	0.91	0.33	42,42,42,42	0
85	MG	c8	201	1/1	0.91	0.11	91,91,91,91	0
85	MG	1	3467	1/1	0.91	0.14	42,42,42,42	0
85	MG	5	3773	1/1	0.91	0.12	52,52,52,52	0
86	OHX	7	222	7/7	0.91	0.18	38,38,38,38	4
86	OHX	7	223	7/7	0.91	0.16	54,54,54,54	4
86	OHX	1	4074	7/7	0.91	0.20	38,38,38,38	3
85	MG	5	3496	1/1	0.91	0.18	35,35,35,35	0
85	MG	5	3497	1/1	0.91	0.21	36,36,36,36	0
86	OHX	8	226	7/7	0.91	0.13	47,47,47,47	3
85	MG	5	3623	1/1	0.91	0.06	42,42,42,42	0
85	MG	1	3639	1/1	0.91	0.25	56,56,56,56	0
85	MG	1	3524	1/1	0.91	0.28	44,44,44,44	0
85	MG	5	3788	1/1	0.91	0.24	68,68,68,68	0
86	OHX	l3	404	7/7	0.91	0.09	72,72,72,72	4
86	OHX	1	4083	7/7	0.91	0.09	45,45,45,45	4
86	OHX	1	4084	7/7	0.91	0.24	42,42,42,42	5
85	MG	6	1914	1/1	0.91	0.27	62,62,62,62	0
85	MG	1	3420	1/1	0.91	0.29	45,45,45,45	0
86	OHX	5	3917	7/7	0.91	0.23	49,49,49,49	3
85	MG	5	3506	1/1	0.91	0.36	27,27,27,27	0
85	MG	3	204	1/1	0.91	0.35	33,33,33,33	0
85	MG	5	3793	1/1	0.91	0.20	37,37,37,37	0
85	MG	5	3797	1/1	0.91	0.13	39,39,39,39	0
85	MG	1	3707	1/1	0.91	0.27	48,48,48,48	0
85	MG	1	3479	1/1	0.92	0.16	45,45,45,45	0
86	OHX	5	3991	7/7	0.92	0.11	37,37,37,37	3
86	OHX	5	3993	7/7	0.92	0.16	38,38,38,38	4
85	MG	6	1925	1/1	0.92	0.24	49,49,49,49	0
86	OHX	2	2053	7/7	0.92	0.15	107,107,107,107	4
86	OHX	1	3939	7/7	0.92	0.13	54,54,54,54	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3613	1/1	0.92	0.24	42,42,42,42	0
86	OHX	2	2061	7/7	0.92	0.24	88,88,88,88	5
86	OHX	1	3951	7/7	0.92	0.12	159,159,159,159	7
85	MG	5	3517	1/1	0.92	0.18	28,28,28,28	0
85	MG	1	3711	1/1	0.92	0.20	54,54,54,54	0
85	MG	5	3519	1/1	0.92	0.32	35,35,35,35	0
86	OHX	3	213	7/7	0.92	0.16	82,82,82,82	5
85	MG	M7	202	1/1	0.92	0.34	40,40,40,40	0
86	OHX	5	4031	7/7	0.92	0.12	85,85,85,85	4
85	MG	5	3620	1/1	0.92	0.33	39,39,39,39	0
86	OHX	2	2077	7/7	0.92	0.14	108,108,108,108	7
85	MG	5	3621	1/1	0.92	0.13	36,36,36,36	0
86	OHX	1	3970	7/7	0.92	0.11	68,68,68,68	1
85	MG	6	1966	1/1	0.92	0.22	56,56,56,56	0
85	MG	5	3725	1/1	0.92	0.15	51,51,51,51	0
85	MG	5	3624	1/1	0.92	0.11	31,31,31,31	0
85	MG	5	3527	1/1	0.92	0.21	32,32,32,32	0
85	MG	M7	203	1/1	0.92	0.17	46,46,46,46	0
85	MG	5	3461	1/1	0.92	0.33	57,57,57,57	0
85	MG	1	3675	1/1	0.92	0.20	49,49,49,49	0
86	OHX	M0	303	7/7	0.92	0.19	55,55,55,55	4
85	MG	1	3558	1/1	0.92	0.23	35,35,35,35	0
86	OHX	2	2097	7/7	0.92	0.12	73,73,73,73	5
85	MG	1	3480	1/1	0.92	0.39	46,46,46,46	0
86	OHX	O3	201	7/7	0.92	0.22	52,52,52,52	4
85	MG	1	3679	1/1	0.92	0.20	59,59,59,59	0
85	MG	5	3634	1/1	0.92	0.10	36,36,36,36	0
85	MG	1	3418	1/1	0.92	0.16	47,47,47,47	0
86	OHX	1	3993	7/7	0.92	0.15	94,94,94,94	7
85	MG	1	3720	1/1	0.92	0.20	48,48,48,48	0
86	OHX	1	3998	7/7	0.92	0.15	107,107,107,107	4
85	MG	1	3470	1/1	0.92	0.21	46,46,46,46	0
85	MG	5	3642	1/1	0.92	0.11	39,39,39,39	0
86	OHX	1	4004	7/7	0.92	0.17	75,75,75,75	5
85	MG	1	3655	1/1	0.92	0.22	44,44,44,44	0
85	MG	1	3724	1/1	0.92	0.19	55,55,55,55	0
86	OHX	1	4012	7/7	0.92	0.15	64,64,64,64	1
86	OHX	6	2103	7/7	0.92	0.15	67,67,67,67	4
86	OHX	5	4089	7/7	0.92	0.24	47,47,47,47	3
86	OHX	6	2107	7/7	0.92	0.12	81,81,81,81	5
85	MG	5	3763	1/1	0.92	0.12	38,38,38,38	0
85	MG	5	3473	1/1	0.92	0.22	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3412	1/1	0.92	0.20	47,47,47,47	0
86	OHX	5	4097	7/7	0.92	0.13	75,75,75,75	6
85	MG	5	3475	1/1	0.92	0.16	51,51,51,51	0
85	MG	5	3651	1/1	0.92	0.08	42,42,42,42	0
85	MG	5	3552	1/1	0.92	0.26	52,52,52,52	0
85	MG	5	3653	1/1	0.92	0.14	47,47,47,47	0
86	OHX	1	4025	7/7	0.92	0.13	56,56,56,56	3
85	MG	3	207	1/1	0.92	0.34	66,66,66,66	0
85	MG	1	3548	1/1	0.92	0.25	30,30,30,30	0
85	MG	5	3661	1/1	0.92	0.15	64,64,64,64	0
86	OHX	5	4112	7/7	0.92	0.19	51,51,51,51	6
85	MG	6	1941	1/1	0.92	0.29	57,57,57,57	0
86	OHX	6	2130	7/7	0.92	0.09	153,153,153,153	7
85	MG	1	3463	1/1	0.92	0.25	39,39,39,39	0
86	OHX	1	4031	7/7	0.92	0.12	65,65,65,65	6
85	MG	1	3584	1/1	0.92	0.30	33,33,33,33	0
85	MG	1	3477	1/1	0.92	0.28	41,41,41,41	0
85	MG	5	3669	1/1	0.92	0.22	36,36,36,36	1
85	MG	5	3794	1/1	0.92	0.10	45,45,45,45	0
86	OHX	5	4126	7/7	0.92	0.12	98,98,98,98	3
85	MG	1	3629	1/1	0.92	0.13	33,33,33,33	0
85	MG	4	206	1/1	0.92	0.23	44,44,44,44	0
86	OHX	6	2145	7/7	0.92	0.11	92,92,92,92	4
85	MG	5	3801	1/1	0.92	0.25	44,44,44,44	0
85	MG	5	3427	1/1	0.92	0.27	40,40,40,40	0
85	MG	5	3580	1/1	0.92	0.38	38,38,38,38	0
85	MG	5	3675	1/1	0.92	0.28	34,34,34,34	1
86	OHX	5	4135	7/7	0.92	0.16	54,54,54,54	4
85	MG	4	207	1/1	0.92	0.30	41,41,41,41	0
85	MG	1	3663	1/1	0.92	0.29	44,44,44,44	0
85	MG	5	3499	1/1	0.92	0.14	42,42,42,42	0
85	MG	4	210	1/1	0.92	0.24	63,63,63,63	0
85	MG	7	209	1/1	0.92	0.20	54,54,54,54	0
86	OHX	1	4056	7/7	0.92	0.15	85,85,85,85	5
86	OHX	1	4057	7/7	0.92	0.09	109,109,109,109	5
86	OHX	2	2144	7/7	0.92	0.16	103,103,103,103	6
86	OHX	6	2160	7/7	0.92	0.18	69,69,69,69	5
85	MG	1	3695	1/1	0.92	0.31	58,58,58,58	0
85	MG	1	3665	1/1	0.92	0.24	48,48,48,48	0
85	MG	7	213	1/1	0.92	0.13	49,49,49,49	0
86	OHX	2	2148	7/7	0.92	0.29	69,69,69,69	6
86	OHX	1	4064	7/7	0.92	0.23	39,39,39,39	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	S2	301	1/1	0.92	0.31	62,62,62,62	0
85	MG	5	3439	1/1	0.92	0.26	30,30,30,30	0
85	MG	8	206	1/1	0.92	0.15	47,47,47,47	0
85	MG	8	209	1/1	0.92	0.24	55,55,55,55	0
85	MG	6	1956	1/1	0.92	0.30	44,44,44,44	0
85	MG	5	3688	1/1	0.92	0.19	47,47,47,47	0
85	MG	5	3595	1/1	0.92	0.38	28,28,28,28	0
86	OHX	D9	102	7/7	0.92	0.14	97,97,97,97	6
86	OHX	1	3849	7/7	0.92	0.19	48,48,48,48	5
85	MG	1	3556	1/1	0.92	0.22	29,29,29,29	0
85	MG	5	3597	1/1	0.92	0.16	44,44,44,44	0
85	MG	m0	301	1/1	0.92	0.20	33,33,33,33	0
86	OHX	1	4081	7/7	0.92	0.34	43,43,43,43	5
86	OHX	1	3875	7/7	0.92	0.23	53,53,53,53	3
86	OHX	1	3877	7/7	0.92	0.13	95,95,95,95	2
85	MG	m5	301	1/1	0.92	0.11	56,56,56,56	0
85	MG	5	3443	1/1	0.92	0.23	44,44,44,44	0
85	MG	m7	201	1/1	0.92	0.10	36,36,36,36	0
85	MG	n3	201	1/1	0.92	0.25	25,25,25,25	0
86	OHX	1	3900	7/7	0.92	0.14	57,57,57,57	3
86	OHX	8	222	7/7	0.92	0.13	100,100,100,100	5
86	OHX	1	4091	7/7	0.92	0.11	42,42,42,42	4
86	OHX	5	3916	7/7	0.92	0.15	77,77,77,77	3
86	OHX	1	3904	7/7	0.92	0.20	59,59,59,59	3
85	MG	5	3512	1/1	0.92	0.35	28,28,28,28	0
85	MG	1	3573	1/1	0.92	0.35	40,40,40,40	0
86	OHX	5	3938	7/7	0.92	0.15	50,50,50,50	3
86	OHX	1	3912	7/7	0.92	0.13	126,126,126,126	4
85	MG	q1	101	1/1	0.92	0.29	50,50,50,50	0
86	OHX	5	3949	7/7	0.92	0.20	56,56,56,56	4
86	OHX	5	3950	7/7	0.92	0.17	95,95,95,95	4
86	OHX	5	3963	7/7	0.92	0.13	62,62,62,62	5
86	OHX	5	3967	7/7	0.92	0.21	49,49,49,49	5
85	MG	1	3590	1/1	0.92	0.20	43,43,43,43	0
86	OHX	1	3916	7/7	0.92	0.19	54,54,54,54	4
86	OHX	1	4100	7/7	0.92	0.17	38,38,38,38	3
86	OHX	5	3977	7/7	0.92	0.24	58,58,58,58	4
85	MG	5	3708	1/1	0.92	0.09	50,50,50,50	0
85	MG	5	3410	1/1	0.93	0.15	29,29,29,29	0
85	MG	5	3570	1/1	0.93	0.25	29,29,29,29	0
86	OHX	1	4087	7/7	0.93	0.18	44,44,44,44	6
85	MG	8	203	1/1	0.93	0.16	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3411	1/1	0.93	0.31	44,44,44,44	0
86	OHX	5	3957	7/7	0.93	0.20	46,46,46,46	3
85	MG	5	3575	1/1	0.93	0.32	36,36,36,36	0
85	MG	8	207	1/1	0.93	0.18	43,43,43,43	0
85	MG	5	3484	1/1	0.93	0.35	28,28,28,28	0
85	MG	5	3578	1/1	0.93	0.29	35,35,35,35	0
86	OHX	1	3886	7/7	0.93	0.19	56,56,56,56	4
85	MG	1	3482	1/1	0.93	0.30	33,33,33,33	0
