



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 11:17 PM BST

PDB ID : 4V88
Title : The structure of the eukaryotic ribosome at 3.0 Å resolution.
Authors : Ben-Shem, A.; Garreau de Loubresse, N.; Melnikov, S.; Jenner, L.; Yusupova, G.; Yusupov, M.
Deposited on : 2011-10-11
Resolution : 3.00 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

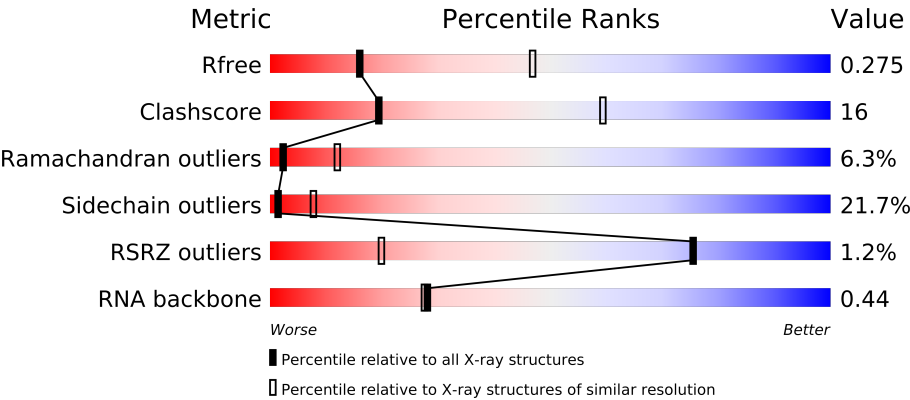
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A2	1800	
2	AA	252	
2	CA	252	
3	AB	255	
3	CB	255	
4	AC	254	
4	CC	254	
5	AD	240	
5	CD	240	
6	AE	261	
6	CE	261	
7	AF	225	

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Mol	Chain	Length	Quality of chain
7	CF	225	
8	AG	236	
8	CG	236	
9	AH	190	
9	CH	190	
10	AI	200	
10	CI	200	
11	AJ	197	
11	CJ	197	
12	AK	105	
12	CK	105	
13	AL	156	
13	CL	156	
14	AM	143	
14	CM	143	
15	AN	151	
15	CN	151	
16	AO	137	
16	CO	137	
17	AP	142	
17	CP	142	
18	AQ	143	
18	CQ	143	
19	AR	136	
19	CR	136	
20	AS	146	
20	CS	146	
21	AT	144	
21	CT	144	
22	AU	121	
22	CU	121	
23	AV	87	
23	CV	87	
24	AW	130	
24	CW	130	
25	AX	145	
25	CX	145	
26	AY	135	
26	CY	135	
27	AZ	108	
27	CZ	108	
28	Aa	119	

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Mol	Chain	Length	Quality of chain
28	Ca	119	
29	Ab	82	
29	Cb	82	
30	Ac	67	
30	Cc	67	
31	Ad	56	
31	Cd	56	
32	Ae	63	
32	Ce	63	
33	Af	152	
34	Ag	319	
34	Cg	319	
35	Ah	273	
36	A1	3396	
36	A5	3396	
37	A3	121	
37	A7	121	
38	A4	158	
38	A8	158	
39	BA	254	
39	DA	254	
40	BB	387	
40	DB	387	
41	BC	362	
41	DC	362	
42	BD	297	
42	DD	297	
43	BE	176	
43	DE	176	
44	BF	244	
44	DF	244	
45	BG	256	
45	DG	256	
46	BH	191	
46	DH	191	
47	BI	221	
47	DI	221	
48	BJ	174	
48	DJ	174	
49	BL	199	
49	DL	199	
50	BM	138	

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Mol	Chain	Length	Quality of chain
50	DM	138	
51	BN	204	
51	DN	204	
52	BO	219	
52	DO	219	
53	BP	184	
53	DP	184	
54	BQ	186	
54	DQ	186	
55	BR	189	
55	DR	189	
56	BS	172	
56	DS	172	
57	BT	160	
57	DT	160	
58	BU	121	
58	DU	121	
59	BV	137	
59	DV	137	
60	BW	155	
60	DW	155	
61	BX	142	
61	DX	142	
62	BY	127	
62	DY	127	
63	BZ	136	
63	DZ	136	
64	Ba	149	
64	Da	149	
65	Bb	59	
65	Db	59	
66	Bc	105	
66	Dc	105	
67	Bd	113	
67	Dd	113	
68	Be	130	
68	De	130	
69	Bf	107	
69	Df	107	
70	Bg	121	
70	Dg	121	
71	Bh	120	

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Mol	Chain	Length	Quality of chain
71	Dh	120	
72	Bi	100	
72	Di	100	
73	Bj	88	
73	Dj	88	
74	Bk	78	
74	Dk	78	
75	Bl	51	
75	Dl	51	
76	Bm	128	
76	Dm	128	
77	Bn	25	
77	Dn	25	
78	Bo	106	
78	Do	106	
79	Bp	92	
79	Dp	92	
80	A6	1800	
81	Cf	152	
82	Ch	273	
83	DK	155	
84	Dq	312	
85	Dr	47	
86	Ds	46	

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 416785 atoms, of which 0 are hydrogen and 0 are deuterium.

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	A2	1781	Total	C	N	O	P	0	1	0
			37835	16910	6661	12482	1782			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AA	206	Total	C	N	O	S	0	0	0
			1577	1014	278	283	2			
2	CA	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	AB	214	Total	C	N	O	S	0	0	0
			1709	1084	310	311	4			
3	CB	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	AC	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			
4	CC	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	AD	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	CD	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	AE	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			
6	CE	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	AF	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			
7	CF	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	AG	226	Total	C	N	O	S	0	0	0
			1799	1129	346	321	3			
8	CG	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	AH	184	Total	C	N	O	0	0	0
			1481	951	265	265			
9	CH	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	AI	188	Total	C	N	O	0	0	0
			1489	925	298	264			
10	CI	188	Total	C	N	O	0	0	0
			1489	925	298	264			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AJ	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			
11	CJ	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	AK	96	Total	C	N	O	S	0	0	0
			772	499	126	145	2			
12	CK	96	Total	C	N	O	S	0	0	0
			761	490	125	144	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AN	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			
15	CN	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	AO	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			
16	CO	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	AP	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			
17	CP	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	AQ	141	Total	C	N	O		0	0	0
			1105	708	203	194				
18	CQ	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	AR	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			
19	CR	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	AS	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			
20	CS	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	AT	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	CT	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	AU	107	Total	C	N	O	S	0	0	0
			855	539	156	159	1			
22	CU	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	AV	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			
23	CV	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	AW	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			
24	CW	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	AX	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			
25	CX	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	AY	134	Total	C	N	O	0	0	0
			1073	676	208	189			
26	CY	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	AZ	70	Total	C	N	O	0	0	0
			563	360	104	99			
27	CZ	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	Aa	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			
28	Ca	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	Ab	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			
29	Cb	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	Ac	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			
30	Cc	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	Ad	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			
31	Cd	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	Ae	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			
32	Ce	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	Af	71	Total	C	N	O	S	0	0	0
			516	328	93	91	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Af	82	UNK	LYS	SEE REMARK 999	UNP P05759
Af	83	UNK	LYS	SEE REMARK 999	UNP P05759
Af	84	UNK	VAL	SEE REMARK 999	UNP P05759
Af	85	UNK	TYR	SEE REMARK 999	UNP P05759
Af	86	UNK	THR	SEE REMARK 999	UNP P05759
Af	87	UNK	THR	SEE REMARK 999	UNP P05759
Af	88	UNK	PRO	SEE REMARK 999	UNP P05759
Af	89	UNK	LYS	SEE REMARK 999	UNP P05759
Af	90	UNK	LYS	SEE REMARK 999	UNP P05759
Af	91	UNK	ILE	SEE REMARK 999	UNP P05759
Af	92	UNK	LYS	SEE REMARK 999	UNP P05759
Af	93	UNK	HIS	SEE REMARK 999	UNP P05759
Af	94	UNK	LYS	SEE REMARK 999	UNP P05759
Af	95	UNK	HIS	SEE REMARK 999	UNP P05759
Af	96	UNK	LYS	SEE REMARK 999	UNP P05759
Af	97	UNK	LYS	SEE REMARK 999	UNP P05759
Af	98	UNK	VAL	SEE REMARK 999	UNP P05759
Af	99	UNK	LYS	SEE REMARK 999	UNP P05759
Af	100	UNK	LEU	SEE REMARK 999	UNP P05759
Af	101	UNK	ALA	SEE REMARK 999	UNP P05759

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein (ASC1, RACK1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	Ag	318	Total	C	N	O	S	0	0	0
			2437	1541	418	470	8			
34	Cg	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	Ah	159	Total	C	N	O	0	0	0
			1105	653	221	231			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ah	9	UNK	GLY	SEE REMARK 999	UNP P39015
Ah	10	UNK	ASN	SEE REMARK 999	UNP P39015
Ah	11	UNK	ASP	SEE REMARK 999	UNP P39015
Ah	12	UNK	VAL	SEE REMARK 999	UNP P39015
Ah	13	UNK	GLU	SEE REMARK 999	UNP P39015
Ah	14	UNK	ASP	SEE REMARK 999	UNP P39015
Ah	15	UNK	ALA	SEE REMARK 999	UNP P39015
Ah	16	UNK	ASP	SEE REMARK 999	UNP P39015
Ah	17	UNK	VAL	SEE REMARK 999	UNP P39015
Ah	18	UNK	VAL	SEE REMARK 999	UNP P39015
Ah	19	UNK	VAL	SEE REMARK 999	UNP P39015
Ah	20	UNK	LEU	SEE REMARK 999	UNP P39015
Ah	151	UNK	LEU	SEE REMARK 999	UNP P39015
Ah	152	UNK	GLN	SEE REMARK 999	UNP P39015
Ah	153	UNK	ASP	SEE REMARK 999	UNP P39015
Ah	154	UNK	TYR	SEE REMARK 999	UNP P39015
Ah	155	UNK	LEU	SEE REMARK 999	UNP P39015
Ah	156	UNK	ASN	SEE REMARK 999	UNP P39015
Ah	157	UNK	GLN	SEE REMARK 999	UNP P39015
Ah	158	UNK	GLN	SEE REMARK 999	UNP P39015
Ah	159	UNK	ALA	SEE REMARK 999	UNP P39015
Ah	160	UNK	ASN	SEE REMARK 999	UNP P39015
Ah	161	UNK	ASN	SEE REMARK 999	UNP P39015
Ah	162	UNK	GLN	SEE REMARK 999	UNP P39015
Ah	163	UNK	PHE	SEE REMARK 999	UNP P39015
Ah	164	UNK	ASN	SEE REMARK 999	UNP P39015
Ah	165	UNK	LYS	SEE REMARK 999	UNP P39015
Ah	166	UNK	VAL	SEE REMARK 999	UNP P39015
Ah	167	UNK	PRO	SEE REMARK 999	UNP P39015
Ah	168	UNK	GLU	SEE REMARK 999	UNP P39015
Ah	169	UNK	ALA	SEE REMARK 999	UNP P39015
Ah	170	UNK	LYS	SEE REMARK 999	UNP P39015
Ah	171	UNK	LYS	SEE REMARK 999	UNP P39015
Ah	172	UNK	VAL	SEE REMARK 999	UNP P39015
Ah	173	UNK	GLU	SEE REMARK 999	UNP P39015
Ah	174	UNK	LEU	SEE REMARK 999	UNP P39015

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Chain	Residue	Modelled	Actual	Comment	Reference
Ah	175	UNK	ASP	SEE REMARK 999	UNP P39015
Ah	176	UNK	ALA	SEE REMARK 999	UNP P39015

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	A1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			
36	A5	3150	Total	C	N	O	P	0	0	0
			67376	30095	12145	21987	3149			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	A3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
37	A7	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	A4	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			
38	A8	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	BA	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	DA	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	BB	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
40	DB	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	BC	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
41	DC	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	BD	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
42	DD	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	BE	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
43	DE	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	BF	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
44	DF	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	BG	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	DG	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BH	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
46	DH	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	BI	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			
47	DI	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	BJ	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			
48	DJ	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BL	193	Total	C	N	O	S	0	0	0
			1543	962	315	266				
49	DL	194	Total	C	N	O	S	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	BM	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			
50	DM	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	BN	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	DN	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, 60S ribosomal protein L16-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BO	197	Total	C	N	O	S	0	197	0
			3119	2008	581	528	2			
52	DO	197	Total	C	N	O	S	0	197	0
			3119	2008	581	528	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BP	183	Total	C	N	O	S	0	0	0
			1420	882	281	257				
53	DP	155	Total	C	N	O	S	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	BQ	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			
54	DQ	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	BR	188	Total	C	N	O	S	0	0	0
			1521	935	326	260				
55	DR	188	Total	C	N	O	S	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	BS	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
56	DS	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	BT	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			
57	DT	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	BU	100	Total	C	N	O		0	0	0
			796	516	131	149				
58	DU	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	BV	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
59	DV	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	BW	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			
60	DW	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	BX	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			
61	DX	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	BY	126	Total	C	N	O	0	0	0
			993	625	192	176			
62	DY	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	BZ	135	Total	C	N	O	0	0	0
			1092	710	202	180			
63	DZ	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	Ba	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			
64	Da	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	Bb	58	Total	C	N	O	0	0	0
			462	289	100	73			
65	Db	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	Bc	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			
66	Dc	100	Total	C	N	O	S	0	0	0
			767	492	128	146	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	Bd	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	Dd	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	Be	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			
68	De	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	Bf	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			
69	Df	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	Bg	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			
70	Dg	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	Bh	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			
71	Dh	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	Bi	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			
72	Di	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	Bj	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			
73	Dj	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	Bk	77	Total	C	N	O		0	0	0
			612	391	115	106				
74	Dk	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	Bl	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			
75	Dl	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	Bm	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			
76	Dm	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	Bn	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			
77	Dn	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	Bo	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			
78	Do	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	Bp	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			
79	Dp	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	A6	1795	Total	C	N	O	P	0	1	0
			38021	16989	6669	12567	1796			

- Molecule 81 is a protein called 40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	Cf	76	Total	C	N	O	S	0	0	0
			544	346	98	96	4			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cf	77	UNK	GLY	SEE REMARK 999	UNP P05759
Cf	78	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	79	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	80	UNK	ARG	SEE REMARK 999	UNP P05759
Cf	81	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	82	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	83	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	84	UNK	VAL	SEE REMARK 999	UNP P05759
Cf	85	UNK	TYR	SEE REMARK 999	UNP P05759
Cf	86	UNK	THR	SEE REMARK 999	UNP P05759
Cf	87	UNK	THR	SEE REMARK 999	UNP P05759
Cf	88	UNK	PRO	SEE REMARK 999	UNP P05759
Cf	89	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	90	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	91	UNK	ILE	SEE REMARK 999	UNP P05759

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Chain	Residue	Modelled	Actual	Comment	Reference
Cf	92	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	93	UNK	HIS	SEE REMARK 999	UNP P05759
Cf	94	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	95	UNK	HIS	SEE REMARK 999	UNP P05759
Cf	96	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	97	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	98	UNK	VAL	SEE REMARK 999	UNP P05759
Cf	99	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	100	UNK	LEU	SEE REMARK 999	UNP P05759
Cf	101	UNK	ALA	SEE REMARK 999	UNP P05759

- Molecule 82 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
82	Ch	104	Total	C	N	O	0	0	0
			680	403	140	137			

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ch	119	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	120	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	121	UNK	LYS	SEE REMARK 999	UNP P39015
Ch	122	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	123	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	124	UNK	GLN	SEE REMARK 999	UNP P39015
Ch	125	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	126	UNK	ASP	SEE REMARK 999	UNP P39015
Ch	127	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	128	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	129	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	130	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	131	UNK	ILE	SEE REMARK 999	UNP P39015
Ch	132	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	133	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	134	UNK	ASP	SEE REMARK 999	UNP P39015
Ch	135	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	136	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	137	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	138	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	139	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	155	UNK	LEU	SEE REMARK 999	UNP P39015

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Chain	Residue	Modelled	Actual	Comment	Reference
Ch	156	UNK	ASN	SEE REMARK 999	UNP P39015
Ch	157	UNK	GLN	SEE REMARK 999	UNP P39015
Ch	158	UNK	GLN	SEE REMARK 999	UNP P39015
Ch	159	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	160	UNK	ASN	SEE REMARK 999	UNP P39015
Ch	161	UNK	ASN	SEE REMARK 999	UNP P39015
Ch	162	UNK	GLN	SEE REMARK 999	UNP P39015
Ch	163	UNK	PHE	SEE REMARK 999	UNP P39015
Ch	164	UNK	ASN	SEE REMARK 999	UNP P39015
Ch	165	UNK	LYS	SEE REMARK 999	UNP P39015
Ch	166	UNK	VAL	SEE REMARK 999	UNP P39015
Ch	167	UNK	PRO	SEE REMARK 999	UNP P39015
Ch	168	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	169	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	170	UNK	LYS	SEE REMARK 999	UNP P39015
Ch	171	UNK	LYS	SEE REMARK 999	UNP P39015
Ch	172	UNK	VAL	SEE REMARK 999	UNP P39015
Ch	173	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	174	UNK	LEU	SEE REMARK 999	UNP P39015

- Molecule 83 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
83	DK	150	Total	C	N	O	0	0	0
			750	450	150	150			

- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

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

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Dq	199	UNK	SER	SEE REMARK 999	UNP P05317
Dq	200	UNK	SER	SEE REMARK 999	UNP P05317
Dq	201	UNK	ILE	SEE REMARK 999	UNP P05317
Dq	202	UNK	LEU	SEE REMARK 999	UNP P05317
Dq	203	UNK	ASP	SEE REMARK 999	UNP P05317
Dq	204	UNK	ILE	SEE REMARK 999	UNP P05317
Dq	205	UNK	THR	SEE REMARK 999	UNP P05317

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Chain	Residue	Modelled	Actual	Comment	Reference
Dq	206	UNK	ASP	SEE REMARK 999	UNP P05317
Dq	207	UNK	GLU	SEE REMARK 999	UNP P05317
Dq	208	UNK	GLU	SEE REMARK 999	UNP P05317
Dq	209	UNK	LEU	SEE REMARK 999	UNP P05317
Dq	210	UNK	VAL	SEE REMARK 999	UNP P05317
Dq	211	UNK	SER	SEE REMARK 999	UNP P05317
Dq	212	UNK	HIS	SEE REMARK 999	UNP P05317
Dq	213	UNK	PHE	SEE REMARK 999	UNP P05317
Dq	214	UNK	VAL	SEE REMARK 999	UNP P05317
Dq	215	UNK	SER	SEE REMARK 999	UNP P05317
Dq	216	UNK	ALA	SEE REMARK 999	UNP P05317
Dq	217	UNK	VAL	SEE REMARK 999	UNP P05317
Dq	218	UNK	SER	SEE REMARK 999	UNP P05317
Dq	219	UNK	THR	SEE REMARK 999	UNP P05317
Dq	220	UNK	ILE	SEE REMARK 999	UNP P05317
Dq	221	UNK	ALA	SEE REMARK 999	UNP P05317

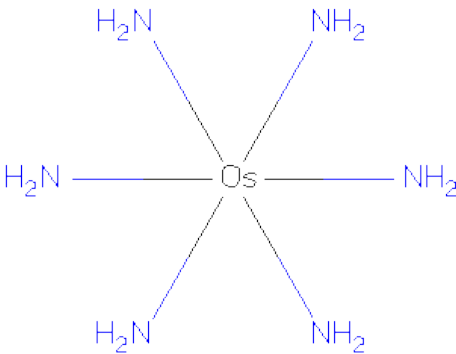
- Molecule 85 is a protein called Ribosomal protein P1 alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
85	Dr	47	Total	C	N	O	0	0	0
			235	141	47	47			

- Molecule 86 is a protein called Ribosomal protein P2 beta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
86	Ds	46	Total	C	N	O	0	0	0
			230	138	46	46			

- Molecule 87 is osmium (III) hexammine (three-letter code: OHX) (formula: H₁₂N₆Os).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	A2	1	Total	N	Os	0	0
			7	6	1		
87	A2	1	Total	N	Os	0	0
			7	6	1		
87	A2	1	Total	N	Os	0	0
			7	6	1		
87	A2	1	Total	N	Os	0	0
			7	6	1		
87	A2	1	Total	N	Os	0	0
			7	6	1		
87	A2	1	Total	N	Os	0	0
			7	6	1		
87	A2	1	Total	N	Os	0	0
			7	6	1		
87	A2	1	Total	N	Os	0	0
			7	6	1		
87	A2	1	Total	N	Os	0	0
			7	6	1		
87	A2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	A2	1	Total	N	Os	0	0
			7	6	1		
87	A2	1	Total	N	Os	0	0
			7	6	1		
87	A2	1	Total	N	Os	0	0
			7	6	1		
87	A2	1	Total	N	Os	0	0
			7	6	1		
87	A2	1	Total	N	Os	0	0
			7	6	1		
87	A2	1	Total	N	Os	0	0
			7	6	1		
87	A2	1	Total	N	Os	0	0
			7	6	1		
87	A2	1	Total	N	Os	0	0
			7	6	1		
87	A2	1	Total	N	Os	0	0
			7	6	1		
87	A2	1	Total	N	Os	0	0
			7	6	1		
87	A2	1	Total	N	Os	0	0
			7	6	1		
87	A2	1	Total	N	Os	0	0
			7	6	1		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	A2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	A1	1	Total	N	Os	0	0
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87	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	A1	1	Total	N	Os	0	0
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87	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	A1	1	Total	N	Os	0	0
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87	A1	1	Total	N	Os	0	0
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87	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	A1	1	Total	N	Os	0	0
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87	A1	1	Total	N	Os	0	0
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87	A1	1	Total	N	Os	0	0
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87	A1	1	Total	N	Os	0	0
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87	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	A1	1	Total	N	Os	0	0
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87	A1	1	Total	N	Os	0	0
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87	A1	1	Total	N	Os	0	0
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87	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	A1	1	Total	N	Os	0	0
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87	A1	1	Total	N	Os	0	0
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87	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	A1	1	Total	N	Os	0	0
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87	A1	1	Total	N	Os	0	0
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87	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	A1	1	Total	N	Os	0	0
			7	6	1		
87	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	A1	1	Total	N	Os	0	0
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87	A1	1	Total	N	Os	0	0
			7	6	1		
87	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	A1	1	Total	N	Os	0	0
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			7	6	1		
87	A1	1	Total	N	Os	0	0
			7	6	1		
87	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	A1	1	Total	N	Os	0	0
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87	A1	1	Total	N	Os	0	0
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87	A1	1	Total	N	Os	0	0
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87	A1	1	Total	N	Os	0	0
			7	6	1		
87	A1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	A1	1	Total	N	Os	0	0
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			7	6	1		
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87	A3	1	Total	N	Os	0	0
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87	A3	1	Total	N	Os	0	0
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87	A3	1	Total	N	Os	0	0
			7	6	1		
87	A4	1	Total	N	Os	0	0
			7	6	1		
87	A4	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	A4	1	Total	N	Os	0	0
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87	A4	1	Total	N	Os	0	0
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87	A4	1	Total	N	Os	0	0
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87	A4	1	Total	N	Os	0	0
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87	A4	1	Total	N	Os	0	0
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87	A4	1	Total	N	Os	0	0
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87	A4	1	Total	N	Os	0	0
			7	6	1		
87	BA	1	Total	N	Os	0	0
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87	BB	1	Total	N	Os	0	0
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87	BB	1	Total	N	Os	0	0
			7	6	1		
87	BC	1	Total	N	Os	0	0
			7	6	1		
87	BD	1	Total	N	Os	0	0
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87	BI	1	Total	N	Os	0	0
			7	6	1		
87	BI	1	Total	N	Os	0	0
			7	6	1		
87	BI	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	BN	1	Total	N	Os	0	0
			7	6	1		
87	BO	1	Total	N	Os	0	0
			7	6	1		
87	BP	1	Total	N	Os	0	0
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87	BP	1	Total	N	Os	0	0
			7	6	1		
87	BR	1	Total	N	Os	0	0
			7	6	1		
87	BT	1	Total	N	Os	0	0
			7	6	1		
87	Bb	1	Total	N	Os	0	0
			7	6	1		
87	Bf	1	Total	N	Os	0	0
			7	6	1		
87	Bj	1	Total	N	Os	0	0
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87	Bj	1	Total	N	Os	0	0
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87	Bj	1	Total	N	Os	0	0
			7	6	1		
87	Bo	1	Total	N	Os	0	0
			7	6	1		
87	A6	1	Total	N	Os	0	0
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87	A6	1	Total	N	Os	0	0
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87	A6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	A7	1	Total	N	Os	0	0
			7	6	1		
87	A7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	A7	1	Total	N	Os	0	0
			7	6	1		
87	A7	1	Total	N	Os	0	0
			7	6	1		
87	A7	1	Total	N	Os	0	0
			7	6	1		
87	A7	1	Total	N	Os	0	0
			7	6	1		
87	A7	1	Total	N	Os	0	0
			7	6	1		
87	A7	1	Total	N	Os	0	0
			7	6	1		
87	A8	1	Total	N	Os	0	0
			7	6	1		
87	A8	1	Total	N	Os	0	0
			7	6	1		
87	A8	1	Total	N	Os	0	0
			7	6	1		
87	A8	1	Total	N	Os	0	0
			7	6	1		
87	A8	1	Total	N	Os	0	0
			7	6	1		
87	A8	1	Total	N	Os	0	0
			7	6	1		
87	A8	1	Total	N	Os	0	0
			7	6	1		
87	A8	1	Total	N	Os	0	0
			7	6	1		
87	A8	1	Total	N	Os	0	0
			7	6	1		
87	A8	1	Total	N	Os	0	0
			7	6	1		
87	A8	1	Total	N	Os	0	0
			7	6	1		
87	A8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	A8	1	Total	N	Os	0	0
			7	6	1		
87	A8	1	Total	N	Os	0	0
			7	6	1		
87	A8	1	Total	N	Os	0	0
			7	6	1		
87	A8	1	Total	N	Os	0	0
			7	6	1		
87	A8	1	Total	N	Os	0	0
			7	6	1		
87	DA	1	Total	N	Os	0	0
			7	6	1		
87	DB	1	Total	N	Os	0	0
			7	6	1		
87	DB	1	Total	N	Os	0	0
			7	6	1		
87	DC	1	Total	N	Os	0	0
			7	6	1		
87	DC	1	Total	N	Os	0	0
			7	6	1		
87	DD	1	Total	N	Os	0	0
			7	6	1		
87	DG	1	Total	N	Os	0	0
			7	6	1		
87	DH	1	Total	N	Os	0	0
			7	6	1		
87	DI	1	Total	N	Os	0	0
			7	6	1		
87	DI	1	Total	N	Os	0	0
			7	6	1		
87	DJ	1	Total	N	Os	0	0
			7	6	1		
87	DM	1	Total	N	Os	0	0
			7	6	1		
87	DO	1	Total	N	Os	0	0
			7	6	1		
87	DP	1	Total	N	Os	0	0
			7	6	1		
87	DQ	1	Total	N	Os	0	0
			7	6	1		
87	DR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	DV	1	Total	N	Os	0	0
			7	6	1		
87	Db	1	Total	N	Os	0	0
			7	6	1		
87	De	1	Total	N	Os	0	0
			7	6	1		
87	Df	1	Total	N	Os	0	0
			7	6	1		
87	Dg	1	Total	N	Os	0	0
			7	6	1		
87	Dh	1	Total	N	Os	0	0
			7	6	1		
87	Dj	1	Total	N	Os	0	0
			7	6	1		
87	Do	1	Total	N	Os	0	0
			7	6	1		

- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	De	2	Total	Mg	0	0
			2	2		
88	Dp	3	Total	Mg	0	0
			3	3		
88	AB	2	Total	Mg	0	0
			2	2		
88	DO	8	Total	Mg	0	0
			8	8		
88	AX	1	Total	Mg	0	0
			1	1		
88	BI	4	Total	Mg	0	0
			4	4		
88	Af	1	Total	Mg	0	0
			1	1		
88	BT	1	Total	Mg	0	0
			1	1		
88	Df	4	Total	Mg	0	0
			4	4		
88	Be	2	Total	Mg	0	0
			2	2		
88	CQ	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	BC	6	Total 6	Mg 6	0	0
88	BN	6	Total 6	Mg 6	0	0
88	BY	2	Total 2	Mg 2	0	0
88	Dl	1	Total 1	Mg 1	0	0
88	A4	34	Total 34	Mg 34	0	0
88	Bj	7	Total 7	Mg 7	0	0
88	AL	2	Total 2	Mg 2	0	0
88	DP	7	Total 7	Mg 7	0	0
88	BS	2	Total 2	Mg 2	0	0
88	Da	4	Total 4	Mg 4	0	0
88	CE	1	Total 1	Mg 1	0	0
88	A3	19	Total 19	Mg 19	0	0
88	CZ	1	Total 1	Mg 1	0	0
88	Bo	3	Total 3	Mg 3	0	0
88	DF	4	Total 4	Mg 4	0	0
88	BE	1	Total 1	Mg 1	0	0
88	BP	10	Total 10	Mg 10	0	0
88	Db	1	Total 1	Mg 1	0	0
88	Ba	8	Total 8	Mg 8	0	0
88	Dq	1	Total 1	Mg 1	0	0
88	AE	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	Bl	1	Total 1	Mg 1	0	0
88	DL	1	Total 1	Mg 1	0	0
88	Cd	1	Total 1	Mg 1	0	0
88	BJ	1	Total 1	Mg 1	0	0
88	DV	3	Total 3	Mg 3	0	0
88	Dg	2	Total 2	Mg 2	0	0
88	Bf	1	Total 1	Mg 1	0	0
88	CP	1	Total 1	Mg 1	0	0
88	DA	4	Total 4	Mg 4	0	0
88	BO	8	Total 8	Mg 8	0	0
88	Ad	3	Total 3	Mg 3	0	0
88	Dm	1	Total 1	Mg 1	0	0
88	CI	2	Total 2	Mg 2	0	0
88	A7	26	Total 26	Mg 26	0	0
88	A8	20	Total 20	Mg 20	0	0
88	CS	2	Total 2	Mg 2	0	0
88	DB	13	Total 13	Mg 13	0	0
88	AP	1	Total 1	Mg 1	0	0
88	BA	5	Total 5	Mg 5	0	0
88	DQ	1	Total 1	Mg 1	0	0
88	BL	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	Dn	1	Total 1	Mg 1	0	0
88	A2	171	Total 171	Mg 171	0	0
88	CY	2	Total 2	Mg 2	0	0
88	DH	2	Total 2	Mg 2	0	0
88	AJ	1	Total 1	Mg 1	0	0
88	DG	1	Total 1	Mg 1	0	0
88	Ch	2	Total 2	Mg 2	0	0
88	BF	2	Total 2	Mg 2	0	0
88	DR	1	Total 1	Mg 1	0	0
88	BQ	4	Total 4	Mg 4	0	0
88	CG	2	Total 2	Mg 2	0	0
88	A1	695	Total 695	Mg 695	0	0
88	Bm	1	Total 1	Mg 1	0	0
88	DM	2	Total 2	Mg 2	0	0
88	AI	2	Total 2	Mg 2	0	0
88	DW	1	Total 1	Mg 1	0	0
88	BV	5	Total 5	Mg 5	0	0
88	Dd	1	Total 1	Mg 1	0	0
88	CB	1	Total 1	Mg 1	0	0
88	Bg	1	Total 1	Mg 1	0	0
88	AC	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	DN	1	Total 1	Mg 1	0	0
88	Dj	3	Total 3	Mg 3	0	0
88	A6	239	Total 239	Mg 239	0	0
88	Bd	1	Total 1	Mg 1	0	0
88	AN	1	Total 1	Mg 1	0	0
88	DC	5	Total 5	Mg 5	0	0
88	AS	2	Total 2	Mg 2	0	0
88	BB	4	Total 4	Mg 4	0	0
88	Ca	1	Total 1	Mg 1	0	0
88	Do	1	Total 1	Mg 1	0	0
88	A5	763	Total 763	Mg 763	0	0
88	CX	2	Total 2	Mg 2	0	0
88	DD	7	Total 7	Mg 7	0	0
88	BG	1	Total 1	Mg 1	0	0
88	DS	4	Total 4	Mg 4	0	0
88	BR	4	Total 4	Mg 4	0	0
88	Aa	1	Total 1	Mg 1	0	0
88	CF	2	Total 2	Mg 2	0	0
88	DJ	2	Total 2	Mg 2	0	0
88	DY	2	Total 2	Mg 2	0	0
88	BD	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	DT	3	Total 3	Mg 3	0	0
88	CL	3	Total 3	Mg 3	0	0

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
89	Bo	1	Total 1	Zn 1	0	0
89	Ad	1	Total 1	Zn 1	0	0
89	Ca	1	Total 1	Zn 1	0	0
89	Dj	1	Total 1	Zn 1	0	0
89	Bm	1	Total 1	Zn 1	0	0
89	Dp	1	Total 1	Zn 1	0	0
89	Ab	1	Total 1	Zn 1	0	0
89	Do	1	Total 1	Zn 1	0	0
89	Cb	1	Total 1	Zn 1	0	0
89	Aa	1	Total 1	Zn 1	0	0
89	Cd	1	Total 1	Zn 1	0	0
89	Bp	1	Total 1	Zn 1	0	0
89	Bj	1	Total 1	Zn 1	0	0
89	Cf	1	Total 1	Zn 1	0	0
89	Dm	1	Total 1	Zn 1	0	0
89	Af	1	Total 1	Zn 1	0	0

- Molecule 90 is water.