86	OHX	5	3978	7/7	0.93	0.13	69,69,69,69	4
86	OHX	5	3979	7/7	0.93	0.18	67,67,67,67	3
86	OHX	5	3982	7/7	0.93	0.14	58,58,58,58	3
86	OHX	1	4097	7/7	0.93	0.13	42,42,42,42	6
85	MG	5	3488	1/1	0.93	0.29	44,44,44,44	0
85	MG	5	3490	1/1	0.93	0.17	40,40,40,40	0
85	MG	5	3491	1/1	0.93	0.13	41,41,41,41	0
85	MG	5	3587	1/1	0.93	0.26	30,30,30,30	0
86	OHX	1	3907	7/7	0.93	0.16	71,71,71,71	3
85	MG	5	3492	1/1	0.93	0.22	30,30,30,30	0
85	MG	L7	303	1/1	0.93	0.13	50,50,50,50	0
85	MG	5	3691	1/1	0.93	0.23	38,38,38,38	0
86	OHX	5	4013	7/7	0.93	0.11	119,119,119,119	4
85	MG	m7	202	1/1	0.93	0.34	33,33,33,33	0
85	MG	1	3740	1/1	0.93	0.15	62,62,62,62	0
85	MG	5	3694	1/1	0.93	0.17	55,55,55,55	0
86	OHX	1	3925	7/7	0.93	0.11	96,96,96,96	5
85	MG	6	1976	1/1	0.93	0.07	32,32,32,32	0
85	MG	o4	201	1/1	0.93	0.39	53,53,53,53	0
85	MG	6	1977	1/1	0.93	0.11	57,57,57,57	0
85	MG	1	3691	1/1	0.93	0.18	64,64,64,64	0
85	MG	1	3651	1/1	0.93	0.19	49,49,49,49	0
86	OHX	2	2022	7/7	0.93	0.18	78,78,78,78	4
86	OHX	3	218	7/7	0.93	0.16	54,54,54,54	5
86	OHX	5	4042	7/7	0.93	0.15	43,43,43,43	3
86	OHX	2	2035	7/7	0.93	0.11	116,116,116,116	5
85	MG	1	3442	1/1	0.93	0.25	52,52,52,52	0
86	OHX	1	3953	7/7	0.93	0.12	58,58,58,58	2
86	OHX	2	2043	7/7	0.93	0.14	100,100,100,100	4
86	OHX	1	3958	7/7	0.93	0.14	45,45,45,45	4
86	OHX	2	2047	7/7	0.93	0.15	80,80,80,80	4
85	MG	5	3706	1/1	0.93	0.24	32,32,32,32	0
85	MG	5	3425	1/1	0.93	0.15	41,41,41,41	0
86	OHX	2	2054	7/7	0.93	0.17	103,103,103,103	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	3967	7/7	0.93	0.09	82,82,82,82	3
86	OHX	2	2057	7/7	0.93	0.10	79,79,79,79	1
86	OHX	M8	201	7/7	0.93	0.14	47,47,47,47	3
86	OHX	5	4063	7/7	0.93	0.15	39,39,39,39	3
85	MG	1	3654	1/1	0.93	0.21	39,39,39,39	0
85	MG	1	3745	1/1	0.93	0.13	53,53,53,53	0
85	MG	5	3711	1/1	0.93	0.20	32,32,32,32	0
86	OHX	5	4074	7/7	0.93	0.14	77,77,77,77	6
85	MG	1	3747	1/1	0.93	0.11	48,48,48,48	0
86	OHX	2	2068	7/7	0.93	0.16	103,103,103,103	7
86	OHX	6	2043	7/7	0.93	0.17	90,90,90,90	5
86	OHX	6	2051	7/7	0.93	0.12	131,131,131,131	5
85	MG	5	3604	1/1	0.93	0.21	33,33,33,33	0
86	OHX	6	2073	7/7	0.93	0.18	69,69,69,69	5
86	OHX	6	2077	7/7	0.93	0.17	98,98,98,98	5
86	OHX	6	2078	7/7	0.93	0.15	60,60,60,60	5
86	OHX	2	2072	7/7	0.93	0.08	187,187,187,187	7
85	MG	2	1903	1/1	0.93	0.22	43,43,43,43	0
85	MG	5	3607	1/1	0.93	0.15	36,36,36,36	0
85	MG	1	3591	1/1	0.93	0.39	53,53,53,53	0
85	MG	5	3610	1/1	0.93	0.16	49,49,49,49	0
85	MG	5	3720	1/1	0.93	0.23	34,34,34,34	0
86	OHX	6	2092	7/7	0.93	0.23	69,69,69,69	4
85	MG	5	3721	1/1	0.93	0.25	36,36,36,36	0
85	MG	1	3699	1/1	0.93	0.16	49,49,49,49	0
85	MG	1	3554	1/1	0.93	0.28	37,37,37,37	0
85	MG	1	3416	1/1	0.93	0.29	43,43,43,43	0
86	OHX	2	2089	7/7	0.93	0.11	116,116,116,116	7
86	OHX	1	3999	7/7	0.93	0.08	215,215,215,215	2
86	OHX	5	4106	7/7	0.93	0.14	32,32,32,32	4
86	OHX	2	2090	7/7	0.93	0.11	94,94,94,94	6
85	MG	1	3757	1/1	0.93	0.19	55,55,55,55	0
86	OHX	5	4110	7/7	0.93	0.11	133,133,133,133	5
86	OHX	1	4003	7/7	0.93	0.13	63,63,63,63	3
86	OHX	6	2117	7/7	0.93	0.10	65,65,65,65	3
86	OHX	5	4114	7/7	0.93	0.11	55,55,55,55	4
85	MG	5	3731	1/1	0.93	0.31	55,55,55,55	0
86	OHX	1	4005	7/7	0.93	0.18	40,40,40,40	4
85	MG	1	3596	1/1	0.93	0.28	46,46,46,46	0
85	MG	6	1991	1/1	0.93	0.11	77,77,77,77	0
86	OHX	1	4011	7/7	0.93	0.09	62,62,62,62	3
85	MG	1	3759	1/1	0.93	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3738	1/1	0.93	0.08	42,42,42,42	0
86	OHX	1	4014	7/7	0.93	0.09	60,60,60,60	3
85	MG	1	3431	1/1	0.93	0.09	47,47,47,47	0
86	OHX	1	4017	7/7	0.93	0.09	46,46,46,46	2
85	MG	1	3509	1/1	0.93	0.28	33,33,33,33	0
86	OHX	5	4129	7/7	0.93	0.19	37,37,37,37	3
85	MG	5	3744	1/1	0.93	0.25	57,57,57,57	0
85	MG	1	3626	1/1	0.93	0.22	46,46,46,46	0
85	MG	5	3520	1/1	0.93	0.26	30,30,30,30	0
85	MG	5	3627	1/1	0.93	0.24	47,47,47,47	0
85	MG	5	3449	1/1	0.93	0.11	32,32,32,32	0
86	OHX	6	2140	7/7	0.93	0.10	74,74,74,74	6
85	MG	5	3524	1/1	0.93	0.25	48,48,48,48	0
86	OHX	6	2144	7/7	0.93	0.13	85,85,85,85	7
86	OHX	5	4138	7/7	0.93	0.20	44,44,44,44	5
85	MG	1	3541	1/1	0.93	0.32	28,28,28,28	0
85	MG	5	3452	1/1	0.93	0.24	29,29,29,29	0
85	MG	5	3453	1/1	0.93	0.19	33,33,33,33	0
85	MG	6	1952	1/1	0.93	0.51	53,53,53,53	0
86	OHX	2	2118	7/7	0.93	0.09	143,143,143,143	7
85	MG	5	3760	1/1	0.93	0.07	53,53,53,53	0
85	MG	1	3628	1/1	0.93	0.21	41,41,41,41	0
85	MG	5	3635	1/1	0.93	0.07	50,50,50,50	0
85	MG	5	3537	1/1	0.93	0.25	26,26,26,26	0
85	MG	1	3579	1/1	0.93	0.10	35,35,35,35	0
85	MG	5	3459	1/1	0.93	0.20	34,34,34,34	0
85	MG	1	3716	1/1	0.93	0.07	65,65,65,65	0
85	MG	5	3780	1/1	0.93	0.16	30,30,30,30	0
86	OHX	2	2127	7/7	0.93	0.10	128,128,128,128	7
85	MG	1	3601	1/1	0.93	0.15	72,72,72,72	0
85	MG	1	3559	1/1	0.93	0.28	22,22,22,22	0
85	MG	6	2010	1/1	0.93	0.19	53,53,53,53	0
85	MG	5	3647	1/1	0.93	0.17	55,55,55,55	0
86	OHX	2	2132	7/7	0.93	0.13	87,87,87,87	3
85	MG	1	3634	1/1	0.93	0.28	41,41,41,41	0
85	MG	1	3498	1/1	0.93	0.32	45,45,45,45	0
85	MG	5	3650	1/1	0.93	0.34	29,29,29,29	0
85	MG	1	3636	1/1	0.93	0.35	53,53,53,53	0
85	MG	1	3637	1/1	0.93	0.36	46,46,46,46	0
86	OHX	6	2172	7/7	0.93	0.14	69,69,69,69	3
85	MG	1	3725	1/1	0.93	0.12	38,38,38,38	0
85	MG	5	3796	1/1	0.93	0.21	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3530	1/1	0.93	0.27	41,41,41,41	0
85	MG	5	3554	1/1	0.93	0.28	32,32,32,32	0
85	MG	6	1965	1/1	0.93	0.10	48,48,48,48	0
85	MG	5	3662	1/1	0.93	0.25	42,42,42,42	0
85	MG	5	3556	1/1	0.93	0.22	33,33,33,33	0
85	MG	5	3804	1/1	0.93	0.28	49,49,49,49	0
85	MG	1	3459	1/1	0.93	0.24	60,60,60,60	0
85	MG	5	3558	1/1	0.93	0.31	31,31,31,31	0
85	MG	5	3561	1/1	0.93	0.33	26,26,26,26	0
85	MG	1	3412	1/1	0.93	0.10	68,68,68,68	0
86	OHX	s9	201	7/7	0.93	0.15	71,71,71,71	5
85	MG	5	3816	1/1	0.93	0.20	39,39,39,39	0
86	OHX	c5	201	7/7	0.93	0.07	129,129,129,129	6
85	MG	1	3503	1/1	0.93	0.30	37,37,37,37	0
85	MG	7	205	1/1	0.93	0.34	26,26,26,26	0
86	OHX	d9	102	7/7	0.93	0.17	106,106,106,106	6
85	MG	5	3671	1/1	0.93	0.09	84,84,84,84	0
86	OHX	5	3876	7/7	0.93	0.20	43,43,43,43	3
86	OHX	5	3889	7/7	0.93	0.27	42,42,42,42	3
85	MG	1	3646	1/1	0.93	0.10	39,39,39,39	0
86	OHX	C5	201	7/7	0.93	0.08	122,122,122,122	7
85	MG	1	3737	1/1	0.93	0.26	63,63,63,63	0
86	OHX	SR	401	7/7	0.93	0.09	144,144,144,144	6
86	OHX	6	2113	7/7	0.94	0.11	67,67,67,67	3
85	MG	1	3562	1/1	0.94	0.34	33,33,33,33	0
86	OHX	2	2094	7/7	0.94	0.17	87,87,87,87	5
86	OHX	5	4036	7/7	0.94	0.17	38,38,38,38	5
86	OHX	5	4038	7/7	0.94	0.12	106,106,106,106	4
86	OHX	5	4039	7/7	0.94	0.17	72,72,72,72	4
85	MG	5	3660	1/1	0.94	0.17	46,46,46,46	0
85	MG	5	3456	1/1	0.94	0.18	31,31,31,31	0
85	MG	7	203	1/1	0.94	0.29	54,54,54,54	0
85	MG	5	3418	1/1	0.94	0.19	36,36,36,36	0
86	OHX	2	2102	7/7	0.94	0.10	118,118,118,118	5
85	MG	1	3563	1/1	0.94	0.14	41,41,41,41	0
86	OHX	1	3932	7/7	0.94	0.17	57,57,57,57	5
86	OHX	5	4053	7/7	0.94	0.08	65,65,65,65	5
86	OHX	1	3933	7/7	0.94	0.09	91,91,91,91	4
86	OHX	1	3938	7/7	0.94	0.16	53,53,53,53	3
86	OHX	1	4072	7/7	0.94	0.28	47,47,47,47	3
85	MG	L2	301	1/1	0.94	0.16	37,37,37,37	0
86	OHX	1	3945	7/7	0.94	0.18	57,57,57,57	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	7	211	1/1	0.94	0.07	57,57,57,57	0
85	MG	5	3606	1/1	0.94	0.07	39,39,39,39	1
86	OHX	2	2108	7/7	0.94	0.12	79,79,79,79	5
86	OHX	5	4067	7/7	0.94	0.16	34,34,34,34	4