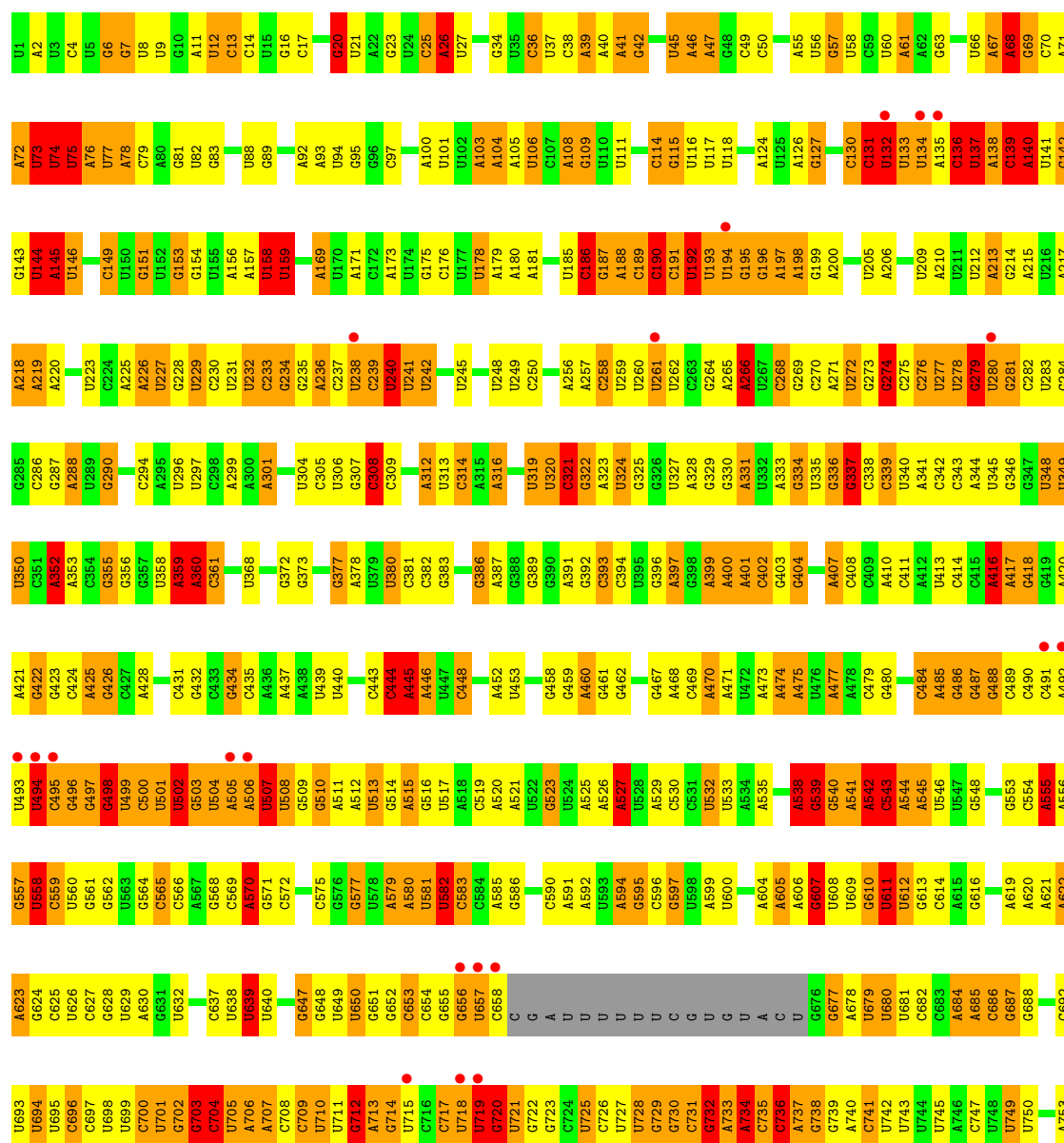
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
90	CI	1	Total 1	O 1	0	0
90	DB	1	Total 1	O 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

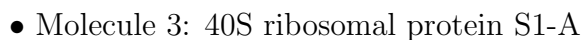
• Molecule 1: 18S RIBOSOMAL RNA

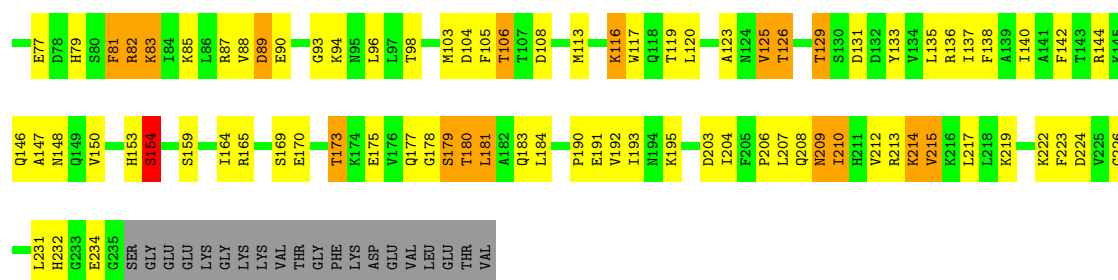
Chain A2: 



G1737	U1738	C1739	A1740	U1741		G1745	A1746	G1747	A1748	G1749	C1751	U1752	A1753	G1754	A1755	U1756	G1757	U1758	C1759	G1760	U1761	A1762	A1763	G1764	A1765	G1766	A1767	G1768	U1769	C1770	A1771	G1772	C1773	A1774	G1775	G1776	C1777	G1778	U1779	A1780	U1781	C1782	G1783	A1784	U1785	A1786	G1787	A1788	U1789	C1790	A1791	G1792	U1793	A1794	U1795	C1796	A1797	U1798	U	A		
A1671	G1672	G1673		U1676	C1677	A1678	U1679	G1680	A1681	U1682	C1683	U1684	G1685	A1686	U1687	A1688	U1689	G1690	A1691	G1692	A1693	U1694	G1695	U1696	A1697	U1698	A1699	U1700	G1701	U1702	A1703	U1704	A1705	U1706	U1707	U1708	C1709	U1710	C1711	A1712	G1713	A1714	C1715	U1716	G1717		G1720	A1721	U1722		G1727	A1728	C1729	U1730	G1663	U1734	U1735	G1736				
A1600	G1601	C1602	G1605	C1606	G1607	U1608		A1611	U1612	G1613	A1614	G1615	U1616	A1617	C1618	G1619	C1620	A1621	U1622	C1623	G1624	C1625		U1628	G1629	U1630	A1631	C1632	A1633	C1634	A1635	C1636		C1639		G1642	U1643	C1644	G1645	C1646	U1647	A1648	G1649	A1650	A1651	C1652	C1653	G1654		U1657	G1658	C1659	A1662	U1666	C1670							
U1532	C1533	G1534	U1535	G1536	C1537	U1538	G1539	U1540	G1541	G1542	A1547	G1548	C1549	A1550	U1551	U1552	U1553	U1554	A1555	U1556	U1557	U1558	A1559	U1560	U1561	C1562	U1563	C1564		C1568	A1569	A1570	C1571	G1572	U1573	A1574	G1575		U1578	U1579		U1582	A1583	U1584	U1585	U1586	A1587	G1588		U1589	G1590	C1591	A1592	A1593	U1594	U1595	C1596					
C1465		A1471	U1472	U1473	U1474	A1475	C1476	G1477	G1478	A1479	U1480	C1481	C1482	A1483	U1484	C1485	G1486	A1487	G1488	U1489	C1490	U1491	A1492	A1493		U1497	G1498	C1499	U1500	C1501	G1502	A1503	U1504	A1505	G1506	U1507	U1508	C1509	U1510	U1511	G1512	U1513	A1514	A1515	A1516	U1517	U1518	U1519	U1520	A1521	U1522	G1523	A1524	A1525		U1528	U1529					
C1393	G1394	U1395	A1396	U1397	U1398	C1399	A1400	A1401	G1402	C1403	U1404	C1405	A1410	A1411	A1412	U1413	U1414	U1415	G1416	A1417		C1420	A1421	A1422		A1427	G1428	C1429	U1430	C1431	G1432	U1433	U1434	U1435	A1436	U1437		C1441	U1442	U1443	A1444	C1445	A1446	C1447	A1448	U1449	U1450	C1451		G1454	G1455	G1456	C1457	G1458	C1459	A1460	C1461	G1462				
A1329	G1330	A1331	C1332	C1333	U1334	U1335	A1336	A1337	C1338	C1339	U1340	A1341	A1344	A1345	A1346	U1347	A1348	G1349	U1350	G1351	U1352	U1353	G1354	C1355		G1358	C1359	A1360	U1361	U1362	U1363	G1364	C1365	U1366	G1367	C1368	U1369	U1370	A1371	U1372		A1375	C1376	U1377	U1378	C1379	U1380	A1381	A1382	G1383	A1384	G1385	U1386	G1387	A1388	U1389	U1390					
U1249	U1250	U1251	C1252	U1253	U1254	G1255	U1256	U1257	U1258	U1259	U1260		G1267	U1268	U1269	G1270		C1274	U1275	G1276	G1277	C1278	C1279	G1280	G1281	U1282		U1286	A1287		U1290	U1291	G1292	U1293	G1294		U1297		U1301	U1302		U1305		U1310	U1311		U1314	U1315	G1316	C1317	G1318	A1319	U1320	A1321	A1322	C1323	A1325					
A1183	A1184	U1185	U1186	U1187	G1188	A1189	C1190	U1191	C1192	U1193	A1194	C1195	A1196	C1197	G1198	G1199	G1200	G1201	A1202	A1203		U1206	C1207	A1208	C1209	C1210		U1214	C1215	C1216	A1217	G1218	A1219	C1220	A1221		U1225	A1226	A1227	G1228	G1229	A1230	U1231	U1232	G1233	A1234	C1235		U1238	U1239	G1240	G1241	A1242	G1243	A1244	G1245	U1246	U1247	C1248			
G1114	U1115	A1116		G1119	U1120	C1121		G1127	C1128	U1129	G1130	A1131	A1132	A1133	C1134		A1137	U1138	A1139		A1142	U1143	U1144	U1145	G1146	A1147		U1157	C1158	C1159	A1160	C1161	C1162	A1163	G1164	G1165	A1166	G1167	U1168	G1169	G1170	A1171	G1172	C1173	C1174			G1178	G1179	C1180	G1181	G1182										
C1034		A1039	G1040	G1041	G1042	A1043		G1046		U1049	G1050	G1051	U1052	G1053		U1057	U1058	U1059	U1060	A1061	A1062	U1063	G1064	U1065	C1066		U1071	C1072	G1073	U1074	C1075		U1079	U1080	A1081	C1082	G1083	A1084	G1085	A1086	A1087		A1091	A1092	A1093		C1096	U1097	U1098	U1099	G1100	A1026	A1027	U959	U960	C1028	U1029	A1030	U1031	G1032	A1113	
U968	C969	A970	G971	G972	A973	U974	C975	G976	A977	U978	A979	G980	U981	U982		G986	G987	A988	U989	C990	A992	A993	G994	A995	U996	U997	U1071	C1072	G1073	G1074	C1075		U1079	U1080	C931	A1081	C1082	G1083	A1084	G1085	A1086	A1087		A1091	A1092	A1093		C1096	U1097	U1098	U1099	G1100	A1026	A1027	U959	U960	C1028	U1029	A1030	U1031	G1032	A1113
A824	G885	U886	U887		A892	U893	U894	G895	A897	U898	A899		G901	G902		G986	G987	A988	U989	C990	A992	A993	G994	A995	U996	U997	U1071	C1072	G1073	G1074	C1075		U1079	U1080	C931	A1081	C1082	G1083	A1084	G1085	A1086	A1087		A1091	A1092	A1093		C1096	U1097	U1098	U1099	G1100	A1026	A1027	U959	U960	C1028	U1029	A1030	U1031	G1032	A1113
U821	U822	G823	G824		C827	U828	A829	U830	U831	U832	U833		U836	G837		G838	U839	U840	U841	C842	U843	G844	G845	G846	A847	C848	C849	U850	U851	C852	U853	U854	A855	U856	U857	G858	A859	U860	U861	A862	A863	U864	A865	G866	G867	G868		G871	U872	U873	C874	G875	U876	U877	U878	U879	C880	A881	U882	C883		
A754	A755	A756	A757	U758	U759	A760		G763	U764	G765	U766	U767	C768			A771	G772	U773	A774	G775	G776	C777	G778	U779	A780	U781	U782	U783	U784	U785	C786	G787	A788	U789	U790		A793	U794	U795	A796		A799	U800	G801	G802		U805	A806		G810	A811	A812	U813	G814	U815	G816	A817	C818	U819	U820		

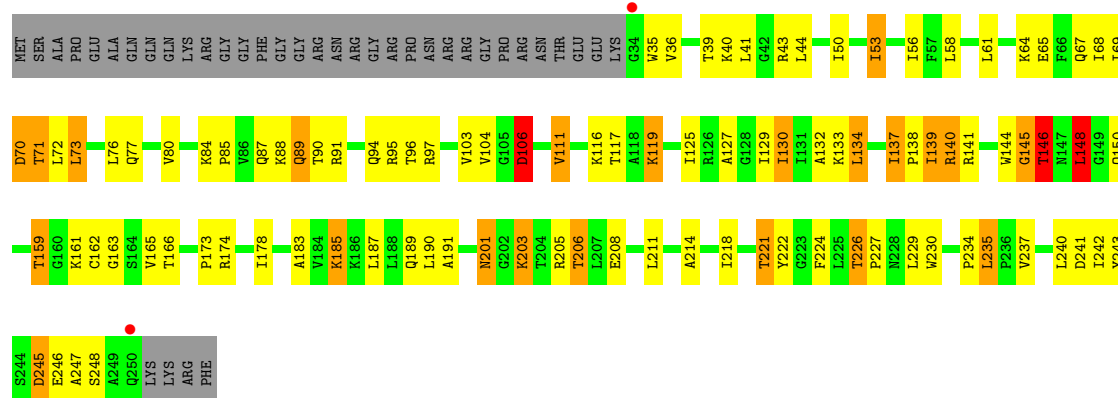
- Molecule 2: 40S ribosomal protein S0-A





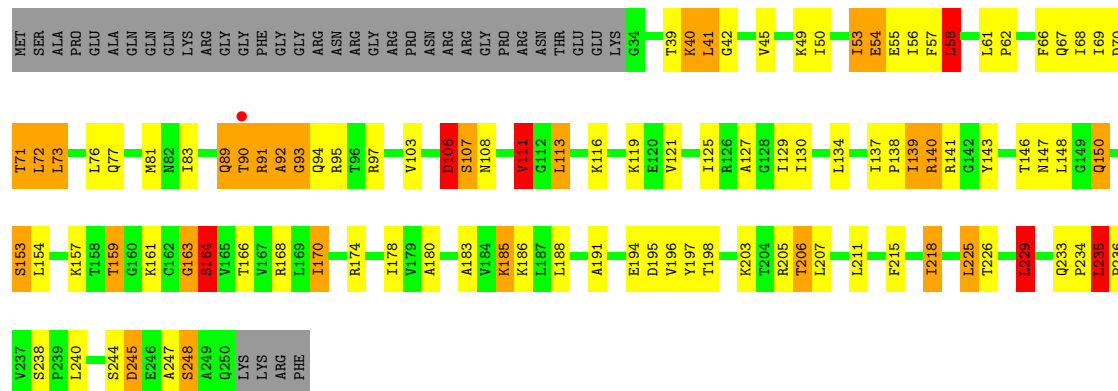
• Molecule 4: 40S ribosomal protein S2

Chain AC:



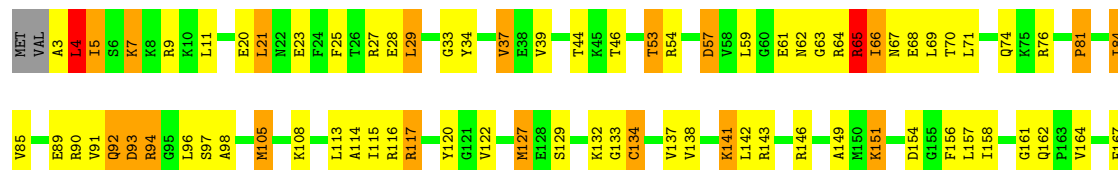
• Molecule 4: 40S ribosomal protein S2

Chain CC:



• Molecule 5: 40S ribosomal protein S3

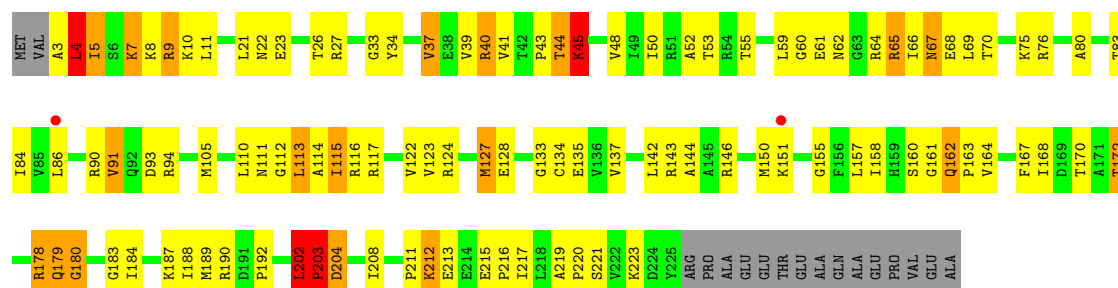
Chain AD:





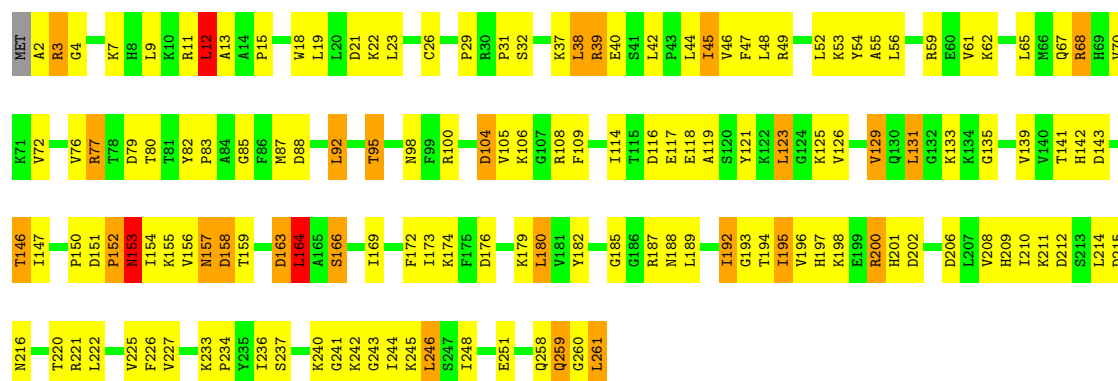
• Molecule 5: 40S ribosomal protein S3

Chain CD:



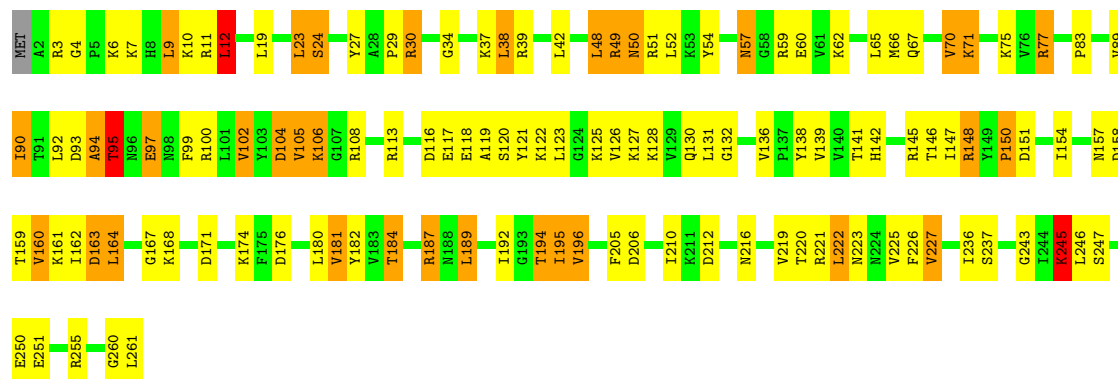
• Molecule 6: 40S ribosomal protein S4-A

Chain AE:



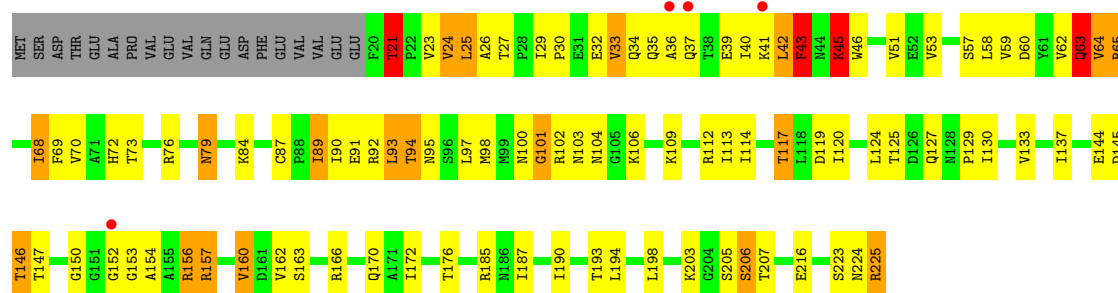
• Molecule 6: 40S ribosomal protein S4-A

Chain CE:



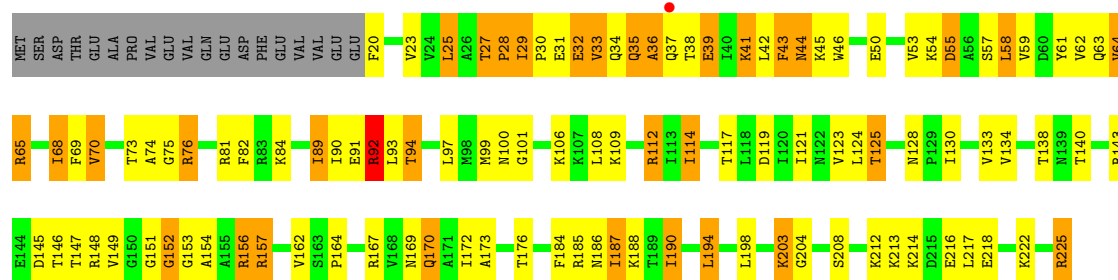
• Molecule 7: 40S ribosomal protein S5

Chain AF:



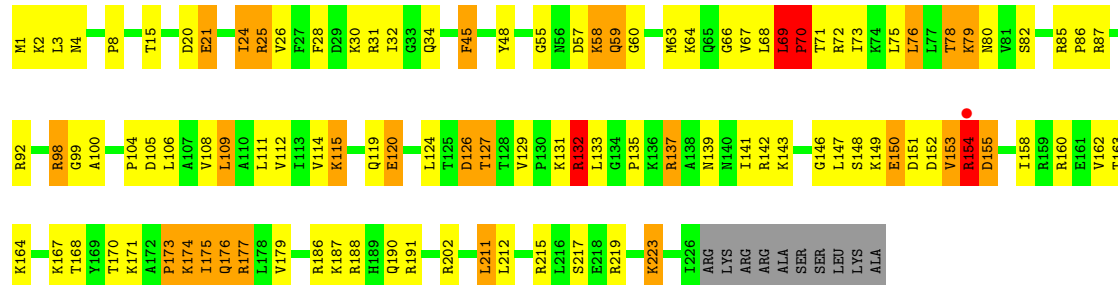
• Molecule 7: 40S ribosomal protein S5

Chain CF:



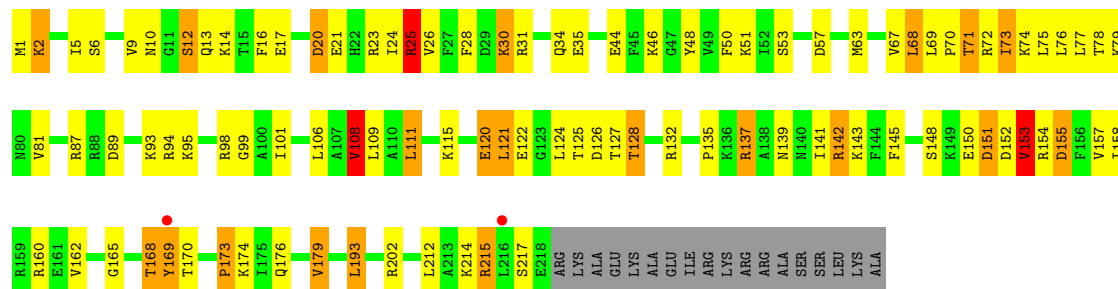
• Molecule 8: 40S ribosomal protein S6-A

Chain AG:



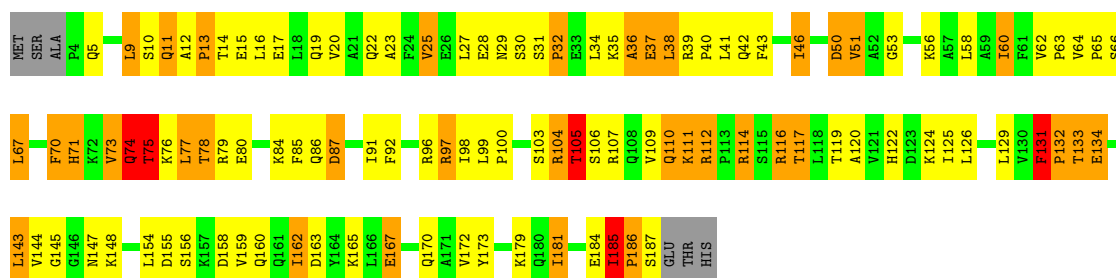
• Molecule 8: 40S ribosomal protein S6-A

Chain CG:



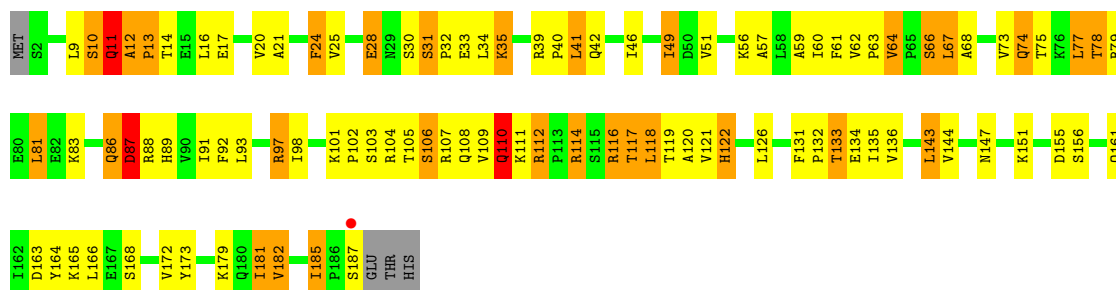
• Molecule 9: 40S ribosomal protein S7-A

Chain AH:



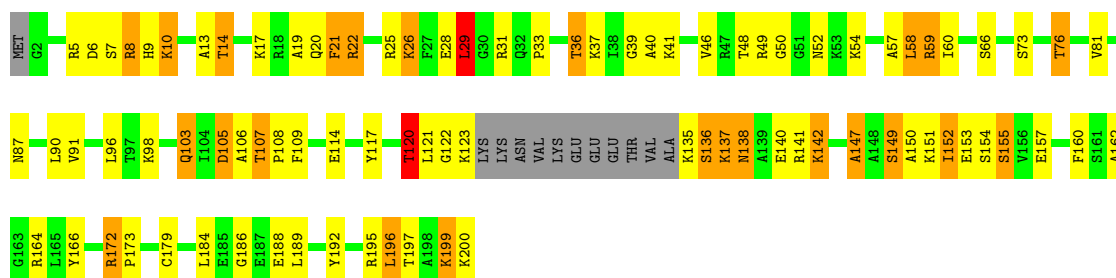
• Molecule 9: 40S ribosomal protein S7-A

Chain CH:



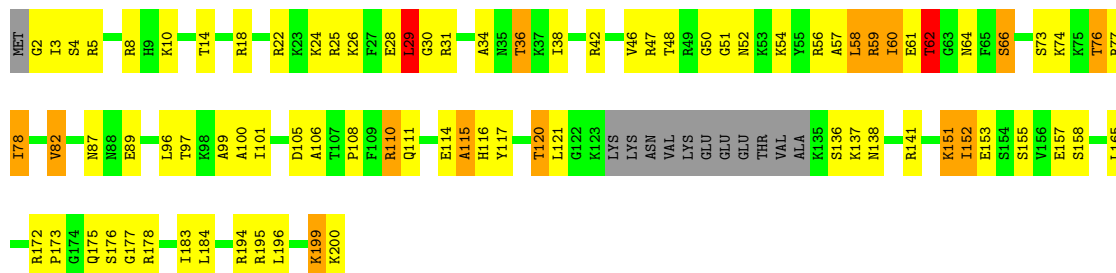
• Molecule 10: 40S ribosomal protein S8-A

Chain AI:



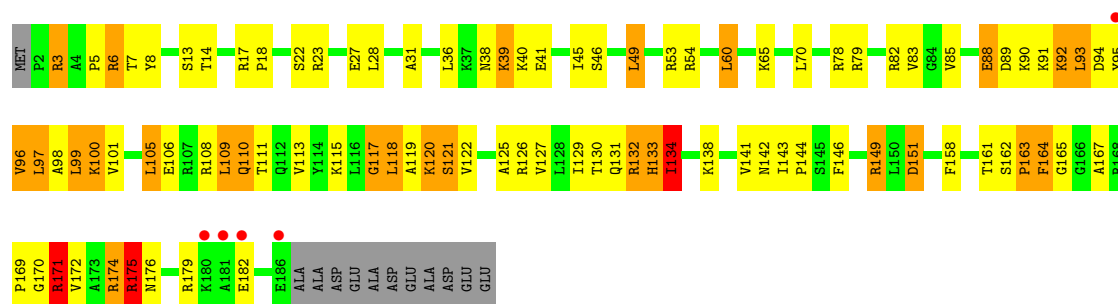
• Molecule 10: 40S ribosomal protein S8-A

Chain CI:



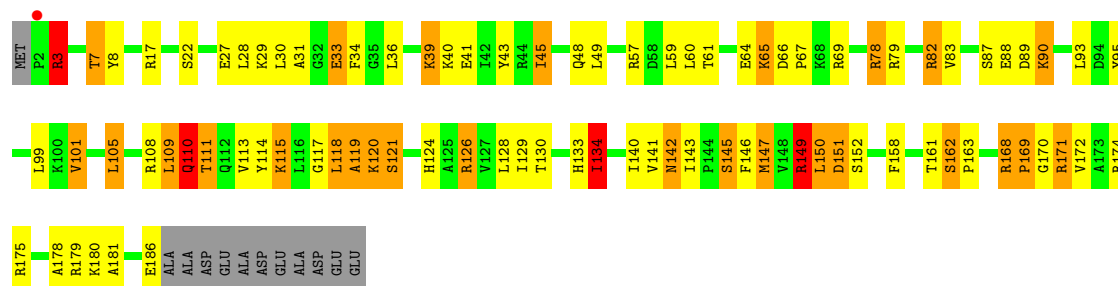
• Molecule 11: 40S ribosomal protein S9-A

Chain AJ:



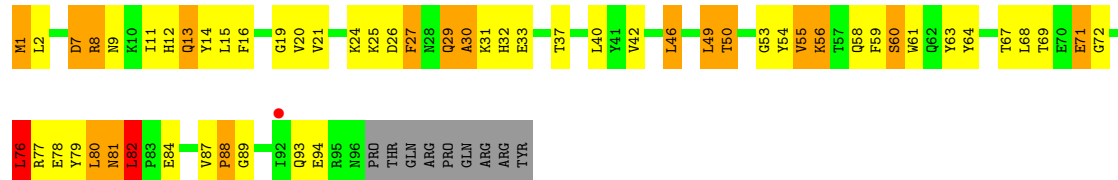
- Molecule 11: 40S ribosomal protein S9-A

Chain CJ:



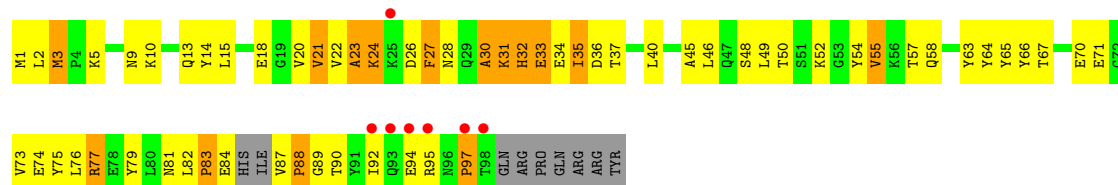
- Molecule 12: 40S ribosomal protein S10-A

Chain AK:



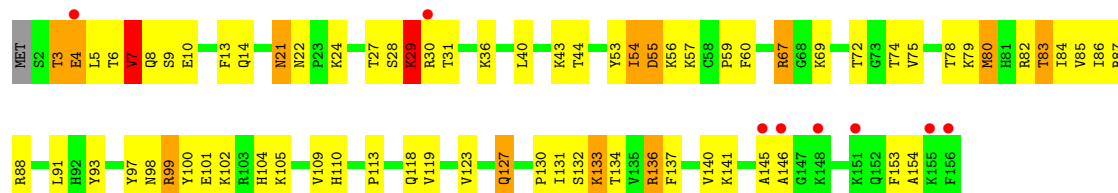
- Molecule 12: 40S ribosomal protein S10-A

Chain CK:



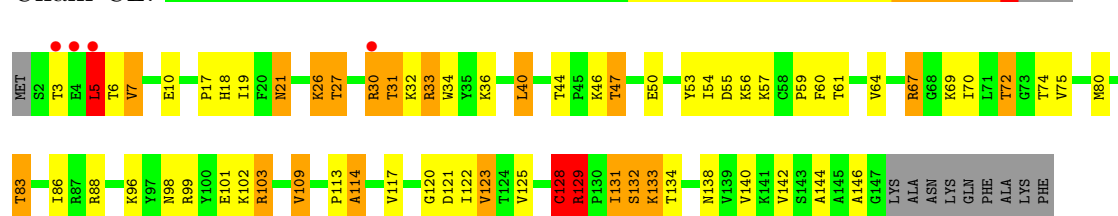
- Molecule 13: 40S ribosomal protein S11-A

Chain AL:



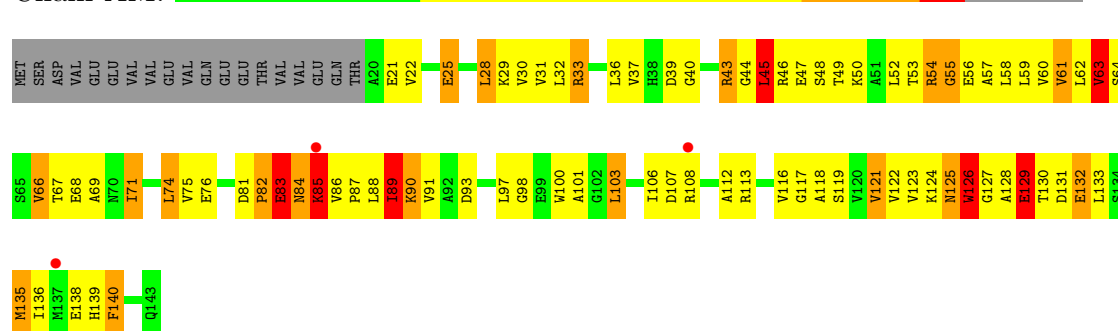
- Molecule 13: 40S ribosomal protein S11-A

Chain CL:



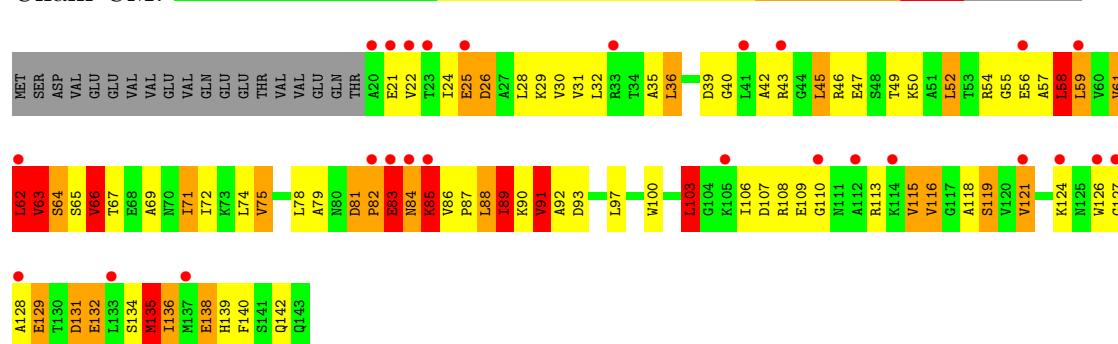
- Molecule 14: 40S ribosomal protein S12

Chain AM:



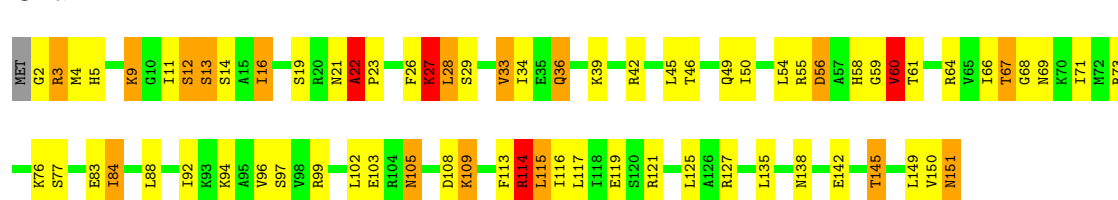
- Molecule 14: 40S ribosomal protein S12

Chain CM:



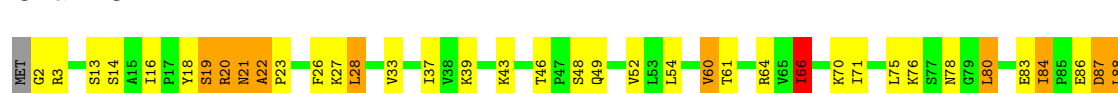
- Molecule 15: 40S ribosomal protein S13

Chain AN:



- Molecule 15: 40S ribosomal protein S13

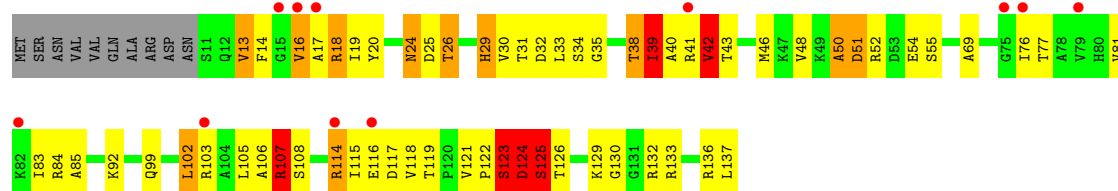
Chain CN:





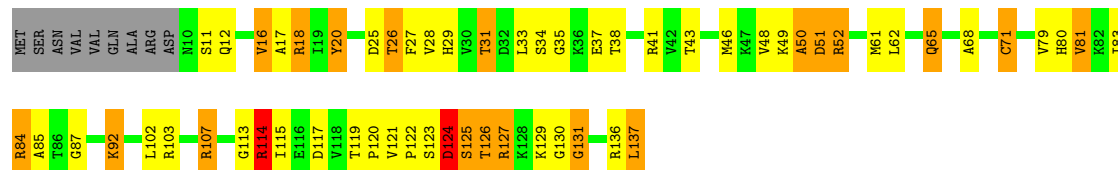
• Molecule 16: 40S ribosomal protein S14-A

Chain AO:



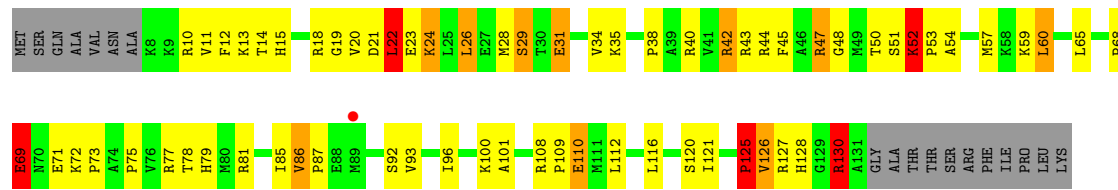
• Molecule 16: 40S ribosomal protein S14-A

Chain CO:



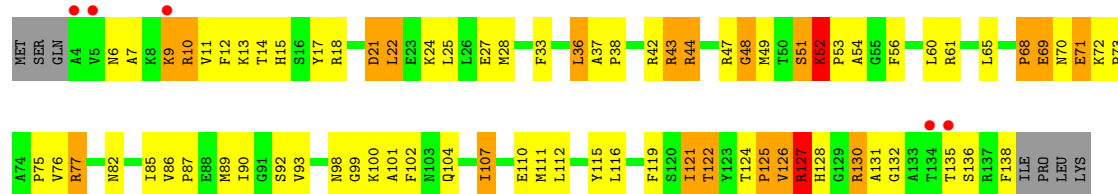
• Molecule 17: 40S ribosomal protein S15

Chain AP:



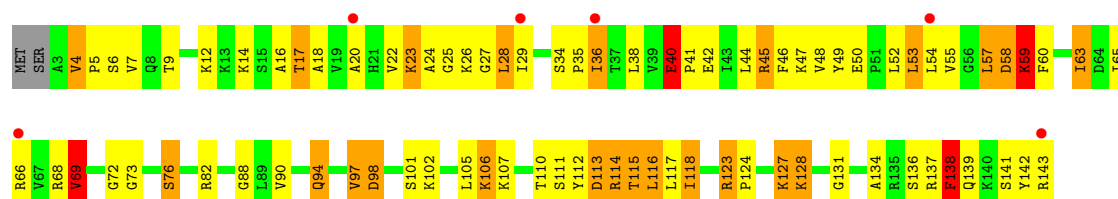
• Molecule 17: 40S ribosomal protein S15

Chain CP:



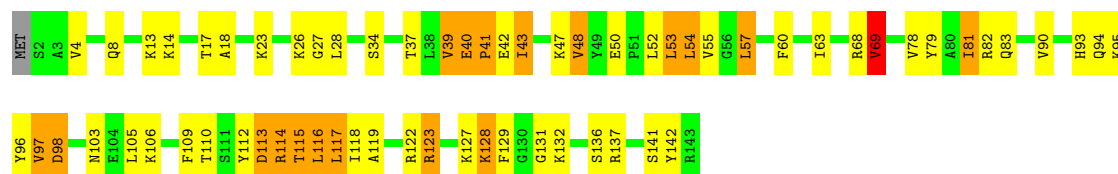
• Molecule 18: 40S ribosomal protein S16-A

Chain AQ:



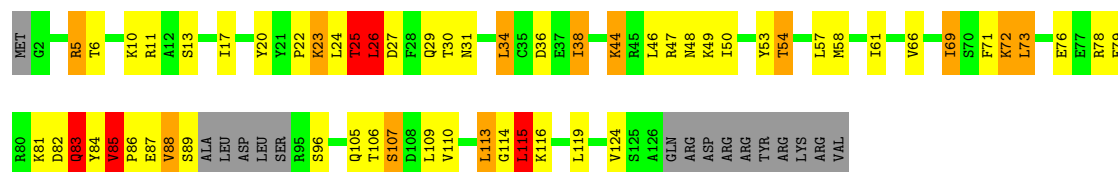
- Molecule 18: 40S ribosomal protein S16-A

Chain CQ:



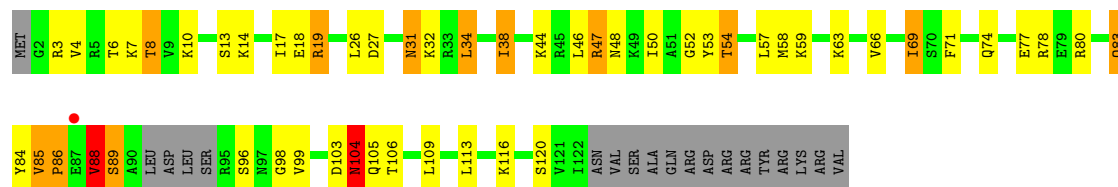
- Molecule 19: 40S ribosomal protein S17-A

Chain AR:



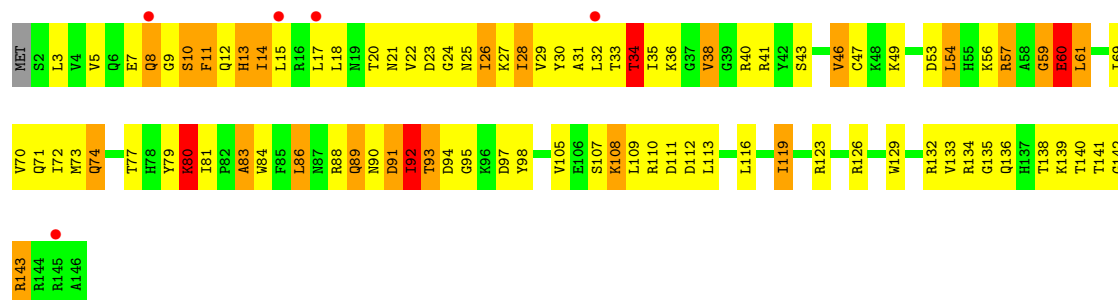
- Molecule 19: 40S ribosomal protein S17-A

Chain CR:



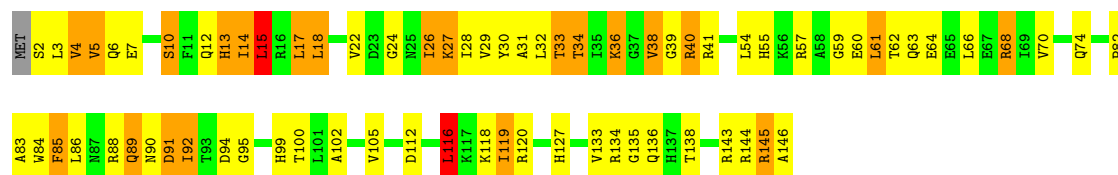
- Molecule 20: 40S ribosomal protein S18-A

Chain AS:

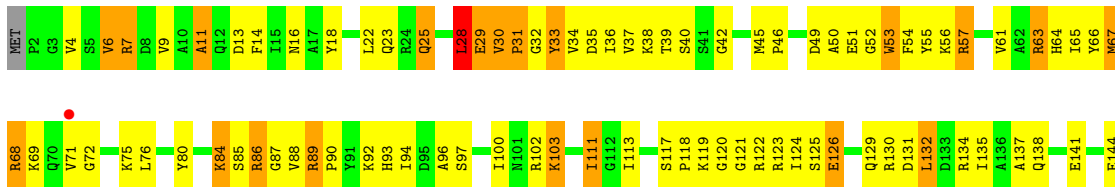


- Molecule 20: 40S ribosomal protein S18-A

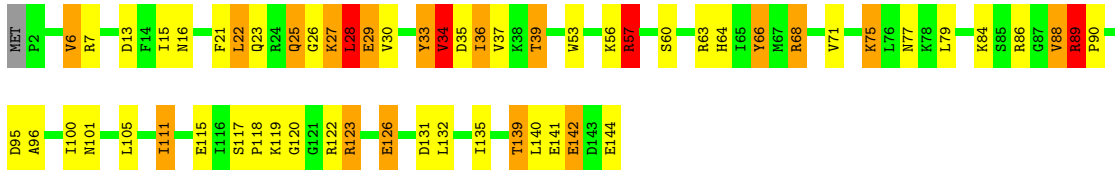
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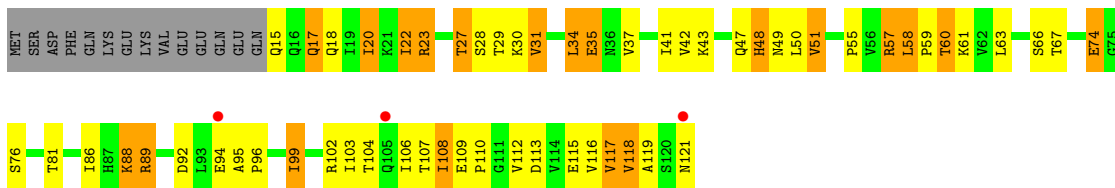
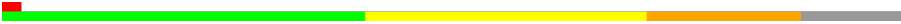
- Molecule 21: 40S ribosomal protein S19-A



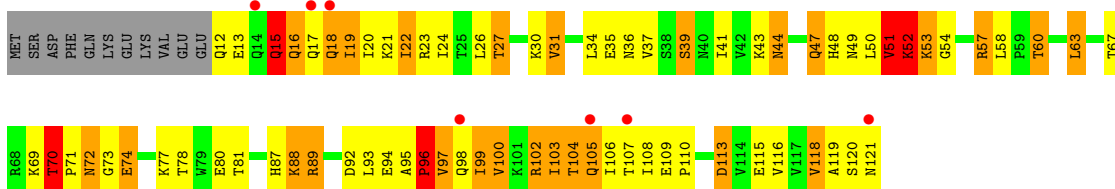
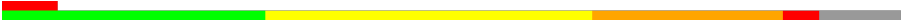
- Chain CT:



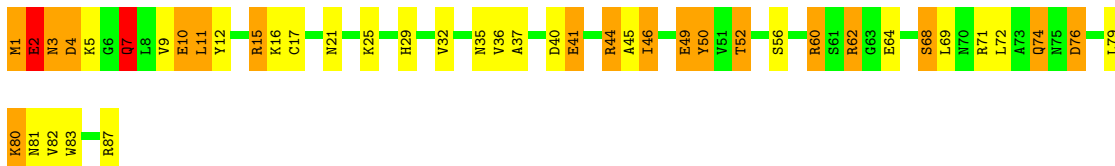
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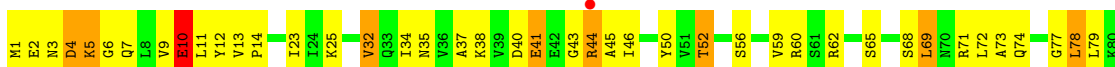
- Chain CU:

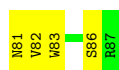


- Chain AV:



- Chain CV:





- Molecule 24: 40S ribosomal protein S22-A

Chain AW:



- Molecule 24: 40S ribosomal protein S22-A

Chain CW:



- Molecule 25: 40S ribosomal protein S23-A

Chain AX:



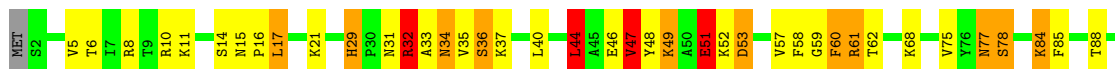
- Molecule 25: 40S ribosomal protein S23-A

Chain CX:



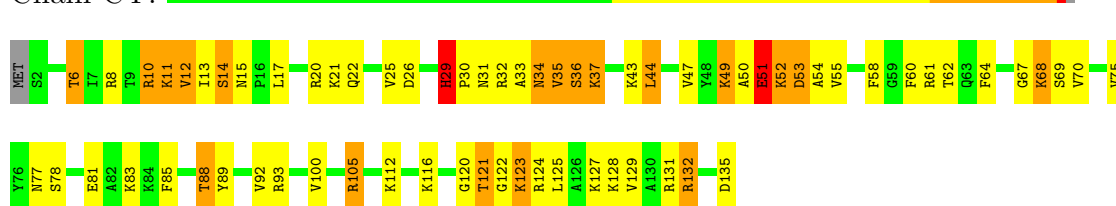
- Molecule 26: 40S ribosomal protein S24-A

Chain AY:



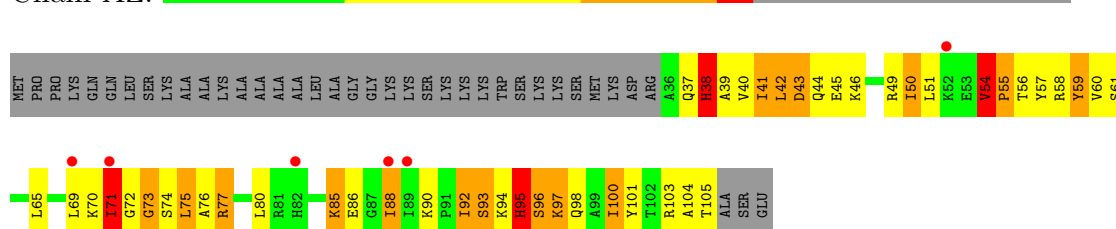
- Molecule 26: 40S ribosomal protein S24-A

Chain CY:



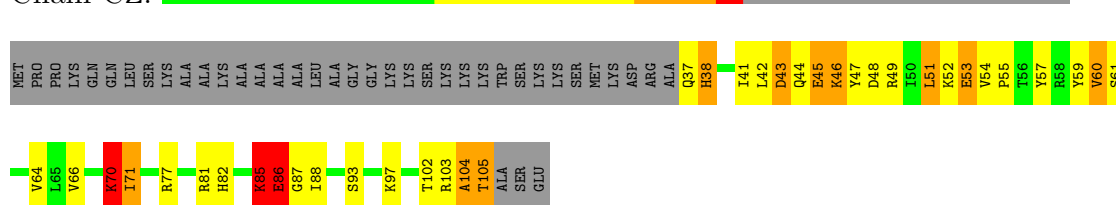
- Molecule 27: 40S ribosomal protein S25-A

Chain AZ:



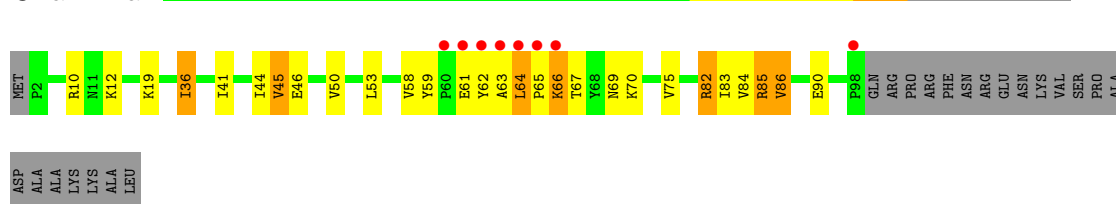
- Molecule 27: 40S ribosomal protein S25-A

Chain CZ:



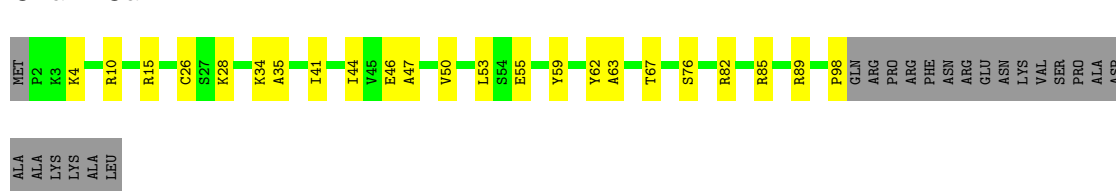
- Molecule 28: 40S ribosomal protein S26-A

Chain Aa:



- Molecule 28: 40S ribosomal protein S26-A

Chain Ca:



- Molecule 29: 40S ribosomal protein S27-A

Chain Ab:



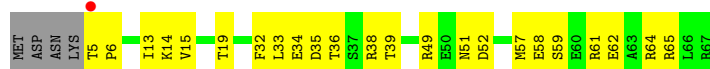
- Molecule 29: 40S ribosomal protein S27-A

Chain Cb: 



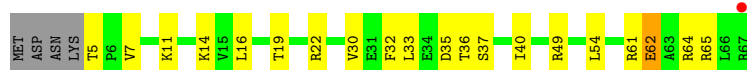
- Molecule 30: 40S ribosomal protein S28-A

Chain Ac: 



- Molecule 30: 40S ribosomal protein S28-A

Chain Cc: 



- Molecule 31: 40S ribosomal protein S29-A

Chain Ad: 



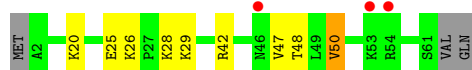
- Molecule 31: 40S ribosomal protein S29-A

Chain Cd: 



- Molecule 32: 40S ribosomal protein S30-A

Chain Ae: 



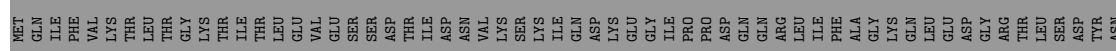
- Molecule 32: 40S ribosomal protein S30-A

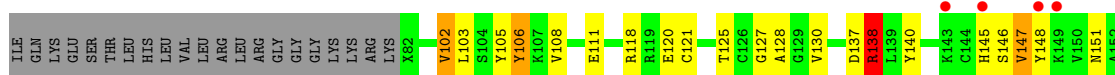
Chain Ce: 



- Molecule 33: 40S ribosomal protein S31

Chain Af: 





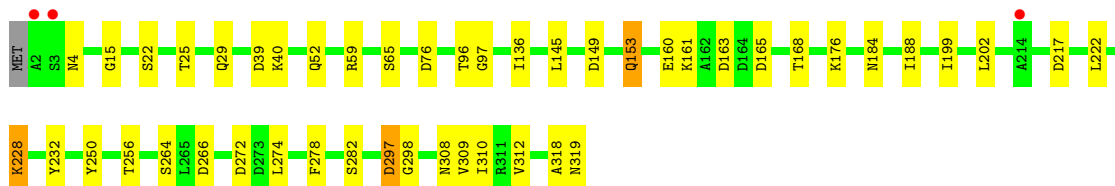
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein (ASC1, RACK1)

Chain Ag:



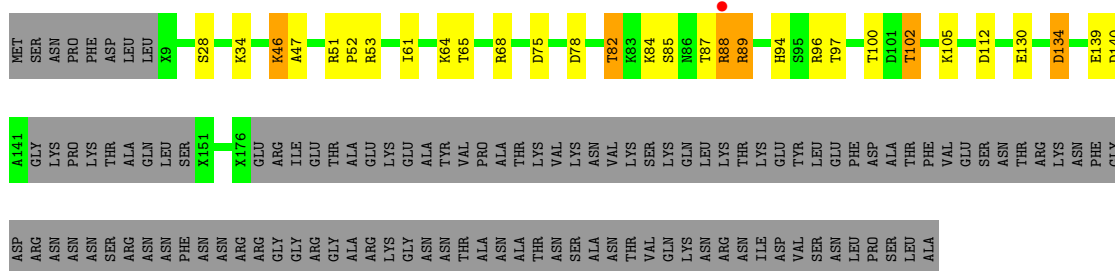
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein (ASC1, RACK1)

Chain Cg:



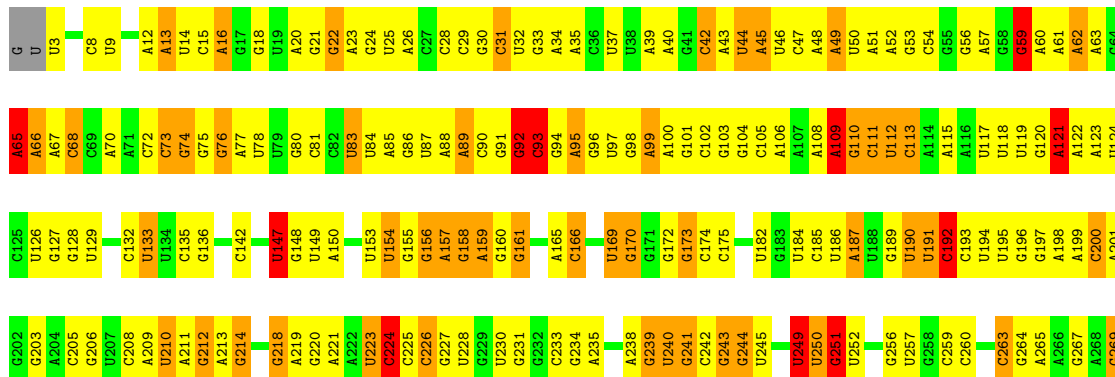
- Molecule 35: Suppressor protein STM1

Chain Ah:



- Molecule 36: 25S rRNA

Chain A1:





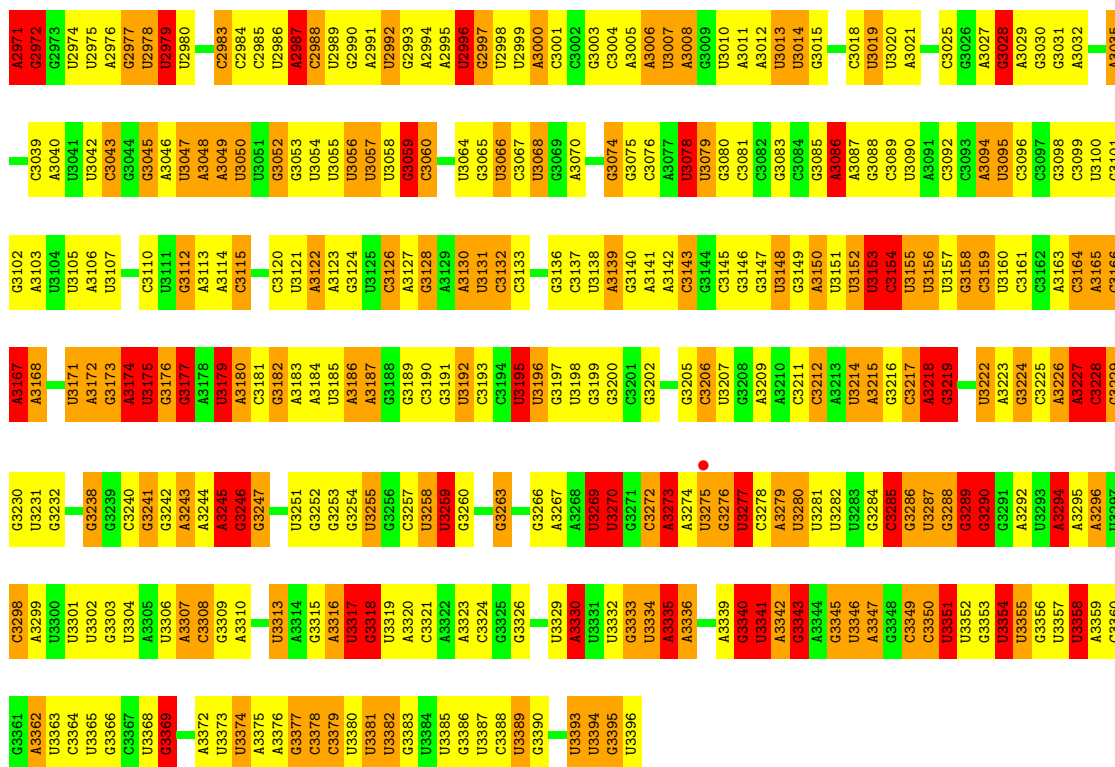






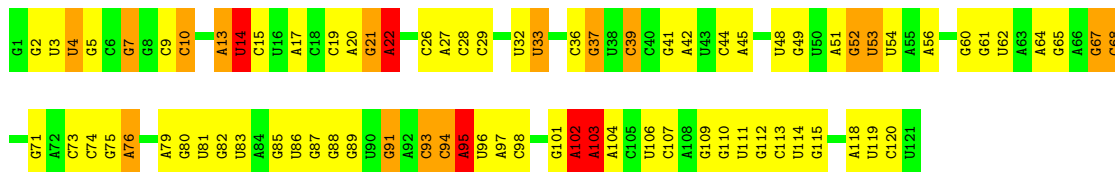


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G2960	A2896	U2834	U2763	C2696	C2631	U2563	G2440	U2380	U2318	G2250	U2184	C	U	
C2961	U2897	G2835	G2764	A2697	U2632	U2565	A2441	C2381	U2319			C	G	
U2962	G2898	C2836	C2765	G2698	U2633	C2566	G2442	G2382	A2320	G2253	A2188	U	A	
C2963	C2899	A2837	U2767	U2699	U2634	C2567	A2443	C2383	A2321	U2254	A2189	U	C	
U2964	U2900	U2838	U2768	G2700	U2635	U2568	C2444	G2384	A2322	A2255	A2190	G	A	
G2965	U2901	A2839	A2769	U2701	A2636	A2569	U2504	A2385	G2323	G2256	U2191	G	U	
C2966	C2906	C2840	G2770	A2702	U2636	U2570	U2505	C2386	G2324	C2257	C2192	U	C	
A2967	G2907	U2841	U2771	A2703	A2637	U2571	U2506	A2387	A2325	U2258	G2124	U	U	
C2968	U2908	C2772	C2772	A2704	U2638	C2572	A	U2388	G2326			A	U	
C2970	U2909	C2773	C2773	A2705	G2639	G2573	U2509	C2389	U2327	G2261	C2195	G	G	



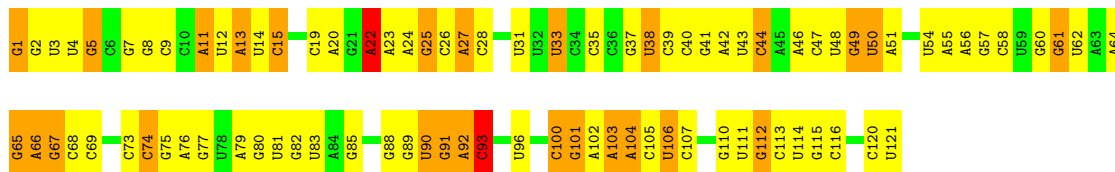
- Molecule 37: 5S rRNA

Chain A3:



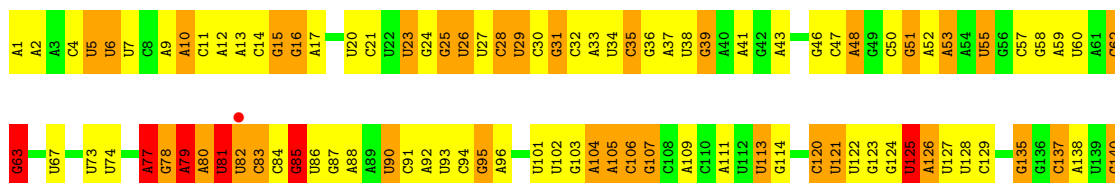
- Molecule 37: 5S rRNA

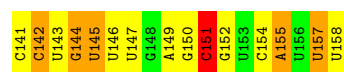
Chain A7:



- Molecule 38: 5.8S rRNA

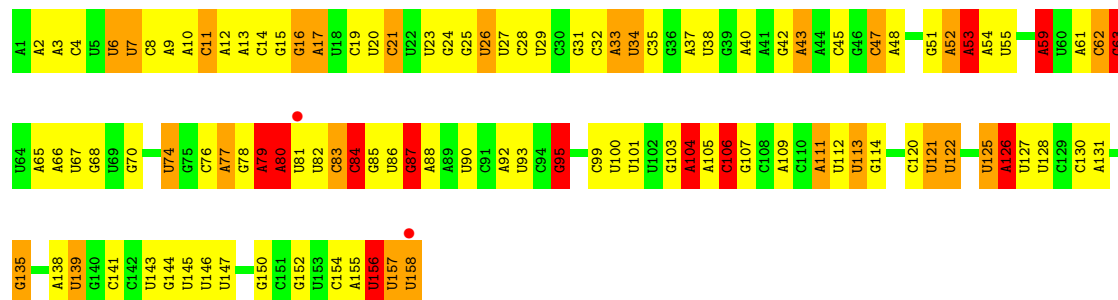
Chain A4:





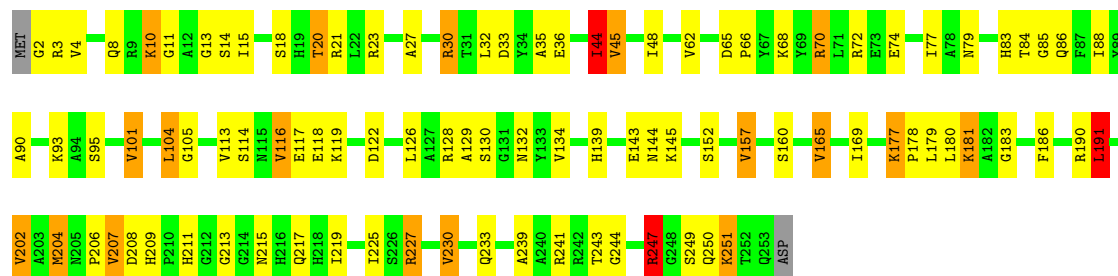
• Molecule 38: 5.8S rRNA

Chain A8:



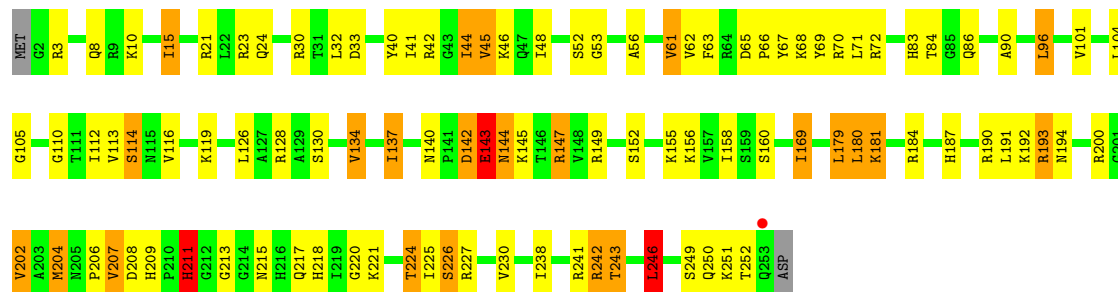
• Molecule 39: 60S ribosomal protein L2-A

Chain BA:



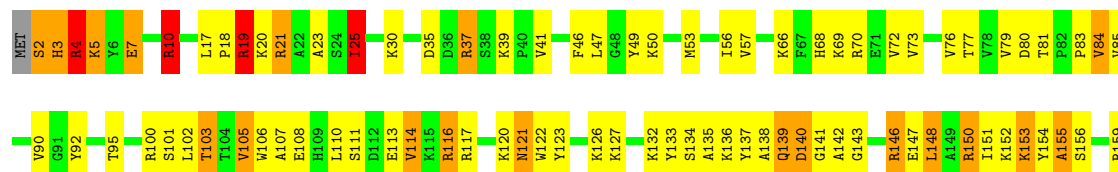
• Molecule 39: 60S ribosomal protein L2-A

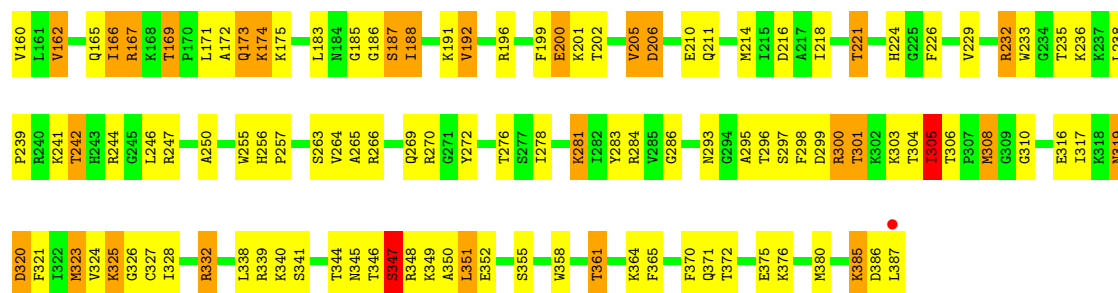
Chain DA:



• Molecule 40: 60S ribosomal protein L3

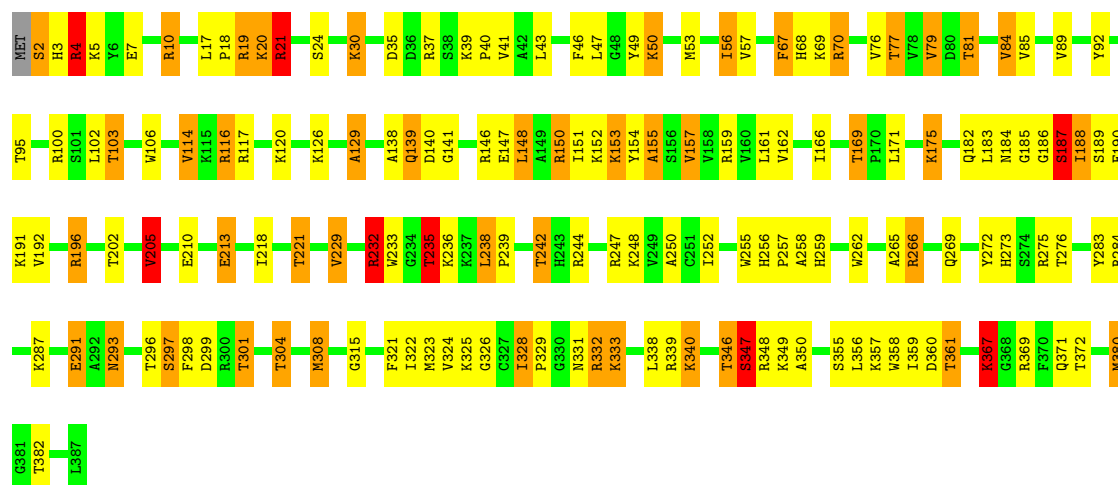
Chain BB:





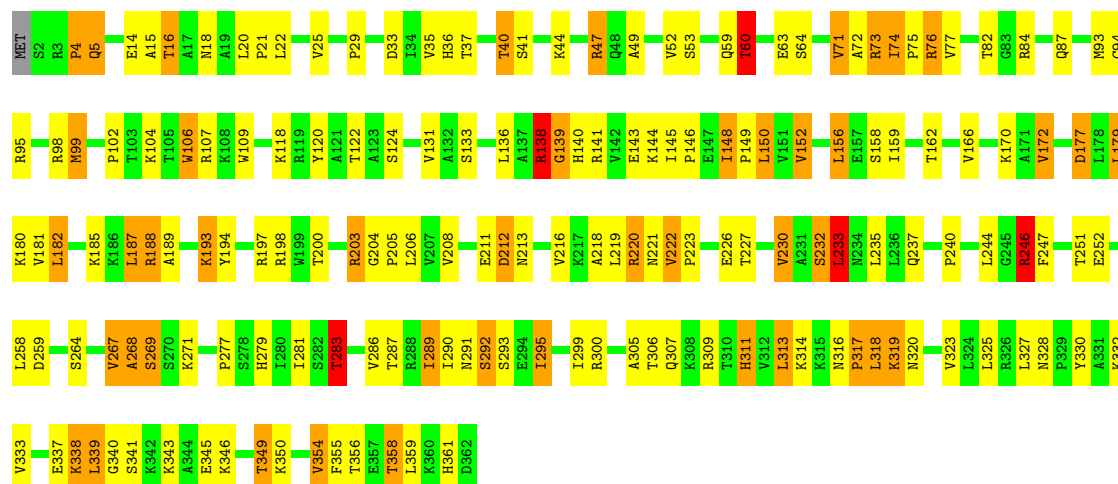
- Molecule 40: 60S ribosomal protein L3

Chain DB:



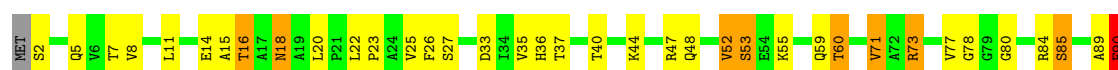
- Molecule 41: 60S ribosomal protein L4-A

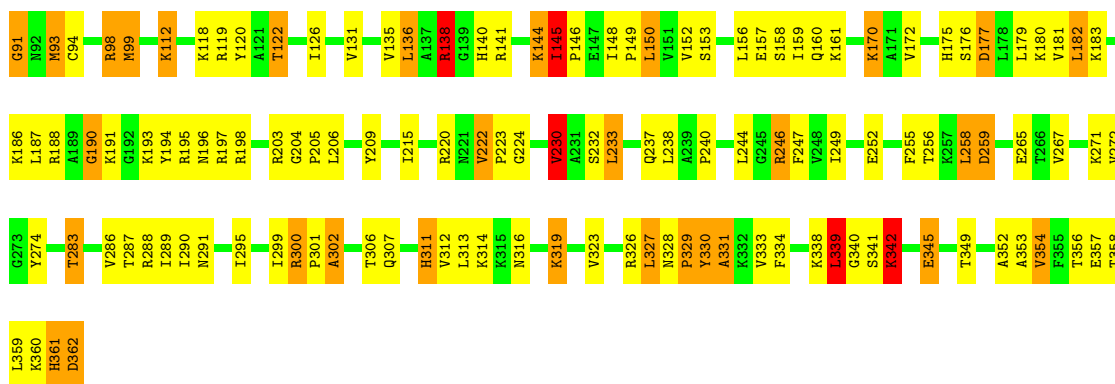
Chain BC:



- Molecule 41: 60S ribosomal protein L4-A

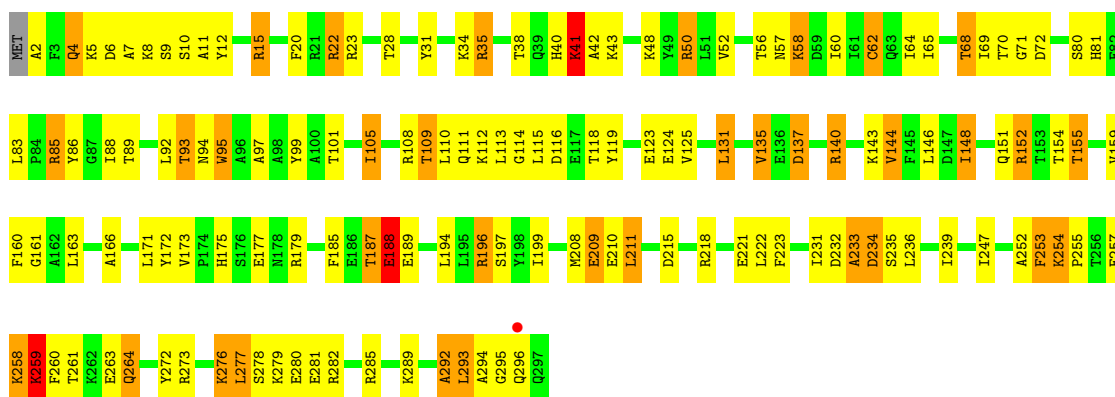
Chain DC:





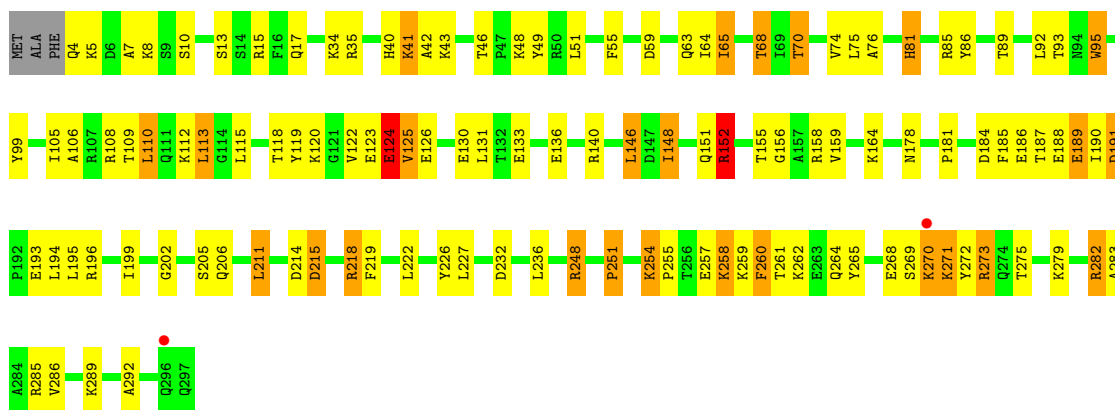
• Molecule 42: 60S ribosomal protein L5

Chain BD:



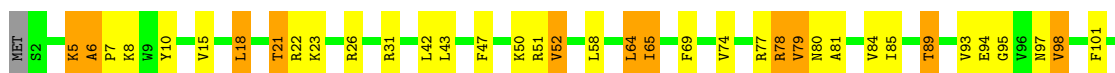
• Molecule 42: 60S ribosomal protein L5

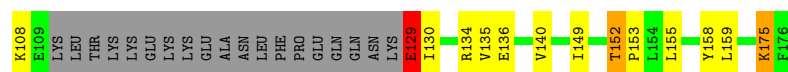
Chain DD:



• Molecule 43: 60S ribosomal protein L6-A

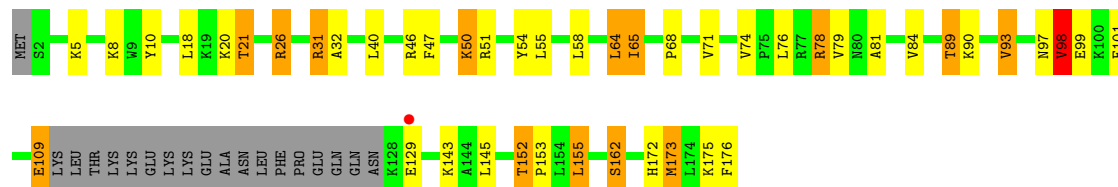
Chain BE:





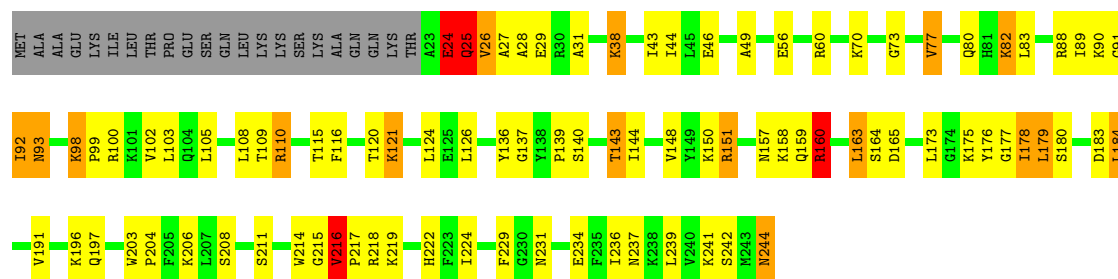
• Molecule 43: 60S ribosomal protein L6-A

Chain DE:



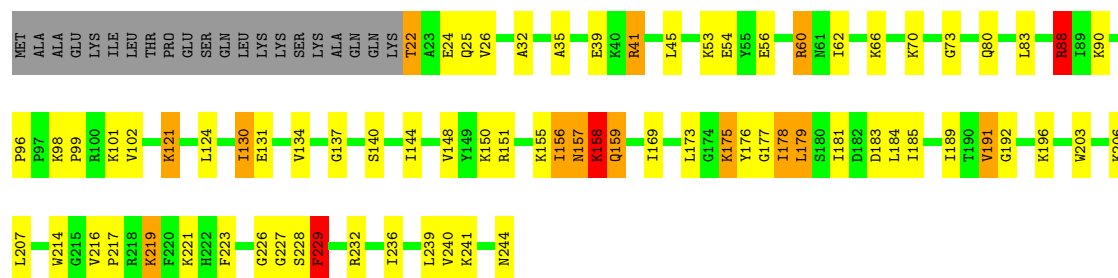
• Molecule 44: 60S ribosomal protein L7-A