85	MG	5	3550	1/1	0.94	0.37	44,44,44,44	0
86	OHX	6	2139	7/7	0.94	0.10	86,86,86,86	3
85	MG	5	3737	1/1	0.94	0.17	40,40,40,40	0
86	OHX	5	4073	7/7	0.94	0.15	44,44,44,44	4
86	OHX	6	2142	7/7	0.94	0.14	95,95,95,95	7
85	MG	5	3668	1/1	0.94	0.07	33,33,33,33	0
86	OHX	5	4077	7/7	0.94	0.18	32,32,32,32	3
86	OHX	1	3956	7/7	0.94	0.12	57,57,57,57	5
85	MG	8	204	1/1	0.94	0.31	44,44,44,44	0
86	OHX	2	2113	7/7	0.94	0.08	152,152,152,152	7
85	MG	1	3643	1/1	0.94	0.22	38,38,38,38	0
85	MG	5	3741	1/1	0.94	0.14	66,66,66,66	0
85	MG	5	3742	1/1	0.94	0.11	31,31,31,31	1
86	OHX	6	2151	7/7	0.94	0.12	65,65,65,65	4
85	MG	1	3499	1/1	0.94	0.21	37,37,37,37	0
85	MG	5	3611	1/1	0.94	0.12	38,38,38,38	0
85	MG	5	3505	1/1	0.94	0.41	25,25,25,25	0
85	MG	1	3605	1/1	0.94	0.18	44,44,44,44	0
85	MG	M5	301	1/1	0.94	0.17	42,42,42,42	0
85	MG	6	1973	1/1	0.94	0.42	51,51,51,51	0
86	OHX	5	4093	7/7	0.94	0.14	55,55,55,55	6
85	MG	1	3730	1/1	0.94	0.12	36,36,36,36	0
85	MG	5	3751	1/1	0.94	0.30	53,53,53,53	0
85	MG	5	3678	1/1	0.94	0.27	37,37,37,37	0
85	MG	m5	303	1/1	0.94	0.21	67,67,67,67	0
85	MG	5	3755	1/1	0.94	0.23	55,55,55,55	0
86	OHX	1	3984	7/7	0.94	0.08	127,127,127,127	7
86	OHX	1	3985	7/7	0.94	0.17	38,38,38,38	2
85	MG	1	3731	1/1	0.94	0.14	57,57,57,57	0
85	MG	5	3563	1/1	0.94	0.32	44,44,44,44	0
85	MG	1	3606	1/1	0.94	0.17	43,43,43,43	0
85	MG	n8	201	1/1	0.94	0.18	37,37,37,37	0
85	MG	n8	202	1/1	0.94	0.23	50,50,50,50	0
85	MG	5	3622	1/1	0.94	0.18	62,62,62,62	0
85	MG	1	3461	1/1	0.94	0.15	57,57,57,57	0
85	MG	5	3765	1/1	0.94	0.13	39,39,39,39	0
85	MG	5	3766	1/1	0.94	0.08	27,27,27,27	0
86	OHX	2	2010	7/7	0.94	0.15	101,101,101,101	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	3	211	7/7	0.94	0.15	64,64,64,64	3
85	MG	5	3767	1/1	0.94	0.13	43,43,43,43	0
85	MG	5	3471	1/1	0.94	0.16	51,51,51,51	0
86	OHX	2	2034	7/7	0.94	0.13	119,119,119,119	4
86	OHX	6	2180	7/7	0.94	0.12	97,97,97,97	6
85	MG	6	1920	1/1	0.94	0.31	46,46,46,46	0
85	MG	5	3568	1/1	0.94	0.26	22,22,22,22	0
85	MG	1	3708	1/1	0.94	0.11	42,42,42,42	0
86	OHX	2	2044	7/7	0.94	0.13	98,98,98,98	6
86	OHX	s4	602	7/7	0.94	0.11	76,76,76,76	3
85	MG	1	3404	1/1	0.94	0.23	57,57,57,57	0
85	MG	5	3438	1/1	0.94	0.29	39,39,39,39	0
86	OHX	2	2050	7/7	0.94	0.11	129,129,129,129	6
86	OHX	2	2051	7/7	0.94	0.15	101,101,101,101	5
86	OHX	2	2052	7/7	0.94	0.16	90,90,90,90	5
86	OHX	c8	203	7/7	0.94	0.14	99,99,99,99	5
85	MG	5	3572	1/1	0.94	0.22	21,21,21,21	0
86	OHX	L4	401	7/7	0.94	0.08	67,67,67,67	7
85	MG	1	3569	1/1	0.94	0.27	39,39,39,39	0
86	OHX	5	3871	7/7	0.94	0.17	72,72,72,72	2
86	OHX	2	2055	7/7	0.94	0.10	63,63,63,63	5
85	MG	5	3576	1/1	0.94	0.16	28,28,28,28	0
86	OHX	5	3909	7/7	0.94	0.12	77,77,77,77	4
86	OHX	5	3910	7/7	0.94	0.17	57,57,57,57	3
86	OHX	M7	205	7/7	0.94	0.13	57,57,57,57	5
85	MG	6	1924	1/1	0.94	0.34	48,48,48,48	0
86	OHX	5	3919	7/7	0.94	0.18	73,73,73,73	3
85	MG	5	3521	1/1	0.94	0.32	44,44,44,44	0
86	OHX	5	4151	7/7	0.94	0.12	53,53,53,53	4
85	MG	5	3579	1/1	0.94	0.15	17,17,17,17	0
85	MG	1	3611	1/1	0.94	0.10	41,41,41,41	0
86	OHX	1	3825	7/7	0.94	0.18	91,91,91,91	5
86	OHX	5	3942	7/7	0.94	0.16	50,50,50,50	5
86	OHX	5	4156	7/7	0.94	0.14	49,49,49,49	6
86	OHX	2	2067	7/7	0.94	0.08	132,132,132,132	4
86	OHX	6	2029	7/7	0.94	0.15	68,68,68,68	2
85	MG	1	3547	1/1	0.94	0.32	32,32,32,32	0
86	OHX	6	2050	7/7	0.94	0.12	87,87,87,87	5
85	MG	1	3440	1/1	0.94	0.40	49,49,49,49	0
86	OHX	6	2066	7/7	0.94	0.10	162,162,162,162	3
86	OHX	5	3969	7/7	0.94	0.14	105,105,105,105	5
85	MG	2	1982	1/1	0.94	0.24	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	6	2072	7/7	0.94	0.19	76,76,76,76	3
86	OHX	5	4167	7/7	0.94	0.16	38,38,38,38	3
86	OHX	5	3972	7/7	0.94	0.13	89,89,89,89	1
85	MG	5	3795	1/1	0.94	0.10	41,41,41,41	0
86	OHX	5	3976	7/7	0.94	0.10	115,115,115,115	3
85	MG	5	3486	1/1	0.94	0.18	51,51,51,51	0
85	MG	5	3447	1/1	0.94	0.17	31,31,31,31	0
85	MG	5	3489	1/1	0.94	0.23	39,39,39,39	0
86	OHX	5	3981	7/7	0.94	0.11	69,69,69,69	3
85	MG	1	3686	1/1	0.94	0.16	35,35,35,35	0
86	OHX	1	4041	7/7	0.94	0.16	46,46,46,46	4
86	OHX	8	219	7/7	0.94	0.13	80,80,80,80	2
85	MG	1	3615	1/1	0.94	0.27	68,68,68,68	0
86	OHX	5	3989	7/7	0.94	0.12	158,158,158,158	5
86	OHX	8	224	7/7	0.94	0.14	95,95,95,95	7
86	OHX	1	3897	7/7	0.94	0.16	49,49,49,49	5
86	OHX	6	2090	7/7	0.94	0.12	91,91,91,91	7
86	OHX	5	3994	7/7	0.94	0.11	42,42,42,42	4
86	OHX	1	3898	7/7	0.94	0.17	89,89,89,89	5
86	OHX	2	2084	7/7	0.94	0.16	95,95,95,95	5
85	MG	1	3511	1/1	0.94	0.33	36,36,36,36	0
86	OHX	14	403	7/7	0.94	0.11	51,51,51,51	7
86	OHX	1	4048	7/7	0.94	0.11	116,116,116,116	5
86	OHX	15	303	7/7	0.94	0.12	90,90,90,90	6
86	OHX	6	2098	7/7	0.94	0.17	87,87,87,87	5
86	OHX	1	3903	7/7	0.94	0.16	53,53,53,53	3
86	OHX	m0	303	7/7	0.94	0.15	96,96,96,96	5
85	MG	1	3638	1/1	0.94	0.27	48,48,48,48	0
86	OHX	6	2104	7/7	0.94	0.12	91,91,91,91	5
86	OHX	m7	204	7/7	0.94	0.12	47,47,47,47	5
86	OHX	6	2106	7/7	0.94	0.12	85,85,85,85	4
85	MG	1	3553	1/1	0.94	0.23	24,24,24,24	0
86	OHX	o3	202	7/7	0.94	0.16	52,52,52,52	3
85	MG	1	3666	1/1	0.94	0.29	65,65,65,65	0
85	MG	5	3544	1/1	0.94	0.33	48,48,48,48	0
85	MG	5	3810	1/1	0.94	0.12	50,50,50,50	0
86	OHX	5	3985	7/7	0.95	0.11	55,55,55,55	2
85	MG	o2	201	1/1	0.95	0.15	35,35,35,35	1
86	OHX	6	2039	7/7	0.95	0.13	126,126,126,126	5
85	MG	1	3702	1/1	0.95	0.14	45,45,45,45	0
85	MG	1	3704	1/1	0.95	0.15	59,59,59,59	0
85	MG	5	3761	1/1	0.95	0.18	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	6	2057	7/7	0.95	0.14	58,58,58,58	2
86	OHX	6	2060	7/7	0.95	0.09	96,96,96,96	1
86	OHX	5	3997	7/7	0.95	0.11	62,62,62,62	5
86	OHX	5	3999	7/7	0.95	0.21	38,38,38,38	5
86	OHX	5	4001	7/7	0.95	0.18	41,41,41,41	4
85	MG	q2	201	1/1	0.95	0.06	43,43,43,43	1
86	OHX	2	2136	7/7	0.95	0.17	74,74,74,74	6
85	MG	B	102	1/1	0.95	0.23	38,38,38,38	0
86	OHX	5	4009	7/7	0.95	0.23	41,41,41,41	3
85	MG	1	3738	1/1	0.95	0.13	41,41,41,41	0
86	OHX	6	2074	7/7	0.95	0.11	70,70,70,70	2
85	MG	5	3764	1/1	0.95	0.17	43,43,43,43	0
85	MG	5	3562	1/1	0.95	0.22	27,27,27,27	0
86	OHX	2	2019	7/7	0.95	0.13	81,81,81,81	3
86	OHX	5	4020	7/7	0.95	0.18	47,47,47,47	1
86	OHX	5	4022	7/7	0.95	0.16	37,37,37,37	1
86	OHX	6	2081	7/7	0.95	0.11	74,74,74,74	6
86	OHX	6	2082	7/7	0.95	0.12	99,99,99,99	5
86	OHX	5	4027	7/7	0.95	0.14	49,49,49,49	3
86	OHX	5	4028	7/7	0.95	0.15	72,72,72,72	4
85	MG	5	3404	1/1	0.95	0.24	33,33,33,33	0
86	OHX	2	2027	7/7	0.95	0.14	75,75,75,75	4
86	OHX	2	2030	7/7	0.95	0.10	98,98,98,98	5
86	OHX	2	2032	7/7	0.95	0.14	102,102,102,102	6
85	MG	4	201	1/1	0.95	0.17	36,36,36,36	0
85	MG	5	3768	1/1	0.95	0.18	34,34,34,34	0
86	OHX	5	4037	7/7	0.95	0.10	93,93,93,93	5
85	MG	1	3677	1/1	0.95	0.12	46,46,46,46	0
86	OHX	6	2094	7/7	0.95	0.15	109,109,109,109	6
86	OHX	1	4022	7/7	0.95	0.12	71,71,71,71	6
86	OHX	2	2037	7/7	0.95	0.17	73,73,73,73	4
86	OHX	1	4024	7/7	0.95	0.14	42,42,42,42	3
86	OHX	2	2040	7/7	0.95	0.15	89,89,89,89	3
85	MG	1	3550	1/1	0.95	0.24	33,33,33,33	0
86	OHX	5	4047	7/7	0.95	0.10	28,28,28,28	1
85	MG	5	3689	1/1	0.95	0.28	40,40,40,40	0
86	OHX	6	2105	7/7	0.95	0.10	81,81,81,81	4
86	OHX	5	4051	7/7	0.95	0.13	64,64,64,64	6
85	MG	5	3774	1/1	0.95	0.30	55,55,55,55	0
86	OHX	2	2048	7/7	0.95	0.08	141,141,141,141	5
86	OHX	S9	201	7/7	0.95	0.13	94,94,94,94	6
85	MG	1	3468	1/1	0.95	0.27	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3489	1/1	0.95	0.22	67,67,67,67	0
85	MG	1	3500	1/1	0.95	0.33	30,30,30,30	0
85	MG	1	3527	1/1	0.95	0.25	31,31,31,31	0
86	OHX	6	2115	7/7	0.95	0.11	58,58,58,58	2
86	OHX	6	2116	7/7	0.95	0.14	61,61,61,61	2
86	OHX	5	4064	7/7	0.95	0.11	52,52,52,52	3
86	OHX	1	3807	7/7	0.95	0.21	73,73,73,73	2
86	OHX	1	4037	7/7	0.95	0.15	84,84,84,84	7
86	OHX	6	2119	7/7	0.95	0.16	60,60,60,60	3
86	OHX	5	4071	7/7	0.95	0.10	45,45,45,45	3
85	MG	2	1990	1/1	0.95	0.17	49,49,49,49	0
86	OHX	1	3843	7/7	0.95	0.15	55,55,55,55	2
85	MG	4	209	1/1	0.95	0.22	51,51,51,51	0
85	MG	5	3786	1/1	0.95	0.12	35,35,35,35	0
86	OHX	5	4076	7/7	0.95	0.08	43,43,43,43	3
86	OHX	1	3859	7/7	0.95	0.17	53,53,53,53	2
86	OHX	1	3862	7/7	0.95	0.10	83,83,83,83	3
86	OHX	1	3866	7/7	0.95	0.14	69,69,69,69	3
86	OHX	6	2128	7/7	0.95	0.14	53,53,53,53	4
86	OHX	6	2129	7/7	0.95	0.11	58,58,58,58	5
86	OHX	2	2056	7/7	0.95	0.17	99,99,99,99	4
86	OHX	1	3870	7/7	0.95	0.17	67,67,67,67	3
86	OHX	5	4084	7/7	0.95	0.20	35,35,35,35	6
85	MG	5	3698	1/1	0.95	0.24	42,42,42,42	0
85	MG	5	3573	1/1	0.95	0.35	48,48,48,48	0
86	OHX	6	2134	7/7	0.95	0.07	163,163,163,163	7
86	OHX	1	4051	7/7	0.95	0.13	58,58,58,58	3
86	OHX	2	2060	7/7	0.95	0.14	89,89,89,89	6
86	OHX	1	4054	7/7	0.95	0.20	77,77,77,77	6
85	MG	5	3702	1/1	0.95	0.12	54,54,54,54	0
85	MG	5	3574	1/1	0.95	0.25	37,37,37,37	0
86	OHX	5	4094	7/7	0.95	0.16	36,36,36,36	3
85	MG	5	3704	1/1	0.95	0.25	2,2,2,2	0
86	OHX	5	4096	7/7	0.95	0.07	119,119,119,119	7
86	OHX	1	3887	7/7	0.95	0.10	131,131,131,131	5
86	OHX	1	3888	7/7	0.95	0.15	71,71,71,71	3
86	OHX	1	3890	7/7	0.95	0.12	48,48,48,48	3
85	MG	5	3415	1/1	0.95	0.28	44,44,44,44	0
86	OHX	5	4101	7/7	0.95	0.11	69,69,69,69	3
86	OHX	5	4103	7/7	0.95	0.15	40,40,40,40	5
86	OHX	1	3893	7/7	0.95	0.10	155,155,155,155	6
86	OHX	6	2147	7/7	0.95	0.13	64,64,64,64	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3416	1/1	0.95	0.26	31,31,31,31	0
85	MG	5	3637	1/1	0.95	0.09	36,36,36,36	0
86	OHX	2	2070	7/7	0.95	0.09	108,108,108,108	5
86	OHX	5	4109	7/7	0.95	0.15	53,53,53,53	5
86	OHX	2	2071	7/7	0.95	0.10	72,72,72,72	6
86	OHX	1	4068	7/7	0.95	0.11	39,39,39,39	3
86	OHX	1	3902	7/7	0.95	0.22	53,53,53,53	3
86	OHX	5	4113	7/7	0.95	0.15	52,52,52,52	6
85	MG	1	3617	1/1	0.95	0.18	41,41,41,41	0
86	OHX	1	4071	7/7	0.95	0.19	42,42,42,42	3
85	MG	1	3687	1/1	0.95	0.35	46,46,46,46	0
86	OHX	2	2075	7/7	0.95	0.11	80,80,80,80	6
86	OHX	5	4118	7/7	0.95	0.20	49,49,49,49	4
86	OHX	1	3906	7/7	0.95	0.15	65,65,65,65	4
85	MG	5	3419	1/1	0.95	0.12	36,36,36,36	0
86	OHX	1	4076	7/7	0.95	0.24	45,45,45,45	5
85	MG	4	213	1/1	0.95	0.23	64,64,64,64	0
85	MG	5	3581	1/1	0.95	0.29	24,24,24,24	0
85	MG	6	1951	1/1	0.95	0.43	43,43,43,43	0
85	MG	5	3645	1/1	0.95	0.24	31,31,31,31	0
85	MG	5	3717	1/1	0.95	0.31	16,16,16,16	0
86	OHX	1	3919	7/7	0.95	0.10	106,106,106,106	3
86	OHX	1	3920	7/7	0.95	0.14	43,43,43,43	3
85	MG	1	3749	1/1	0.95	0.20	17,17,17,17	0
85	MG	1	3750	1/1	0.95	0.27	48,48,48,48	0
86	OHX	6	2170	7/7	0.95	0.09	83,83,83,83	7
85	MG	1	3688	1/1	0.95	0.23	39,39,39,39	0
85	MG	5	3814	1/1	0.95	0.23	42,42,42,42	0
85	MG	L3	401	1/1	0.95	0.20	41,41,41,41	0
85	MG	1	3406	1/1	0.95	0.15	44,44,44,44	0
86	OHX	1	4090	7/7	0.95	0.15	47,47,47,47	4
85	MG	5	3723	1/1	0.95	0.28	52,52,52,52	0
86	OHX	1	3935	7/7	0.95	0.11	71,71,71,71	2
86	OHX	1	3937	7/7	0.95	0.12	110,110,110,110	6
85	MG	5	3532	1/1	0.95	0.22	35,35,35,35	0
85	MG	7	204	1/1	0.95	0.23	44,44,44,44	0
85	MG	1	3514	1/1	0.95	0.18	35,35,35,35	0
86	OHX	5	4145	7/7	0.95	0.14	70,70,70,70	7
85	MG	7	208	1/1	0.95	0.30	45,45,45,45	0
86	OHX	2	2099	7/7	0.95	0.08	185,185,185,185	7
86	OHX	2	2100	7/7	0.95	0.11	83,83,83,83	4
85	MG	6	1958	1/1	0.95	0.21	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3728	1/1	0.95	0.12	44,44,44,44	0
86	OHX	1	3954	7/7	0.95	0.10	122,122,122,122	3
85	MG	5	3730	1/1	0.95	0.07	41,41,41,41	0
85	MG	5	3654	1/1	0.95	0.30	31,31,31,31	0
85	MG	5	3430	1/1	0.95	0.21	36,36,36,36	0
86	OHX	1	3959	7/7	0.95	0.09	112,112,112,112	3
86	OHX	1	3961	7/7	0.95	0.17	45,45,45,45	5
86	OHX	2	2106	7/7	0.95	0.11	78,78,78,78	3
85	MG	1	3640	1/1	0.95	0.21	62,62,62,62	0
85	MG	1	3484	1/1	0.95	0.17	52,52,52,52	0
85	MG	M5	302	1/1	0.95	0.22	47,47,47,47	0
85	MG	5	3487	1/1	0.95	0.17	37,37,37,37	0
86	OHX	5	4163	7/7	0.95	0.14	36,36,36,36	4
86	OHX	3	212	7/7	0.95	0.14	86,86,86,86	3
85	MG	5	3599	1/1	0.95	0.23	39,39,39,39	0
86	OHX	5	3914	7/7	0.95	0.15	74,74,74,74	4
86	OHX	1	3969	7/7	0.95	0.13	65,65,65,65	4
85	MG	1	3438	1/1	0.95	0.09	33,33,33,33	0
86	OHX	3	216	7/7	0.95	0.14	49,49,49,49	5
86	OHX	5	4170	7/7	0.95	0.17	71,71,71,71	3
86	OHX	5	3922	7/7	0.95	0.09	119,119,119,119	6
85	MG	1	3494	1/1	0.95	0.17	42,42,42,42	0
86	OHX	5	3928	7/7	0.95	0.09	146,146,146,146	3
86	OHX	5	3932	7/7	0.95	0.10	139,139,139,139	5
85	MG	5	3603	1/1	0.95	0.21	50,50,50,50	0
85	MG	l3	402	1/1	0.95	0.16	39,39,39,39	1
86	OHX	8	215	7/7	0.95	0.14	60,60,60,60	3
86	OHX	5	3939	7/7	0.95	0.13	92,92,92,92	2
86	OHX	5	3940	7/7	0.95	0.13	62,62,62,62	2
86	OHX	8	221	7/7	0.95	0.13	62,62,62,62	3
85	MG	1	3625	1/1	0.95	0.12	41,41,41,41	0
86	OHX	4	227	7/7	0.95	0.12	103,103,103,103	6
86	OHX	5	3945	7/7	0.95	0.14	46,46,46,46	3
86	OHX	1	3977	7/7	0.95	0.09	72,72,72,72	7
85	MG	5	3745	1/1	0.95	0.27	34,34,34,34	0
85	MG	1	3456	1/1	0.95	0.18	32,32,32,32	0
86	OHX	5	3951	7/7	0.95	0.17	67,67,67,67	5
86	OHX	5	3952	7/7	0.95	0.10	100,100,100,100	2
85	MG	1	3697	1/1	0.95	0.10	42,42,42,42	0
85	MG	1	3457	1/1	0.95	0.17	32,32,32,32	0
85	MG	m3	201	1/1	0.95	0.17	40,40,40,40	0
85	MG	6	1968	1/1	0.95	0.18	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	3	203	1/1	0.95	0.26	42,42,42,42	0
85	MG	5	3445	1/1	0.95	0.19	38,38,38,38	0
85	MG	5	3752	1/1	0.95	0.25	40,40,40,40	0
86	OHX	5	3974	7/7	0.95	0.13	53,53,53,53	4
85	MG	s8	302	1/1	0.95	0.32	49,49,49,49	0
85	MG	1	3649	1/1	0.95	0.17	37,37,37,37	0
86	OHX	1	3992	7/7	0.95	0.10	52,52,52,52	3
85	MG	1	3610	1/1	0.95	0.09	45,45,45,45	0
85	MG	5	3615	1/1	0.95	0.29	35,35,35,35	0
86	OHX	1	3996	7/7	0.95	0.12	64,64,64,64	5
85	MG	5	3758	1/1	0.95	0.06	36,36,36,36	0
86	OHX	5	3983	7/7	0.95	0.16	46,46,46,46	3
89	PRO	1	4114	7/8	0.95	0.17	41,41,51,51	0
85	MG	6	1995	1/1	0.96	0.22	47,47,47,47	0
85	MG	1	3705	1/1	0.96	0.16	33,33,33,33	0
86	OHX	1	3829	7/7	0.96	0.16	59,59,59,59	2
86	OHX	1	3834	7/7	0.96	0.13	62,62,62,62	3
86	OHX	5	4056	7/7	0.96	0.14	40,40,40,40	6
86	OHX	1	3997	7/7	0.96	0.12	55,55,55,55	5
86	OHX	5	4058	7/7	0.96	0.32	36,36,36,36	6
86	OHX	3	210	7/7	0.96	0.16	51,51,51,51	5
86	OHX	1	3841	7/7	0.96	0.17	70,70,70,70	3
85	MG	12	301	1/1	0.96	0.24	37,37,37,37	0
86	OHX	1	3848	7/7	0.96	0.13	76,76,76,76	3
86	OHX	1	4001	7/7	0.96	0.11	61,61,61,61	4
85	MG	12	302	1/1	0.96	0.25	45,45,45,45	0
86	OHX	1	3853	7/7	0.96	0.13	54,54,54,54	3
85	MG	4	212	1/1	0.96	0.07	60,60,60,60	0
86	OHX	1	3858	7/7	0.96	0.10	98,98,98,98	4
85	MG	5	3553	1/1	0.96	0.18	26,26,26,26	0
86	OHX	4	222	7/7	0.96	0.09	61,61,61,61	3
86	OHX	2	2080	7/7	0.96	0.15	91,91,91,91	4
85	MG	6	1998	1/1	0.96	0.21	42,42,42,42	0
86	OHX	2	2082	7/7	0.96	0.10	90,90,90,90	5
86	OHX	4	229	7/7	0.96	0.10	60,60,60,60	3
85	MG	6	1999	1/1	0.96	0.29	36,36,36,36	0
85	MG	5	3655	1/1	0.96	0.23	42,42,42,42	0
86	OHX	1	4015	7/7	0.96	0.14	47,47,47,47	2