Chain BF:



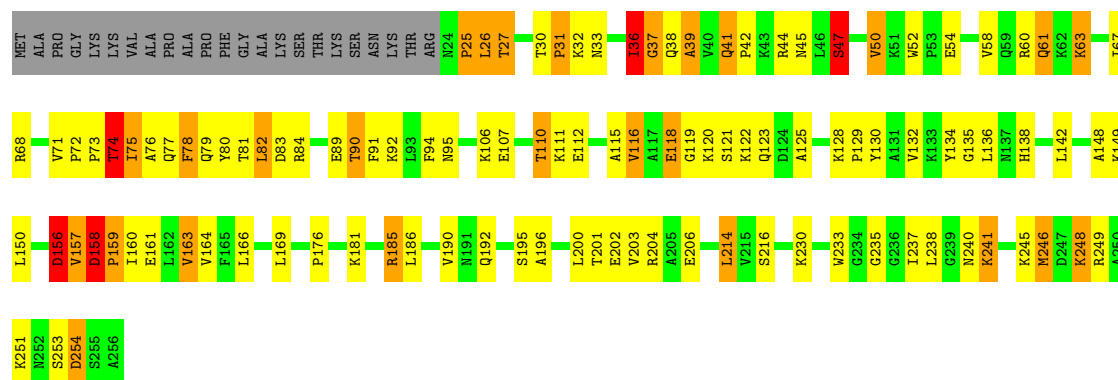
• Molecule 44: 60S ribosomal protein L7-A

Chain DF:



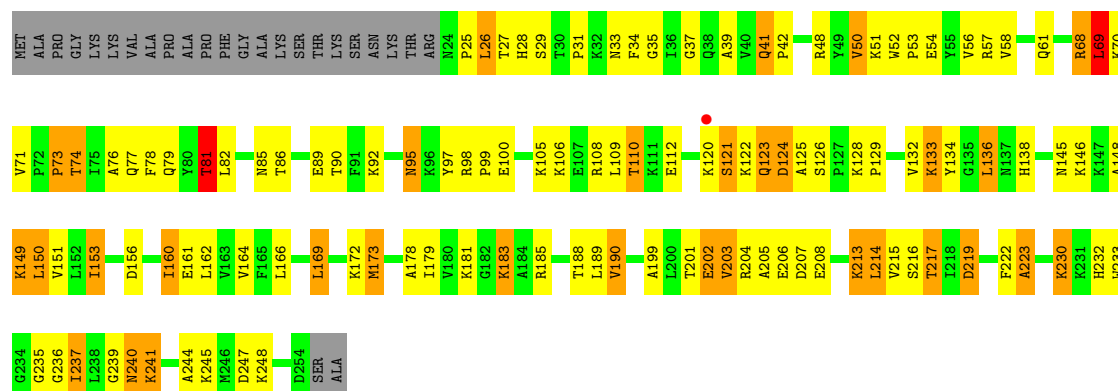
• Molecule 45: 60S ribosomal protein L8-A

Chain BG:



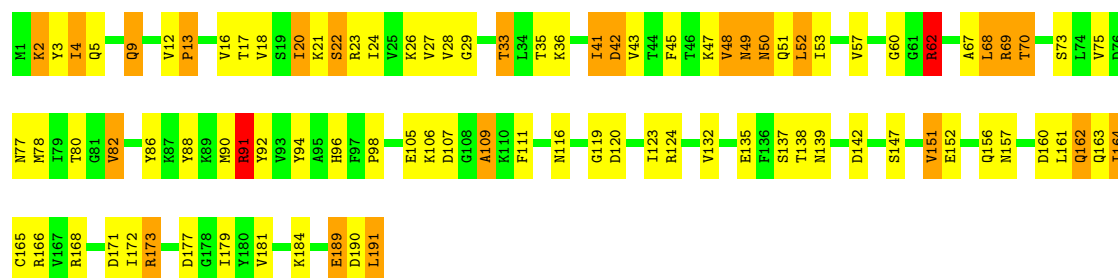
- Molecule 45: 60S ribosomal protein L8-A

Chain DG:



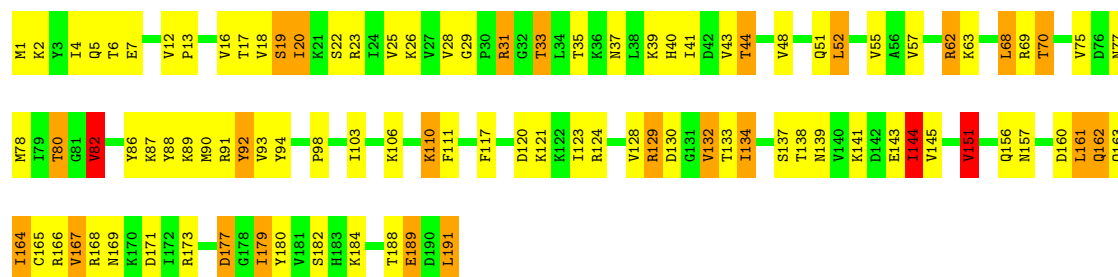
- Molecule 46: 60S ribosomal protein L9-A

Chain BH:



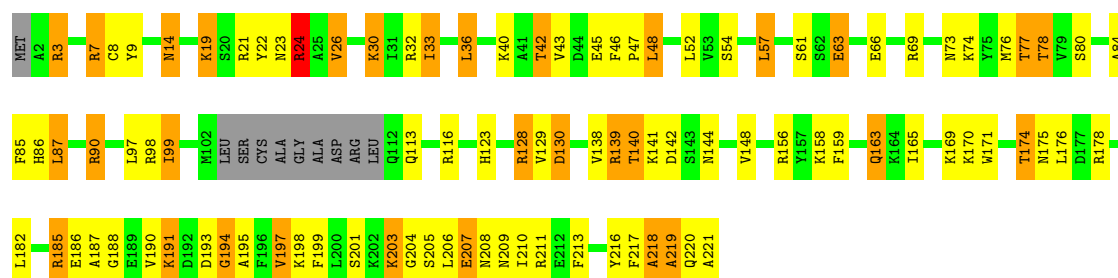
- Molecule 46: 60S ribosomal protein L9-A

Chain DH:



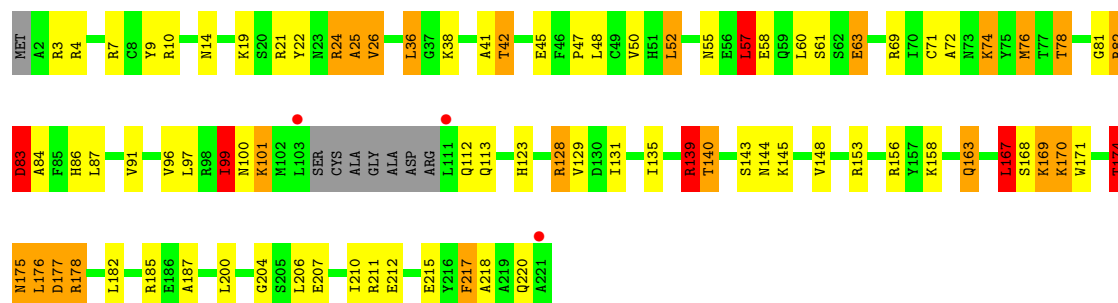
- Molecule 47: 60S ribosomal protein L10

Chain BI:



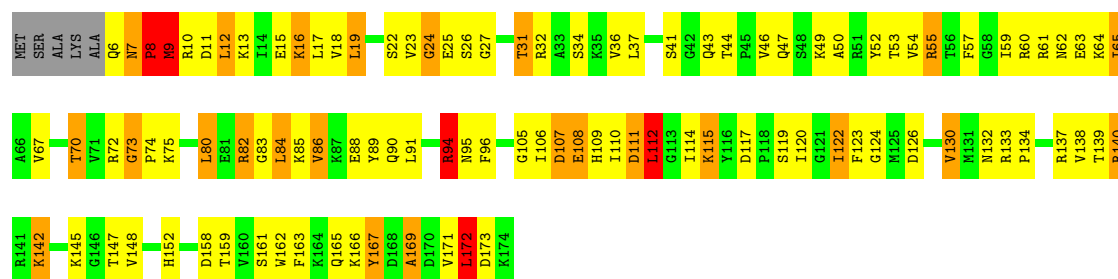
- Molecule 47: 60S ribosomal protein L10

Chain DI:



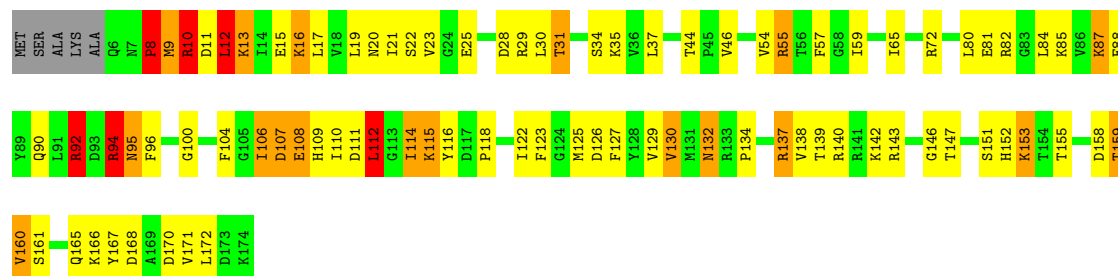
- Molecule 48: 60S ribosomal protein L11-A

Chain BJ:



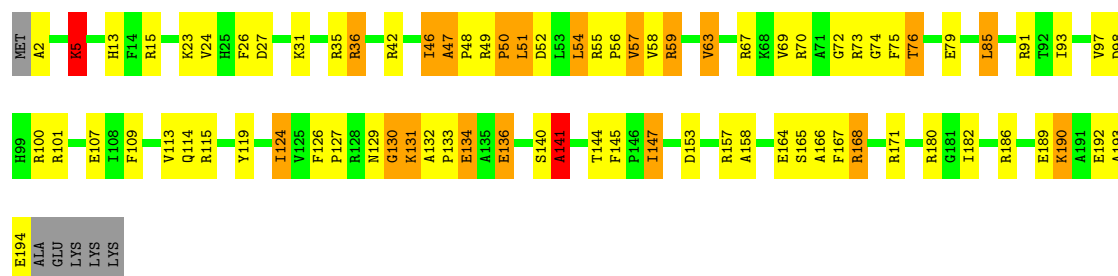
- Molecule 48: 60S ribosomal protein L11-A

Chain DJ:



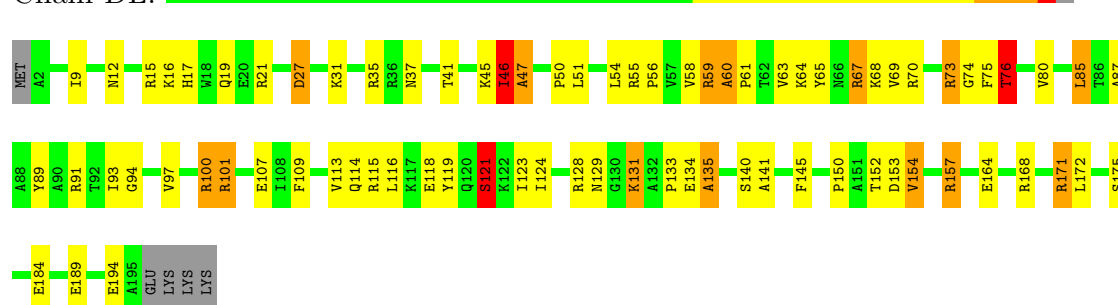
- Molecule 49: 60S ribosomal protein L13-A

Chain BL:



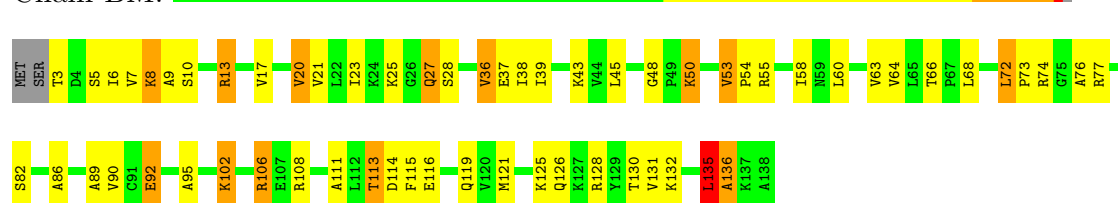
- Molecule 49: 60S ribosomal protein L13-A

Chain DL:



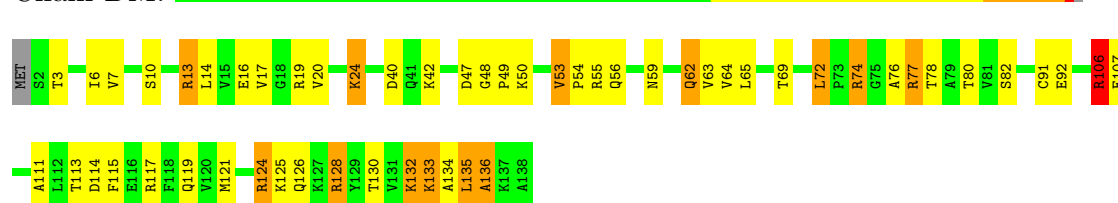
- Molecule 50: 60S ribosomal protein L14-A

Chain BM:



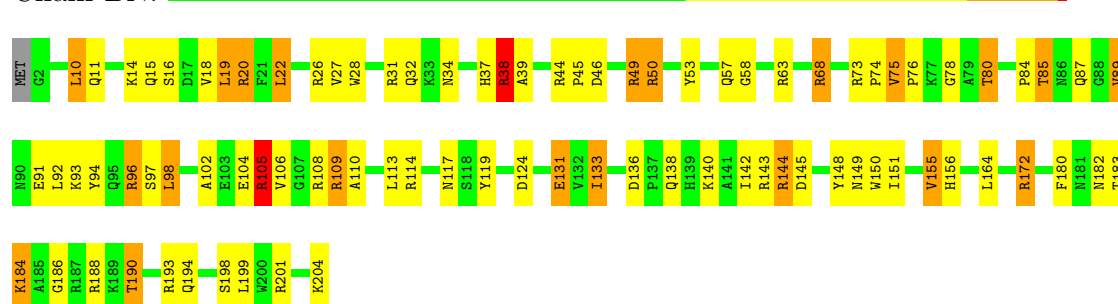
- Molecule 50: 60S ribosomal protein L14-A

Chain DM:



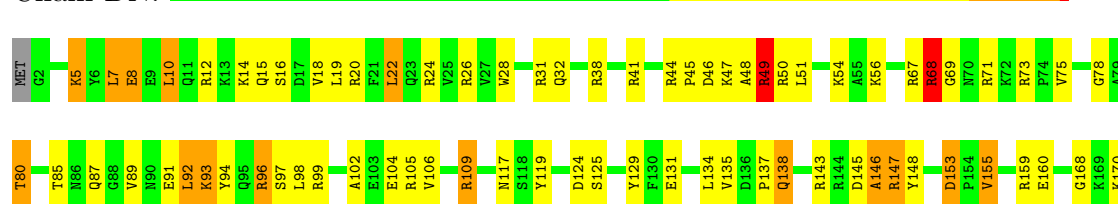
- Molecule 51: 60S ribosomal protein L15-A

Chain BN:



- Molecule 51: 60S ribosomal protein L15-A

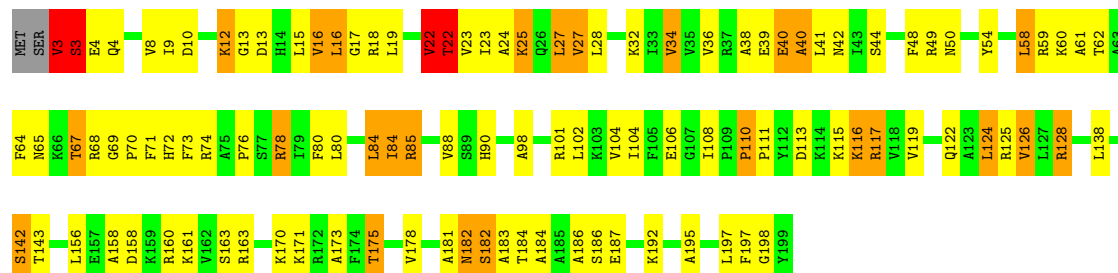
Chain DN:





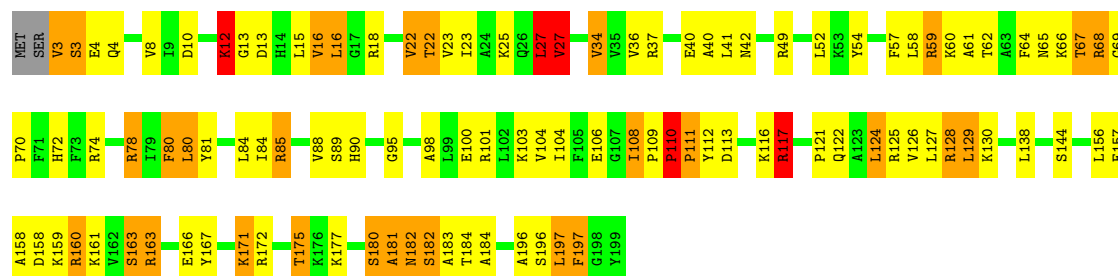
- Molecule 52: 60S ribosomal protein L16-A, 60S ribosomal protein L16-B

Chain BO:



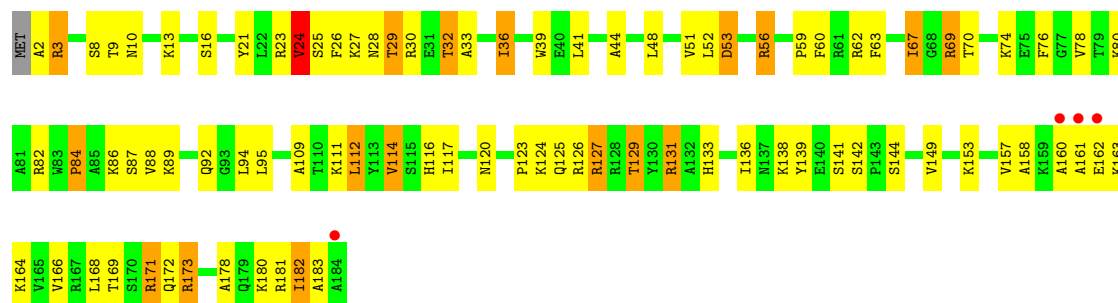
- Molecule 52: 60S ribosomal protein L16-A, 60S ribosomal protein L16-B

Chain DO:



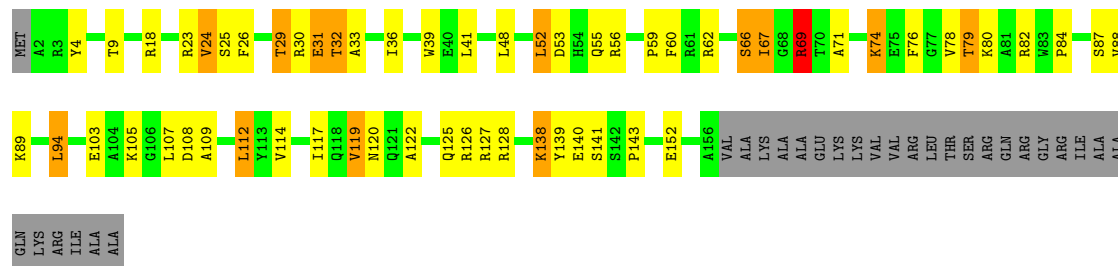
- Molecule 53: 60S ribosomal protein L17-A

Chain BP:



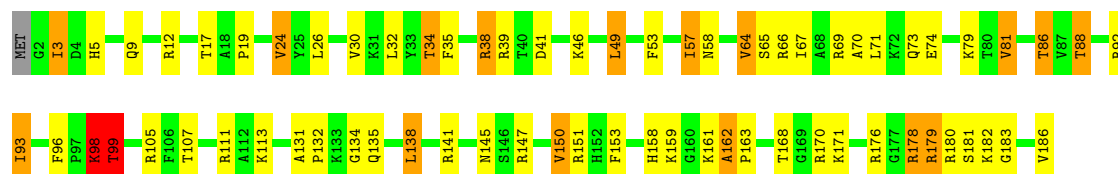
- Molecule 53: 60S ribosomal protein L17-A

Chain DP:



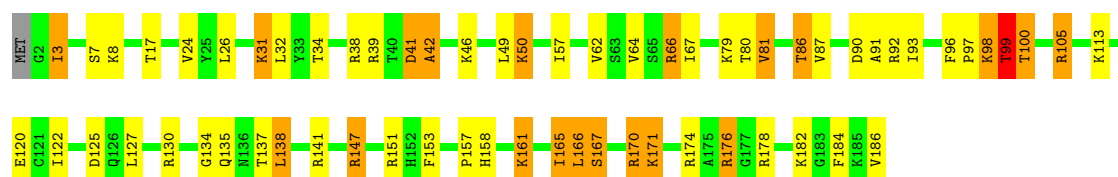
- Molecule 54: 60S ribosomal protein L18-A

Chain BQ:



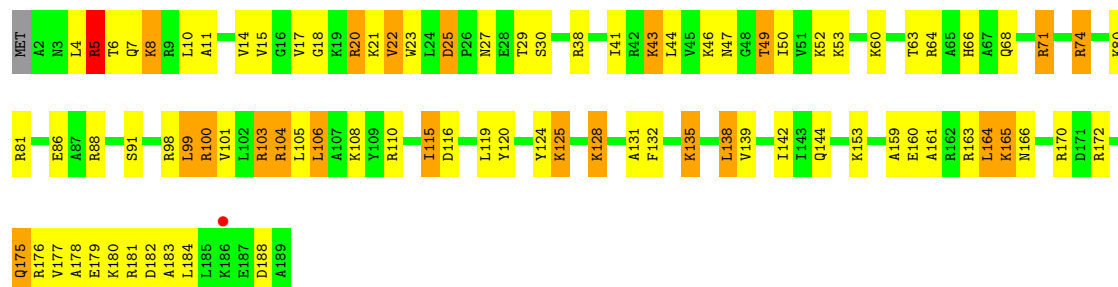
- Molecule 54: 60S ribosomal protein L18-A

Chain DQ:



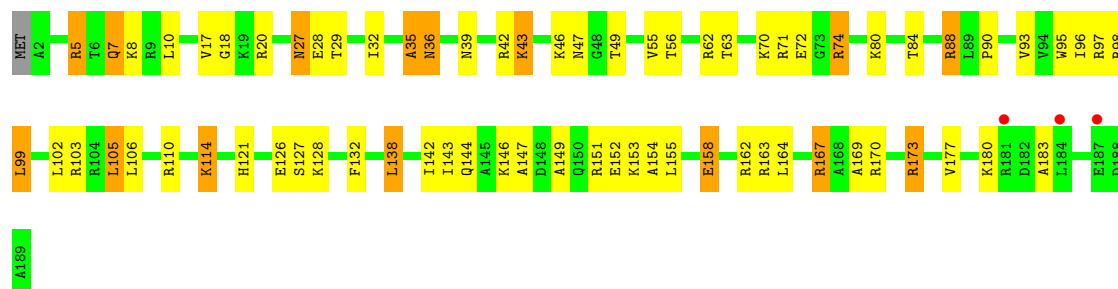
- Molecule 55: 60S ribosomal protein L19-A

Chain BR:



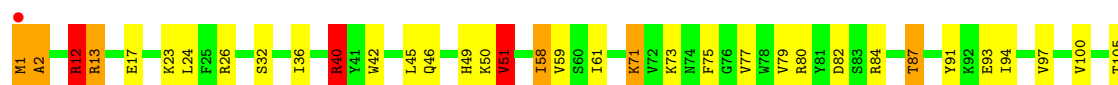
- Molecule 55: 60S ribosomal protein L19-A

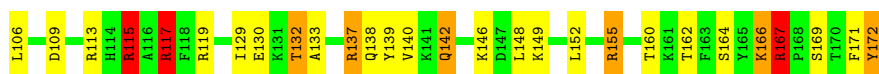
Chain DR:



- Molecule 56: 60S ribosomal protein L20-A

Chain BS:





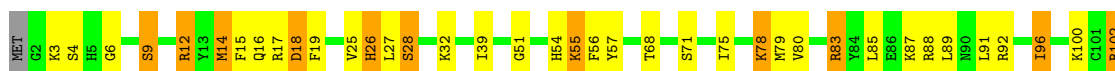
• Molecule 56: 60S ribosomal protein L20-A

Chain DS:



• Molecule 57: 60S ribosomal protein L21-A

Chain BT:



• Molecule 57: 60S ribosomal protein L21-A

Chain DT:



• Molecule 58: 60S ribosomal protein L22-A

Chain BU:



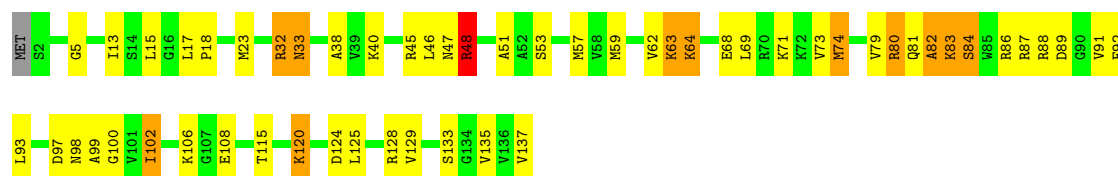
• Molecule 58: 60S ribosomal protein L22-A

Chain DU:



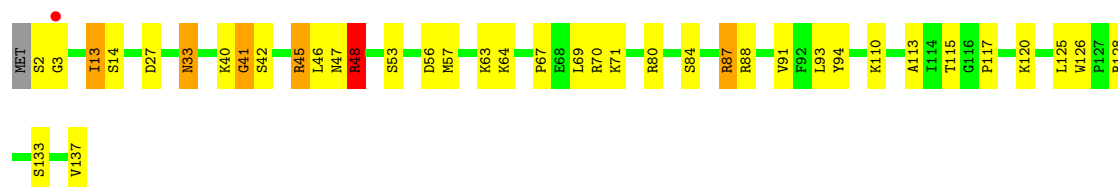
• Molecule 59: 60S ribosomal protein L23-A

Chain BV:



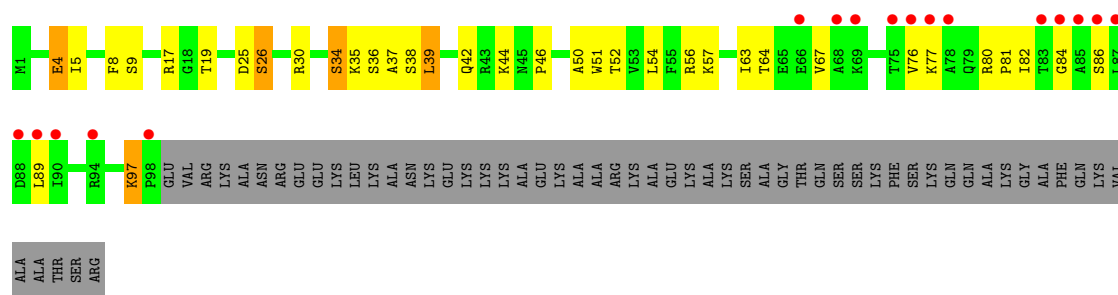
- Molecule 59: 60S ribosomal protein L23-A

Chain DV:



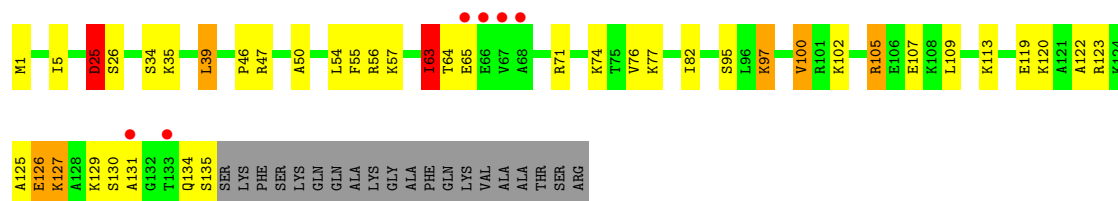
- Molecule 60: 60S ribosomal protein L24-A

Chain BW:



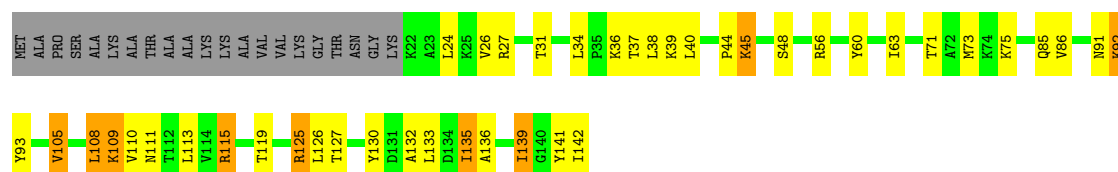
- Molecule 60: 60S ribosomal protein L24-A

Chain DW:



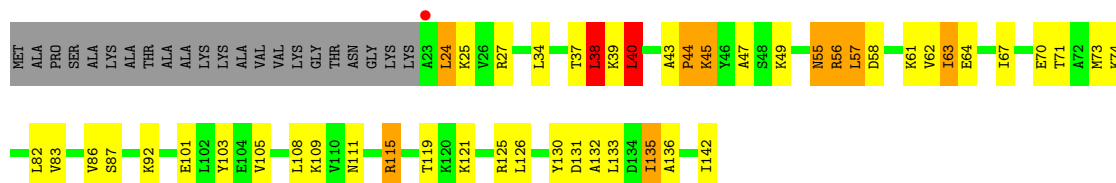
- Molecule 61: 60S ribosomal protein L25

Chain BX:



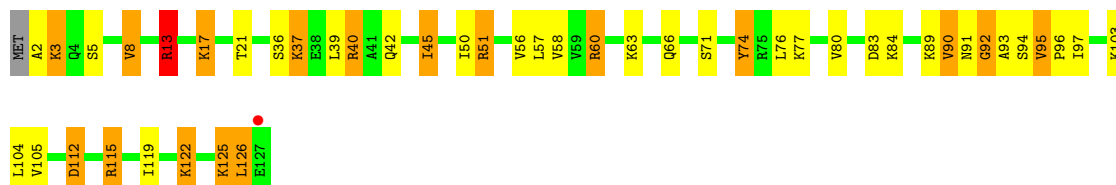
- Molecule 61: 60S ribosomal protein L25

Chain DX:



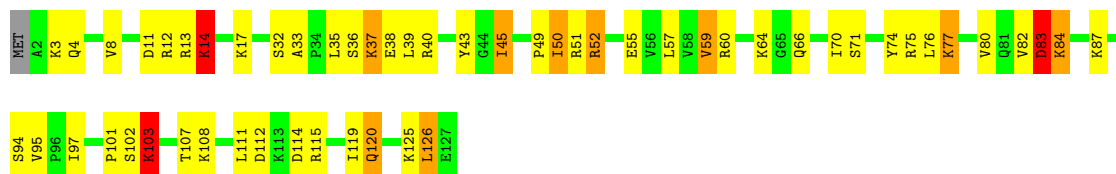
- Molecule 62: 60S ribosomal protein L26-A

Chain BY:



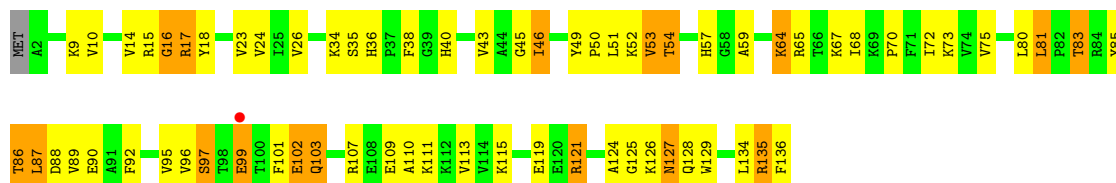
- Molecule 62: 60S ribosomal protein L26-A

Chain DY:



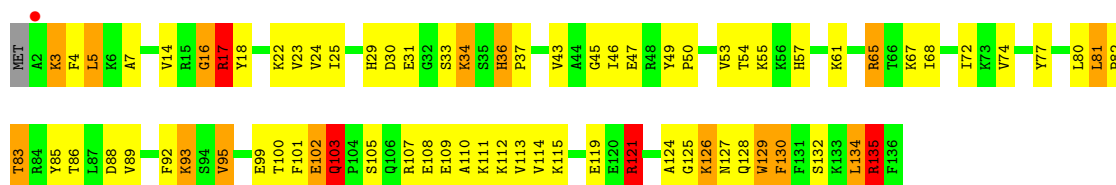
- Molecule 63: 60S ribosomal protein L27-A

Chain BZ:



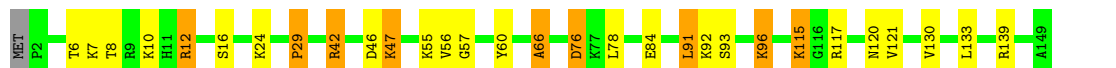
- Molecule 63: 60S ribosomal protein L27-A

Chain DZ:



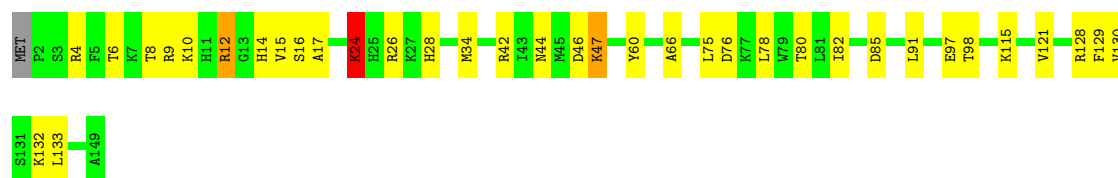
- Molecule 64: 60S ribosomal protein L28

Chain Ba:



- Molecule 64: 60S ribosomal protein L28

Chain Da:



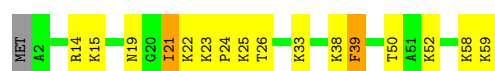
- Molecule 65: 60S ribosomal protein L29

Chain Bb:



- Molecule 65: 60S ribosomal protein L29

Chain Db:



- Molecule 66: 60S ribosomal protein L30

Chain Bc:



- Molecule 66: 60S ribosomal protein L30

Chain Dc:



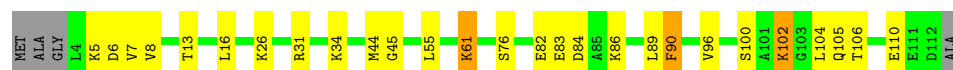
- Molecule 67: 60S ribosomal protein L31-A

Chain Bd:



- Molecule 67: 60S ribosomal protein L31-A

Chain Dd:



- Molecule 68: 60S ribosomal protein L32

Chain Be:



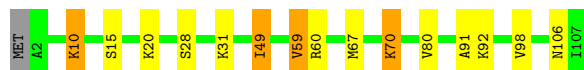
- Molecule 68: 60S ribosomal protein L32

Chain De:



- Molecule 69: 60S ribosomal protein L33-A

Chain Bf:



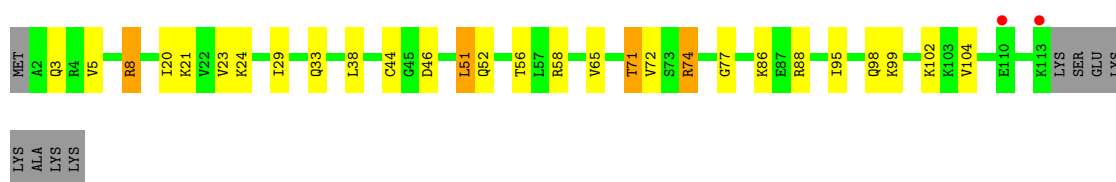
- Molecule 69: 60S ribosomal protein L33-A

Chain Df:



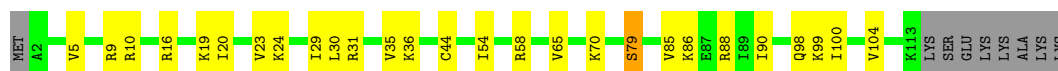
- Molecule 70: 60S ribosomal protein L34-A

Chain Bg:



- Molecule 70: 60S ribosomal protein L34-A

Chain Dg:



- Molecule 71: 60S ribosomal protein L35-A

Chain Bh:



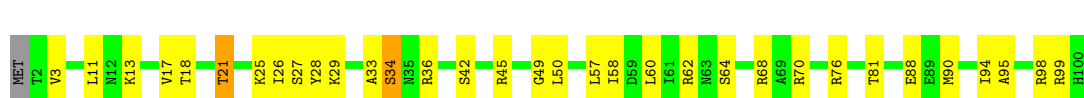
- Molecule 71: 60S ribosomal protein L35-A

Chain Dh:



- Molecule 72: 60S ribosomal protein L36-A

Chain Bi:



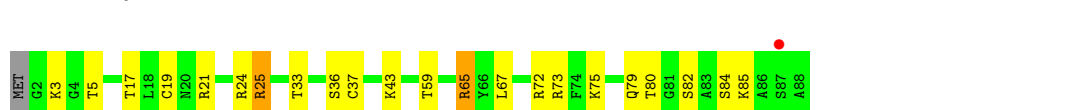
- Molecule 72: 60S ribosomal protein L36-A

Chain Di:



- Molecule 73: 60S ribosomal protein L37-A

Chain Bj:



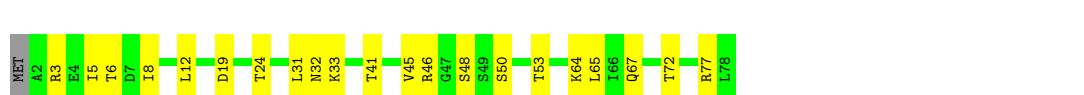
- Molecule 73: 60S ribosomal protein L37-A

Chain Dj:



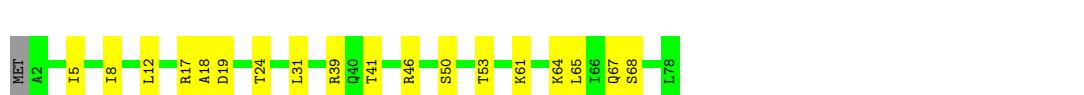
- Molecule 74: 60S ribosomal protein L38

Chain Bk:



- Molecule 74: 60S ribosomal protein L38

Chain Dk:



- Molecule 75: 60S ribosomal protein L39

Chain Bl:



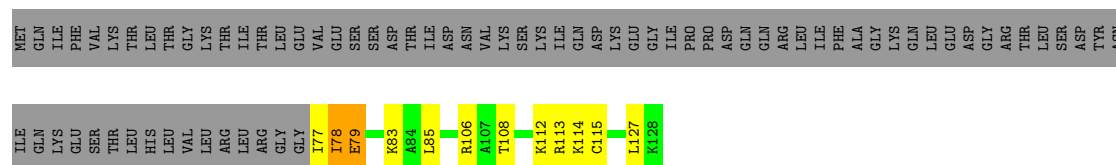
- Molecule 75: 60S ribosomal protein L39

Chain Dl:



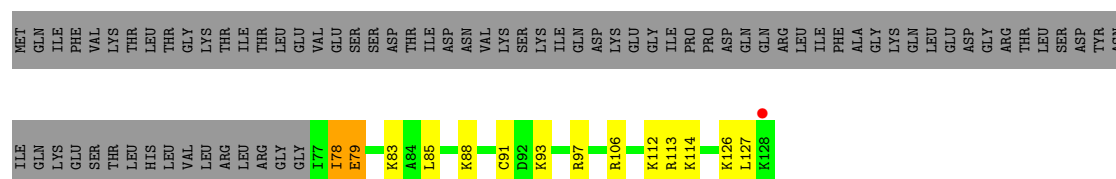
- Molecule 76: 60S ribosomal protein L40

Chain Bm:



- Molecule 76: 60S ribosomal protein L40

Chain Dm:



- Molecule 77: 60S ribosomal protein L41-A

Chain Bn:



- Molecule 77: 60S ribosomal protein L41-A

Chain Dn:



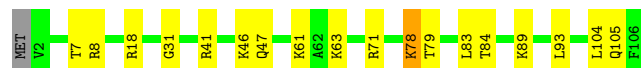
- Molecule 78: 60S ribosomal protein L42-A

Chain Bo:



- Molecule 78: 60S ribosomal protein L42-A

Chain Do:



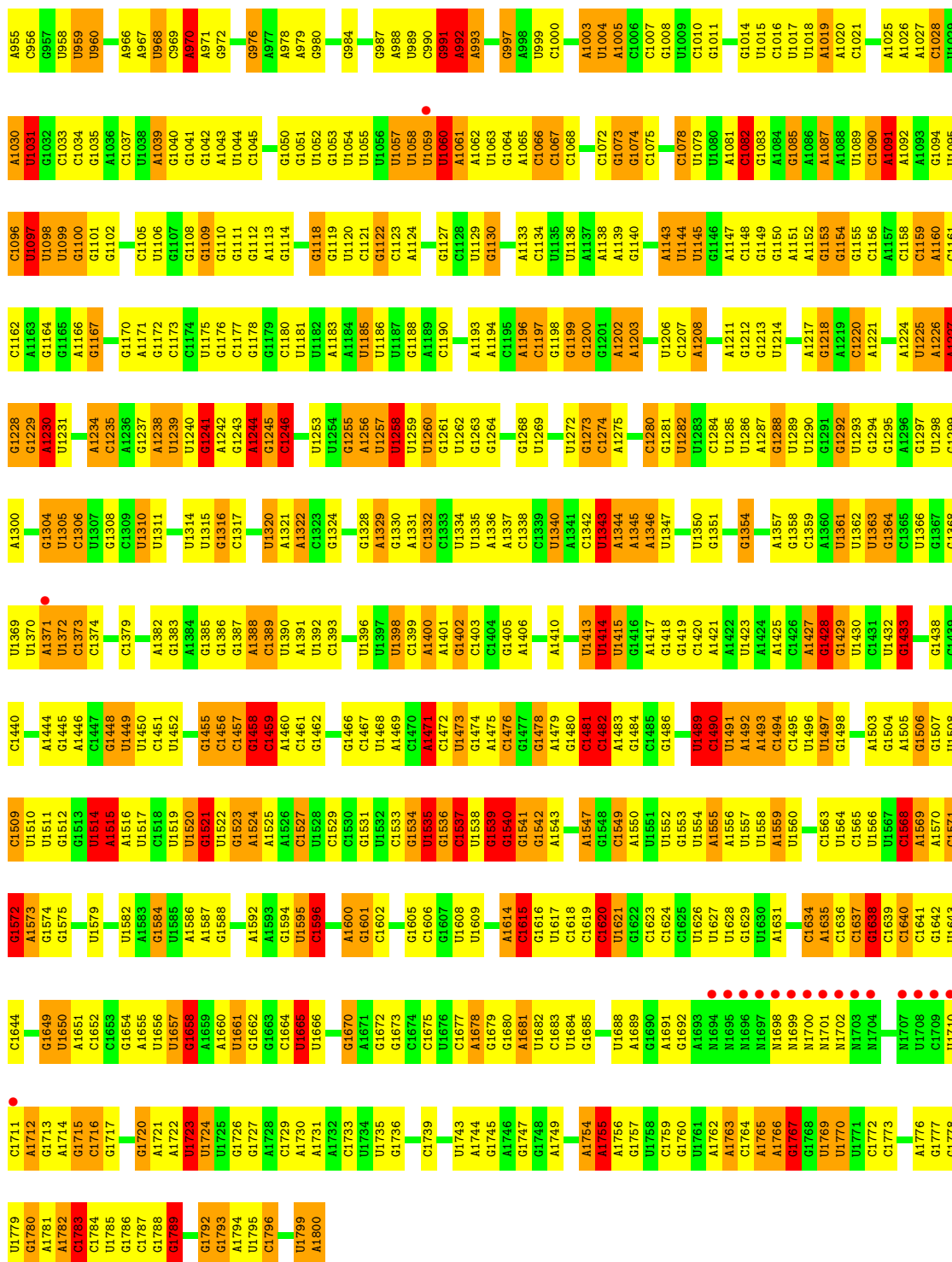
- Molecule 79: 60S ribosomal protein L43-A

Chain Bp:



- Molecule 79: 60S ribosomal protein L43-A





- Molecule 81: 40S ribosomal protein S31

Chain Cf:

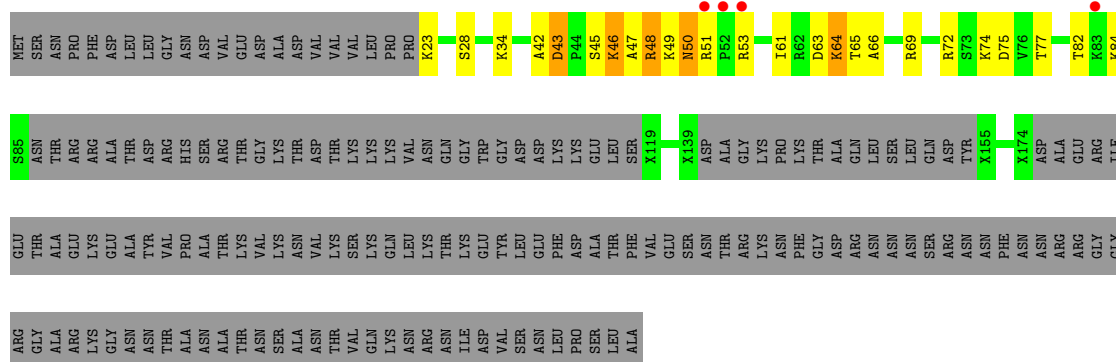


MET	GLN	ILE	PHE	VAL	LYS	THR	THR	THR	LYS	THR	ILE	THR	GLU	GLU	VAL	VAL	ASP	ILE	THR	THR	ASP	SER	SER	ASN	VAL	LYS	LYS	LYS	ILE	GLN	ASP	LYS	GLU	GLY	ILE	GLY	PRO	PRO	PRO	ASP	ASP	GLN	GLN	ARG	LEU	ILE	PHE	ALA	GLY	GLY	LYS	GLN	LEU	GLU	ASP	ASP	GLY	GLY	ARG	THR	LEU	SER	ASP	TYR	ASN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



• Molecule 82: Suppressor protein STM1

Chain Ch:



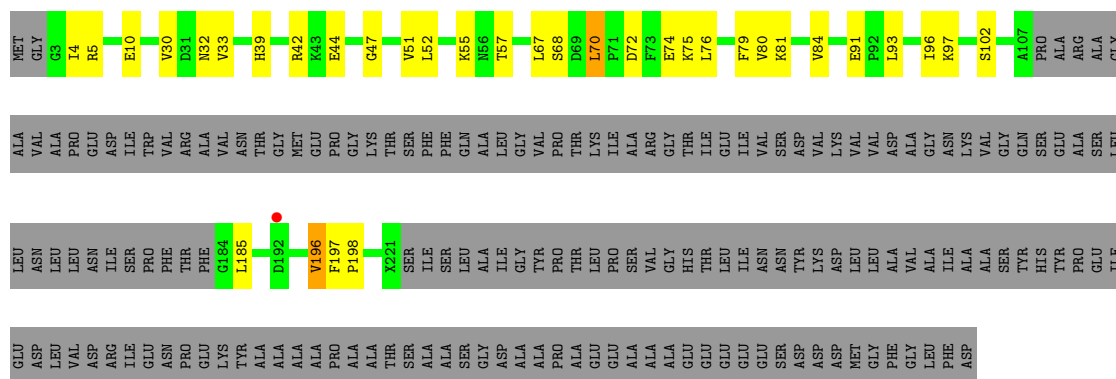
• Molecule 83: Ribosomal protein L12

Chain DK:



• Molecule 84: 60S acidic ribosomal protein P0

Chain Dq:



• Molecule 85: Ribosomal protein P1 alpha

Chain Dr:

There are no outlier residues recorded for this chain.

• Molecule 86: Ribosomal protein P2 beta

Chain Ds:

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	436.43Å 288.22Å 305.08Å 90.00° 98.99° 90.00°	Depositor
Resolution (Å)	300.00 – 3.00 301.33 – 2.90	Depositor EDS
% Data completeness (in resolution range)	2.0 (300.00-3.00) 99.9 (301.33-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.181 , 0.229 0.235 , 0.275	Depositor DCC
R_{free} test set	22543 reflections (1.38%)	DCC
Wilson B-factor (Å ²)	68.6	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 1639309 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	416785	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, OHX, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A2	0.92	36/42128 (0.1%)	1.49	822/65642 (1.3%)
2	AA	0.54	0/1617	0.80	0/2215
2	CA	0.64	0/1623	0.88	0/2222
3	AB	0.45	0/1735	0.81	0/2335
3	CB	0.61	0/1748	0.80	1/2352 (0.0%)
4	AC	0.60	0/1665	0.77	0/2263
4	CC	0.70	0/1665	0.93	6/2263 (0.3%)
5	AD	0.59	0/1759	0.74	0/2368
5	CD	0.54	0/1759	0.76	1/2368 (0.0%)
6	AE	0.57	0/2109	0.86	1/2839 (0.0%)
6	CE	0.70	0/2109	0.94	2/2839 (0.1%)
7	AF	0.49	0/1629	0.72	0/2202
7	CF	0.62	0/1629	0.86	2/2202 (0.1%)
8	AG	0.55	0/1823	0.75	0/2439
8	CG	0.68	0/1779	0.87	2/2379 (0.1%)
9	AH	0.52	0/1506	0.77	0/2028
9	CH	0.59	0/1516	0.85	0/2043
10	AI	0.68	0/1514	0.89	3/2021 (0.1%)
10	CI	0.75	0/1514	0.99	2/2021 (0.1%)
11	AJ	0.59	0/1519	0.81	1/2035 (0.0%)
11	CJ	0.70	0/1519	0.91	3/2035 (0.1%)
12	AK	0.55	0/789	0.83	3/1067 (0.3%)
12	CK	0.51	0/776	0.83	3/1047 (0.3%)
13	AL	0.70	0/1239	0.81	0/1673
13	CL	0.76	0/1194	0.98	5/1610 (0.3%)
14	AM	0.49	0/898	0.76	0/1220
14	CM	0.44	0/898	0.77	2/1220 (0.2%)
15	AN	0.61	0/1215	0.83	3/1638 (0.2%)
15	CN	0.67	0/1215	0.89	1/1638 (0.1%)
16	AO	0.48	0/901	0.82	1/1217 (0.1%)
16	CO	0.70	0/960	0.92	0/1290
17	AP	0.60	0/998	0.86	2/1341 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	CP	0.57	0/1060	0.83	0/1426
18	AQ	0.56	0/1125	0.85	3/1510 (0.2%)
18	CQ	0.66	0/1131	0.85	1/1518 (0.1%)
19	AR	0.54	0/935	0.82	0/1254
19	CR	0.60	0/914	0.86	0/1224
20	AS	0.59	0/1211	0.80	0/1628
20	CS	0.63	0/1211	0.92	3/1628 (0.2%)
21	AT	0.57	0/1130	0.81	0/1517
21	CT	0.66	0/1130	0.86	3/1517 (0.2%)
22	AU	0.55	0/865	0.76	0/1169
22	CU	0.62	0/892	0.86	0/1205
23	AV	0.52	0/693	0.75	0/935
23	CV	0.65	0/693	0.86	0/935
24	AW	0.65	0/1038	0.86	3/1395 (0.2%)
24	CW	0.81	0/1038	0.89	1/1395 (0.1%)
25	AX	0.72	0/1139	0.91	2/1518 (0.1%)
25	CX	0.86	0/1139	0.99	3/1518 (0.2%)
26	AY	0.56	0/1087	0.77	1/1449 (0.1%)
26	CY	0.65	0/1087	0.84	0/1449
27	AZ	0.49	0/571	0.85	1/768 (0.1%)
27	CZ	0.51	0/566	0.80	1/761 (0.1%)
28	Aa	0.54	0/782	0.77	0/1047
28	Ca	0.63	0/782	0.84	0/1047
29	Ab	0.53	0/620	0.82	1/838 (0.1%)
29	Cb	0.55	0/620	0.87	0/838
30	Ac	0.43	0/499	0.72	0/670
30	Cc	0.53	0/499	0.84	0/670
31	Ad	0.71	1/452 (0.2%)	0.94	1/600 (0.2%)
31	Cd	0.77	1/452 (0.2%)	0.94	1/600 (0.2%)
32	Ae	0.50	0/483	0.71	0/643
32	Ce	0.62	0/499	0.89	1/665 (0.2%)
33	Af	0.53	0/404	0.99	2/542 (0.4%)
34	Ag	0.49	0/2490	0.70	0/3389
34	Cg	0.51	0/2495	0.69	0/3395
35	Ah	0.86	2/925 (0.2%)	0.87	2/1240 (0.2%)
36	A1	1.42	515/75394 (0.7%)	1.91	3591/117545 (3.1%)
36	A5	1.46	607/75414 (0.8%)	1.88	3500/117575 (3.0%)
37	A3	1.15	5/2883 (0.2%)	1.59	68/4491 (1.5%)
37	A7	1.38	13/2883 (0.5%)	1.80	121/4491 (2.7%)
38	A4	1.31	18/3746 (0.5%)	1.79	159/5832 (2.7%)
38	A8	1.16	4/3746 (0.1%)	1.70	130/5832 (2.2%)
39	BA	0.84	0/1948	1.01	5/2617 (0.2%)
39	DA	0.87	1/1946 (0.1%)	1.05	4/2614 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
40	BB	0.92	3/3146 (0.1%)	1.05	11/4228 (0.3%)
40	DB	1.02	4/3146 (0.1%)	1.11	13/4228 (0.3%)
41	BC	0.96	3/2800 (0.1%)	1.14	17/3790 (0.4%)
41	DC	0.87	0/2800	1.07	11/3790 (0.3%)
42	BD	0.71	2/2425 (0.1%)	0.87	1/3271 (0.0%)
42	DD	0.89	1/2408 (0.0%)	0.96	3/3248 (0.1%)
43	BE	0.88	0/1260	1.02	3/1694 (0.2%)
43	DE	0.90	1/1269 (0.1%)	1.00	3/1705 (0.2%)
44	BF	0.96	1/1821 (0.1%)	1.06	7/2451 (0.3%)
44	DF	0.99	1/1828 (0.1%)	1.04	6/2461 (0.2%)
45	BG	0.64	0/1836	0.82	1/2481 (0.0%)
45	DG	0.64	0/1795	0.81	1/2429 (0.0%)
46	BH	0.80	0/1539	0.97	5/2073 (0.2%)
46	DH	0.97	2/1539 (0.1%)	1.01	1/2073 (0.0%)
47	BI	0.90	2/1741 (0.1%)	0.97	5/2335 (0.2%)
47	DI	0.92	1/1758 (0.1%)	1.08	12/2358 (0.5%)
48	BJ	0.65	0/1374	0.85	1/1842 (0.1%)
48	DJ	0.81	1/1374 (0.1%)	0.99	4/1842 (0.2%)
49	BL	0.89	0/1568	1.02	8/2106 (0.4%)
49	DL	0.82	0/1573	1.04	6/2113 (0.3%)
50	BM	0.88	0/1068	0.91	0/1438
50	DM	0.95	0/1074	1.01	4/1446 (0.3%)
51	BN	0.88	0/1757	1.05	5/2354 (0.2%)
51	DN	0.83	1/1757 (0.1%)	1.00	6/2354 (0.3%)
52	BO	0.92	10/3160 (0.3%)	1.16	10/4208 (0.2%)
52	DO	0.98	11/3159 (0.3%)	1.02	25/4205 (0.6%)
53	BP	0.97	2/1443 (0.1%)	1.02	3/1944 (0.2%)
53	DP	1.05	1/1250 (0.1%)	1.09	5/1683 (0.3%)
54	BQ	0.98	0/1465	1.13	8/1965 (0.4%)
54	DQ	0.89	1/1465 (0.1%)	1.12	8/1965 (0.4%)
55	BR	0.71	1/1538 (0.1%)	0.87	1/2050 (0.0%)
55	DR	0.78	1/1538 (0.1%)	0.87	3/2050 (0.1%)
56	BS	0.89	0/1481	1.06	9/1990 (0.5%)
56	DS	1.02	0/1481	1.09	7/1990 (0.4%)
57	BT	0.93	0/1300	0.98	1/1743 (0.1%)
57	DT	1.01	2/1300 (0.2%)	1.01	1/1743 (0.1%)
58	BU	0.52	0/812	0.70	0/1099
58	DU	0.56	0/794	0.77	0/1076
59	BV	0.86	0/1018	1.03	3/1369 (0.2%)
59	DV	0.98	0/1018	1.09	4/1369 (0.3%)
60	BW	0.68	0/712	0.86	1/958 (0.1%)
60	DW	0.80	0/1052	0.90	1/1398 (0.1%)
61	BX	0.73	0/979	0.87	0/1321

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
61	DX	0.72	0/974	0.86	0/1314
62	BY	0.78	0/1004	1.10	5/1341 (0.4%)
62	DY	0.79	1/1004 (0.1%)	0.98	2/1341 (0.1%)
63	BZ	0.59	0/1118	0.81	1/1497 (0.1%)
63	DZ	0.55	0/1118	0.83	2/1497 (0.1%)
64	Ba	0.97	2/1204 (0.2%)	1.16	7/1612 (0.4%)
64	Da	0.94	2/1204 (0.2%)	1.14	9/1612 (0.6%)
65	Bb	0.83	0/473	0.85	0/629
65	Db	0.91	0/473	1.14	1/629 (0.2%)
66	Bc	0.59	0/751	0.73	0/1008
66	Dc	0.61	0/775	0.77	0/1040
67	Bd	0.73	0/890	0.89	1/1196 (0.1%)
67	Dd	0.94	2/897 (0.2%)	0.95	1/1205 (0.1%)
68	Be	1.02	2/1041 (0.2%)	1.19	9/1394 (0.6%)
68	De	1.03	0/1041	1.27	11/1394 (0.8%)
69	Bf	1.19	4/868 (0.5%)	1.08	2/1168 (0.2%)
69	Df	1.12	1/868 (0.1%)	1.09	3/1168 (0.3%)
70	Bg	0.70	0/890	0.98	4/1189 (0.3%)
70	Dg	0.72	0/890	0.92	0/1189
71	Bh	0.83	0/978	0.94	2/1301 (0.2%)
71	Dh	0.67	0/974	0.80	0/1297
72	Bi	0.77	0/778	0.98	1/1034 (0.1%)
72	Di	0.67	0/777	0.85	0/1033
73	Bj	0.98	2/696 (0.3%)	1.19	6/923 (0.7%)
73	Dj	0.87	0/696	1.04	3/923 (0.3%)
74	Bk	0.59	0/618	0.75	0/826
74	Dk	0.50	0/614	0.70	0/822
75	Bl	0.90	1/443 (0.2%)	1.07	1/588 (0.2%)
75	Dl	0.90	0/443	1.02	1/588 (0.2%)
76	Bm	0.89	1/423 (0.2%)	0.97	1/562 (0.2%)
76	Dm	1.08	2/423 (0.5%)	1.13	1/562 (0.2%)
77	Bn	0.78	0/234	1.18	2/300 (0.7%)
77	Dn	0.90	0/234	1.15	1/300 (0.3%)
78	Bo	0.87	1/860 (0.1%)	0.97	2/1136 (0.2%)
78	Do	0.83	0/860	0.88	1/1136 (0.1%)
79	Bp	0.80	0/701	0.96	1/934 (0.1%)
79	Dp	0.86	0/701	0.98	1/934 (0.1%)
80	A6	1.13	97/42174 (0.2%)	1.61	1103/65711 (1.7%)
81	Cf	0.46	0/404	0.84	0/542
82	Ch	0.64	0/480	0.85	0/642
84	Dq	0.54	0/977	0.75	1/1313 (0.1%)
All	All	1.11	1373/432157 (0.3%)	1.51	9884/634038 (1.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	CA	0	1
3	AB	0	1
5	CD	0	1
7	CF	0	2
9	AH	0	1
11	CJ	0	3
13	AL	0	1
16	AO	0	1
16	CO	0	1
17	CP	0	1
18	CQ	0	1
19	AR	0	2
22	CU	0	1
25	CX	0	1
27	AZ	0	3
27	CZ	0	2
29	Ab	0	1
33	Af	0	2
35	Ah	0	1
36	A1	0	3
36	A5	0	1
39	DA	0	2
40	BB	0	1
41	BC	0	1
41	DC	0	1
42	DD	0	1
43	BE	0	2
43	DE	0	1
44	BF	0	1
44	DF	0	2
45	BG	0	3
46	BH	0	1
48	BJ	0	1
52	BO	0	2
52	DO	0	2
56	DS	0	1
57	BT	0	1
59	DV	0	1
62	DY	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
63	DZ	0	1
64	Da	0	3
65	Bb	0	2
65	Db	0	1
67	Bd	0	1
78	Bo	0	1
81	Cf	0	2
All	All	0	67

The worst 5 of 1373 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	BO	3[A]	VAL	C-N	26.80	1.95	1.34
36	A1	2777	G	C5-C6	-23.22	1.19	1.42
52	DO	197[B]	PHE	C-N	-21.96	0.93	1.33
52	DO	182[B]	SER	C-N	18.04	1.75	1.34
36	A5	1152	G	N9-C8	15.01	1.48	1.37

The worst 5 of 9884 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2777	G	C4-C5-N7	50.47	130.99	110.80
36	A1	2777	G	N9-C4-C5	-40.53	89.19	105.40
36	A1	2777	G	C5-C6-O6	-39.10	105.14	128.60
52	BO	3[A]	VAL	CA-C-N	-39.08	31.23	117.20
36	A5	1152	G	N3-C4-C5	33.63	145.41	128.60

There are no chirality outliers.

5 of 67 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AB	131	ASP	Peptide
9	AH	131	PHE	Peptide
13	AL	127	GLN	Peptide
16	AO	124	ASP	Peptide
19	AR	22	PRO	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A2	37835	0	19062	1052	0
2	AA	1577	0	1567	102	0
2	CA	1583	0	1578	87	0
3	AB	1709	0	1784	122	0
3	CB	1722	0	1793	75	0
4	AC	1635	0	1723	53	0
4	CC	1635	0	1723	60	0
5	AD	1734	0	1817	66	0
5	CD	1734	0	1817	50	0
6	AE	2068	0	2154	71	0
6	CE	2068	0	2154	89	0
7	AF	1609	0	1675	67	0
7	CF	1609	0	1675	70	0
8	AG	1799	0	1879	88	0
8	CG	1755	0	1846	57	0
9	AH	1481	0	1572	82	0
9	CH	1491	0	1578	65	0
10	AI	1489	0	1525	67	0
10	CI	1489	0	1525	47	0
11	AJ	1494	0	1573	81	0
11	CJ	1494	0	1573	78	0
12	AK	772	0	727	43	0
12	CK	761	0	697	35	0
13	AL	1213	0	1257	49	0
13	CL	1168	0	1233	39	0
14	AM	890	0	887	46	0
14	CM	890	0	887	51	0
15	AN	1192	0	1255	42	0
15	CN	1192	0	1255	40	0
16	AO	891	0	883	57	0
16	CO	949	0	985	43	0
17	AP	977	0	1002	44	0
17	CP	1039	0	1050	67	0
18	AQ	1105	0	1166	68	0
18	CQ	1111	0	1171	49	0
19	AR	926	0	930	40	0
19	CR	906	0	909	38	0
20	AS	1192	0	1222	63	1
20	CS	1192	0	1222	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	AT	1112	0	1124	65	0
21	CT	1112	0	1124	45	0
22	AU	855	0	917	38	0
22	CU	882	0	939	55	0
23	AV	684	0	672	39	0
23	CV	684	0	672	30	0
24	AW	1021	0	1060	55	0
24	CW	1021	0	1060	28	0
25	AX	1121	0	1196	48	0
25	CX	1121	0	1196	32	0
26	AY	1073	0	1132	40	0
26	CY	1073	0	1132	49	0
27	AZ	563	0	603	42	0
27	CZ	558	0	598	29	0
28	Aa	769	0	814	0	0
28	Ca	769	0	815	0	0
29	Ab	610	0	630	0	0
29	Cb	610	0	631	0	0
30	Ac	497	0	535	0	0
30	Cc	497	0	535	0	0
31	Ad	442	0	428	0	0
31	Cd	442	0	428	0	0
32	Ae	475	0	525	0	0
32	Ce	491	0	542	0	0
33	Af	516	0	517	0	0
34	Ag	2437	0	2386	0	0
34	Cg	2442	0	2392	0	0
35	Ah	1105	0	960	0	0
36	A1	67355	0	33821	1318	0
36	A5	67376	0	33831	1282	0
37	A3	2579	0	1304	38	0
37	A7	2579	0	1303	43	0
38	A4	3353	0	1691	54	0
38	A8	3353	0	1695	56	0
39	BA	1914	0	1981	65	0
39	DA	1912	0	1976	82	0
40	BB	3075	0	3142	158	0
40	DB	3075	0	3142	119	0
41	BC	2748	0	2859	97	0
41	DC	2748	0	2859	95	0
42	BD	2375	0	2325	100	0
42	DD	2359	0	2311	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	BE	1239	0	1326	37	0
43	DE	1248	0	1339	33	0
44	BF	1784	0	1862	72	0
44	DF	1791	0	1869	45	0
45	BG	1804	0	1877	81	0
45	DG	1763	0	1819	73	0
46	BH	1518	0	1587	63	0
46	DH	1518	0	1587	67	0
47	BI	1705	0	1736	83	0
47	DI	1722	0	1755	51	1
48	BJ	1353	0	1383	65	0
48	DJ	1353	0	1383	56	0
49	BL	1543	0	1608	50	0
49	DL	1548	0	1613	45	0
50	BM	1053	0	1149	42	0
50	DM	1059	0	1154	41	0
51	BN	1720	0	1779	65	0
51	DN	1720	0	1779	68	0
52	BO	3119	0	3302	75	0
52	DO	3119	0	3302	89	0
53	BP	1420	0	1437	67	0
53	DP	1227	0	1236	34	0
54	BQ	1441	0	1543	51	0
54	DQ	1441	0	1543	40	0
55	BR	1521	0	1617	64	0
55	DR	1521	0	1617	39	0
56	BS	1445	0	1487	50	0
56	DS	1445	0	1487	49	0
57	BT	1276	0	1323	37	0
57	DT	1276	0	1323	50	0
58	BU	796	0	812	21	0
58	DU	778	0	791	25	0
59	BV	1003	0	1048	50	0
59	DV	1003	0	1048	28	0
60	BW	699	0	640	17	0
60	DW	1038	0	1071	21	0
61	BX	964	0	1025	22	0
61	DX	959	0	1023	24	0
62	BY	993	0	1081	31	0
62	DY	993	0	1081	27	0
63	BZ	1092	0	1155	43	0
63	DZ	1092	0	1155	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	Ba	1173	0	1215	0	0
64	Da	1173	0	1215	0	0
65	Bb	462	0	491	0	0
65	Db	462	0	491	0	0
66	Bc	743	0	797	0	0
66	Dc	767	0	816	0	0
67	Bd	876	0	912	0	0
67	Dd	883	0	918	0	0
68	Be	1020	0	1090	0	0
68	De	1020	0	1090	0	0
69	Bf	850	0	880	0	0
69	Df	850	0	880	0	0
70	Bg	880	0	945	0	0
70	Dg	880	0	945	0	0
71	Bh	969	0	1078	0	0
71	Dh	965	0	1067	0	0
72	Bi	771	0	849	0	0
72	Di	770	0	846	0	0
73	Bj	681	0	683	0	0
73	Dj	681	0	683	0	0
74	Bk	612	0	682	0	0
74	Dk	608	0	671	0	0
75	Bl	436	0	475	0	0
75	Dl	436	0	475	0	0
76	Bm	417	0	456	0	0
76	Dm	417	0	455	0	0
77	Bn	233	0	284	0	0
77	Dn	233	0	284	0	0
78	Bo	847	0	916	0	0
78	Do	847	0	915	0	0
79	Bp	694	0	734	0	0
79	Dp	694	0	734	0	0
80	A6	38021	0	19178	890	0
81	Cf	544	0	546	0	0
82	Ch	680	0	542	0	0
83	DK	750	0	185	12	0
84	Dq	1077	0	1012	0	0
85	Dr	235	0	50	0	0
86	Ds	230	0	49	0	0
87	A1	2891	0	0	486	1
87	A2	1316	0	0	231	0
87	A3	91	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	A4	105	0	0	9	0
87	A5	2926	0	0	479	0
87	A6	1399	0	0	209	0
87	A7	91	0	0	13	0
87	A8	133	0	0	24	0
87	AC	7	0	0	5	0
87	AI	7	0	0	1	0
87	AL	7	0	0	6	0
87	AN	7	0	0	1	0
87	AP	7	0	0	3	0
87	Ad	7	0	0	0	0
87	Ag	7	0	0	0	0
87	BA	7	0	0	5	0
87	BB	14	0	0	2	0
87	BC	7	0	0	2	0
87	BD	7	0	0	1	0
87	BI	28	0	0	21	0
87	BN	7	0	0	0	0
87	BO	7	0	0	1	0
87	BP	14	0	0	2	0
87	BR	7	0	0	1	0
87	BT	7	0	0	0	0
87	Bb	7	0	0	0	0
87	Bf	7	0	0	0	0
87	Bj	21	0	0	0	0
87	Bo	7	0	0	0	0
87	CB	7	0	0	0	0
87	CG	14	0	0	4	1
87	CI	7	0	0	1	0
87	CJ	7	0	0	3	0
87	CL	7	0	0	5	0
87	CN	7	0	0	2	0
87	CP	14	0	0	7	0
87	CS	7	0	0	0	0
87	CY	14	0	0	0	0
87	Cd	7	0	0	0	0
87	Cg	7	0	0	0	0
87	DA	7	0	0	6	0
87	DB	14	0	0	1	0
87	DC	14	0	0	2	0
87	DD	7	0	0	1	0
87	DG	7	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	DH	7	0	0	0	0
87	DI	14	0	0	1	0
87	DJ	7	0	0	1	0
87	DM	7	0	0	0	0
87	DO	7	0	0	0	0
87	DP	7	0	0	1	0
87	DQ	7	0	0	0	0
87	DR	7	0	0	1	0
87	DV	7	0	0	1	0
87	Db	7	0	0	0	0
87	De	7	0	0	0	0
87	Df	7	0	0	0	0
87	Dg	7	0	0	0	0
87	Dh	7	0	0	0	0
87	Dj	7	0	0	0	0
87	Do	7	0	0	0	0
88	A1	695	0	0	0	0
88	A2	171	0	0	0	0
88	A3	19	0	0	0	0
88	A4	34	0	0	0	0
88	A5	763	0	0	0	0
88	A6	239	0	0	0	0
88	A7	26	0	0	0	0
88	A8	20	0	0	0	0
88	AB	2	0	0	0	0
88	AC	1	0	0	0	0
88	AE	1	0	0	0	0
88	AI	2	0	0	0	0
88	AJ	1	0	0	0	0
88	AL	2	0	0	0	0
88	AN	1	0	0	0	0
88	AP	1	0	0	0	0
88	AS	2	0	0	0	0
88	AX	1	0	0	0	0
88	Aa	1	0	0	0	0
88	Ad	3	0	0	0	0
88	Af	1	0	0	0	0
88	BA	5	0	0	0	0
88	BB	4	0	0	0	0
88	BC	6	0	0	0	0
88	BD	1	0	0	0	0
88	BE	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	BF	2	0	0	0	0
88	BG	1	0	0	0	0
88	BI	4	0	0	0	0
88	BJ	1	0	0	0	0
88	BL	5	0	0	0	0
88	BN	6	0	0	0	0
88	BO	8	0	0	0	0
88	BP	10	0	0	0	0
88	BQ	4	0	0	0	0
88	BR	4	0	0	0	0
88	BS	2	0	0	0	0
88	BT	1	0	0	0	0
88	BV	5	0	0	0	0
88	BY	2	0	0	0	0
88	Ba	8	0	0	0	0
88	Bd	1	0	0	0	0
88	Be	2	0	0	0	0
88	Bf	1	0	0	0	0
88	Bg	1	0	0	0	0
88	Bj	7	0	0	0	0
88	Bl	1	0	0	0	0
88	Bm	1	0	0	0	0
88	Bo	3	0	0	0	0
88	CB	1	0	0	0	0
88	CE	1	0	0	0	0
88	CF	2	0	0	0	0
88	CG	2	0	0	0	0
88	CI	2	0	0	0	0
88	CL	3	0	0	0	0
88	CP	1	0	0	0	0
88	CQ	2	0	0	0	0
88	CS	2	0	0	0	0
88	CX	2	0	0	0	0
88	CY	2	0	0	0	0
88	CZ	1	0	0	0	0
88	Ca	1	0	0	0	0
88	Cd	1	0	0	0	0
88	Ch	2	0	0	0	0
88	DA	4	0	0	0	0
88	DB	13	0	0	0	0
88	DC	5	0	0	0	0
88	DD	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	DF	4	0	0	0	0
88	DG	1	0	0	0	0
88	DH	2	0	0	0	0
88	DJ	2	0	0	0	0
88	DL	1	0	0	0	0
88	DM	2	0	0	0	0
88	DN	1	0	0	0	0
88	DO	8	0	0	0	0
88	DP	7	0	0	0	0
88	DQ	1	0	0	0	0
88	DR	1	0	0	0	0
88	DS	4	0	0	0	0
88	DT	3	0	0	0	0
88	DV	3	0	0	0	0
88	DW	1	0	0	0	0
88	DY	2	0	0	0	0
88	Da	4	0	0	0	0
88	Db	1	0	0	0	0
88	Dd	1	0	0	0	0
88	De	2	0	0	0	0
88	Df	4	0	0	0	0
88	Dg	2	0	0	0	0
88	Dj	3	0	0	0	0
88	Di	1	0	0	0	0
88	Dm	1	0	0	0	0
88	Dn	1	0	0	0	0
88	Do	1	0	0	0	0
88	Dp	3	0	0	0	0
88	Dq	1	0	0	0	0
89	Aa	1	0	0	0	0
89	Ab	1	0	0	0	0
89	Ad	1	0	0	0	0
89	Af	1	0	0	0	0
89	Bj	1	0	0	0	0
89	Bm	1	0	0	0	0
89	Bo	1	0	0	0	0
89	Bp	1	0	0	0	0
89	Ca	1	0	0	0	0
89	Cb	1	0	0	0	0
89	Cd	1	0	0	0	0
89	Cf	1	0	0	0	0
89	Dj	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	Dm	1	0	0	0	0
89	Do	1	0	0	0	0
89	Dp	1	0	0	0	0
90	CI	1	0	0	0	0
90	DB	1	0	0	0	0
All	All	416785	0	300420	10055	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

The worst 5 of 10055 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
54:DQ:171:LYS:NZ	54:DQ:171:LYS:CE	1.67	1.52
48:DJ:8:PRO:CG	48:DJ:8:PRO:CB	1.75	1.50
1:A2:1686:C:H2'	1:A2:1687:U:H6	1.07	1.16
36:A1:1733:G:OP2	87:A1:3811:OHX:N6	1.84	1.10
80:A6:1636:C:H4'	80:A6:1637:C:H5'	1.34	1.09