85	MG	5	3656	1/1	0.96	0.42	41,41,41,41	0
85	MG	1	3633	1/1	0.96	0.11	59,59,59,59	0
85	MG	5	3658	1/1	0.96	0.20	27,27,27,27	0
85	MG	1	3732	1/1	0.96	0.21	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3465	1/1	0.96	0.30	44,44,44,44	0
86	OHX	2	2091	7/7	0.96	0.15	89,89,89,89	5
86	OHX	M5	304	7/7	0.96	0.17	72,72,72,72	4
85	MG	1	3667	1/1	0.96	0.16	58,58,58,58	0
85	MG	5	3511	1/1	0.96	0.22	43,43,43,43	0
85	MG	m7	203	1/1	0.96	0.23	34,34,34,34	0
85	MG	6	1907	1/1	0.96	0.32	51,51,51,51	0
86	OHX	2	2096	7/7	0.96	0.10	108,108,108,108	6
85	MG	1	3648	1/1	0.96	0.11	42,42,42,42	0
85	MG	1	3565	1/1	0.96	0.38	40,40,40,40	0
86	OHX	6	2025	7/7	0.96	0.15	62,62,62,62	2
85	MG	1	3650	1/1	0.96	0.17	47,47,47,47	0
86	OHX	1	3901	7/7	0.96	0.14	62,62,62,62	4
85	MG	6	1911	1/1	0.96	0.35	49,49,49,49	0
86	OHX	5	3869	7/7	0.96	0.14	35,35,35,35	4
86	OHX	6	2044	7/7	0.96	0.10	46,46,46,46	2
86	OHX	5	3874	7/7	0.96	0.14	62,62,62,62	3
86	OHX	5	4102	7/7	0.96	0.09	45,45,45,45	5
86	OHX	6	2045	7/7	0.96	0.15	91,91,91,91	5
85	MG	1	3443	1/1	0.96	0.14	46,46,46,46	0
86	OHX	5	3895	7/7	0.96	0.15	63,63,63,63	3
86	OHX	5	3902	7/7	0.96	0.13	72,72,72,72	3
85	MG	1	3552	1/1	0.96	0.38	37,37,37,37	0
86	OHX	1	4034	7/7	0.96	0.15	75,75,75,75	3
85	MG	5	3727	1/1	0.96	0.19	44,44,44,44	0
86	OHX	6	2064	7/7	0.96	0.12	98,98,98,98	5
86	OHX	6	2065	7/7	0.96	0.10	138,138,138,138	5
85	MG	s8	301	1/1	0.96	0.12	52,52,52,52	0
86	OHX	6	2067	7/7	0.96	0.10	154,154,154,154	3
85	MG	q3	502	1/1	0.96	0.27	48,48,48,48	0
85	MG	5	3729	1/1	0.96	0.07	47,47,47,47	0
86	OHX	5	3929	7/7	0.96	0.20	41,41,41,41	4
85	MG	1	3623	1/1	0.96	0.17	57,57,57,57	0
86	OHX	1	3913	7/7	0.96	0.06	54,54,54,54	3
86	OHX	6	2076	7/7	0.96	0.10	52,52,52,52	5
86	OHX	5	4120	7/7	0.96	0.15	64,64,64,64	5
86	OHX	2	1999	7/7	0.96	0.11	113,113,113,113	2
86	OHX	1	4043	7/7	0.96	0.10	39,39,39,39	2
86	OHX	2	2004	7/7	0.96	0.11	135,135,135,135	5
86	OHX	2	2007	7/7	0.96	0.13	94,94,94,94	5
86	OHX	1	3918	7/7	0.96	0.10	91,91,91,91	5
85	MG	1	3568	1/1	0.96	0.24	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3522	1/1	0.96	0.31	36,36,36,36	0
86	OHX	1	3922	7/7	0.96	0.10	82,82,82,82	3
86	OHX	2	2016	7/7	0.96	0.12	96,96,96,96	4
86	OHX	2	2017	7/7	0.96	0.14	74,74,74,74	4
86	OHX	5	3955	7/7	0.96	0.09	149,149,149,149	4
85	MG	5	3437	1/1	0.96	0.34	34,34,34,34	0
86	OHX	5	3960	7/7	0.96	0.20	44,44,44,44	3
86	OHX	1	4053	7/7	0.96	0.09	43,43,43,43	3
86	OHX	5	3964	7/7	0.96	0.10	107,107,107,107	2
86	OHX	5	3966	7/7	0.96	0.14	50,50,50,50	4
86	OHX	6	2093	7/7	0.96	0.09	45,45,45,45	2
86	OHX	2	2020	7/7	0.96	0.10	117,117,117,117	3
86	OHX	2	2021	7/7	0.96	0.11	99,99,99,99	5
85	MG	5	3480	1/1	0.96	0.07	47,47,47,47	0
86	OHX	2	2023	7/7	0.96	0.09	106,106,106,106	4
86	OHX	6	2099	7/7	0.96	0.11	81,81,81,81	5
86	OHX	1	3934	7/7	0.96	0.12	54,54,54,54	3
85	MG	5	3736	1/1	0.96	0.17	35,35,35,35	1
86	OHX	1	3936	7/7	0.96	0.16	54,54,54,54	3
86	OHX	2	2029	7/7	0.96	0.14	98,98,98,98	5
85	MG	2	1902	1/1	0.96	0.27	49,49,49,49	0
85	MG	5	3806	1/1	0.96	0.18	37,37,37,37	0
86	OHX	6	2108	7/7	0.96	0.08	109,109,109,109	6
86	OHX	1	3941	7/7	0.96	0.10	51,51,51,51	3
86	OHX	1	3942	7/7	0.96	0.12	94,94,94,94	4
85	MG	1	3718	1/1	0.96	0.20	52,52,52,52	0
85	MG	5	3528	1/1	0.96	0.36	21,21,21,21	0
86	OHX	1	3948	7/7	0.96	0.10	37,37,37,37	2
85	MG	5	3440	1/1	0.96	0.15	36,36,36,36	0
85	MG	d3	201	1/1	0.96	0.17	50,50,50,50	0
86	OHX	2	2039	7/7	0.96	0.14	103,103,103,103	7
85	MG	5	3811	1/1	0.96	0.12	30,30,30,30	0
86	OHX	5	3996	7/7	0.96	0.14	52,52,52,52	3
86	OHX	2	2041	7/7	0.96	0.08	141,141,141,141	6
86	OHX	5	3998	7/7	0.96	0.17	43,43,43,43	5
86	OHX	2	2042	7/7	0.96	0.11	68,68,68,68	5
85	MG	5	3812	1/1	0.96	0.13	32,32,32,32	0
86	OHX	5	4003	7/7	0.96	0.13	54,54,54,54	3
85	MG	5	3813	1/1	0.96	0.19	31,31,31,31	0
86	OHX	2	2045	7/7	0.96	0.12	95,95,95,95	4
86	OHX	6	2124	7/7	0.96	0.09	103,103,103,103	6
86	OHX	2	2046	7/7	0.96	0.14	83,83,83,83	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	3962	7/7	0.96	0.12	59,59,59,59	2
86	OHX	5	4012	7/7	0.96	0.15	41,41,41,41	4
86	OHX	7	216	7/7	0.96	0.14	62,62,62,62	3
85	MG	M6	204	1/1	0.96	0.10	37,37,37,37	0
86	OHX	5	4015	7/7	0.96	0.10	36,36,36,36	4
85	MG	5	3533	1/1	0.96	0.33	28,28,28,28	0
85	MG	1	3402	1/1	0.96	0.27	36,36,36,36	0
85	MG	2	1918	1/1	0.96	0.27	68,68,68,68	0
86	OHX	8	217	7/7	0.96	0.09	78,78,78,78	5
85	MG	5	3636	1/1	0.96	0.27	43,43,43,43	0
85	MG	1	3698	1/1	0.96	0.13	42,42,42,42	0
85	MG	M7	204	1/1	0.96	0.10	46,46,46,46	0
86	OHX	5	4025	7/7	0.96	0.14	50,50,50,50	2
85	MG	7	207	1/1	0.96	0.20	55,55,55,55	0
85	MG	1	3593	1/1	0.96	0.25	50,50,50,50	0
86	OHX	1	3972	7/7	0.96	0.10	55,55,55,55	4
86	OHX	5	4029	7/7	0.96	0.09	76,76,76,76	4
85	MG	5	3692	1/1	0.96	0.11	38,38,38,38	0
85	MG	1	3594	1/1	0.96	0.24	48,48,48,48	0
85	MG	1	3682	1/1	0.96	0.14	36,36,36,36	0
86	OHX	2	2059	7/7	0.96	0.13	101,101,101,101	4
86	OHX	6	2141	7/7	0.96	0.07	151,151,151,151	7
86	OHX	5	4035	7/7	0.96	0.13	40,40,40,40	3
85	MG	N8	201	1/1	0.96	0.11	33,33,33,33	0
86	OHX	1	3979	7/7	0.96	0.08	197,197,197,197	5
85	MG	5	3696	1/1	0.96	0.15	45,45,45,45	0
86	OHX	2	2062	7/7	0.96	0.14	109,109,109,109	6
86	OHX	2	2063	7/7	0.96	0.07	153,153,153,153	7
86	OHX	5	4041	7/7	0.96	0.10	73,73,73,73	4
85	MG	N8	202	1/1	0.96	0.32	47,47,47,47	0
85	MG	1	3522	1/1	0.96	0.24	31,31,31,31	0
85	MG	1	3703	1/1	0.96	0.08	40,40,40,40	0
85	MG	5	3701	1/1	0.96	0.15	38,38,38,38	0
85	MG	1	3754	1/1	0.96	0.34	71,71,71,71	0
86	OHX	o7	502	7/7	0.96	0.15	83,83,83,83	4
85	MG	1	3427	1/1	0.96	0.30	42,42,42,42	0
86	OHX	5	4049	7/7	0.96	0.19	37,37,37,37	3
85	MG	8	208	1/1	0.96	0.26	51,51,51,51	0
89	PRO	B	101	7/8	0.96	0.13	32,32,56,56	0
86	OHX	1	3864	7/7	0.97	0.12	104,104,104,104	3
86	OHX	2	2033	7/7	0.97	0.16	78,78,78,78	3
85	MG	5	3762	1/1	0.97	0.29	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	1	3869	7/7	0.97	0.10	92,92,92,92	3
85	MG	1	3510	1/1	0.97	0.15	39,39,39,39	0
85	MG	L7	301	1/1	0.97	0.18	38,38,38,38	0
86	OHX	1	3872	7/7	0.97	0.12	44,44,44,44	4
86	OHX	1	3873	7/7	0.97	0.15	53,53,53,53	5
86	OHX	1	3874	7/7	0.97	0.10	50,50,50,50	3
86	OHX	1	3994	7/7	0.97	0.10	54,54,54,54	5
85	MG	L7	302	1/1	0.97	0.11	50,50,50,50	0
86	OHX	1	3876	7/7	0.97	0.14	41,41,41,41	2
85	MG	1	3408	1/1	0.97	0.19	25,25,25,25	0
86	OHX	5	4044	7/7	0.97	0.11	51,51,51,51	3
86	OHX	1	3879	7/7	0.97	0.15	44,44,44,44	2
86	OHX	1	3881	7/7	0.97	0.12	86,86,86,86	4
86	OHX	1	3882	7/7	0.97	0.12	64,64,64,64	3
85	MG	8	201	1/1	0.97	0.11	43,43,43,43	0
85	MG	1	3685	1/1	0.97	0.17	43,43,43,43	0
86	OHX	1	3885	7/7	0.97	0.13	53,53,53,53	3
85	MG	5	3665	1/1	0.97	0.18	43,43,43,43	0
86	OHX	5	4052	7/7	0.97	0.12	67,67,67,67	5
85	MG	M0	302	1/1	0.97	0.17	50,50,50,50	0
86	OHX	1	4006	7/7	0.97	0.14	48,48,48,48	5
86	OHX	1	4007	7/7	0.97	0.08	43,43,43,43	4
86	OHX	4	217	7/7	0.97	0.12	61,61,61,61	3
86	OHX	4	220	7/7	0.97	0.09	81,81,81,81	2
86	OHX	4	221	7/7	0.97	0.12	84,84,84,84	3
86	OHX	1	4008	7/7	0.97	0.13	47,47,47,47	5
86	OHX	4	223	7/7	0.97	0.09	61,61,61,61	3
86	OHX	4	224	7/7	0.97	0.09	86,86,86,86	3
86	OHX	4	225	7/7	0.97	0.12	44,44,44,44	3
85	MG	1	3722	1/1	0.97	0.05	43,43,43,43	0
86	OHX	1	3889	7/7	0.97	0.12	48,48,48,48	2
86	OHX	5	4066	7/7	0.97	0.12	38,38,38,38	4
85	MG	5	3529	1/1	0.97	0.23	45,45,45,45	0
86	OHX	5	4068	7/7	0.97	0.10	49,49,49,49	3
85	MG	5	3414	1/1	0.97	0.16	33,33,33,33	0
86	OHX	1	3892	7/7	0.97	0.11	65,65,65,65	3
85	MG	5	3775	1/1	0.97	0.09	40,40,40,40	0
86	OHX	1	3895	7/7	0.97	0.12	57,57,57,57	4
86	OHX	1	3896	7/7	0.97	0.18	49,49,49,49	2
86	OHX	L3	403	7/7	0.97	0.10	72,72,72,72	5
85	MG	5	3450	1/1	0.97	0.31	45,45,45,45	0
85	MG	2	1984	1/1	0.97	0.08	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	5	3779	1/1	0.97	0.23	35,35,35,35	0
85	MG	5	3626	1/1	0.97	0.24	42,42,42,42	0
85	MG	l3	401	1/1	0.97	0.31	27,27,27,27	0
85	MG	6	2001	1/1	0.97	0.10	48,48,48,48	0
86	OHX	M6	203	7/7	0.97	0.15	43,43,43,43	2
85	MG	1	3746	1/1	0.97	0.23	43,43,43,43	0
85	MG	5	3536	1/1	0.97	0.38	29,29,29,29	0
85	MG	5	3785	1/1	0.97	0.16	57,57,57,57	0
85	MG	6	1942	1/1	0.97	0.41	43,43,43,43	0
86	OHX	O1	201	7/7	0.97	0.14	93,93,93,93	3
85	MG	5	3787	1/1	0.97	0.06	33,33,33,33	0
86	OHX	5	4088	7/7	0.97	0.10	39,39,39,39	4
85	MG	5	3583	1/1	0.97	0.43	23,23,23,23	0
86	OHX	O7	104	7/7	0.97	0.12	78,78,78,78	4
86	OHX	1	3909	7/7	0.97	0.12	73,73,73,73	4
86	OHX	1	3910	7/7	0.97	0.10	81,81,81,81	4
86	OHX	1	3911	7/7	0.97	0.12	61,61,61,61	3
86	OHX	6	2037	7/7	0.97	0.10	101,101,101,101	3
85	MG	5	3538	1/1	0.97	0.29	32,32,32,32	0
86	OHX	6	2041	7/7	0.97	0.16	56,56,56,56	4
85	MG	1	3670	1/1	0.97	0.32	38,38,38,38	0
86	OHX	5	3845	7/7	0.97	0.13	48,48,48,48	2
86	OHX	5	3846	7/7	0.97	0.14	37,37,37,37	3
86	OHX	5	3856	7/7	0.97	0.15	65,65,65,65	3
86	OHX	5	3858	7/7	0.97	0.14	72,72,72,72	3
86	OHX	5	3866	7/7	0.97	0.14	60,60,60,60	3
85	MG	1	3653	1/1	0.97	0.11	55,55,55,55	0
85	MG	1	3521	1/1	0.97	0.35	43,43,43,43	0
86	OHX	5	3872	7/7	0.97	0.16	82,82,82,82	3
86	OHX	6	2046	7/7	0.97	0.11	60,60,60,60	2
86	OHX	5	3875	7/7	0.97	0.12	49,49,49,49	2
86	OHX	6	2049	7/7	0.97	0.10	97,97,97,97	3
85	MG	1	3727	1/1	0.97	0.18	48,48,48,48	0
86	OHX	1	3917	7/7	0.97	0.08	54,54,54,54	4
86	OHX	5	3900	7/7	0.97	0.15	52,52,52,52	3
86	OHX	6	2052	7/7	0.97	0.11	67,67,67,67	3
86	OHX	5	3905	7/7	0.97	0.11	51,51,51,51	4
86	OHX	6	2053	7/7	0.97	0.13	92,92,92,92	5
86	OHX	6	2054	7/7	0.97	0.09	87,87,87,87	3
86	OHX	6	2055	7/7	0.97	0.09	113,113,113,113	4
86	OHX	5	3915	7/7	0.97	0.16	39,39,39,39	4
86	OHX	6	2056	7/7	0.97	0.10	73,73,73,73	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3435	1/1	0.97	0.32	25,25,25,25	0
86	OHX	5	3918	7/7	0.97	0.10	36,36,36,36	2
86	OHX	5	4121	7/7	0.97	0.13	68,68,68,68	7
86	OHX	6	2059	7/7	0.97	0.10	61,61,61,61	3
86	OHX	2	2066	7/7	0.97	0.08	160,160,160,160	7
86	OHX	5	3924	7/7	0.97	0.15	43,43,43,43	5
86	OHX	6	2061	7/7	0.97	0.10	86,86,86,86	4
86	OHX	6	2062	7/7	0.97	0.09	117,117,117,117	4
86	OHX	6	2063	7/7	0.97	0.07	147,147,147,147	6
86	OHX	5	3930	7/7	0.97	0.10	55,55,55,55	2
86	OHX	1	4040	7/7	0.97	0.13	52,52,52,52	4
85	MG	n0	201	1/1	0.97	0.15	41,41,41,41	0
85	MG	5	3500	1/1	0.97	0.05	40,40,40,40	0
85	MG	1	3656	1/1	0.97	0.18	46,46,46,46	0
86	OHX	6	2068	7/7	0.97	0.11	103,103,103,103	4
86	OHX	6	2069	7/7	0.97	0.11	73,73,73,73	4
86	OHX	6	2070	7/7	0.97	0.12	87,87,87,87	3
86	OHX	5	3943	7/7	0.97	0.12	44,44,44,44	2
85	MG	1	3620	1/1	0.97	0.13	32,32,32,32	0
86	OHX	5	3946	7/7	0.97	0.10	109,109,109,109	4
86	OHX	1	3926	7/7	0.97	0.18	57,57,57,57	4
85	MG	5	3798	1/1	0.97	0.16	42,42,42,42	0
85	MG	5	3799	1/1	0.97	0.21	42,42,42,42	0
86	OHX	6	2075	7/7	0.97	0.09	76,76,76,76	3
85	MG	5	3641	1/1	0.97	0.31	55,55,55,55	0
85	MG	5	3740	1/1	0.97	0.18	45,45,45,45	0
86	OHX	5	3956	7/7	0.97	0.08	40,40,40,40	2
86	OHX	5	4146	7/7	0.97	0.09	71,71,71,71	5
85	MG	1	3658	1/1	0.97	0.11	42,42,42,42	0
85	MG	5	3504	1/1	0.97	0.25	28,28,28,28	0
86	OHX	5	3961	7/7	0.97	0.10	74,74,74,74	1
86	OHX	5	3962	7/7	0.97	0.09	47,47,47,47	4
86	OHX	2	2078	7/7	0.97	0.07	115,115,115,115	7
85	MG	1	3436	1/1	0.97	0.22	39,39,39,39	0
86	OHX	5	3965	7/7	0.97	0.11	49,49,49,49	4
85	MG	f	1001	1/1	0.97	0.13	53,53,53,53	0
86	OHX	6	2084	7/7	0.97	0.12	104,104,104,104	5
86	OHX	5	3968	7/7	0.97	0.11	47,47,47,47	4
85	MG	5	3428	1/1	0.97	0.35	45,45,45,45	0
85	MG	1	3756	1/1	0.97	0.22	53,53,53,53	0
86	OHX	1	3940	7/7	0.97	0.12	77,77,77,77	5
86	OHX	6	2089	7/7	0.97	0.10	56,56,56,56	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	MG	1	3733	1/1	0.97	0.12	40,40,40,40	0
86	OHX	2	2002	7/7	0.97	0.12	101,101,101,101	3
86	OHX	1	3944	7/7	0.97	0.11	48,48,48,48	4
86	OHX	2	2085	7/7	0.97	0.09	103,103,103,103	4
86	OHX	1	3946	7/7	0.97	0.07	69,69,69,69	3
85	MG	N8	203	1/1	0.97	0.15	30,30,30,30	0
86	OHX	5	3980	7/7	0.97	0.13	55,55,55,55	3
86	OHX	6	2096	7/7	0.97	0.13	94,94,94,94	5
85	MG	1	3713	1/1	0.97	0.22	40,40,40,40	0
85	MG	d2	201	1/1	0.97	0.20	59,59,59,59	0
86	OHX	5	3984	7/7	0.97	0.12	56,56,56,56	4
86	OHX	C8	201	7/7	0.97	0.10	111,111,111,111	4
86	OHX	6	2101	7/7	0.97	0.10	62,62,62,62	2
85	MG	5	3699	1/1	0.97	0.26	39,39,39,39	0
86	OHX	7	221	7/7	0.97	0.12	50,50,50,50	4
85	MG	O7	101	1/1	0.97	0.08	62,62,62,62	0
85	MG	5	3435	1/1	0.97	0.15	33,33,33,33	0
86	OHX	1	3808	7/7	0.97	0.12	74,74,74,74	3
86	OHX	1	3811	7/7	0.97	0.14	79,79,79,79	2
86	OHX	8	216	7/7	0.97	0.10	85,85,85,85	3
86	OHX	1	3957	7/7	0.97	0.09	49,49,49,49	5
86	OHX	1	3817	7/7	0.97	0.12	109,109,109,109	5
86	OHX	6	2109	7/7	0.97	0.10	99,99,99,99	6
86	OHX	1	3820	7/7	0.97	0.18	47,47,47,47	4
86	OHX	1	3960	7/7	0.97	0.11	42,42,42,42	4
86	OHX	1	3821	7/7	0.97	0.14	66,66,66,66	5
86	OHX	5	4002	7/7	0.97	0.12	70,70,70,70	4
86	OHX	2	2018	7/7	0.97	0.09	74,74,74,74	5
86	OHX	8	227	7/7	0.97	0.11	59,59,59,59	3
85	MG	1	3645	1/1	0.97	0.32	51,51,51,51	0
86	OHX	1	3831	7/7	0.97	0.15	48,48,48,48	3
86	OHX	1	3832	7/7	0.97	0.13	80,80,80,80	3
86	OHX	1	3833	7/7	0.97	0.11	71,71,71,71	4
86	OHX	5	4010	7/7	0.97	0.07	72,72,72,72	5
86	OHX	14	402	7/7	0.97	0.08	69,69,69,69	5
85	MG	1	3471	1/1	0.97	0.31	45,45,45,45	0
85	MG	5	3402	1/1	0.97	0.10	54,54,54,54	0
86	OHX	1	3842	7/7	0.97	0.10	80,80,80,80	3
86	OHX	5	4014	7/7	0.97	0.10	48,48,48,48	3
85	MG	7	202	1/1	0.97	0.36	19,19,19,19	0
86	OHX	1	3845	7/7	0.97	0.09	123,123,123,123	3
85	MG	1	3441	1/1	0.97	0.08	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	2	2024	7/7	0.97	0.10	100,100,100,100	6
86	OHX	m5	306	7/7	0.97	0.10	76,76,76,76	3
86	OHX	1	3852	7/7	0.97	0.12	70,70,70,70	3
86	OHX	2	2026	7/7	0.97	0.11	103,103,103,103	4
86	OHX	5	4023	7/7	0.97	0.11	39,39,39,39	2
86	OHX	1	3976	7/7	0.97	0.11	41,41,41,41	4
86	OHX	1	3855	7/7	0.97	0.11	87,87,87,87	3
85	MG	5	3477	1/1	0.97	0.25	27,27,27,27	0
86	OHX	q2	203	7/7	0.97	0.15	47,47,47,47	2
86	OHX	1	3857	7/7	0.97	0.14	54,54,54,54	4
87	ZN	E1	501	1/1	0.97	0.04	145,145,145,145	0
85	MG	5	3707	1/1	0.97	0.32	64,64,64,64	0
88	SPS	5	3403	23/23	0.97	0.10	35,38,52,54	23
85	MG	1	3582	1/1	0.97	0.42	27,27,27,27	0
89	PRO	5	4173	7/8	0.97	0.11	35,35,45,45	0
85	MG	1	3536	1/1	0.97	0.21	29,29,29,29	0
86	OHX	1	3931	7/7	0.98	0.12	43,43,43,43	4
86	OHX	5	3903	7/7	0.98	0.12	91,91,91,91	2
86	OHX	5	4065	7/7	0.98	0.13	39,39,39,39	3
86	OHX	5	3904	7/7	0.98	0.16	49,49,49,49	2
86	OHX	1	3836	7/7	0.98	0.12	98,98,98,98	3
86	OHX	5	3906	7/7	0.98	0.11	60,60,60,60	4
86	OHX	6	2100	7/7	0.98	0.10	71,71,71,71	3
86	OHX	1	3839	7/7	0.98	0.12	64,64,64,64	3
86	OHX	5	3912	7/7	0.98	0.10	107,107,107,107	2
86	OHX	5	3913	7/7	0.98	0.08	77,77,77,77	3
86	OHX	1	3840	7/7	0.98	0.11	85,85,85,85	3
86	OHX	2	2025	7/7	0.98	0.11	79,79,79,79	5