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:AS:97:ASP:OD2	87:A1:3788:OHX:N2[2.545]	2.06	0.14
47:DI:218:ALA:O	87:CG:301:OHX:N3[2.647]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AA	204/252 (81%)	143 (70%)	35 (17%)	26 (13%)	0 2
2	CA	204/252 (81%)	146 (72%)	33 (16%)	25 (12%)	1 2
3	AB	212/255 (83%)	133 (63%)	41 (19%)	38 (18%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	CB	214/255 (84%)	174 (81%)	25 (12%)	15 (7%)	2	9
4	AC	215/254 (85%)	187 (87%)	16 (7%)	12 (6%)	3	16
4	CC	215/254 (85%)	188 (87%)	14 (6%)	13 (6%)	2	14
5	AD	221/240 (92%)	180 (81%)	28 (13%)	13 (6%)	2	14
5	CD	221/240 (92%)	177 (80%)	23 (10%)	21 (10%)	1	4
6	AE	258/261 (99%)	201 (78%)	36 (14%)	21 (8%)	1	7
6	CE	258/261 (99%)	219 (85%)	19 (7%)	20 (8%)	1	7
7	AF	204/225 (91%)	154 (76%)	31 (15%)	19 (9%)	1	5
7	CF	204/225 (91%)	155 (76%)	32 (16%)	17 (8%)	1	6
8	AG	224/236 (95%)	190 (85%)	22 (10%)	12 (5%)	3	17
8	CG	216/236 (92%)	183 (85%)	21 (10%)	12 (6%)	3	16
9	AH	182/190 (96%)	127 (70%)	28 (15%)	27 (15%)	0	1
9	CH	184/190 (97%)	143 (78%)	23 (12%)	18 (10%)	1	4
10	AI	184/200 (92%)	155 (84%)	14 (8%)	15 (8%)	1	6
10	CI	184/200 (92%)	160 (87%)	17 (9%)	7 (4%)	5	27
11	AJ	183/197 (93%)	152 (83%)	19 (10%)	12 (7%)	2	10
11	CJ	183/197 (93%)	152 (83%)	17 (9%)	14 (8%)	1	7
12	AK	94/105 (90%)	66 (70%)	18 (19%)	10 (11%)	1	3
12	CK	92/105 (88%)	59 (64%)	15 (16%)	18 (20%)	0	0
13	AL	153/156 (98%)	125 (82%)	19 (12%)	9 (6%)	2	14
13	CL	144/156 (92%)	118 (82%)	15 (10%)	11 (8%)	2	7
14	AM	122/143 (85%)	66 (54%)	23 (19%)	33 (27%)	0	0
14	CM	122/143 (85%)	60 (49%)	31 (25%)	31 (25%)	0	0
15	AN	148/151 (98%)	125 (84%)	15 (10%)	8 (5%)	3	17
15	CN	148/151 (98%)	129 (87%)	10 (7%)	9 (6%)	2	14
16	AO	125/137 (91%)	94 (75%)	16 (13%)	15 (12%)	1	2
16	CO	126/137 (92%)	101 (80%)	20 (16%)	5 (4%)	5	25
17	AP	122/142 (86%)	92 (75%)	15 (12%)	15 (12%)	1	2
17	CP	133/142 (94%)	91 (68%)	20 (15%)	22 (16%)	0	1
18	AQ	139/143 (97%)	114 (82%)	14 (10%)	11 (8%)	1	7
18	CQ	140/143 (98%)	122 (87%)	10 (7%)	8 (6%)	3	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AR	116/136 (85%)	87 (75%)	17 (15%)	12 (10%)	1	4
19	CR	113/136 (83%)	92 (81%)	12 (11%)	9 (8%)	1	7
20	AS	143/146 (98%)	110 (77%)	19 (13%)	14 (10%)	1	4
20	CS	143/146 (98%)	111 (78%)	25 (18%)	7 (5%)	3	20
21	AT	141/144 (98%)	111 (79%)	18 (13%)	12 (8%)	1	6
21	CT	141/144 (98%)	125 (89%)	9 (6%)	7 (5%)	3	19
22	AU	105/121 (87%)	87 (83%)	13 (12%)	5 (5%)	4	20
22	CU	108/121 (89%)	81 (75%)	12 (11%)	15 (14%)	0	2
23	AV	85/87 (98%)	64 (75%)	11 (13%)	10 (12%)	1	2
23	CV	85/87 (98%)	71 (84%)	7 (8%)	7 (8%)	1	6
24	AW	127/130 (98%)	114 (90%)	10 (8%)	3 (2%)	9	42
24	CW	127/130 (98%)	115 (91%)	12 (9%)	0	100	100
25	AX	142/145 (98%)	111 (78%)	13 (9%)	18 (13%)	0	2
25	CX	142/145 (98%)	127 (89%)	13 (9%)	2 (1%)	16	60
26	AY	132/135 (98%)	106 (80%)	13 (10%)	13 (10%)	1	4
26	CY	132/135 (98%)	100 (76%)	17 (13%)	15 (11%)	1	3
27	AZ	68/108 (63%)	46 (68%)	11 (16%)	11 (16%)	0	1
27	CZ	67/108 (62%)	50 (75%)	10 (15%)	7 (10%)	1	4
28	Aa	95/119 (80%)	57 (60%)	21 (22%)	17 (18%)	0	1
28	Ca	95/119 (80%)	67 (70%)	20 (21%)	8 (8%)	1	6
29	Ab	79/82 (96%)	62 (78%)	13 (16%)	4 (5%)	3	18
29	Cb	79/82 (96%)	62 (78%)	9 (11%)	8 (10%)	1	4
30	Ac	61/67 (91%)	47 (77%)	9 (15%)	5 (8%)	1	6
30	Cc	61/67 (91%)	41 (67%)	17 (28%)	3 (5%)	3	20
31	Ad	51/56 (91%)	43 (84%)	6 (12%)	2 (4%)	5	26
31	Cd	51/56 (91%)	45 (88%)	2 (4%)	4 (8%)	1	7
32	Ae	58/63 (92%)	49 (84%)	7 (12%)	2 (3%)	6	31
32	Ce	60/63 (95%)	45 (75%)	9 (15%)	6 (10%)	1	4
33	Af	50/152 (33%)	30 (60%)	9 (18%)	11 (22%)	0	0
34	Ag	316/319 (99%)	273 (86%)	30 (10%)	13 (4%)	4	24
34	Cg	316/319 (99%)	262 (83%)	38 (12%)	16 (5%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	Ah	120/273 (44%)	92 (77%)	17 (14%)	11 (9%)	1	5
39	BA	250/254 (98%)	230 (92%)	14 (6%)	6 (2%)	9	42
39	DA	250/254 (98%)	213 (85%)	30 (12%)	7 (3%)	8	37
40	BB	384/387 (99%)	333 (87%)	37 (10%)	14 (4%)	5	29
40	DB	384/387 (99%)	341 (89%)	34 (9%)	9 (2%)	10	43
41	BC	359/362 (99%)	304 (85%)	34 (10%)	21 (6%)	3	15
41	DC	359/362 (99%)	306 (85%)	32 (9%)	21 (6%)	3	15
42	BD	294/297 (99%)	242 (82%)	31 (10%)	21 (7%)	2	9
42	DD	292/297 (98%)	267 (91%)	19 (6%)	6 (2%)	11	47
43	BE	152/176 (86%)	137 (90%)	11 (7%)	4 (3%)	8	39
43	DE	153/176 (87%)	134 (88%)	15 (10%)	4 (3%)	8	39
44	BF	220/244 (90%)	200 (91%)	11 (5%)	9 (4%)	4	24
44	DF	221/244 (91%)	201 (91%)	15 (7%)	5 (2%)	10	43
45	BG	231/256 (90%)	186 (80%)	26 (11%)	19 (8%)	1	6
45	DG	229/256 (90%)	180 (79%)	28 (12%)	21 (9%)	1	5
46	BH	189/191 (99%)	166 (88%)	17 (9%)	6 (3%)	6	33
46	DH	189/191 (99%)	172 (91%)	13 (7%)	4 (2%)	11	47
47	BI	207/221 (94%)	181 (87%)	19 (9%)	7 (3%)	6	31
47	DI	209/221 (95%)	175 (84%)	22 (10%)	12 (6%)	3	16
48	BJ	167/174 (96%)	120 (72%)	26 (16%)	21 (13%)	0	2
48	DJ	167/174 (96%)	135 (81%)	19 (11%)	13 (8%)	1	7
49	BL	191/199 (96%)	161 (84%)	18 (9%)	12 (6%)	2	12
49	DL	192/199 (96%)	161 (84%)	20 (10%)	11 (6%)	3	16
50	BM	134/138 (97%)	117 (87%)	8 (6%)	9 (7%)	2	10
50	DM	135/138 (98%)	124 (92%)	10 (7%)	1 (1%)	30	78
51	BN	201/204 (98%)	184 (92%)	10 (5%)	7 (4%)	6	30
51	DN	201/204 (98%)	182 (90%)	13 (6%)	6 (3%)	7	34
52	BO	353/219 (161%)	332 (94%)	14 (4%)	7 (2%)	11	48
52	DO	352/219 (161%)	324 (92%)	18 (5%)	10 (3%)	8	37
53	BP	181/184 (98%)	155 (86%)	17 (9%)	9 (5%)	3	19
53	DP	153/184 (83%)	142 (93%)	9 (6%)	2 (1%)	18	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	BQ	183/186 (98%)	162 (88%)	17 (9%)	4 (2%)	10	45
54	DQ	183/186 (98%)	168 (92%)	9 (5%)	6 (3%)	6	32
55	BR	186/189 (98%)	170 (91%)	12 (6%)	4 (2%)	10	45
55	DR	186/189 (98%)	167 (90%)	16 (9%)	3 (2%)	14	56
56	BS	170/172 (99%)	154 (91%)	12 (7%)	4 (2%)	9	42
56	DS	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	33	81
57	BT	157/160 (98%)	140 (89%)	10 (6%)	7 (4%)	4	22
57	DT	157/160 (98%)	146 (93%)	9 (6%)	2 (1%)	18	62
58	BU	98/121 (81%)	75 (76%)	14 (14%)	9 (9%)	1	5
58	DU	96/121 (79%)	80 (83%)	13 (14%)	3 (3%)	7	34
59	BV	134/137 (98%)	124 (92%)	9 (7%)	1 (1%)	30	78
59	DV	134/137 (98%)	124 (92%)	8 (6%)	2 (2%)	15	58
60	BW	96/155 (62%)	69 (72%)	16 (17%)	11 (12%)	1	3
60	DW	133/155 (86%)	106 (80%)	19 (14%)	8 (6%)	2	14
61	BX	119/142 (84%)	106 (89%)	11 (9%)	2 (2%)	14	54
61	DX	118/142 (83%)	103 (87%)	7 (6%)	8 (7%)	2	10
62	BY	124/127 (98%)	107 (86%)	15 (12%)	2 (2%)	14	56
62	DY	124/127 (98%)	107 (86%)	12 (10%)	5 (4%)	5	25
63	BZ	133/136 (98%)	114 (86%)	9 (7%)	10 (8%)	2	8
63	DZ	133/136 (98%)	107 (80%)	13 (10%)	13 (10%)	1	4
64	Ba	146/149 (98%)	120 (82%)	15 (10%)	11 (8%)	2	8
64	Da	146/149 (98%)	123 (84%)	18 (12%)	5 (3%)	6	31
65	Bb	56/59 (95%)	44 (79%)	9 (16%)	3 (5%)	3	17
65	Db	56/59 (95%)	44 (79%)	7 (12%)	5 (9%)	1	5
66	Bc	95/105 (90%)	86 (90%)	8 (8%)	1 (1%)	21	67
66	Dc	98/105 (93%)	87 (89%)	8 (8%)	3 (3%)	7	34
67	Bd	107/113 (95%)	94 (88%)	8 (8%)	5 (5%)	4	21
67	Dd	107/113 (95%)	88 (82%)	13 (12%)	6 (6%)	3	16
68	Be	125/130 (96%)	111 (89%)	10 (8%)	4 (3%)	6	33
68	De	125/130 (96%)	110 (88%)	9 (7%)	6 (5%)	4	20
69	Bf	104/107 (97%)	100 (96%)	2 (2%)	2 (2%)	12	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	Df	104/107 (97%)	96 (92%)	5 (5%)	3 (3%)	7	35
70	Bg	110/121 (91%)	97 (88%)	9 (8%)	4 (4%)	5	29
70	Dg	110/121 (91%)	93 (84%)	13 (12%)	4 (4%)	5	29
71	Bh	117/120 (98%)	99 (85%)	10 (8%)	8 (7%)	2	10
71	Dh	117/120 (98%)	99 (85%)	14 (12%)	4 (3%)	6	31
72	Bi	97/100 (97%)	75 (77%)	11 (11%)	11 (11%)	1	3
72	Di	97/100 (97%)	77 (79%)	13 (13%)	7 (7%)	2	8
73	Bj	85/88 (97%)	70 (82%)	12 (14%)	3 (4%)	6	30
73	Dj	85/88 (97%)	75 (88%)	8 (9%)	2 (2%)	9	42
74	Bk	75/78 (96%)	66 (88%)	8 (11%)	1 (1%)	18	62
74	Dk	75/78 (96%)	61 (81%)	10 (13%)	4 (5%)	3	18
75	Bl	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
75	Dl	48/51 (94%)	41 (85%)	6 (12%)	1 (2%)	11	47
76	Bm	50/128 (39%)	45 (90%)	3 (6%)	2 (4%)	5	25
76	Dm	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	11	48
77	Bn	23/25 (92%)	20 (87%)	3 (13%)	0	100	100
77	Dn	23/25 (92%)	22 (96%)	0	1 (4%)	4	23
78	Bo	103/106 (97%)	86 (84%)	13 (13%)	4 (4%)	5	26
78	Do	103/106 (97%)	90 (87%)	11 (11%)	2 (2%)	12	51
79	Bp	89/92 (97%)	77 (86%)	9 (10%)	3 (3%)	6	31
79	Dp	89/92 (97%)	81 (91%)	8 (9%)	0	100	100
81	Cf	50/152 (33%)	26 (52%)	13 (26%)	11 (22%)	0	0
82	Ch	61/273 (22%)	38 (62%)	9 (15%)	14 (23%)	0	0
84	Dq	117/312 (38%)	93 (80%)	18 (15%)	6 (5%)	3	18
All	All	22511/24658 (91%)	18787 (84%)	2329 (10%)	1395 (6%)	2	13

5 of 1395 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AA	4	PRO
2	AA	29	VAL
2	AA	30	GLN
2	AA	39	ASN
2	AA	66	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AA	164/210 (78%)	122 (74%)	42 (26%)	1	4
2	CA	165/210 (79%)	131 (79%)	34 (21%)	2	9
3	AB	191/224 (85%)	137 (72%)	54 (28%)	0	3
3	CB	192/224 (86%)	148 (77%)	44 (23%)	1	6
4	AC	176/205 (86%)	130 (74%)	46 (26%)	1	4
4	CC	176/205 (86%)	133 (76%)	43 (24%)	1	5
5	AD	182/195 (93%)	138 (76%)	44 (24%)	1	5
5	CD	182/195 (93%)	140 (77%)	42 (23%)	1	6
6	AE	221/222 (100%)	166 (75%)	55 (25%)	1	4
6	CE	221/222 (100%)	178 (80%)	43 (20%)	2	11
7	AF	173/191 (91%)	137 (79%)	36 (21%)	2	8
7	CF	173/191 (91%)	132 (76%)	41 (24%)	1	5
8	AG	188/201 (94%)	149 (79%)	39 (21%)	2	8
8	CG	187/201 (93%)	143 (76%)	44 (24%)	1	5
9	AH	165/170 (97%)	124 (75%)	41 (25%)	1	4
9	CH	165/170 (97%)	127 (77%)	38 (23%)	1	6
10	AI	150/161 (93%)	118 (79%)	32 (21%)	1	8
10	CI	150/161 (93%)	117 (78%)	33 (22%)	1	7
11	AJ	158/166 (95%)	117 (74%)	41 (26%)	1	4
11	CJ	158/166 (95%)	124 (78%)	34 (22%)	1	8
12	AK	77/98 (79%)	58 (75%)	19 (25%)	1	4
12	CK	73/98 (74%)	56 (77%)	17 (23%)	1	6
13	AL	129/137 (94%)	105 (81%)	24 (19%)	2	13
13	CL	129/137 (94%)	100 (78%)	29 (22%)	1	7
14	AM	88/119 (74%)	55 (62%)	33 (38%)	0	1
14	CM	88/119 (74%)	55 (62%)	33 (38%)	0	1
15	AN	127/128 (99%)	91 (72%)	36 (28%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	CN	127/128 (99%)	103 (81%)	24 (19%)	2	12
16	AO	81/105 (77%)	57 (70%)	24 (30%)	0	2
16	CO	97/105 (92%)	71 (73%)	26 (27%)	1	4
17	AP	101/118 (86%)	82 (81%)	19 (19%)	2	12
17	CP	103/118 (87%)	81 (79%)	22 (21%)	1	8
18	AQ	117/119 (98%)	84 (72%)	33 (28%)	0	3
18	CQ	118/119 (99%)	92 (78%)	26 (22%)	1	7
19	AR	94/124 (76%)	70 (74%)	24 (26%)	1	4
19	CR	92/124 (74%)	74 (80%)	18 (20%)	2	11
20	AS	128/129 (99%)	87 (68%)	41 (32%)	0	2
20	CS	128/129 (99%)	98 (77%)	30 (23%)	1	5
21	AT	115/116 (99%)	84 (73%)	31 (27%)	1	3
21	CT	115/116 (99%)	88 (76%)	27 (24%)	1	5
22	AU	100/114 (88%)	71 (71%)	29 (29%)	0	3
22	CU	103/114 (90%)	69 (67%)	34 (33%)	0	2
23	AV	74/74 (100%)	56 (76%)	18 (24%)	1	5
23	CV	74/74 (100%)	57 (77%)	17 (23%)	1	6
24	AW	110/111 (99%)	84 (76%)	26 (24%)	1	5
24	CW	110/111 (99%)	96 (87%)	14 (13%)	6	27
25	AX	119/120 (99%)	97 (82%)	22 (18%)	2	13
25	CX	119/120 (99%)	101 (85%)	18 (15%)	4	20
26	AY	112/113 (99%)	84 (75%)	28 (25%)	1	4
26	CY	112/113 (99%)	90 (80%)	22 (20%)	2	11
27	AZ	61/89 (68%)	43 (70%)	18 (30%)	0	2
27	CZ	61/89 (68%)	44 (72%)	17 (28%)	0	3
28	Aa	83/101 (82%)	65 (78%)	18 (22%)	1	8
28	Ca	83/101 (82%)	68 (82%)	15 (18%)	2	13
29	Ab	70/71 (99%)	62 (89%)	8 (11%)	8	33
29	Cb	70/71 (99%)	57 (81%)	13 (19%)	2	13
30	Ac	56/60 (93%)	38 (68%)	18 (32%)	0	2
30	Cc	56/60 (93%)	38 (68%)	18 (32%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	Ad	47/49 (96%)	38 (81%)	9 (19%)	2	12
31	Cd	47/49 (96%)	36 (77%)	11 (23%)	1	5
32	Ae	51/54 (94%)	43 (84%)	8 (16%)	4	18
32	Ce	53/54 (98%)	37 (70%)	16 (30%)	0	2
33	Af	43/116 (37%)	32 (74%)	11 (26%)	1	4
34	Ag	259/262 (99%)	222 (86%)	37 (14%)	5	22
34	Cg	260/262 (99%)	226 (87%)	34 (13%)	6	25
35	Ah	97/195 (50%)	74 (76%)	23 (24%)	1	5
39	BA	193/196 (98%)	160 (83%)	33 (17%)	3	15
39	DA	192/196 (98%)	154 (80%)	38 (20%)	2	11
40	BB	321/323 (99%)	240 (75%)	81 (25%)	1	4
40	DB	321/323 (99%)	251 (78%)	70 (22%)	1	8
41	BC	288/289 (100%)	227 (79%)	61 (21%)	1	8
41	DC	288/289 (100%)	222 (77%)	66 (23%)	1	6
42	BD	244/245 (100%)	189 (78%)	55 (22%)	1	7
42	DD	243/245 (99%)	195 (80%)	48 (20%)	2	11
43	BE	134/153 (88%)	116 (87%)	18 (13%)	6	24
43	DE	135/153 (88%)	115 (85%)	20 (15%)	4	21
44	BF	186/205 (91%)	165 (89%)	21 (11%)	9	33
44	DF	187/205 (91%)	158 (84%)	29 (16%)	4	19
45	BG	187/208 (90%)	151 (81%)	36 (19%)	2	12
45	DG	177/208 (85%)	138 (78%)	39 (22%)	1	7
46	BH	171/171 (100%)	131 (77%)	40 (23%)	1	5
46	DH	171/171 (100%)	132 (77%)	39 (23%)	1	6
47	BI	177/187 (95%)	143 (81%)	34 (19%)	2	12
47	DI	179/187 (96%)	142 (79%)	37 (21%)	2	8
48	BJ	147/150 (98%)	111 (76%)	36 (24%)	1	5
48	DJ	147/150 (98%)	114 (78%)	33 (22%)	1	7
49	BL	154/159 (97%)	123 (80%)	31 (20%)	2	10
49	DL	154/159 (97%)	124 (80%)	30 (20%)	2	11
50	BM	107/109 (98%)	84 (78%)	23 (22%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	DM	108/109 (99%)	84 (78%)	24 (22%)	1	7
51	BN	175/176 (99%)	146 (83%)	29 (17%)	3	16
51	DN	175/176 (99%)	142 (81%)	33 (19%)	2	12
52	BO	323/179 (180%)	276 (85%)	47 (15%)	5	21
52	DO	323/179 (180%)	267 (83%)	56 (17%)	3	14
53	BP	140/146 (96%)	109 (78%)	31 (22%)	1	7
53	DP	125/146 (86%)	103 (82%)	22 (18%)	3	14
54	BQ	150/151 (99%)	126 (84%)	24 (16%)	3	17
54	DQ	150/151 (99%)	124 (83%)	26 (17%)	3	14
55	BR	153/154 (99%)	116 (76%)	37 (24%)	1	5
55	DR	153/154 (99%)	121 (79%)	32 (21%)	1	8
56	BS	156/156 (100%)	127 (81%)	29 (19%)	2	13
56	DS	156/156 (100%)	123 (79%)	33 (21%)	1	8
57	BT	136/137 (99%)	103 (76%)	33 (24%)	1	5
57	DT	136/137 (99%)	109 (80%)	27 (20%)	2	10
58	BU	87/107 (81%)	73 (84%)	14 (16%)	3	17
58	DU	85/107 (79%)	62 (73%)	23 (27%)	1	3
59	BV	104/105 (99%)	88 (85%)	16 (15%)	4	19
59	DV	104/105 (99%)	96 (92%)	8 (8%)	18	56
60	BW	57/129 (44%)	49 (86%)	8 (14%)	5	23
60	DW	100/129 (78%)	85 (85%)	15 (15%)	4	20
61	BX	104/118 (88%)	78 (75%)	26 (25%)	1	4
61	DX	104/118 (88%)	81 (78%)	23 (22%)	1	7
62	BY	109/110 (99%)	87 (80%)	22 (20%)	2	10
62	DY	109/110 (99%)	85 (78%)	24 (22%)	1	7
63	BZ	115/116 (99%)	88 (76%)	27 (24%)	1	5
63	DZ	115/116 (99%)	89 (77%)	26 (23%)	1	6
64	Ba	118/119 (99%)	97 (82%)	21 (18%)	2	14
64	Da	118/119 (99%)	95 (80%)	23 (20%)	2	11
65	Bb	46/47 (98%)	36 (78%)	10 (22%)	1	8
65	Db	46/47 (98%)	35 (76%)	11 (24%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
66	Bc	81/88 (92%)	63 (78%)	18 (22%)	1	7
66	Dc	84/88 (96%)	68 (81%)	16 (19%)	2	12
67	Bd	92/97 (95%)	73 (79%)	19 (21%)	2	8
67	Dd	94/97 (97%)	73 (78%)	21 (22%)	1	7
68	Be	109/111 (98%)	87 (80%)	22 (20%)	2	10
68	De	109/111 (98%)	89 (82%)	20 (18%)	2	13
69	Bf	90/91 (99%)	77 (86%)	13 (14%)	5	22
69	Df	90/91 (99%)	79 (88%)	11 (12%)	7	29
70	Bg	95/103 (92%)	70 (74%)	25 (26%)	1	4
70	Dg	95/103 (92%)	71 (75%)	24 (25%)	1	4
71	Bh	104/105 (99%)	79 (76%)	25 (24%)	1	5
71	Dh	103/105 (98%)	77 (75%)	26 (25%)	1	4
72	Bi	81/82 (99%)	58 (72%)	23 (28%)	0	3
72	Di	80/82 (98%)	51 (64%)	29 (36%)	0	1
73	Bj	70/71 (99%)	56 (80%)	14 (20%)	2	10
73	Dj	70/71 (99%)	53 (76%)	17 (24%)	1	5
74	Bk	68/69 (99%)	48 (71%)	20 (29%)	0	2
74	Dk	67/69 (97%)	53 (79%)	14 (21%)	1	8
75	Bl	45/46 (98%)	36 (80%)	9 (20%)	2	10
75	Dl	45/46 (98%)	34 (76%)	11 (24%)	1	5
76	Bm	47/116 (40%)	37 (79%)	10 (21%)	1	8
76	Dm	47/116 (40%)	34 (72%)	13 (28%)	0	3
77	Bn	23/23 (100%)	15 (65%)	8 (35%)	0	1
77	Dn	23/23 (100%)	16 (70%)	7 (30%)	0	2
78	Bo	90/91 (99%)	68 (76%)	22 (24%)	1	5
78	Do	90/91 (99%)	74 (82%)	16 (18%)	2	14
79	Bp	71/72 (99%)	56 (79%)	15 (21%)	1	8
79	Dp	71/72 (99%)	61 (86%)	10 (14%)	5	23
81	Cf	43/112 (38%)	32 (74%)	11 (26%)	1	4
82	Ch	54/199 (27%)	38 (70%)	16 (30%)	0	2
84	Dq	105/233 (45%)	76 (72%)	29 (28%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	19013/20587 (92%)	14917 (78%)	4096 (22%)	1 8

5 of 4096 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
67	Bd	26	LYS
7	CF	70	VAL
63	DZ	89	VAL
70	Bg	23	VAL
2	CA	41	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
59	BV	33	ASN
4	CC	250	GLN
54	DQ	9	GLN
59	BV	98	ASN
74	Bk	40	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	1764/1800 (98%)	545 (30%)	86 (4%)
36	A1	3146/3396 (92%)	738 (23%)	127 (4%)
36	A5	3145/3396 (92%)	731 (23%)	129 (4%)
37	A3	120/121 (99%)	22 (18%)	3 (2%)
37	A7	120/121 (99%)	18 (15%)	0
38	A4	157/158 (99%)	38 (24%)	5 (3%)
38	A8	157/158 (99%)	32 (20%)	3 (1%)
80	A6	1766/1800 (98%)	499 (28%)	60 (3%)
All	All	10375/10950 (94%)	2623 (25%)	413 (3%)

5 of 2623 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	2	A
1	A2	4	C
1	A2	8	U
1	A2	16	G

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Mol	Chain	Res	Type
1	A2	20	G

5 of 413 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	A1	2818	U
80	A6	187	G
36	A5	2728	G
36	A1	3121	U
36	A1	3350	C

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3566 ligands modelled in this entry, 2221 are monoatomic - leaving 1345 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	$\# Z > 2$
87	OHX	A1	3401	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3402	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3407	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3408	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3409	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3410	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A1	3411	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3412	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3413	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3414	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3415	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3416	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3417	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3418	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3419	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3420	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3421	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3422	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3423	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3424	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3426	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3427	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3428	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3429	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3430	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3431	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3432	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3433	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3434	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3435	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3437	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3438	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3439	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3440	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3441	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3442	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3443	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3444	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3445	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3446	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3447	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3448	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3449	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3450	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3451	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3452	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3453	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A1	3454	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3455	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3456	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3457	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3458	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3459	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3460	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3461	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3462	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3463	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3464	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3465	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3466	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3467	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3468	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3469	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3470	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3471	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3472	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3473	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3474	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3475	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3476	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3477	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3478	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3479	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3480	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3481	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3482	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3483	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3485	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3486	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3487	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3488	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3489	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3491	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3492	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3493	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3494	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3495	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3496	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A1	3497	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3498	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3499	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3500	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3501	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3502	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3503	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3504	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3505	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3506	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3507	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3508	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3509	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3510	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3511	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3512	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3513	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3514	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3515	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3516	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3517	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3518	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3519	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3520	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3521	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3522	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3523	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3524	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3525	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3526	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3527	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3528	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3529	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3530	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3531	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3532	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3533	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3534	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3535	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3536	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3537	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3538	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3539	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A1	3540	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3541	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3542	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3543	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3544	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3545	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3546	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3547	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3548	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3549	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3550	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3551	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3552	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3553	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3554	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3555	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3556	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3557	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3558	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3559	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3560	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3561	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3562	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3563	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3564	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3565	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3566	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3567	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3568	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3569	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3570	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3571	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3572	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3573	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3574	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3575	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3576	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3577	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3578	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3579	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3580	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3581	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3582	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A1	3583	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3584	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3585	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3586	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3587	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3588	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3589	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3590	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3591	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3592	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3593	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3594	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3595	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3596	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3597	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3598	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3599	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3600	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3601	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3602	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3603	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3604	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3605	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3606	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3607	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3608	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3609	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3610	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3611	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3612	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3613	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3614	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3615	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3616	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3617	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3618	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3619	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3620	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3621	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3622	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3623	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3624	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3625	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A1	3626	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3627	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3628	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3629	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3630	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3631	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3632	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3633	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3634	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3635	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3636	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3637	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3638	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3639	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3640	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3641	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3642	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3643	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3644	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3645	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3646	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3647	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3648	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3649	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3650	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3651	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3652	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3653	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3654	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3655	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3656	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3657	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3658	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3659	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3660	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3661	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3662	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3663	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3664	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3665	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3666	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3667	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3668	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A1	3669	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3670	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3671	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3672	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3673	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3674	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3675	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3676	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3677	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3678	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3679	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3680	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3681	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3682	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3683	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3684	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3685	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3686	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3687	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3688	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3689	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3690	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3691	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3692	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3693	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3694	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3695	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3696	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3697	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3698	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3699	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3700	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3701	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3702	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3703	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3704	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3705	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3706	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3707	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3708	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3709	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3710	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3711	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A1	3712	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3713	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3714	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3715	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3716	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3717	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3718	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3719	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3720	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3721	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3722	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3723	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3724	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3725	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3726	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3727	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3728	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3729	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3730	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3731	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3732	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3733	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3734	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3735	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3736	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3737	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3738	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3739	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3740	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3741	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3742	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3743	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3744	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3745	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3746	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3747	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3748	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3749	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3750	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3751	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3752	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3753	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3754	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A1	3755	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3756	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3757	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3758	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3759	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3760	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3761	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3762	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3763	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3764	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3765	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3766	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3767	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3768	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3769	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3770	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3771	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3772	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3773	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3774	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3775	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3776	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3777	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3778	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3779	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3780	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3781	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3782	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3783	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3784	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3785	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3786	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3787	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3788	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3789	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3790	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3791	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3792	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3793	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3794	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3795	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3796	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3797	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A1	3798	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3799	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3800	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3801	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3802	36,87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3803	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3804	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3805	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3806	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3807	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3808	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3809	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3810	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3811	36	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3812	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3813	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3814	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3815	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A1	3816	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1901	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1902	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1903	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1904	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1905	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1906	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1907	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1908	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1909	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1910	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1911	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1912	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1913	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1914	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1915	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1916	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1917	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1918	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1919	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1920	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1921	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1922	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1923	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1924	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A2	1925	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1926	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1927	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1928	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1929	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1930	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1931	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1932	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1933	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1934	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1935	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1936	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1937	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1938	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1939	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1940	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1941	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1942	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1943	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1944	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1945	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1946	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1947	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1948	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1949	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1950	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1951	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1952	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1953	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1954	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1955	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1956	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1957	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1958	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1959	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1960	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1961	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1962	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1963	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1964	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1965	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1966	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1967	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A2	1968	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1969	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1970	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1971	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1972	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1973	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1974	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1975	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1976	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1977	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1978	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1979	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1980	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1981	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1982	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1983	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1984	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1985	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1986	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1987	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1988	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1989	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1990	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1991	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1992	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1993	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1994	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1995	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1996	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1997	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1998	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	1999	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2000	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2001	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2002	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2003	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2004	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2005	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2006	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2007	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2008	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2009	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2010	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A2	2011	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2012	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2013	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2014	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2015	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2016	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2017	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2018	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2019	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2020	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2021	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2033	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2053	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A2	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2067	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2074	1	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A2	2258	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A3	204	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A3	205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A3	206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A3	207	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A3	208	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A3	209	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A3	210	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A3	211	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A3	212	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A3	213	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A4	203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A4	204	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A4	205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A4	206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A4	207	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A4	208	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A4	209	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A4	210	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A4	211	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A4	212	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A4	213	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A4	214	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A4	215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3401	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3402	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3404	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3405	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3406	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3407	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3413	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3414	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3415	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3416	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3417	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3418	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3419	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3420	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3421	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3422	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3423	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3424	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3426	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3427	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3428	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A5	3429	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3430	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3431	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3432	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3433	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3434	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3435	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3437	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3438	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3439	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3440	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3441	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3442	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3443	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3444	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3445	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3446	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3447	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3448	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3449	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3450	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3451	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3452	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3453	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3454	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3455	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3456	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3457	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3458	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3459	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3460	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3461	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3462	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3463	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3464	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3465	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3466	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3467	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3468	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3469	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3470	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3471	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A5	3472	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3473	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3474	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3475	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3476	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3477	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3478	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3479	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3480	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3481	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3482	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3483	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3485	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3486	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3487	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3488	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3489	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3491	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3492	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3493	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3494	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3495	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3496	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3497	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3498	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3499	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3500	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3501	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3502	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3503	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3504	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3505	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3506	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3507	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3508	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3509	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3510	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3511	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3512	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3513	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3514	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A5	3515	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3516	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3517	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3518	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3519	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3520	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3521	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3522	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3523	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3524	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3525	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3526	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3527	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3528	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3529	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3530	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3531	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3532	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3533	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3534	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3535	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3536	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3537	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3538	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3539	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3540	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3541	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3542	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3543	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3544	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3545	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3546	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3547	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3548	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3549	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3550	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3551	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3552	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3553	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3554	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3555	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3556	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3557	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A5	3558	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3559	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3560	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3561	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3562	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3563	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3564	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3565	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3566	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3567	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3568	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3569	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3570	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3571	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3572	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3573	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3574	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3575	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3576	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3577	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3578	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3579	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3580	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3581	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3582	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3583	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3584	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3585	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3586	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3587	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3588	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3589	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3590	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3591	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3592	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3593	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3594	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3595	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3596	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3597	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3598	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3599	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3600	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A5	3601	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3602	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3603	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3604	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3605	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3606	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3607	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3608	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3609	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3610	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3611	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3612	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3613	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3614	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3615	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3616	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3617	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3618	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3619	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3620	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3621	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3622	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3623	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3624	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3625	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3626	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3627	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3628	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3629	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3630	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3631	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3632	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3633	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3634	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3635	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3636	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3637	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3638	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3639	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3640	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3641	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3642	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3643	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A5	3644	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3645	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3646	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3647	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3648	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3649	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3650	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3651	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3652	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3653	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3654	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3655	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3656	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3657	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3658	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3659	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3660	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3661	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3662	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3663	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3664	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3665	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3666	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3667	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3668	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3669	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3670	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3671	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3672	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3673	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3674	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3675	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3676	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3677	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3678	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3679	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3680	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3681	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3682	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3683	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3684	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3685	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3686	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A5	3687	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3688	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3689	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3690	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3691	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3692	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3693	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3694	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3695	36	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3696	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3697	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3698	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3699	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3700	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3701	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3702	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3703	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3704	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3705	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3706	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3707	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3708	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3709	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3710	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3711	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3712	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3713	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3714	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3715	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3716	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3717	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3718	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3719	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3720	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3721	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3722	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3723	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3724	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3725	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3726	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3727	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3728	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3729	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A5	3730	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3731	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3732	36	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3733	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3734	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3735	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3736	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3737	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3738	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3739	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3740	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3741	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3742	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3743	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3744	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3745	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3746	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3747	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3748	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3749	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3750	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3751	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3752	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3753	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3754	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3755	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3756	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3757	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3758	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3759	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3760	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3761	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3762	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3763	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3764	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3765	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3766	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3767	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3768	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3769	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3770	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3771	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3772	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A5	3773	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3774	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3775	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3776	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3777	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3778	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3779	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3780	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3781	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3782	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3783	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3784	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3785	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3786	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3787	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3788	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3789	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3790	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3791	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3792	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3793	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3794	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3795	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3796	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3797	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3798	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3799	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3800	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3801	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3802	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3803	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3804	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3805	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3806	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3807	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3808	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3809	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3810	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3811	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3812	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3813	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3814	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3815	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A5	3816	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3817	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3818	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3819	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3820	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3821	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3822	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A5	3823	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1901	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1902	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1903	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1904	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1905	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1906	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1907	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1908	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1909	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1910	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1911	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1912	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1913	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1914	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1915	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1916	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1917	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1918	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1919	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1920	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1921	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1922	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1923	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1924	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1925	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1926	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1927	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1928	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1929	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1930	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1931	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1932	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1933	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1934	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1935	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A6	1936	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1937	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1938	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1939	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1940	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1941	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1942	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1943	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1944	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1945	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1946	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1947	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1948	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1949	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1950	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1951	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1952	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1953	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1954	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1955	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1956	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1957	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1958	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1959	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1960	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1961	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1962	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1963	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1964	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1965	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1966	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1967	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1968	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1969	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1970	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1971	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1972	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1973	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1974	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1975	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1976	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1977	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1978	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A6	1979	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1980	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1981	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1982	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1983	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1984	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1985	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1986	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1987	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1988	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1989	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1990	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1991	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1992	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1993	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1994	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1995	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1996	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1997	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1998	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	1999	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2000	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2001	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2002	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2003	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2004	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2005	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2006	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2007	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2008	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2009	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2010	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2011	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2012	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2013	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2014	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2015	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2016	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2017	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2018	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2019	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2020	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2021	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A6	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2031	-	0,5,6	0.00	-	0,10,15	0.00	-
87	OHX	A6	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2064	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A6	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2076	87	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A6	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A7	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A7	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A7	203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A7	204	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A7	205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A7	207	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	A7	208	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A7	209	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A7	210	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A7	211	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A7	212	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A7	213	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A8	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A8	203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A8	204	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A8	205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A8	206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A8	207	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A8	208	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A8	209	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A8	210	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A8	211	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A8	212	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A8	213	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A8	214	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A8	215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A8	216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	A8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	AC	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	AI	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	AL	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	AN	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	AP	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Ad	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Ag	401	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	BA	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	BB	401	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	BB	402	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	BC	401	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	BD	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	BI	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	BI	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	BI	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	BI	304	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	BN	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	BO	201	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	BP	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	BP	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	BR	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	BT	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Bb	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Bf	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Bj	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Bj	102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Bj	103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Bo	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	CB	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	CG	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	CG	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	CI	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	CJ	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	CL	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	CN	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	CP	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	CP	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	CS	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	CY	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	CY	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Cd	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Cg	401	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	DA	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	DB	401	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	DB	402	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	DC	401	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	DC	402	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	DD	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	DG	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	DH	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	DI	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	DI	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	DJ	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	DM	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	DO	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	DP	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	DQ	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	DR	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	DV	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Db	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	De	201	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	Df	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Dg	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Dh	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Dj	104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Do	201	-	0,6,6	0.00	-	0,15,15	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A1	3401	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3402	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3403	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3407	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3408	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3409	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3410	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3411	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3412	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3413	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3414	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3415	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3416	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3417	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3418	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3419	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3420	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3421	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3422	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3423	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3424	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3425	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3426	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3427	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3428	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3429	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3430	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3431	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3432	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3433	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3434	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A1	3435	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3436	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3437	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3438	87	-	0/0/0/0	0/0/0/0
87	OHX	A1	3439	87	-	0/0/0/0	0/0/0/0
87	OHX	A1	3440	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3441	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3442	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3443	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3444	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3445	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3446	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3447	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3448	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3449	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3450	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3451	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3452	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3453	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3454	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3455	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3456	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3457	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3458	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3459	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3460	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3461	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3462	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3463	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3464	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3465	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3466	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3467	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3468	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3469	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3470	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3471	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3472	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3473	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3474	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3475	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3476	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A1	3477	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3478	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3479	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3480	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3481	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3482	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3483	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3484	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3485	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3486	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3487	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3488	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3489	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3490	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3491	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3492	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3493	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3494	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3495	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3496	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3497	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3498	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3499	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3500	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3501	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3502	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3503	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3504	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3505	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3506	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3507	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3508	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3509	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3510	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3511	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3512	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3513	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3514	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3515	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3516	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3517	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3518	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A1	3519	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3520	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3521	87	-	0/0/0/0	0/0/0/0
87	OHX	A1	3522	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3523	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3524	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3525	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3526	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3527	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3528	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3529	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3530	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3531	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3532	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3533	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3534	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3535	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3536	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3537	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3538	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3539	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3540	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3541	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3542	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3543	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3544	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3545	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3546	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3547	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3548	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3549	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3550	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3551	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3552	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3553	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3554	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3555	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3556	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3557	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3558	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3559	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3560	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A1	3561	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3562	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3563	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3564	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3565	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3566	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3567	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3568	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3569	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3570	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3571	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3572	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3573	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3574	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3575	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3576	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3577	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3578	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3579	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3580	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3581	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3582	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3583	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3584	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3585	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3586	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3587	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3588	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3589	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3590	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3591	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3592	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3593	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3594	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3595	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3596	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3597	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3598	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3599	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3600	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3601	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3602	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A1	3603	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3604	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3605	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3606	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3607	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3608	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3609	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3610	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3611	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3612	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3613	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3614	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3615	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3616	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3617	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3618	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3619	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3620	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3621	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3622	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3623	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3624	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3625	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3626	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3627	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3628	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3629	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3630	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3631	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3632	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3633	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3634	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3635	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3636	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3637	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3638	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3639	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3640	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3641	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3642	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3643	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3644	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A1	3645	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3646	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3647	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3648	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3649	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3650	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3651	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3652	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3653	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3654	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3655	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3656	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3657	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3658	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3659	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3660	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3661	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3662	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3663	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3664	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3665	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3666	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3667	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3668	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3669	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3670	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3671	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3672	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3673	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3674	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3675	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3676	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3677	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3678	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3679	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3680	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3681	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3682	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3683	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3684	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3685	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3686	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A1	3687	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3688	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3689	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3690	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3691	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3692	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3693	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3694	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3695	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3696	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3697	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3698	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3699	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3700	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3701	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3702	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3703	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3704	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3705	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3706	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3707	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3708	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3709	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3710	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3711	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3712	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3713	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3714	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3715	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3716	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3717	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3718	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3719	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3720	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3721	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3722	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3723	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3724	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3725	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3726	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3727	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3728	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A1	3729	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3730	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3731	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3732	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3733	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3734	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3735	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3736	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3737	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3738	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3739	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3740	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3741	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3742	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3743	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3744	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3745	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3746	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3747	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3748	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3749	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3750	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3751	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3752	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3753	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3754	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3755	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3756	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3757	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3758	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3759	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3760	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3761	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3762	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3763	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3764	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3765	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3766	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3767	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3768	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3769	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3770	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A1	3771	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3772	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3773	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3774	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3775	87	-	0/0/0/0	0/0/0/0
87	OHX	A1	3776	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3777	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3778	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3779	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3780	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3781	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3782	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3783	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3784	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3785	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3786	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3787	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3788	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3789	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3790	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3791	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3792	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3793	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3794	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3795	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3796	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3797	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3798	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3799	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3800	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3801	87	-	0/0/0/0	0/0/0/0
87	OHX	A1	3802	36,87	-	0/0/0/0	0/0/0/0
87	OHX	A1	3803	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3804	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3805	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3806	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3807	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3808	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3809	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3810	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3811	36	-	0/0/0/0	0/0/0/0
87	OHX	A1	3812	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A1	3813	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3814	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3815	-	-	0/0/0/0	0/0/0/0
87	OHX	A1	3816	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1901	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1902	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1903	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1904	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1905	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1906	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1907	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1908	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1909	87	-	0/0/0/0	0/0/0/0
87	OHX	A2	1910	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1911	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1912	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1913	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1914	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1915	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1916	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1917	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1918	87	-	0/0/0/0	0/0/0/0
87	OHX	A2	1919	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1920	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1921	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1922	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1923	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1924	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1925	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1926	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1927	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1928	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1929	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1930	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1931	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1932	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1933	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1934	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1935	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1936	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1937	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1938	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A2	1939	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1940	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1941	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1942	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1943	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1944	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1945	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1946	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1947	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1948	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1949	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1950	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1951	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1952	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1953	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1954	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1955	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1956	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1957	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1958	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1959	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1960	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1961	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1962	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1963	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1964	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1965	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1966	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1967	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1968	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1969	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1970	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1971	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1972	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1973	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1974	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1975	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1976	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1977	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1978	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1979	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1980	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A2	1981	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1982	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1983	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1984	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1985	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1986	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1987	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1988	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1989	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1990	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1991	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1992	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1993	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1994	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1995	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1996	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1997	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1998	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	1999	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2000	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2001	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2002	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2003	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2004	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2005	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2006	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2007	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2008	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2009	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2010	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2011	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2012	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2013	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2014	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2015	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2016	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2017	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2018	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2019	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2020	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2021	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2022	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A2	2023	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2024	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2025	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2026	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2027	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2028	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2029	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2030	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2031	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2032	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2033	87	-	0/0/0/0	0/0/0/0
87	OHX	A2	2034	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2035	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2036	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2037	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2038	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2039	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2040	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2041	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2042	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2043	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2044	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2045	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2046	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2047	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2048	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2049	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2050	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2051	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2052	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2053	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2054	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2055	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2056	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2057	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2058	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2059	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2060	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2061	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2062	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2063	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2064	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A2	2065	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2066	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2067	87	-	0/0/0/0	0/0/0/0
87	OHX	A2	2068	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2069	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2070	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2071	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2072	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2073	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2074	1	-	0/0/0/0	0/0/0/0
87	OHX	A2	2075	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2076	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2077	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2078	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2079	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2080	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2081	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2082	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2083	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2084	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2085	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2086	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2087	-	-	0/0/0/0	0/0/0/0
87	OHX	A2	2258	-	-	0/0/0/0	0/0/0/0
87	OHX	A3	201	-	-	0/0/0/0	0/0/0/0
87	OHX	A3	202	-	-	0/0/0/0	0/0/0/0
87	OHX	A3	203	-	-	0/0/0/0	0/0/0/0
87	OHX	A3	204	-	-	0/0/0/0	0/0/0/0
87	OHX	A3	205	-	-	0/0/0/0	0/0/0/0
87	OHX	A3	206	-	-	0/0/0/0	0/0/0/0
87	OHX	A3	207	-	-	0/0/0/0	0/0/0/0
87	OHX	A3	208	-	-	0/0/0/0	0/0/0/0
87	OHX	A3	209	-	-	0/0/0/0	0/0/0/0
87	OHX	A3	210	-	-	0/0/0/0	0/0/0/0
87	OHX	A3	211	-	-	0/0/0/0	0/0/0/0
87	OHX	A3	212	-	-	0/0/0/0	0/0/0/0
87	OHX	A3	213	-	-	0/0/0/0	0/0/0/0
87	OHX	A4	201	-	-	0/0/0/0	0/0/0/0
87	OHX	A4	202	-	-	0/0/0/0	0/0/0/0
87	OHX	A4	203	-	-	0/0/0/0	0/0/0/0
87	OHX	A4	204	-	-	0/0/0/0	0/0/0/0
87	OHX	A4	205	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A4	206	-	-	0/0/0/0	0/0/0/0
87	OHX	A4	207	-	-	0/0/0/0	0/0/0/0
87	OHX	A4	208	-	-	0/0/0/0	0/0/0/0
87	OHX	A4	209	-	-	0/0/0/0	0/0/0/0
87	OHX	A4	210	-	-	0/0/0/0	0/0/0/0
87	OHX	A4	211	-	-	0/0/0/0	0/0/0/0
87	OHX	A4	212	-	-	0/0/0/0	0/0/0/0
87	OHX	A4	213	-	-	0/0/0/0	0/0/0/0
87	OHX	A4	214	-	-	0/0/0/0	0/0/0/0
87	OHX	A4	215	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3401	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3402	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3403	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3404	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3405	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3406	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3407	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3413	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3414	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3415	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3416	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3417	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3418	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3419	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3420	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3421	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3422	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3423	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3424	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3425	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3426	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3427	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3428	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3429	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3430	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3431	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3432	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3433	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3434	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3435	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3436	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3437	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A5	3438	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3439	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3440	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3441	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3442	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3443	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3444	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3445	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3446	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3447	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3448	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3449	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3450	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3451	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3452	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3453	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3454	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3455	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3456	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3457	87	-	0/0/0/0	0/0/0/0
87	OHX	A5	3458	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3459	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3460	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3461	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3462	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3463	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3464	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3465	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3466	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3467	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3468	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3469	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3470	87	-	0/0/0/0	0/0/0/0
87	OHX	A5	3471	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3472	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3473	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3474	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3475	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3476	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3477	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3478	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3479	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A5	3480	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3481	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3482	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3483	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3484	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3485	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3486	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3487	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3488	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3489	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3490	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3491	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3492	87	-	0/0/0/0	0/0/0/0
87	OHX	A5	3493	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3494	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3495	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3496	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3497	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3498	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3499	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3500	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3501	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3502	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3503	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3504	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3505	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3506	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3507	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3508	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3509	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3510	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3511	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3512	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3513	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3514	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3515	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3516	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3517	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3518	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3519	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3520	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3521	87	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A5	3522	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3523	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3524	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3525	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3526	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3527	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3528	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3529	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3530	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3531	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3532	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3533	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3534	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3535	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3536	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3537	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3538	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3539	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3540	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3541	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3542	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3543	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3544	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3545	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3546	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3547	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3548	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3549	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3550	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3551	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3552	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3553	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3554	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3555	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3556	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3557	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3558	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3559	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3560	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3561	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3562	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3563	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A5	3564	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3565	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3566	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3567	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3568	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3569	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3570	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3571	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3572	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3573	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3574	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3575	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3576	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3577	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3578	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3579	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3580	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3581	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3582	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3583	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3584	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3585	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3586	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3587	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3588	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3589	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3590	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3591	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3592	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3593	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3594	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3595	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3596	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3597	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3598	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3599	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3600	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3601	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3602	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3603	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3604	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3605	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A5	3606	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3607	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3608	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3609	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3610	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3611	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3612	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3613	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3614	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3615	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3616	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3617	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3618	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3619	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3620	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3621	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3622	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3623	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3624	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3625	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3626	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3627	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3628	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3629	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3630	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3631	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3632	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3633	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3634	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3635	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3636	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3637	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3638	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3639	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3640	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3641	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3642	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3643	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3644	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3645	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3646	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3647	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A5	3648	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3649	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3650	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3651	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3652	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3653	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3654	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3655	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3656	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3657	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3658	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3659	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3660	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3661	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3662	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3663	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3664	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3665	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3666	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3667	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3668	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3669	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3670	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3671	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3672	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3673	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3674	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3675	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3676	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3677	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3678	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3679	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3680	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3681	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3682	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3683	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3684	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3685	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3686	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3687	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3688	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3689	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A5	3690	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3691	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3692	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3693	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3694	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3695	36	-	0/0/0/0	0/0/0/0
87	OHX	A5	3696	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3697	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3698	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3699	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3700	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3701	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3702	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3703	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3704	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3705	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3706	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3707	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3708	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3709	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3710	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3711	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3712	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3713	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3714	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3715	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3716	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3717	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3718	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3719	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3720	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3721	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3722	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3723	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3724	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3725	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3726	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3727	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3728	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3729	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3730	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3731	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A5	3732	36	-	0/0/0/0	0/0/0/0
87	OHX	A5	3733	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3734	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3735	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3736	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3737	87	-	0/0/0/0	0/0/0/0
87	OHX	A5	3738	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3739	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3740	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3741	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3742	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3743	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3744	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3745	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3746	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3747	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3748	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3749	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3750	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3751	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3752	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3753	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3754	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3755	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3756	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3757	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3758	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3759	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3760	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3761	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3762	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3763	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3764	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3765	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3766	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3767	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3768	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3769	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3770	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3771	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3772	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3773	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A5	3774	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3775	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3776	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3777	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3778	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3779	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3780	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3781	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3782	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3783	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3784	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3785	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3786	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3787	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3788	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3789	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3790	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3791	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3792	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3793	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3794	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3795	87	-	0/0/0/0	0/0/0/0
87	OHX	A5	3796	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3797	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3798	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3799	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3800	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3801	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3802	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3803	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3804	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3805	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3806	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3807	87	-	0/0/0/0	0/0/0/0
87	OHX	A5	3808	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3809	87	-	0/0/0/0	0/0/0/0
87	OHX	A5	3810	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3811	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3812	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3813	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3814	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3815	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A5	3816	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3817	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3818	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3819	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3820	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3821	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3822	-	-	0/0/0/0	0/0/0/0
87	OHX	A5	3823	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1901	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1902	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1903	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1904	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1905	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1906	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1907	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1908	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1909	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1910	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1911	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1912	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1913	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1914	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1915	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1916	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1917	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1918	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1919	87	-	0/0/0/0	0/0/0/0
87	OHX	A6	1920	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1921	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1922	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1923	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1924	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1925	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1926	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1927	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1928	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1929	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1930	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1931	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1932	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1933	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1934	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A6	1935	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1936	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1937	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1938	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1939	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1940	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1941	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1942	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1943	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1944	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1945	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1946	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1947	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1948	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1949	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1950	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1951	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1952	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1953	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1954	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1955	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1956	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1957	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1958	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1959	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1960	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1961	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1962	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1963	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1964	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1965	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1966	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1967	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1968	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1969	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1970	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1971	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1972	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1973	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1974	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1975	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1976	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A6	1977	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1978	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1979	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1980	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1981	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1982	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1983	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1984	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1985	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1986	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1987	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1988	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1989	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1990	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1991	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1992	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1993	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1994	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1995	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1996	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1997	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1998	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	1999	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2000	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2001	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2002	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2003	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2004	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2005	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2006	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2007	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2008	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2009	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2010	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2011	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2012	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2013	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2014	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2015	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2016	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2017	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2018	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A6	2019	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2020	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2021	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2022	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2023	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2024	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2025	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2026	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2027	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2028	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2029	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2030	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2031	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2032	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2033	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2034	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2035	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2036	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2037	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2038	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2039	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2040	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2041	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2042	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2043	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2044	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2045	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2046	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2047	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2048	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2049	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2050	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2051	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2052	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2053	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2054	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2055	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2056	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2057	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2058	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2059	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2060	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A6	2061	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2062	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2063	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2064	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2065	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2066	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2067	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2068	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2069	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2070	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2071	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2072	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2073	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2074	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2075	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2076	87	-	0/0/0/0	0/0/0/0
87	OHX	A6	2077	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2078	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2079	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2080	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2081	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2082	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2083	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2084	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2085	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2086	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2087	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2088	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2089	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2090	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2091	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2092	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2093	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2094	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2095	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2096	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2097	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2098	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2099	-	-	0/0/0/0	0/0/0/0
87	OHX	A6	2100	-	-	0/0/0/0	0/0/0/0
87	OHX	A7	201	-	-	0/0/0/0	0/0/0/0
87	OHX	A7	202	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	A7	203	-	-	0/0/0/0	0/0/0/0
87	OHX	A7	204	-	-	0/0/0/0	0/0/0/0
87	OHX	A7	205	-	-	0/0/0/0	0/0/0/0
87	OHX	A7	206	-	-	0/0/0/0	0/0/0/0
87	OHX	A7	207	-	-	0/0/0/0	0/0/0/0
87	OHX	A7	208	-	-	0/0/0/0	0/0/0/0
87	OHX	A7	209	-	-	0/0/0/0	0/0/0/0
87	OHX	A7	210	-	-	0/0/0/0	0/0/0/0
87	OHX	A7	211	-	-	0/0/0/0	0/0/0/0
87	OHX	A7	212	-	-	0/0/0/0	0/0/0/0
87	OHX	A7	213	-	-	0/0/0/0	0/0/0/0
87	OHX	A8	202	-	-	0/0/0/0	0/0/0/0
87	OHX	A8	203	-	-	0/0/0/0	0/0/0/0
87	OHX	A8	204	-	-	0/0/0/0	0/0/0/0
87	OHX	A8	205	-	-	0/0/0/0	0/0/0/0
87	OHX	A8	206	-	-	0/0/0/0	0/0/0/0
87	OHX	A8	207	-	-	0/0/0/0	0/0/0/0
87	OHX	A8	208	-	-	0/0/0/0	0/0/0/0
87	OHX	A8	209	-	-	0/0/0/0	0/0/0/0
87	OHX	A8	210	-	-	0/0/0/0	0/0/0/0
87	OHX	A8	211	-	-	0/0/0/0	0/0/0/0
87	OHX	A8	212	-	-	0/0/0/0	0/0/0/0
87	OHX	A8	213	-	-	0/0/0/0	0/0/0/0
87	OHX	A8	214	-	-	0/0/0/0	0/0/0/0
87	OHX	A8	215	-	-	0/0/0/0	0/0/0/0
87	OHX	A8	216	-	-	0/0/0/0	0/0/0/0
87	OHX	A8	217	-	-	0/0/0/0	0/0/0/0
87	OHX	A8	218	-	-	0/0/0/0	0/0/0/0
87	OHX	A8	219	-	-	0/0/0/0	0/0/0/0
87	OHX	A8	220	-	-	0/0/0/0	0/0/0/0
87	OHX	AC	301	-	-	0/0/0/0	0/0/0/0
87	OHX	AI	301	-	-	0/0/0/0	0/0/0/0
87	OHX	AL	201	-	-	0/0/0/0	0/0/0/0
87	OHX	AN	201	-	-	0/0/0/0	0/0/0/0
87	OHX	AP	201	-	-	0/0/0/0	0/0/0/0
87	OHX	Ad	101	-	-	0/0/0/0	0/0/0/0
87	OHX	Ag	401	-	-	0/0/0/0	0/0/0/0
87	OHX	BA	301	-	-	0/0/0/0	0/0/0/0
87	OHX	BB	401	-	-	0/0/0/0	0/0/0/0
87	OHX	BB	402	-	-	0/0/0/0	0/0/0/0
87	OHX	BC	401	-	-	0/0/0/0	0/0/0/0
87	OHX	BD	301	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	BI	301	-	-	0/0/0/0	0/0/0/0
87	OHX	BI	302	-	-	0/0/0/0	0/0/0/0
87	OHX	BI	303	-	-	0/0/0/0	0/0/0/0
87	OHX	BI	304	-	-	0/0/0/0	0/0/0/0
87	OHX	BN	301	-	-	0/0/0/0	0/0/0/0
87	OHX	BO	201	-	-	0/0/0/0	0/0/0/0
87	OHX	BP	201	-	-	0/0/0/0	0/0/0/0
87	OHX	BP	202	-	-	0/0/0/0	0/0/0/0
87	OHX	BR	201	-	-	0/0/0/0	0/0/0/0
87	OHX	BT	201	-	-	0/0/0/0	0/0/0/0
87	OHX	Bb	101	-	-	0/0/0/0	0/0/0/0
87	OHX	Bf	201	-	-	0/0/0/0	0/0/0/0
87	OHX	Bj	101	-	-	0/0/0/0	0/0/0/0
87	OHX	Bj	102	-	-	0/0/0/0	0/0/0/0
87	OHX	Bj	103	-	-	0/0/0/0	0/0/0/0
87	OHX	Bo	201	-	-	0/0/0/0	0/0/0/0
87	OHX	CB	301	-	-	0/0/0/0	0/0/0/0
87	OHX	CG	301	-	-	0/0/0/0	0/0/0/0
87	OHX	CG	302	-	-	0/0/0/0	0/0/0/0
87	OHX	CI	301	-	-	0/0/0/0	0/0/0/0
87	OHX	CJ	201	-	-	0/0/0/0	0/0/0/0
87	OHX	CL	201	-	-	0/0/0/0	0/0/0/0
87	OHX	CN	201	-	-	0/0/0/0	0/0/0/0
87	OHX	CP	201	-	-	0/0/0/0	0/0/0/0
87	OHX	CP	202	-	-	0/0/0/0	0/0/0/0
87	OHX	CS	201	-	-	0/0/0/0	0/0/0/0
87	OHX	CY	201	-	-	0/0/0/0	0/0/0/0
87	OHX	CY	202	-	-	0/0/0/0	0/0/0/0
87	OHX	Cd	101	-	-	0/0/0/0	0/0/0/0
87	OHX	Cg	401	-	-	0/0/0/0	0/0/0/0
87	OHX	DA	302	-	-	0/0/0/0	0/0/0/0
87	OHX	DB	401	-	-	0/0/0/0	0/0/0/0
87	OHX	DB	402	-	-	0/0/0/0	0/0/0/0
87	OHX	DC	401	-	-	0/0/0/0	0/0/0/0
87	OHX	DC	402	-	-	0/0/0/0	0/0/0/0
87	OHX	DD	301	-	-	0/0/0/0	0/0/0/0
87	OHX	DG	301	-	-	0/0/0/0	0/0/0/0
87	OHX	DH	201	-	-	0/0/0/0	0/0/0/0
87	OHX	DI	301	-	-	0/0/0/0	0/0/0/0
87	OHX	DI	302	-	-	0/0/0/0	0/0/0/0
87	OHX	DJ	201	-	-	0/0/0/0	0/0/0/0
87	OHX	DM	201	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	DO	201	-	-	0/0/0/0	0/0/0/0
87	OHX	DP	201	-	-	0/0/0/0	0/0/0/0
87	OHX	DQ	201	-	-	0/0/0/0	0/0/0/0
87	OHX	DR	201	-	-	0/0/0/0	0/0/0/0
87	OHX	DV	201	-	-	0/0/0/0	0/0/0/0
87	OHX	Db	101	-	-	0/0/0/0	0/0/0/0
87	OHX	De	201	-	-	0/0/0/0	0/0/0/0
87	OHX	Df	201	-	-	0/0/0/0	0/0/0/0
87	OHX	Dg	201	-	-	0/0/0/0	0/0/0/0
87	OHX	Dh	201	-	-	0/0/0/0	0/0/0/0
87	OHX	Dj	104	-	-	0/0/0/0	0/0/0/0
87	OHX	Do	201	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A2	1781/1800 (98%)	-0.16	52 (2%)	49	9	49, 89, 231, 373	0
2	AA	206/252 (81%)	0.18	2 (0%)	79	22	71, 111, 170, 202	0
2	CA	206/252 (81%)	0.06	2 (0%)	79	22	60, 90, 133, 228	0
3	AB	214/255 (83%)	0.68	21 (9%)	8	2	79, 144, 219, 256	0
3	CB	216/255 (84%)	0.01	0	100	100	59, 85, 127, 171	0
4	AC	217/254 (85%)	0.01	2 (0%)	81	24	60, 91, 130, 170	0
4	CC	217/254 (85%)	0.00	1 (0%)	88	36	50, 75, 127, 193	0
5	AD	223/240 (92%)	0.20	1 (0%)	90	41	69, 97, 154, 222	0
5	CD	223/240 (92%)	0.15	2 (0%)	81	24	56, 91, 144, 182	0
6	AE	260/261 (99%)	-0.03	0	100	100	60, 89, 131, 187	0
6	CE	260/261 (99%)	-0.09	0	100	100	48, 74, 112, 237	0
7	AF	206/225 (91%)	0.28	4 (1%)	64	13	72, 116, 160, 231	0
7	CF	206/225 (91%)	-0.09	1 (0%)	88	36	53, 87, 143, 207	0
8	AG	226/236 (95%)	0.09	1 (0%)	90	41	58, 102, 153, 209	0
8	CG	218/236 (92%)	0.06	2 (0%)	81	24	49, 83, 140, 239	0
9	AH	184/190 (96%)	0.32	0	100	100	75, 121, 178, 259	0
9	CH	186/190 (97%)	0.10	1 (0%)	88	36	64, 102, 162, 223	0
10	AI	188/200 (94%)	-0.07	0	100	100	48, 76, 132, 165	0
10	CI	188/200 (94%)	-0.15	0	100	100	41, 68, 116, 154	0
11	AJ	185/197 (93%)	0.28	5 (2%)	52	10	70, 101, 163, 231	0
11	CJ	185/197 (93%)	0.01	1 (0%)	88	36	55, 78, 138, 196	0
12	AK	96/105 (91%)	0.17	1 (1%)	79	22	71, 101, 164, 198	0
12	CK	96/105 (91%)	0.42	7 (7%)	15	3	77, 116, 163, 222	0
13	AL	155/156 (99%)	0.20	8 (5%)	26	6	48, 71, 176, 236	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	CL	146/156 (93%)	0.01	4 (2%)	52	10	41, 63, 134, 219	0
14	AM	124/143 (86%)	0.55	3 (2%)	56	11	97, 148, 209, 234	0
14	CM	124/143 (86%)	1.37	26 (20%)	1	1	121, 191, 250, 311	0
15	AN	150/151 (99%)	0.03	0	100	100	57, 89, 127, 183	0
15	CN	150/151 (99%)	-0.20	0	100	100	49, 73, 109, 130	0
16	AO	127/137 (92%)	0.64	11 (8%)	10	3	61, 134, 179, 240	0
16	CO	128/137 (93%)	0.01	0	100	100	50, 84, 118, 140	0
17	AP	124/142 (87%)	0.13	1 (0%)	83	26	68, 93, 167, 197	0
17	CP	135/142 (95%)	0.10	5 (3%)	39	8	61, 93, 166, 196	0
18	AQ	141/143 (98%)	0.47	6 (4%)	34	7	72, 100, 138, 155	0
18	CQ	142/143 (99%)	-0.07	0	100	100	53, 79, 121, 171	0
19	AR	120/136 (88%)	0.07	0	100	100	66, 112, 180, 214	0
19	CR	117/136 (86%)	-0.01	1 (0%)	81	24	58, 88, 142, 199	0
20	AS	145/146 (99%)	0.48	5 (3%)	43	8	57, 104, 156, 182	0
20	CS	145/146 (99%)	-0.12	0	100	100	56, 79, 138, 165	0
21	AT	143/144 (99%)	0.19	1 (0%)	84	28	73, 102, 147, 180	0
21	CT	143/144 (99%)	-0.14	0	100	100	48, 74, 114, 181	0
22	AU	107/121 (88%)	0.37	3 (2%)	50	10	64, 102, 189, 226	0
22	CU	110/121 (90%)	0.38	7 (6%)	19	5	56, 93, 183, 243	0
23	AV	87/87 (100%)	0.13	0	100	100	75, 102, 151, 169	0
23	CV	87/87 (100%)	0.03	1 (1%)	77	21	54, 79, 118, 185	0
24	AW	129/130 (99%)	-0.15	0	100	100	58, 82, 103, 121	0
24	CW	129/130 (99%)	-0.12	0	100	100	40, 62, 77, 98	0
25	AX	144/145 (99%)	-0.09	0	100	100	48, 68, 98, 150	0
25	CX	144/145 (99%)	-0.19	0	100	100	37, 53, 80, 139	0
26	AY	134/135 (99%)	0.07	0	100	100	70, 106, 166, 216	0
26	CY	134/135 (99%)	-0.00	0	100	100	57, 84, 143, 191	0
27	AZ	70/108 (64%)	0.75	6 (8%)	11	3	88, 132, 172, 235	0
27	CZ	69/108 (63%)	0.08	0	100	100	68, 103, 151, 196	0
28	Aa	97/119 (81%)	0.75	8 (8%)	12	3	69, 113, 206, 223	0
28	Ca	97/119 (81%)	-0.07	0	100	100	54, 79, 129, 165	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	Ab	81/82 (98%)	0.35	3 (3%) 39 8	68, 102, 188, 225	0
29	Cb	81/82 (98%)	0.23	1 (1%) 75 20	51, 85, 170, 203	0
30	Ac	63/67 (94%)	0.47	1 (1%) 68 16	86, 130, 182, 204	0
30	Cc	63/67 (94%)	0.22	1 (1%) 68 16	74, 107, 155, 180	0
31	Ad	53/56 (94%)	-0.05	1 (1%) 64 13	64, 76, 106, 155	0
31	Cd	53/56 (94%)	-0.04	2 (3%) 38 7	51, 69, 108, 168	0
32	Ae	60/63 (95%)	0.40	3 (5%) 28 6	56, 103, 179, 270	0
32	Ce	62/63 (98%)	0.05	1 (1%) 68 16	47, 84, 184, 218	0
33	Af	51/152 (33%)	0.45	4 (7%) 13 3	92, 138, 186, 202	0
34	Ag	318/319 (99%)	0.26	2 (0%) 86 32	74, 113, 171, 237	0
34	Cg	318/319 (99%)	0.18	3 (0%) 81 24	73, 105, 158, 232	0
35	Ah	121/273 (44%)	0.10	1 (0%) 83 26	54, 99, 162, 212	0
36	A1	3149/3396 (92%)	-0.32	25 (0%) 83 26	29, 54, 168, 351	0
36	A5	3150/3396 (92%)	-0.31	28 (0%) 81 24	28, 52, 157, 346	0
37	A3	121/121 (100%)	-0.36	0 100 100	34, 72, 92, 118	0
37	A7	121/121 (100%)	-0.27	0 100 100	31, 57, 74, 144	0
38	A4	158/158 (100%)	-0.30	1 (0%) 86 32	37, 58, 112, 223	0
38	A8	158/158 (100%)	-0.35	2 (1%) 74 19	39, 65, 128, 263	0
39	BA	252/254 (99%)	-0.20	0 100 100	27, 53, 78, 150	0
39	DA	252/254 (99%)	-0.15	1 (0%) 90 41	29, 55, 83, 177	0
40	BB	386/387 (99%)	-0.20	1 (0%) 91 48	27, 58, 86, 187	0
40	DB	386/387 (99%)	-0.29	0 100 100	20, 44, 69, 188	0
41	BC	361/362 (99%)	-0.26	0 100 100	26, 50, 86, 132	0
41	DC	361/362 (99%)	-0.22	0 100 100	30, 56, 90, 136	0
42	BD	296/297 (99%)	-0.11	1 (0%) 91 48	47, 81, 132, 223	0
42	DD	294/297 (98%)	-0.17	2 (0%) 84 28	38, 58, 110, 205	0
43	BE	156/176 (88%)	-0.27	0 100 100	34, 52, 89, 152	0
43	DE	157/176 (89%)	-0.16	1 (0%) 86 32	37, 54, 97, 160	0
44	BF	222/244 (90%)	-0.27	0 100 100	31, 46, 87, 247	0
44	DF	223/244 (91%)	-0.31	0 100 100	26, 44, 99, 197	0
45	BG	233/256 (91%)	-0.13	0 100 100	52, 79, 148, 255	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	DG	231/256 (90%)	0.05	1 (0%) 90 41	63, 88, 132, 196	0
46	BH	191/191 (100%)	-0.11	0 100 100	44, 65, 99, 197	0
46	DH	191/191 (100%)	-0.28	0 100 100	30, 47, 83, 206	0
47	BI	211/221 (95%)	-0.22	0 100 100	37, 60, 121, 229	0
47	DI	213/221 (96%)	-0.07	3 (1%) 72 18	34, 60, 106, 207	0
48	BJ	169/174 (97%)	-0.04	0 100 100	50, 84, 123, 151	0
48	DJ	169/174 (97%)	-0.16	0 100 100	40, 64, 98, 123	0
49	BL	193/199 (96%)	-0.25	0 100 100	30, 57, 126, 216	0
49	DL	194/199 (97%)	-0.10	0 100 100	38, 69, 134, 174	0
50	BM	136/138 (98%)	-0.23	0 100 100	37, 55, 92, 132	0
50	DM	137/138 (99%)	-0.29	0 100 100	30, 47, 83, 153	0
51	BN	203/204 (99%)	-0.26	0 100 100	32, 52, 68, 92	0
51	DN	203/204 (99%)	-0.18	0 100 100	37, 60, 82, 104	0
52	BO	217/219 (99%)	-0.17	0 100 100	26, 51, 97, 114	40 (18%)
52	DO	217/219 (99%)	-0.24	0 100 100	22, 41, 91, 118	40 (18%)
53	BP	183/184 (99%)	-0.04	4 (2%) 59 12	30, 49, 149, 224	0
53	DP	155/184 (84%)	-0.31	0 100 100	30, 44, 72, 161	0
54	BQ	185/186 (99%)	-0.25	0 100 100	33, 48, 68, 107	0
54	DQ	185/186 (99%)	-0.27	0 100 100	35, 54, 73, 125	0
55	BR	188/189 (99%)	-0.07	1 (0%) 88 36	45, 71, 170, 201	0
55	DR	188/189 (99%)	-0.13	3 (1%) 68 16	36, 64, 142, 199	0
56	BS	172/172 (100%)	-0.17	1 (0%) 86 32	36, 51, 85, 123	0
56	DS	172/172 (100%)	-0.28	0 100 100	26, 44, 72, 141	0
57	BT	159/160 (99%)	-0.28	0 100 100	33, 52, 111, 149	0
57	DT	159/160 (99%)	-0.28	0 100 100	30, 46, 97, 120	0
58	BU	100/121 (82%)	0.14	1 (1%) 79 22	79, 108, 150, 180	0
58	DU	98/121 (80%)	0.25	1 (1%) 79 22	67, 97, 128, 168	0
59	BV	136/137 (99%)	-0.23	0 100 100	35, 57, 95, 182	0
59	DV	136/137 (99%)	-0.19	1 (0%) 84 28	26, 42, 78, 210	0
60	BW	98/155 (63%)	0.76	17 (17%) 2 1	47, 77, 244, 306	0
60	DW	135/155 (87%)	0.16	6 (4%) 33 7	36, 94, 192, 249	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
61	BX	121/142 (85%)	-0.07	0 100 100	41, 68, 99, 152	0
61	DX	120/142 (84%)	-0.10	1 (0%) 83 26	46, 71, 108, 135	0
62	BY	126/127 (99%)	-0.12	1 (0%) 83 26	38, 59, 91, 150	0
62	DY	126/127 (99%)	-0.05	0 100 100	39, 66, 102, 168	0
63	BZ	135/136 (99%)	0.21	1 (0%) 84 28	68, 94, 138, 162	0
63	DZ	135/136 (99%)	0.34	1 (0%) 84 28	68, 103, 142, 170	0
64	Ba	148/149 (99%)	-0.18	0 100 100	26, 50, 89, 116	0
64	Da	148/149 (99%)	-0.20	0 100 100	28, 55, 93, 142	0
65	Bb	58/59 (98%)	-0.12	0 100 100	33, 58, 119, 142	0
65	Db	58/59 (98%)	-0.17	0 100 100	35, 59, 123, 160	0
66	Bc	97/105 (92%)	-0.03	0 100 100	63, 88, 129, 171	0
66	Dc	100/105 (95%)	0.09	1 (1%) 79 22	59, 86, 154, 173	0
67	Bd	109/113 (96%)	-0.01	2 (1%) 65 14	40, 66, 132, 202	0
67	Dd	109/113 (96%)	-0.20	0 100 100	34, 57, 126, 199	0
68	Be	127/130 (97%)	-0.18	1 (0%) 83 26	22, 42, 65, 149	0
68	De	127/130 (97%)	-0.24	0 100 100	25, 47, 77, 136	0
69	Bf	106/107 (99%)	-0.25	0 100 100	30, 41, 73, 139	0
69	Df	106/107 (99%)	-0.27	0 100 100	27, 40, 75, 119	0
70	Bg	112/121 (92%)	0.05	2 (1%) 65 14	44, 71, 134, 197	0
70	Dg	112/121 (92%)	-0.02	0 100 100	41, 72, 139, 191	0
71	Bh	119/120 (99%)	-0.12	0 100 100	42, 68, 104, 119	0
71	Dh	119/120 (99%)	-0.05	1 (0%) 83 26	51, 75, 109, 149	0
72	Bi	99/100 (99%)	-0.09	0 100 100	45, 69, 111, 172	0
72	Di	99/100 (99%)	0.03	1 (1%) 79 22	57, 75, 116, 171	0
73	Bj	87/88 (98%)	-0.19	1 (1%) 77 21	35, 45, 74, 216	0
73	Dj	87/88 (98%)	-0.11	2 (2%) 57 12	30, 50, 91, 241	0
74	Bk	77/78 (98%)	-0.02	0 100 100	65, 95, 146, 168	0
74	Dk	77/78 (98%)	0.10	0 100 100	64, 98, 138, 153	0
75	Bl	50/51 (98%)	-0.10	0 100 100	37, 59, 80, 95	0
75	Dl	50/51 (98%)	-0.16	0 100 100	44, 59, 82, 102	0
76	Bm	52/128 (40%)	-0.20	0 100 100	42, 55, 82, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
76	Dm	52/128 (40%)	-0.23	1 (1%) 64 13	31, 39, 68, 106	0
77	Bn	25/25 (100%)	-0.10	0 100 100	49, 62, 79, 94	0
77	Dn	25/25 (100%)	-0.10	0 100 100	37, 55, 72, 99	0
78	Bo	105/106 (99%)	-0.11	1 (0%) 79 22	35, 60, 97, 219	0
78	Do	105/106 (99%)	-0.13	0 100 100	37, 59, 101, 157	0
79	Bp	91/92 (98%)	-0.27	0 100 100	40, 61, 104, 126	0
79	Dp	91/92 (98%)	-0.22	0 100 100	29, 60, 96, 111	0
80	A6	1795/1800 (99%)	-0.15	46 (2%) 53 10	38, 72, 214, 360	0
81	Cf	51/152 (33%)	1.21	5 (9%) 8 2	113, 172, 222, 254	0
82	Ch	63/273 (23%)	0.29	4 (6%) 19 5	50, 99, 156, 183	0
83	DK	0/155	-	-	-	-
84	Dq	120/312 (38%)	0.33	1 (0%) 83 26	70, 109, 166, 232	0
85	Dr	0/47	-	-	-	-
86	Ds	0/46	-	-	-	-
All	All	32987/35856 (91%)	-0.09	399 (1%) 75 20	20, 71, 158, 373	80 (0%)

The worst 5 of 399 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A2	1702	N	57.1
1	A2	1699	N	37.6
1	A2	1697	N	30.9
80	A6	663	N	29.8
1	A2	1694	N	29.3