85	MG	5	3713	1/1	0.98	0.23	38,38,38,38	0
85	MG	1	3495	1/1	0.98	0.34	34,34,34,34	0
86	OHX	4	218	7/7	0.98	0.09	55,55,55,55	2
86	OHX	4	219	7/7	0.98	0.13	60,60,60,60	4
86	OHX	5	3920	7/7	0.98	0.08	36,36,36,36	2
86	OHX	5	3921	7/7	0.98	0.11	57,57,57,57	2
86	OHX	1	3844	7/7	0.98	0.10	98,98,98,98	5
85	MG	6	1930	1/1	0.98	0.36	45,45,45,45	0
86	OHX	5	3925	7/7	0.98	0.08	56,56,56,56	3
86	OHX	1	3846	7/7	0.98	0.08	119,119,119,119	3
86	OHX	5	3927	7/7	0.98	0.10	64,64,64,64	5
85	MG	6	2005	1/1	0.98	0.06	88,88,88,88	0
86	OHX	2	2031	7/7	0.98	0.10	81,81,81,81	4
86	OHX	1	3943	7/7	0.98	0.09	97,97,97,97	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	3931	7/7	0.98	0.10	54,54,54,54	4
85	MG	5	3534	1/1	0.98	0.24	25,25,25,25	0
86	OHX	5	3933	7/7	0.98	0.09	94,94,94,94	4
86	OHX	5	3934	7/7	0.98	0.11	38,38,38,38	2
86	OHX	5	3935	7/7	0.98	0.11	45,45,45,45	1
85	MG	1	3664	1/1	0.98	0.22	39,39,39,39	0
86	OHX	5	3937	7/7	0.98	0.09	53,53,53,53	2
85	MG	5	3609	1/1	0.98	0.09	35,35,35,35	0
85	MG	5	3478	1/1	0.98	0.26	21,21,21,21	0
85	MG	5	3771	1/1	0.98	0.22	36,36,36,36	0
85	MG	5	3772	1/1	0.98	0.27	37,37,37,37	0
86	OHX	1	3950	7/7	0.98	0.09	41,41,41,41	4
86	OHX	2	2038	7/7	0.98	0.08	119,119,119,119	6
86	OHX	5	3944	7/7	0.98	0.13	42,42,42,42	3
86	OHX	L3	402	7/7	0.98	0.10	59,59,59,59	4
86	OHX	1	3861	7/7	0.98	0.10	60,60,60,60	3
86	OHX	5	3947	7/7	0.98	0.13	45,45,45,45	3
85	MG	1	3589	1/1	0.98	0.12	40,40,40,40	0
86	OHX	1	3863	7/7	0.98	0.11	42,42,42,42	3
85	MG	1	3528	1/1	0.98	0.28	47,47,47,47	0
85	MG	1	3425	1/1	0.98	0.41	27,27,27,27	0
85	MG	5	3805	1/1	0.98	0.10	37,37,37,37	0
86	OHX	5	3953	7/7	0.98	0.10	45,45,45,45	3
86	OHX	5	3954	7/7	0.98	0.09	49,49,49,49	2
86	OHX	1	3868	7/7	0.98	0.11	53,53,53,53	4
85	MG	5	3776	1/1	0.98	0.05	75,75,75,75	0
85	MG	5	3677	1/1	0.98	0.06	29,29,29,29	0
86	OHX	5	3958	7/7	0.98	0.12	42,42,42,42	2
86	OHX	5	3959	7/7	0.98	0.10	61,61,61,61	4
86	OHX	2	1991	7/7	0.98	0.11	88,88,88,88	0
86	OHX	2	1992	7/7	0.98	0.08	98,98,98,98	1
86	OHX	2	1993	7/7	0.98	0.12	96,96,96,96	2
86	OHX	2	1994	7/7	0.98	0.10	97,97,97,97	2
86	OHX	2	1996	7/7	0.98	0.13	101,101,101,101	5
86	OHX	2	1997	7/7	0.98	0.11	107,107,107,107	5
86	OHX	2	1998	7/7	0.98	0.12	116,116,116,116	2
86	OHX	1	4060	7/7	0.98	0.10	65,65,65,65	4
86	OHX	Q2	503	7/7	0.98	0.12	46,46,46,46	2
86	OHX	6	2016	7/7	0.98	0.11	83,83,83,83	4
86	OHX	6	2020	7/7	0.98	0.11	100,100,100,100	4
86	OHX	1	3878	7/7	0.98	0.10	58,58,58,58	3
85	MG	5	3482	1/1	0.98	0.32	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	3973	7/7	0.98	0.13	39,39,39,39	4
86	OHX	6	2031	7/7	0.98	0.11	80,80,80,80	4
86	OHX	6	2032	7/7	0.98	0.11	117,117,117,117	2
86	OHX	6	2033	7/7	0.98	0.14	56,56,56,56	5
86	OHX	6	2035	7/7	0.98	0.11	82,82,82,82	3
86	OHX	6	2036	7/7	0.98	0.09	58,58,58,58	3
86	OHX	1	3880	7/7	0.98	0.11	47,47,47,47	5
85	MG	5	3679	1/1	0.98	0.17	31,31,31,31	1
86	OHX	6	2040	7/7	0.98	0.09	123,123,123,123	5
85	MG	5	3525	1/1	0.98	0.32	31,31,31,31	0
86	OHX	S1	301	7/7	0.98	0.10	121,121,121,121	2
86	OHX	2	2005	7/7	0.98	0.10	99,99,99,99	3
86	OHX	2	2006	7/7	0.98	0.10	93,93,93,93	3
85	MG	5	3616	1/1	0.98	0.05	42,42,42,42	0
86	OHX	5	3987	7/7	0.98	0.12	41,41,41,41	3
86	OHX	6	2047	7/7	0.98	0.10	67,67,67,67	5
86	OHX	6	2048	7/7	0.98	0.10	65,65,65,65	4
86	OHX	5	3990	7/7	0.98	0.10	44,44,44,44	4
86	OHX	2	2008	7/7	0.98	0.09	89,89,89,89	5
86	OHX	5	3992	7/7	0.98	0.13	80,80,80,80	5
85	MG	5	3754	1/1	0.98	0.23	51,51,51,51	0
85	MG	5	3783	1/1	0.98	0.03	38,38,38,38	0
86	OHX	2	2012	7/7	0.98	0.09	87,87,87,87	3
86	OHX	2	2013	7/7	0.98	0.11	94,94,94,94	4
86	OHX	1	3982	7/7	0.98	0.12	47,47,47,47	5
86	OHX	1	3776	7/7	0.98	0.12	55,55,55,55	1
86	OHX	1	3782	7/7	0.98	0.13	71,71,71,71	4
86	OHX	1	3894	7/7	0.98	0.06	132,132,132,132	7
86	OHX	6	2058	7/7	0.98	0.07	72,72,72,72	2
86	OHX	1	3787	7/7	0.98	0.14	72,72,72,72	3
86	OHX	5	4004	7/7	0.98	0.07	55,55,55,55	2
86	OHX	1	3792	7/7	0.98	0.11	74,74,74,74	3
86	OHX	1	3793	7/7	0.98	0.14	68,68,68,68	4
86	OHX	5	4007	7/7	0.98	0.09	40,40,40,40	3
86	OHX	1	3794	7/7	0.98	0.11	69,69,69,69	2
86	OHX	1	3795	7/7	0.98	0.12	85,85,85,85	2
86	OHX	1	3991	7/7	0.98	0.09	57,57,57,57	3
86	OHX	1	3796	7/7	0.98	0.11	57,57,57,57	4
86	OHX	1	3798	7/7	0.98	0.10	69,69,69,69	1
86	OHX	1	3799	7/7	0.98	0.12	78,78,78,78	3
86	OHX	1	3800	7/7	0.98	0.14	44,44,44,44	3
86	OHX	1	3801	7/7	0.98	0.12	71,71,71,71	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	7	214	7/7	0.98	0.10	70,70,70,70	1
86	OHX	7	215	7/7	0.98	0.11	60,60,60,60	5
86	OHX	1	3805	7/7	0.98	0.09	93,93,93,93	4
86	OHX	7	218	7/7	0.98	0.13	67,67,67,67	3
86	OHX	7	219	7/7	0.98	0.08	67,67,67,67	2
86	OHX	2	2014	7/7	0.98	0.06	130,130,130,130	7
86	OHX	2	2015	7/7	0.98	0.06	90,90,90,90	4
86	OHX	1	3810	7/7	0.98	0.12	62,62,62,62	3
86	OHX	5	4021	7/7	0.98	0.11	36,36,36,36	2
85	MG	5	3457	1/1	0.98	0.17	38,38,38,38	0
86	OHX	8	214	7/7	0.98	0.11	62,62,62,62	4
86	OHX	1	3812	7/7	0.98	0.11	88,88,88,88	3
86	OHX	1	3813	7/7	0.98	0.10	52,52,52,52	2
86	OHX	1	3814	7/7	0.98	0.14	76,76,76,76	3
86	OHX	1	3815	7/7	0.98	0.10	85,85,85,85	3
86	OHX	6	2079	7/7	0.98	0.09	51,51,51,51	3
86	OHX	8	220	7/7	0.98	0.09	44,44,44,44	3
86	OHX	1	3816	7/7	0.98	0.15	62,62,62,62	5
85	MG	5	3559	1/1	0.98	0.31	22,22,22,22	0
86	OHX	1	3819	7/7	0.98	0.09	81,81,81,81	3
85	MG	5	3560	1/1	0.98	0.38	27,27,27,27	0
86	OHX	8	225	7/7	0.98	0.08	40,40,40,40	3
86	OHX	5	3843	7/7	0.98	0.11	64,64,64,64	1
85	MG	1	3632	1/1	0.98	0.25	47,47,47,47	0
86	OHX	6	2085	7/7	0.98	0.12	76,76,76,76	2
86	OHX	5	3855	7/7	0.98	0.13	71,71,71,71	3
85	MG	6	2000	1/1	0.98	0.28	48,48,48,48	0
86	OHX	1	3826	7/7	0.98	0.11	84,84,84,84	4
86	OHX	13	403	7/7	0.98	0.10	50,50,50,50	3
86	OHX	5	3860	7/7	0.98	0.10	88,88,88,88	3
86	OHX	5	3862	7/7	0.98	0.10	47,47,47,47	2
86	OHX	5	3865	7/7	0.98	0.10	86,86,86,86	1
86	OHX	1	3921	7/7	0.98	0.08	82,82,82,82	3
86	OHX	5	3867	7/7	0.98	0.08	126,126,126,126	2
86	OHX	5	3868	7/7	0.98	0.13	74,74,74,74	2
85	MG	5	3601	1/1	0.98	0.23	26,26,26,26	0
86	OHX	1	3923	7/7	0.98	0.09	40,40,40,40	3
86	OHX	1	3830	7/7	0.98	0.12	99,99,99,99	3
85	MG	1	3734	1/1	0.98	0.34	35,35,35,35	1
86	OHX	m5	305	7/7	0.98	0.14	54,54,54,54	3
85	MG	1	3706	1/1	0.98	0.12	38,38,38,38	0
86	OHX	m6	201	7/7	0.98	0.13	36,36,36,36	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	2	2073	7/7	0.98	0.09	63,63,63,63	6
86	OHX	5	3879	7/7	0.98	0.10	59,59,59,59	3
86	OHX	5	3881	7/7	0.98	0.08	96,96,96,96	2
86	OHX	n3	202	7/7	0.98	0.08	60,60,60,60	3
86	OHX	5	3882	7/7	0.98	0.10	89,89,89,89	3
86	OHX	5	3884	7/7	0.98	0.10	63,63,63,63	3
85	MG	7	206	1/1	0.98	0.14	34,34,34,34	0
86	OHX	o7	503	7/7	0.98	0.14	62,62,62,62	1
86	OHX	5	3890	7/7	0.98	0.11	69,69,69,69	3
86	OHX	5	3891	7/7	0.98	0.11	66,66,66,66	4
86	OHX	5	3892	7/7	0.98	0.14	63,63,63,63	3
87	ZN	Q0	500	1/1	0.98	0.03	54,54,54,54	0
86	OHX	5	3894	7/7	0.98	0.15	50,50,50,50	2
87	ZN	e1	501	1/1	0.98	0.05	173,173,173,173	0
87	ZN	q2	202	1/1	0.98	0.08	71,71,71,71	0
88	SPS	1	4113	23/23	0.98	0.07	39,42,55,58	0
86	OHX	1	3929	7/7	0.98	0.10	53,53,53,53	4
86	OHX	5	3896	7/7	0.98	0.10	42,42,42,42	4
86	OHX	5	3899	7/7	0.98	0.12	49,49,49,49	3
86	OHX	1	3835	7/7	0.98	0.14	62,62,62,62	1
89	PRO	C	101	7/8	0.98	0.09	29,29,51,51	0
86	OHX	1	3788	7/7	0.99	0.08	58,58,58,58	4
86	OHX	5	3861	7/7	0.99	0.09	46,46,46,46	3
86	OHX	1	3789	7/7	0.99	0.07	74,74,74,74	2
86	OHX	5	3863	7/7	0.99	0.10	85,85,85,85	3
86	OHX	5	3864	7/7	0.99	0.07	88,88,88,88	3
86	OHX	4	216	7/7	0.99	0.10	59,59,59,59	3
86	OHX	1	3790	7/7	0.99	0.09	48,48,48,48	3
86	OHX	1	3791	7/7	0.99	0.10	41,41,41,41	2
86	OHX	2	2001	7/7	0.99	0.07	120,120,120,120	2
85	MG	5	3582	1/1	0.99	0.35	31,31,31,31	0
86	OHX	5	3870	7/7	0.99	0.12	76,76,76,76	5
86	OHX	2	2003	7/7	0.99	0.11	76,76,76,76	5
85	MG	1	3574	1/1	0.99	0.33	30,30,30,30	0
86	OHX	5	3873	7/7	0.99	0.08	58,58,58,58	4
86	OHX	1	3847	7/7	0.99	0.10	56,56,56,56	3
85	MG	1	3668	1/1	0.99	0.04	38,38,38,38	1
86	OHX	5	4000	7/7	0.99	0.07	45,45,45,45	2
86	OHX	1	3797	7/7	0.99	0.07	54,54,54,54	2
86	OHX	5	3877	7/7	0.99	0.07	62,62,62,62	3
86	OHX	5	3878	7/7	0.99	0.11	73,73,73,73	3
86	OHX	1	3850	7/7	0.99	0.12	47,47,47,47	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	3880	7/7	0.99	0.08	47,47,47,47	3
86	OHX	1	3851	7/7	0.99	0.08	46,46,46,46	3
85	MG	1	3518	1/1	0.99	0.33	31,31,31,31	0
86	OHX	5	3883	7/7	0.99	0.08	53,53,53,53	1
85	MG	5	3593	1/1	0.99	0.30	22,22,22,22	0
86	OHX	5	3885	7/7	0.99	0.07	78,78,78,78	3
86	OHX	5	3886	7/7	0.99	0.12	79,79,79,79	3
86	OHX	5	3887	7/7	0.99	0.08	44,44,44,44	2
86	OHX	5	3888	7/7	0.99	0.10	43,43,43,43	3
86	OHX	1	3854	7/7	0.99	0.09	43,43,43,43	4
86	OHX	2	1995	7/7	0.99	0.13	76,76,76,76	2
86	OHX	2	2009	7/7	0.99	0.10	89,89,89,89	4
86	OHX	1	3802	7/7	0.99	0.08	60,60,60,60	2
86	OHX	5	4018	7/7	0.99	0.09	48,48,48,48	4
86	OHX	5	3893	7/7	0.99	0.10	59,59,59,59	2
86	OHX	1	3803	7/7	0.99	0.09	73,73,73,73	3
86	OHX	1	3804	7/7	0.99	0.11	62,62,62,62	1
85	MG	6	1994	1/1	0.99	0.35	49,49,49,49	0
86	OHX	5	3897	7/7	0.99	0.09	46,46,46,46	5
86	OHX	5	3898	7/7	0.99	0.09	58,58,58,58	4
86	OHX	1	3806	7/7	0.99	0.12	52,52,52,52	2
85	MG	L2	302	1/1	0.99	0.19	41,41,41,41	0
86	OHX	5	3901	7/7	0.99	0.11	43,43,43,43	3
85	MG	5	3732	1/1	0.99	0.14	30,30,30,30	0
86	OHX	1	3865	7/7	0.99	0.08	75,75,75,75	2
86	OHX	1	3809	7/7	0.99	0.11	80,80,80,80	2
86	OHX	1	3763	7/7	0.99	0.10	58,58,58,58	2
86	OHX	1	3765	7/7	0.99	0.11	65,65,65,65	2
86	OHX	5	3907	7/7	0.99	0.09	63,63,63,63	3
86	OHX	5	3908	7/7	0.99	0.09	45,45,45,45	4
86	OHX	1	3766	7/7	0.99	0.09	61,61,61,61	2
86	OHX	1	3767	7/7	0.99	0.11	77,77,77,77	2
86	OHX	5	3911	7/7	0.99	0.10	44,44,44,44	4
86	OHX	1	3769	7/7	0.99	0.07	64,64,64,64	2
86	OHX	N9	101	7/7	0.99	0.08	64,64,64,64	1
86	OHX	1	3771	7/7	0.99	0.07	59,59,59,59	2
86	OHX	1	3772	7/7	0.99	0.08	67,67,67,67	2
86	OHX	1	3773	7/7	0.99	0.10	49,49,49,49	2
86	OHX	1	3818	7/7	0.99	0.09	62,62,62,62	2
86	OHX	1	3774	7/7	0.99	0.09	71,71,71,71	3
86	OHX	1	3775	7/7	0.99	0.12	66,66,66,66	2
86	OHX	6	2012	7/7	0.99	0.12	70,70,70,70	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	6	2013	7/7	0.99	0.08	87,87,87,87	2
86	OHX	6	2014	7/7	0.99	0.09	76,76,76,76	3
86	OHX	5	3923	7/7	0.99	0.13	41,41,41,41	1
86	OHX	7	217	7/7	0.99	0.08	40,40,40,40	1
86	OHX	6	2015	7/7	0.99	0.07	78,78,78,78	3
85	MG	1	3525	1/1	0.99	0.41	35,35,35,35	0
86	OHX	6	2018	7/7	0.99	0.09	90,90,90,90	2
86	OHX	6	2019	7/7	0.99	0.12	79,79,79,79	2
86	OHX	1	3822	7/7	0.99	0.09	50,50,50,50	4
86	OHX	6	2021	7/7	0.99	0.08	69,69,69,69	3
86	OHX	6	2022	7/7	0.99	0.07	67,67,67,67	2
86	OHX	8	212	7/7	0.99	0.10	57,57,57,57	3
86	OHX	8	213	7/7	0.99	0.07	57,57,57,57	2
86	OHX	6	2023	7/7	0.99	0.10	80,80,80,80	3
86	OHX	6	2024	7/7	0.99	0.07	99,99,99,99	3
86	OHX	1	3823	7/7	0.99	0.09	111,111,111,111	4
86	OHX	6	2026	7/7	0.99	0.10	66,66,66,66	1
86	OHX	6	2027	7/7	0.99	0.10	76,76,76,76	2
86	OHX	6	2028	7/7	0.99	0.08	63,63,63,63	2
86	OHX	1	3824	7/7	0.99	0.09	68,68,68,68	3
86	OHX	6	2030	7/7	0.99	0.09	57,57,57,57	2
86	OHX	1	3777	7/7	0.99	0.10	61,61,61,61	3
86	OHX	s1	301	7/7	0.99	0.10	95,95,95,95	2
86	OHX	1	3778	7/7	0.99	0.09	64,64,64,64	1
86	OHX	1	3827	7/7	0.99	0.08	45,45,45,45	4
86	OHX	6	2034	7/7	0.99	0.09	66,66,66,66	5
86	OHX	1	3828	7/7	0.99	0.09	63,63,63,63	2
86	OHX	1	3780	7/7	0.99	0.08	75,75,75,75	1
86	OHX	1	3781	7/7	0.99	0.09	76,76,76,76	2
86	OHX	6	2038	7/7	0.99	0.09	61,61,61,61	5
86	OHX	3	209	7/7	0.99	0.08	76,76,76,76	4
86	OHX	2	2028	7/7	0.99	0.07	108,108,108,108	5
86	OHX	1	3783	7/7	0.99	0.08	83,83,83,83	2
86	OHX	6	2042	7/7	0.99	0.11	62,62,62,62	3
86	OHX	5	3819	7/7	0.99	0.14	51,51,51,51	3
86	OHX	5	3821	7/7	0.99	0.11	64,64,64,64	2
86	OHX	5	3823	7/7	0.99	0.14	53,53,53,53	2
86	OHX	5	3825	7/7	0.99	0.09	58,58,58,58	1
86	OHX	5	3827	7/7	0.99	0.09	80,80,80,80	1
86	OHX	5	3828	7/7	0.99	0.09	50,50,50,50	3
86	OHX	5	3830	7/7	0.99	0.09	67,67,67,67	0
86	OHX	5	3831	7/7	0.99	0.09	61,61,61,61	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
86	OHX	5	3832	7/7	0.99	0.09	56,56,56,56	2
86	OHX	5	3833	7/7	0.99	0.08	59,59,59,59	2
86	OHX	5	3834	7/7	0.99	0.11	51,51,51,51	1
86	OHX	5	3835	7/7	0.99	0.07	54,54,54,54	1
86	OHX	5	3836	7/7	0.99	0.11	65,65,65,65	3
86	OHX	5	3839	7/7	0.99	0.08	64,64,64,64	2
86	OHX	5	3840	7/7	0.99	0.09	65,65,65,65	2
86	OHX	n9	101	7/7	0.99	0.08	62,62,62,62	2
86	OHX	1	3784	7/7	0.99	0.11	73,73,73,73	2
86	OHX	5	3844	7/7	0.99	0.10	62,62,62,62	2
86	OHX	1	3785	7/7	0.99	0.11	59,59,59,59	2
86	OHX	1	3786	7/7	0.99	0.10	94,94,94,94	3
86	OHX	5	3847	7/7	0.99	0.10	48,48,48,48	1
87	ZN	D6	500	1/1	0.99	0.04	103,103,103,103	0
86	OHX	5	3848	7/7	0.99	0.09	54,54,54,54	1
87	ZN	D9	101	1/1	0.99	0.03	89,89,89,89	0
86	OHX	5	3849	7/7	0.99	0.08	100,100,100,100	3
86	OHX	5	3850	7/7	0.99	0.10	51,51,51,51	2
87	ZN	Q2	501	1/1	0.99	0.08	77,77,77,77	0
87	ZN	d6	101	1/1	0.99	0.07	84,84,84,84	0
86	OHX	5	3851	7/7	0.99	0.11	55,55,55,55	4
87	ZN	d9	101	1/1	0.99	0.03	91,91,91,91	0
86	OHX	5	3852	7/7	0.99	0.12	55,55,55,55	2
86	OHX	5	3853	7/7	0.99	0.08	56,56,56,56	3
86	OHX	5	3854	7/7	0.99	0.07	78,78,78,78	2
86	OHX	2	2000	7/7	0.99	0.10	105,105,105,105	3
86	OHX	1	3837	7/7	0.99	0.09	60,60,60,60	2
86	OHX	5	3857	7/7	0.99	0.10	54,54,54,54	1
86	OHX	1	3838	7/7	0.99	0.10	52,52,52,52	3
86	OHX	5	3859	7/7	0.99	0.10	55,55,55,55	1
86	OHX	5	3842	7/7	1.00	0.07	38,38,38,38	3
86	OHX	1	3768	7/7	1.00	0.08	52,52,52,52	2
86	OHX	8	211	7/7	1.00	0.07	64,64,64,64	1
86	OHX	5	3824	7/7	1.00	0.08	62,62,62,62	2
86	OHX	1	3779	7/7	1.00	0.07	49,49,49,49	4
86	OHX	5	3826	7/7	1.00	0.08	46,46,46,46	1
86	OHX	1	3762	7/7	1.00	0.08	55,55,55,55	3
86	OHX	1	3770	7/7	1.00	0.09	61,61,61,61	2
86	OHX	5	3829	7/7	1.00	0.08	44,44,44,44	5
87	ZN	O7	102	1/1	1.00	0.01	47,47,47,47	0
86	OHX	1	3860	7/7	1.00	0.09	38,38,38,38	2
86	OHX	M5	303	7/7	1.00	0.09	61,61,61,61	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	ZN	Q3	501	1/1	1.00	0.02	78,78,78,78	0
86	OHX	1	3761	7/7	1.00	0.08	57,57,57,57	1
86	OHX	5	3817	7/7	1.00	0.10	53,53,53,53	4
86	OHX	m5	304	7/7	1.00	0.08	61,61,61,61	2
86	OHX	5	3818	7/7	1.00	0.06	57,57,57,57	0
87	ZN	o7	501	1/1	1.00	0.02	45,45,45,45	0
87	ZN	q0	500	1/1	1.00	0.02	42,42,42,42	0
86	OHX	1	3764	7/7	1.00	0.10	65,65,65,65	2
87	ZN	q3	501	1/1	1.00	0.02	62,62,62,62	0
86	OHX	5	3820	7/7	1.00	0.10	52,52,52,52	3
86	OHX	5	3837	7/7	1.00	0.07	71,71,71,71	0
86	OHX	5	3838	7/7	1.00	0.07	58,58,58,58	2
86	OHX	6	2017	7/7	1.00	0.09	59,59,59,59	2
86	OHX	5	3822	7/7	1.00	0.09	61,61,61,61	2
86	OHX	5	3841	7/7	1.00	0.06	51,51,51,51	1

5.5 Other polymers [i](#)

There are no such residues in this entry.