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
88	MG	A5	4059	1/1	0.36	-	71,71,71,71	0
88	MG	A5	4429	1/1	0.17	-	58,58,58,58	0
87	OHX	A3	203	7/7	0.15	-	118,118,118,118	7
88	MG	A2	2255	1/1	0.07	-	107,107,107,107	0
87	OHX	A1	3678	7/7	0.14	-	186,186,186,186	7
88	MG	A2	2187	1/1	0.21	-	90,90,90,90	0
88	MG	A1	4388	1/1	0.45	-	78,78,78,78	0
87	OHX	A5	3552	7/7	0.15	-	138,138,138,138	7
88	MG	A1	3861	1/1	0.26	-	34,34,34,34	0
88	MG	A1	3835	1/1	0.15	-	41,41,41,41	0
87	OHX	A2	1994	7/7	0.14	-	118,118,118,118	7
87	OHX	A2	2074	7/7	0.21	-	191,191,191,191	7
88	MG	A1	3892	1/1	0.28	-	75,75,75,75	0
88	MG	A5	4308	1/1	0.63	-	52,52,52,52	0
87	OHX	A6	1991	7/7	0.20	-	149,149,149,149	7
88	MG	A5	4464	1/1	0.43	-	85,85,85,85	0
88	MG	CG	304	1/1	0.29	-	72,72,72,72	0
88	MG	DO	204	1/1	0.41	-	57,57,57,57	0
87	OHX	A6	1974	7/7	0.17	-	116,116,116,116	7
88	MG	A5	4573	1/1	0.53	-	56,56,56,56	0
88	MG	A5	4400	1/1	0.26	-	86,86,86,86	0
87	OHX	A5	3465	7/7	0.18	-	91,91,91,91	7
87	OHX	A2	1985	7/7	0.11	-	144,144,144,144	7
88	MG	A1	4381	1/1	0.44	-	65,65,65,65	0
88	MG	A5	3949	1/1	0.24	-	37,37,37,37	0
88	MG	A5	4149	1/1	0.19	-	63,63,63,63	0
87	OHX	A1	3556	7/7	0.14	-	128,128,128,128	7
88	MG	A7	228	1/1	0.24	-	85,85,85,85	0
88	MG	A8	235	1/1	0.64	-	79,79,79,79	0
88	MG	A1	4025	1/1	0.42	-	39,39,39,39	0
87	OHX	A1	3546	7/7	0.16	-	106,106,106,106	7
88	MG	A1	4331	1/1	0.26	-	62,62,62,62	0
87	OHX	A6	1973	7/7	0.17	-	87,87,87,87	7
87	OHX	A1	3642	7/7	0.10	-	139,139,139,139	7
87	OHX	A2	1981	7/7	0.12	-	132,132,132,132	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	4087	1/1	0.25	-	67,67,67,67	0
88	MG	A5	4263	1/1	0.22	-	72,72,72,72	0
88	MG	A6	2233	1/1	0.27	-	63,63,63,63	0
89	ZN	Dm	202	1/1	0.17	-	41,41,41,41	0
88	MG	A5	3979	1/1	0.41	-	61,61,61,61	0
88	MG	A5	4389	1/1	0.57	-	66,66,66,66	0
88	MG	A5	4545	1/1	0.36	-	94,94,94,94	0
87	OHX	A5	3707	7/7	0.32	-	135,135,135,135	7
88	MG	A2	2192	1/1	0.23	-	66,66,66,66	0
88	MG	A5	3840	1/1	0.17	-	26,26,26,26	0
88	MG	A5	4268	1/1	0.25	-	96,96,96,96	0
87	OHX	A1	3659	7/7	0.13	-	156,156,156,156	7
88	MG	A1	4074	1/1	0.11	-	57,57,57,57	0
87	OHX	A5	3747	7/7	0.16	-	160,160,160,160	7
88	MG	A5	4510	1/1	1.67	-	86,86,86,86	0
88	MG	A1	4310	1/1	0.91	-	67,67,67,67	0
88	MG	A5	4560	1/1	0.32	-	108,108,108,108	0
88	MG	A5	3825	1/1	0.16	-	29,29,29,29	0
88	MG	A1	3859	1/1	0.39	-	78,78,78,78	0
87	OHX	A5	3495	7/7	0.18	-	92,92,92,92	7
88	MG	A5	4273	1/1	0.73	-	75,75,75,75	0
87	OHX	A5	3604	7/7	0.17	-	113,113,113,113	7
87	OHX	A6	1950	7/7	0.13	-	140,140,140,140	0
87	OHX	A1	3526	7/7	0.14	-	126,126,126,126	7
88	MG	A5	4333	1/1	0.38	-	75,75,75,75	0
87	OHX	A6	1904	7/7	0.21	-	88,88,88,88	0
88	MG	A5	3914	1/1	0.42	-	69,69,69,69	0
87	OHX	A1	3537	7/7	0.14	-	119,119,119,119	7
89	ZN	Bp	501	1/1	0.12	-	68,68,68,68	0
88	MG	A5	3913	1/1	0.07	-	68,68,68,68	0
88	MG	A5	4456	1/1	0.27	-	79,79,79,79	0
87	OHX	A5	3761	7/7	0.15	-	146,146,146,146	7
87	OHX	A1	3762	7/7	0.25	-	144,144,144,144	7
88	MG	A5	4123	1/1	0.13	-	39,39,39,39	0
87	OHX	A5	3455	7/7	0.19	-	100,100,100,100	0
88	MG	A6	2141	1/1	0.39	-	78,78,78,78	0
87	OHX	A1	3777	7/7	0.22	-	137,137,137,137	7
87	OHX	A2	2014	7/7	0.19	-	166,166,166,166	7
88	MG	A5	3960	1/1	0.17	-	49,49,49,49	0
88	MG	A4	219	1/1	0.23	-	59,59,59,59	0
88	MG	A1	3913	1/1	0.27	-	86,86,86,86	0
87	OHX	A6	2099	7/7	0.27	-	184,184,184,184	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A1	3753	7/7	0.83	-	243,243,243,243	7
88	MG	A1	4399	1/1	0.43	-	85,85,85,85	0
88	MG	Dp	101	1/1	0.14	-	54,54,54,54	0
87	OHX	A1	3689	7/7	0.25	-	99,99,99,99	7
88	MG	A6	2173	1/1	0.20	-	71,71,71,71	0
87	OHX	A5	3770	7/7	0.23	-	198,198,198,198	7
88	MG	A5	4082	1/1	0.31	-	46,46,46,46	0
88	MG	DD	305	1/1	0.17	-	74,74,74,74	0
88	MG	A5	3874	1/1	0.29	-	32,32,32,32	0
88	MG	A1	4337	1/1	0.28	-	108,108,108,108	0
88	MG	A6	2143	1/1	0.39	-	45,45,45,45	0
87	OHX	A6	2027	7/7	0.10	-	189,189,189,189	7
88	MG	A1	4282	1/1	0.38	-	92,92,92,92	0
87	OHX	A6	2084	7/7	0.16	-	196,196,196,196	7
88	MG	A1	4364	1/1	0.21	-	92,92,92,92	0
88	MG	A5	4069	1/1	0.23	-	88,88,88,88	0
87	OHX	A5	3721	7/7	0.18	-	167,167,167,167	7
87	OHX	A5	3693	7/7	0.24	-	181,181,181,181	7
88	MG	A2	2225	1/1	0.45	-	79,79,79,79	0
88	MG	A1	4473	1/1	0.21	-	111,111,111,111	0
88	MG	CQ	202	1/1	0.28	-	85,85,85,85	0
88	MG	A1	4004	1/1	0.44	-	57,57,57,57	0
88	MG	A1	3907	1/1	0.25	-	50,50,50,50	0
88	MG	A1	4238	1/1	0.17	-	69,69,69,69	0
88	MG	CI	303	1/1	0.16	-	62,62,62,62	0
87	OHX	A6	1906	7/7	0.18	-	85,85,85,85	0
87	OHX	A6	2047	7/7	0.20	-	156,156,156,156	7
88	MG	A5	3848	1/1	0.37	-	77,77,77,77	0
88	MG	A8	226	1/1	0.22	-	62,62,62,62	0
88	MG	A5	3924	1/1	0.33	-	39,39,39,39	0
88	MG	A5	4168	1/1	0.28	-	74,74,74,74	0
88	MG	A1	3910	1/1	0.33	-	58,58,58,58	0
88	MG	A1	3995	1/1	0.28	-	63,63,63,63	0
88	MG	BF	4101	1/1	0.22	-	64,64,64,64	0
88	MG	A5	4075	1/1	0.35	-	60,60,60,60	0
88	MG	A2	2256	1/1	0.54	-	80,80,80,80	0
88	MG	A2	2095	1/1	0.24	-	63,63,63,63	0
87	OHX	A1	3502	7/7	0.16	-	78,78,78,78	7
87	OHX	A5	3457	7/7	0.14	-	86,86,86,86	7
87	OHX	A1	3443	7/7	0.17	-	76,76,76,76	0
88	MG	A6	2188	1/1	0.21	-	38,38,38,38	0
87	OHX	A6	1922	7/7	0.14	-	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A5	3436	7/7	0.16	-	82,82,82,82	0
88	MG	A6	2168	1/1	0.30	-	77,77,77,77	0
88	MG	A5	4405	1/1	0.76	-	69,69,69,69	0
88	MG	A5	4523	1/1	0.26	-	65,65,65,65	0
88	MG	A5	4223	1/1	0.29	-	78,78,78,78	0
89	ZN	Bm	202	1/1	0.17	-	56,56,56,56	0
88	MG	A5	4138	1/1	0.35	-	77,77,77,77	0
88	MG	A6	2331	1/1	0.12	-	79,79,79,79	0
87	OHX	CP	201	7/7	0.13	-	177,177,177,177	7
88	MG	A5	4262	1/1	0.20	-	60,60,60,60	0
88	MG	A1	4288	1/1	0.33	-	81,81,81,81	0
87	OHX	A5	3511	7/7	0.14	-	142,142,142,142	0
87	OHX	A5	3814	7/7	0.17	-	114,114,114,114	7
88	MG	A1	3877	1/1	0.27	-	34,34,34,34	0
87	OHX	A2	1956	7/7	0.17	-	128,128,128,128	7
87	OHX	A5	3745	7/7	0.20	-	131,131,131,131	7
88	MG	A1	4022	1/1	0.26	-	40,40,40,40	0
88	MG	A1	4490	1/1	0.26	-	77,77,77,77	0
87	OHX	A1	3517	7/7	0.12	-	99,99,99,99	7
88	MG	A6	2114	1/1	0.38	-	61,61,61,61	0
87	OHX	A5	3716	7/7	0.30	-	115,115,115,115	7
87	OHX	A6	2057	7/7	0.30	-	134,134,134,134	7
87	OHX	BR	201	7/7	0.18	-	181,181,181,181	7
87	OHX	A2	1934	7/7	0.18	-	123,123,123,123	7
87	OHX	A1	3709	7/7	0.17	-	176,176,176,176	7
87	OHX	A1	3761	7/7	0.10	-	173,173,173,173	7
87	OHX	A3	213	7/7	0.22	-	195,195,195,195	7
87	OHX	A5	3758	7/7	0.15	-	167,167,167,167	7
87	OHX	A1	3576	7/7	0.16	-	83,83,83,83	7
88	MG	A2	2097	1/1	0.21	-	78,78,78,78	0
87	OHX	A6	2089	7/7	0.21	-	212,212,212,212	7
87	OHX	A1	3666	7/7	0.20	-	142,142,142,142	7
88	MG	A1	4141	1/1	0.28	-	53,53,53,53	0
88	MG	A5	3839	1/1	0.19	-	48,48,48,48	0
88	MG	A5	4230	1/1	0.29	-	78,78,78,78	0
88	MG	DA	301	1/1	0.22	-	86,86,86,86	0
87	OHX	A7	204	7/7	0.17	-	75,75,75,75	7
87	OHX	A5	3425	7/7	0.18	-	72,72,72,72	0
88	MG	A5	4413	1/1	0.12	-	80,80,80,80	0
88	MG	A1	4311	1/1	0.20	-	92,92,92,92	0
87	OHX	A5	3681	7/7	0.25	-	112,112,112,112	7
87	OHX	A6	2070	7/7	0.15	-	139,139,139,139	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A5	3507	7/7	0.17	-	75,75,75,75	7
88	MG	A5	4544	1/1	0.34	-	79,79,79,79	0
87	OHX	A1	3673	7/7	0.18	-	154,154,154,154	7
88	MG	A1	4046	1/1	0.33	-	50,50,50,50	0
87	OHX	A5	3762	7/7	0.29	-	153,153,153,153	7
88	MG	A1	4352	1/1	0.21	-	93,93,93,93	0
88	MG	A1	4453	1/1	0.61	-	114,114,114,114	0
87	OHX	A2	1912	7/7	0.17	-	115,115,115,115	0
88	MG	A6	2230	1/1	0.13	-	86,86,86,86	0
87	OHX	A1	3480	7/7	0.17	-	96,96,96,96	7
88	MG	A5	4503	1/1	0.26	-	72,72,72,72	0
88	MG	A6	2228	1/1	0.24	-	89,89,89,89	0
87	OHX	A6	1984	7/7	0.13	-	174,174,174,174	7
88	MG	De	203	1/1	0.85	-	109,109,109,109	0
87	OHX	A2	1906	7/7	0.16	-	98,98,98,98	0
87	OHX	A5	3487	7/7	0.17	-	94,94,94,94	7
87	OHX	A5	3579	7/7	0.16	-	105,105,105,105	7
87	OHX	A1	3601	7/7	0.15	-	184,184,184,184	7
87	OHX	A1	3616	7/7	0.22	-	117,117,117,117	7
88	MG	A1	3968	1/1	0.18	-	68,68,68,68	0
87	OHX	A2	1921	7/7	0.16	-	113,113,113,113	7
87	OHX	A5	3523	7/7	0.17	-	79,79,79,79	7
88	MG	A2	2182	1/1	0.18	-	78,78,78,78	0
88	MG	A5	4461	1/1	0.22	-	62,62,62,62	0
88	MG	A1	4216	1/1	0.23	-	93,93,93,93	0
88	MG	A3	216	1/1	0.17	-	67,67,67,67	0
88	MG	A4	238	1/1	0.28	-	68,68,68,68	0
87	OHX	A2	2057	7/7	0.15	-	173,173,173,173	7
88	MG	A1	3876	1/1	0.32	-	68,68,68,68	0
88	MG	A1	4414	1/1	0.19	-	90,90,90,90	0
88	MG	A1	3904	1/1	0.27	-	43,43,43,43	0
88	MG	A6	2265	1/1	0.17	-	73,73,73,73	0
88	MG	A1	4056	1/1	0.27	-	61,61,61,61	0
87	OHX	A6	1985	7/7	0.19	-	114,114,114,114	7
87	OHX	A5	3558	7/7	0.17	-	85,85,85,85	7
87	OHX	A1	3509	7/7	0.16	-	98,98,98,98	7
88	MG	A1	4195	1/1	0.14	-	83,83,83,83	0
88	MG	A5	4457	1/1	0.20	-	78,78,78,78	0
88	MG	A2	2146	1/1	0.27	-	71,71,71,71	0
88	MG	A1	4064	1/1	0.24	-	69,69,69,69	0
87	OHX	A6	1951	7/7	0.15	-	115,115,115,115	7
88	MG	CX	202	1/1	0.37	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A5	4093	1/1	0.18	-	64,64,64,64	0
88	MG	A1	4396	1/1	0.17	-	74,74,74,74	0
87	OHX	A5	3787	7/7	0.22	-	195,195,195,195	7
88	MG	A1	3818	1/1	0.19	-	63,63,63,63	0
88	MG	A1	4100	1/1	0.10	-	34,34,34,34	0
87	OHX	A2	2054	7/7	0.14	-	227,227,227,227	7
87	OHX	A5	3642	7/7	0.17	-	118,118,118,118	7
88	MG	A5	4284	1/1	0.16	-	69,69,69,69	0
88	MG	Ca	201	1/1	0.20	-	67,67,67,67	0
87	OHX	A5	3725	7/7	0.17	-	171,171,171,171	7
87	OHX	A1	3763	7/7	0.25	-	157,157,157,157	7
88	MG	A5	4567	1/1	0.18	-	59,59,59,59	0
87	OHX	A5	3635	7/7	0.12	-	147,147,147,147	7
88	MG	A1	4127	1/1	0.19	-	65,65,65,65	0
88	MG	A1	4361	1/1	0.73	-	126,126,126,126	0
87	OHX	A1	3686	7/7	0.10	-	204,204,204,204	7
88	MG	A6	2311	1/1	0.50	-	76,76,76,76	0
88	MG	A5	4394	1/1	0.17	-	73,73,73,73	0
88	MG	A2	2153	1/1	0.21	-	72,72,72,72	0
87	OHX	A1	3765	7/7	0.24	-	173,173,173,173	7
88	MG	A2	2117	1/1	0.32	-	80,80,80,80	0
87	OHX	A5	3634	7/7	0.16	-	130,130,130,130	7
88	MG	A7	219	1/1	0.24	-	71,71,71,71	0
88	MG	A1	3943	1/1	0.35	-	59,59,59,59	0
87	OHX	A1	3547	7/7	0.17	-	99,99,99,99	7
87	OHX	A5	3704	7/7	0.16	-	141,141,141,141	7
88	MG	A1	3890	1/1	0.34	-	61,61,61,61	0
88	MG	A1	4332	1/1	0.25	-	74,74,74,74	0
88	MG	A5	4362	1/1	0.28	-	60,60,60,60	0
88	MG	DV	202	1/1	0.38	-	35,35,35,35	0
88	MG	A5	3862	1/1	0.48	-	82,82,82,82	0
88	MG	A2	2102	1/1	0.34	-	60,60,60,60	0
88	MG	A5	4244	1/1	0.15	-	82,82,82,82	0
88	MG	A1	3994	1/1	0.35	-	64,64,64,64	0
88	MG	A5	4006	1/1	0.36	-	40,40,40,40	0
88	MG	A1	4275	1/1	0.34	-	74,74,74,74	0
88	MG	A2	2250	1/1	0.13	-	97,97,97,97	0
88	MG	A1	4456	1/1	0.21	-	76,76,76,76	0
88	MG	A5	3882	1/1	0.05	-	74,74,74,74	0
87	OHX	A5	3665	7/7	0.19	-	184,184,184,184	7
88	MG	A3	220	1/1	0.49	-	83,83,83,83	0
87	OHX	A2	2072	7/7	0.30	-	207,207,207,207	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	Be	201	1/1	0.56	-	88,88,88,88	0
88	MG	A1	4257	1/1	0.18	-	88,88,88,88	0
88	MG	A1	3976	1/1	0.48	-	66,66,66,66	0
88	MG	A5	4354	1/1	0.55	-	60,60,60,60	0
88	MG	A5	4312	1/1	0.29	-	87,87,87,87	0
88	MG	A1	4372	1/1	0.18	-	71,71,71,71	0
87	OHX	DG	301	7/7	0.43	-	226,226,226,226	7
87	OHX	A2	2042	7/7	0.11	-	155,155,155,155	7
88	MG	A5	4072	1/1	0.25	-	56,56,56,56	0
88	MG	A2	2090	1/1	0.27	-	53,53,53,53	0
88	MG	A5	4065	1/1	0.22	-	68,68,68,68	0
87	OHX	A6	2090	7/7	0.37	-	212,212,212,212	7
88	MG	A1	4249	1/1	0.26	-	73,73,73,73	0
88	MG	A1	3986	1/1	0.35	-	41,41,41,41	0
88	MG	A5	4430	1/1	0.29	-	95,95,95,95	0
88	MG	A5	4383	1/1	0.22	-	69,69,69,69	0
88	MG	A1	3883	1/1	0.37	-	37,37,37,37	0
88	MG	A1	3888	1/1	0.28	-	67,67,67,67	0
87	OHX	A8	209	7/7	0.15	-	130,130,130,130	7
88	MG	A5	4107	1/1	0.18	-	66,66,66,66	0
88	MG	A5	4310	1/1	0.39	-	69,69,69,69	0
87	OHX	A1	3692	7/7	0.18	-	124,124,124,124	7
87	OHX	Db	101	7/7	0.19	-	86,86,86,86	0
88	MG	A5	4323	1/1	0.26	-	64,64,64,64	0
87	OHX	A2	1931	7/7	0.17	-	143,143,143,143	7
88	MG	A5	3992	1/1	0.32	-	57,57,57,57	0
87	OHX	A6	2045	7/7	0.25	-	124,124,124,124	7
87	OHX	A6	2021	7/7	0.16	-	131,131,131,131	7
87	OHX	A1	3418	7/7	0.18	-	81,81,81,81	0
88	MG	DF	302	1/1	0.45	-	48,48,48,48	0
88	MG	A6	2245	1/1	0.13	-	82,82,82,82	0
88	MG	A6	2244	1/1	0.52	-	97,97,97,97	0
87	OHX	A1	3431	7/7	0.15	-	89,89,89,89	0
87	OHX	A2	1992	7/7	0.14	-	123,123,123,123	7
88	MG	A5	4144	1/1	0.43	-	75,75,75,75	0
87	OHX	A5	3589	7/7	0.15	-	93,93,93,93	7
88	MG	A1	4132	1/1	0.13	-	64,64,64,64	0
88	MG	A1	4506	1/1	0.17	-	77,77,77,77	0
88	MG	A1	4109	1/1	0.29	-	80,80,80,80	0
88	MG	A1	4165	1/1	0.30	-	57,57,57,57	0
88	MG	A5	4533	1/1	0.17	-	83,83,83,83	0
87	OHX	A5	3763	7/7	0.39	-	197,197,197,197	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
88	MG	A1	4247	1/1	0.18	-	74,74,74,74	0
88	MG	A5	3904	1/1	0.18	-	60,60,60,60	0
88	MG	A2	2147	1/1	0.18	-	93,93,93,93	0
88	MG	A1	4309	1/1	0.31	-	99,99,99,99	0
88	MG	A1	4376	1/1	0.43	-	71,71,71,71	0
88	MG	A5	4469	1/1	0.14	-	70,70,70,70	0
88	MG	A1	4316	1/1	0.36	-	65,65,65,65	0
88	MG	A1	4410	1/1	0.40	-	69,69,69,69	0
88	MG	CS	202	1/1	0.40	-	63,63,63,63	0
88	MG	A1	4023	1/1	0.42	-	42,42,42,42	0
88	MG	Bd	201	1/1	0.44	-	106,106,106,106	0
88	MG	A5	4156	1/1	0.26	-	65,65,65,65	0
88	MG	A5	3968	1/1	0.20	-	50,50,50,50	0
87	OHX	A1	3701	7/7	0.30	-	112,112,112,112	7
88	MG	A6	2337	1/1	0.32	-	127,127,127,127	0
88	MG	A5	4443	1/1	0.26	-	64,64,64,64	0
88	MG	A5	4447	1/1	0.19	-	61,61,61,61	0
88	MG	A1	3891	1/1	0.20	-	58,58,58,58	0
87	OHX	A2	2015	7/7	0.19	-	138,138,138,138	7
88	MG	A1	3827	1/1	0.28	-	47,47,47,47	0
87	OHX	A1	3452	7/7	0.15	-	81,81,81,81	7
88	MG	A5	3912	1/1	0.35	-	77,77,77,77	0
87	OHX	A5	3453	7/7	0.17	-	102,102,102,102	0
87	OHX	A4	205	7/7	0.14	-	122,122,122,122	7
88	MG	A7	234	1/1	0.34	-	90,90,90,90	0
88	MG	A6	2185	1/1	0.21	-	71,71,71,71	0
88	MG	A5	4014	1/1	0.35	-	54,54,54,54	0
87	OHX	A6	2074	7/7	0.30	-	176,176,176,176	7
88	MG	AC	302	1/1	0.26	-	74,74,74,74	0
87	OHX	A1	3484	7/7	0.18	-	126,126,126,126	0
88	MG	A1	4059	1/1	0.41	-	84,84,84,84	0
88	MG	DD	303	1/1	0.56	-	67,67,67,67	0
87	OHX	A5	3463	7/7	0.21	-	130,130,130,130	0
87	OHX	A5	3802	7/7	0.27	-	151,151,151,151	7
88	MG	BP	210	1/1	0.45	-	46,46,46,46	0
87	OHX	A5	3459	7/7	0.17	-	100,100,100,100	0
88	MG	A1	3940	1/1	0.39	-	51,51,51,51	0
87	OHX	A1	3600	7/7	0.18	-	100,100,100,100	7
88	MG	A5	3989	1/1	0.38	-	76,76,76,76	0
88	MG	A5	3964	1/1	0.32	-	57,57,57,57	0
88	MG	A6	2229	1/1	0.20	-	65,65,65,65	0
87	OHX	A1	3691	7/7	0.23	-	175,175,175,175	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
88	MG	A5	4254	1/1	0.52	-	103,103,103,103	0
88	MG	A1	3987	1/1	0.21	-	57,57,57,57	0
88	MG	A5	4092	1/1	0.31	-	82,82,82,82	0
88	MG	A5	4115	1/1	0.26	-	69,69,69,69	0
88	MG	A6	2138	1/1	0.31	-	94,94,94,94	0
88	MG	A5	4224	1/1	0.24	-	58,58,58,58	0
88	MG	A1	4032	1/1	0.13	-	46,46,46,46	0
88	MG	Dp	102	1/1	0.28	-	63,63,63,63	0
88	MG	A5	3897	1/1	0.36	-	100,100,100,100	0
88	MG	A7	214	1/1	0.47	-	55,55,55,55	0
87	OHX	A2	1983	7/7	0.14	-	166,166,166,166	7
87	OHX	A4	213	7/7	0.12	-	164,164,164,164	7
87	OHX	A2	1908	7/7	0.18	-	115,115,115,115	0
87	OHX	A2	2082	7/7	0.21	-	225,225,225,225	7
87	OHX	A1	3527	7/7	0.19	-	94,94,94,94	7
88	MG	A5	4324	1/1	0.22	-	80,80,80,80	0
88	MG	A5	4015	1/1	0.41	-	45,45,45,45	0
88	MG	A5	3895	1/1	0.25	-	32,32,32,32	0
88	MG	A5	3939	1/1	0.34	-	42,42,42,42	0
88	MG	DA	305	1/1	0.91	-	69,69,69,69	0
88	MG	A2	2103	1/1	0.37	-	58,58,58,58	0
88	MG	A1	3832	1/1	0.18	-	65,65,65,65	0
88	MG	Df	204	1/1	0.39	-	61,61,61,61	0
87	OHX	A6	1926	7/7	0.17	-	82,82,82,82	7
87	OHX	A2	2078	7/7	0.18	-	169,169,169,169	7
88	MG	A5	4031	1/1	0.42	-	39,39,39,39	0
88	MG	A5	3925	1/1	0.18	-	57,57,57,57	0
87	OHX	A1	3779	7/7	0.37	-	164,164,164,164	7
88	MG	A8	227	1/1	0.17	-	65,65,65,65	0
88	MG	A5	3870	1/1	0.33	-	56,56,56,56	0
88	MG	A6	2256	1/1	0.19	-	73,73,73,73	0
87	OHX	A2	1955	7/7	0.15	-	123,123,123,123	7
87	OHX	A2	1993	7/7	0.10	-	159,159,159,159	7
88	MG	A1	4451	1/1	0.42	-	75,75,75,75	0
87	OHX	A1	3474	7/7	0.16	-	92,92,92,92	7
88	MG	A1	4162	1/1	0.29	-	79,79,79,79	0
87	OHX	A2	1967	7/7	0.14	-	120,120,120,120	7
88	MG	A1	4039	1/1	0.33	-	65,65,65,65	0
88	MG	A5	4446	1/1	0.16	-	64,64,64,64	0
87	OHX	A1	3451	7/7	0.15	-	105,105,105,105	0
88	MG	A1	4116	1/1	0.24	-	65,65,65,65	0
88	MG	A5	4035	1/1	0.12	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	4185	1/1	0.16	-	65,65,65,65	0
88	MG	A5	3959	1/1	0.41	-	61,61,61,61	0
88	MG	A5	4427	1/1	0.31	-	102,102,102,102	0
88	MG	A1	4299	1/1	0.37	-	84,84,84,84	0
87	OHX	A6	2044	7/7	0.13	-	178,178,178,178	7
88	MG	A1	4096	1/1	0.25	-	80,80,80,80	0
87	OHX	A5	3566	7/7	0.19	-	99,99,99,99	7
87	OHX	A5	3592	7/7	0.16	-	102,102,102,102	7
88	MG	A5	4462	1/1	0.43	-	83,83,83,83	0
88	MG	A4	234	1/1	0.26	-	74,74,74,74	0
87	OHX	A5	3703	7/7	0.16	-	123,123,123,123	7
88	MG	A5	4445	1/1	0.26	-	65,65,65,65	0
88	MG	A6	2105	1/1	0.24	-	78,78,78,78	0
88	MG	BY	202	1/1	0.38	-	85,85,85,85	0
88	MG	A1	4228	1/1	0.31	-	82,82,82,82	0
88	MG	DB	406	1/1	0.52	-	47,47,47,47	0
87	OHX	A2	2023	7/7	0.13	-	136,136,136,136	7
88	MG	A5	3835	1/1	0.31	-	49,49,49,49	0
88	MG	A1	4215	1/1	0.17	-	65,65,65,65	0
88	MG	A2	2253	1/1	0.15	-	89,89,89,89	0
88	MG	A5	3983	1/1	0.39	-	47,47,47,47	0
87	OHX	A5	3616	7/7	0.19	-	102,102,102,102	7
88	MG	A1	4280	1/1	0.10	-	51,51,51,51	0
88	MG	A5	4158	1/1	0.27	-	62,62,62,62	0
87	OHX	A1	3732	7/7	0.27	-	166,166,166,166	7
87	OHX	A5	3481	7/7	0.15	-	92,92,92,92	7
87	OHX	A2	2025	7/7	0.14	-	219,219,219,219	7
88	MG	AS	202	1/1	0.50	-	63,63,63,63	0
88	MG	A8	221	1/1	0.14	-	33,33,33,33	0
88	MG	A1	3999	1/1	0.33	-	37,37,37,37	0
88	MG	A5	4269	1/1	0.19	-	66,66,66,66	0
88	MG	A5	3867	1/1	0.20	-	27,27,27,27	0
88	MG	A1	3941	1/1	0.34	-	52,52,52,52	0
88	MG	A5	4329	1/1	0.39	-	86,86,86,86	0
88	MG	BY	201	1/1	0.19	-	56,56,56,56	0
88	MG	A1	4057	1/1	0.22	-	63,63,63,63	0
88	MG	A5	4322	1/1	0.30	-	61,61,61,61	0
88	MG	A1	4366	1/1	0.29	-	86,86,86,86	0
88	MG	A1	4355	1/1	0.25	-	53,53,53,53	0
88	MG	A5	4116	1/1	0.29	-	56,56,56,56	0
87	OHX	A5	3550	7/7	0.18	-	119,119,119,119	7
87	OHX	A1	3617	7/7	0.12	-	144,144,144,144	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A1	3528	7/7	0.18	-	81,81,81,81	7
87	OHX	A6	2062	7/7	0.22	-	163,163,163,163	7
88	MG	A1	4503	1/1	0.80	-	77,77,77,77	0
88	MG	A1	4318	1/1	0.39	-	66,66,66,66	0
88	MG	A2	2199	1/1	0.20	-	72,72,72,72	0
88	MG	A6	2194	1/1	0.15	-	67,67,67,67	0
88	MG	A1	4068	1/1	0.33	-	78,78,78,78	0
88	MG	A1	4172	1/1	0.22	-	54,54,54,54	0
88	MG	A6	2170	1/1	0.20	-	49,49,49,49	0
88	MG	DY	201	1/1	0.22	-	59,59,59,59	0
87	OHX	A5	3427	7/7	0.20	-	79,79,79,79	0
87	OHX	A5	3820	7/7	0.33	-	80,80,80,80	7
88	MG	A6	2292	1/1	0.22	-	75,75,75,75	0
88	MG	A5	3838	1/1	0.38	-	39,39,39,39	0
88	MG	BN	306	1/1	0.43	-	55,55,55,55	0
87	OHX	A5	3444	7/7	0.16	-	74,74,74,74	7
87	OHX	A5	3422	7/7	0.20	-	75,75,75,75	0
88	MG	A5	4017	1/1	0.42	-	62,62,62,62	0
87	OHX	A1	3578	7/7	0.17	-	112,112,112,112	7
87	OHX	A6	1992	7/7	0.11	-	125,125,125,125	7
88	MG	A5	3907	1/1	0.31	-	75,75,75,75	0
88	MG	A1	3996	1/1	0.46	-	48,48,48,48	0
87	OHX	A5	3718	7/7	0.13	-	157,157,157,157	7
88	MG	A1	4294	1/1	0.24	-	78,78,78,78	0
88	MG	A6	2302	1/1	0.21	-	108,108,108,108	0
87	OHX	A1	3440	7/7	0.14	-	86,86,86,86	0
87	OHX	A5	3702	7/7	0.20	-	121,121,121,121	7
87	OHX	A5	3443	7/7	0.15	-	75,75,75,75	7
87	OHX	A2	2080	7/7	0.11	-	191,191,191,191	7
87	OHX	A5	3621	7/7	0.20	-	123,123,123,123	7
88	MG	A5	3920	1/1	0.23	-	83,83,83,83	0
87	OHX	A5	3821	7/7	0.18	-	223,223,223,223	7
88	MG	A6	2196	1/1	0.45	-	83,83,83,83	0
88	MG	A6	2242	1/1	0.36	-	87,87,87,87	0
88	MG	A1	4199	1/1	0.28	-	74,74,74,74	0
87	OHX	A2	1938	7/7	0.13	-	111,111,111,111	7
88	MG	Dj	102	1/1	0.85	-	74,74,74,74	0
87	OHX	A6	2081	7/7	0.10	-	201,201,201,201	7
87	OHX	A5	3549	7/7	0.17	-	107,107,107,107	7
87	OHX	A5	3571	7/7	0.17	-	143,143,143,143	7
88	MG	A6	2110	1/1	0.24	-	65,65,65,65	0
88	MG	Dd	201	1/1	0.23	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A6	2148	1/1	0.34	-	39,39,39,39	0
88	MG	A5	3887	1/1	0.40	-	84,84,84,84	0
87	OHX	A5	3486	7/7	0.15	-	75,75,75,75	7
88	MG	A1	3931	1/1	0.28	-	40,40,40,40	0
88	MG	A5	3883	1/1	0.22	-	36,36,36,36	0
88	MG	A8	234	1/1	0.29	-	64,64,64,64	0
88	MG	A2	2148	1/1	0.21	-	89,89,89,89	0
88	MG	A1	4301	1/1	0.26	-	118,118,118,118	0
87	OHX	A5	3580	7/7	0.14	-	121,121,121,121	7
88	MG	A1	3875	1/1	0.12	-	60,60,60,60	0
87	OHX	A1	3444	7/7	0.16	-	84,84,84,84	0
88	MG	A5	4491	1/1	0.38	-	82,82,82,82	0
88	MG	A5	4426	1/1	0.17	-	70,70,70,70	0
87	OHX	A5	3738	7/7	0.19	-	101,101,101,101	7
88	MG	CS	203	1/1	0.12	-	71,71,71,71	0
88	MG	A1	4175	1/1	0.10	-	69,69,69,69	0
87	OHX	A1	3490	7/7	0.16	-	126,126,126,126	0
88	MG	A5	3998	1/1	0.37	-	41,41,41,41	0
88	MG	A1	3932	1/1	0.27	-	30,30,30,30	0
88	MG	A5	4306	1/1	0.26	-	72,72,72,72	0
87	OHX	A5	3717	7/7	0.37	-	108,108,108,108	7
88	MG	A2	2116	1/1	0.33	-	59,59,59,59	0
88	MG	A1	4177	1/1	0.67	-	76,76,76,76	0
87	OHX	A6	2024	7/7	0.15	-	156,156,156,156	7
87	OHX	A6	2001	7/7	0.15	-	149,149,149,149	7
88	MG	A5	3859	1/1	0.21	-	50,50,50,50	0
87	OHX	A5	3757	7/7	0.09	-	192,192,192,192	7
87	OHX	A6	1977	7/7	0.17	-	128,128,128,128	7
87	OHX	A1	3552	7/7	0.17	-	115,115,115,115	7
88	MG	A1	3992	1/1	0.31	-	41,41,41,41	0
88	MG	DT	203	1/1	0.33	-	80,80,80,80	0
88	MG	A1	4387	1/1	0.49	-	89,89,89,89	0
88	MG	DS	201	1/1	0.20	-	61,61,61,61	0
88	MG	A1	4159	1/1	0.28	-	84,84,84,84	0
88	MG	A5	4459	1/1	0.74	-	84,84,84,84	0
87	OHX	A1	3645	7/7	0.22	-	102,102,102,102	7
87	OHX	A5	3627	7/7	0.20	-	80,80,80,80	7
87	OHX	A3	211	7/7	0.18	-	137,137,137,137	7
88	MG	A1	4107	1/1	0.17	-	74,74,74,74	0
88	MG	A6	2130	1/1	0.32	-	74,74,74,74	0
87	OHX	A5	3724	7/7	0.21	-	124,124,124,124	7
87	OHX	A5	3469	7/7	0.15	-	107,107,107,107	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	A5	3765	7/7	0.20	-	201,201,201,201	7
89	ZN	Cd	103	1/1	0.16	-	71,71,71,71	0
88	MG	A1	4284	1/1	0.27	-	87,87,87,87	0
88	MG	A2	2096	1/1	0.28	-	76,76,76,76	0
87	OHX	A2	2055	7/7	0.23	-	116,116,116,116	7
87	OHX	A1	3677	7/7	0.23	-	115,115,115,115	7
88	MG	A1	3965	1/1	0.37	-	80,80,80,80	0
88	MG	A1	4384	1/1	0.24	-	61,61,61,61	0
87	OHX	A5	3417	7/7	0.23	-	72,72,72,72	0
87	OHX	A1	3764	7/7	0.13	-	159,159,159,159	7
87	OHX	A2	1907	7/7	0.17	-	104,104,104,104	7
88	MG	A5	4062	1/1	0.27	-	37,37,37,37	0
87	OHX	A6	1981	7/7	0.18	-	110,110,110,110	7
88	MG	A1	4239	1/1	0.26	-	60,60,60,60	0
88	MG	A5	4314	1/1	0.17	-	56,56,56,56	0
87	OHX	A1	3473	7/7	0.19	-	85,85,85,85	7
88	MG	A2	2165	1/1	0.27	-	78,78,78,78	0
88	MG	A2	2132	1/1	0.13	-	77,77,77,77	0
87	OHX	A1	3498	7/7	0.21	-	89,89,89,89	7
88	MG	A6	2280	1/1	0.36	-	79,79,79,79	0
88	MG	A3	215	1/1	0.33	-	77,77,77,77	0
87	OHX	A6	2025	7/7	0.13	-	161,161,161,161	7
88	MG	A1	4090	1/1	0.30	-	78,78,78,78	0
88	MG	A5	4291	1/1	0.38	-	78,78,78,78	0
87	OHX	A6	1963	7/7	0.15	-	103,103,103,103	7
87	OHX	A1	3807	7/7	0.15	-	167,167,167,167	7
88	MG	BV	204	1/1	0.36	-	40,40,40,40	0
87	OHX	A2	1941	7/7	0.16	-	117,117,117,117	7
87	OHX	A1	3596	7/7	0.17	-	120,120,120,120	7
88	MG	A6	2179	1/1	0.22	-	47,47,47,47	0
87	OHX	A5	3509	7/7	0.17	-	97,97,97,97	7
88	MG	A6	2104	1/1	0.32	-	68,68,68,68	0
88	MG	A1	4304	1/1	0.38	-	102,102,102,102	0
88	MG	A5	4292	1/1	0.18	-	113,113,113,113	0
88	MG	A1	3934	1/1	0.28	-	46,46,46,46	0
88	MG	DP	208	1/1	0.24	-	42,42,42,42	0
88	MG	A5	4261	1/1	0.21	-	71,71,71,71	0
88	MG	A1	4293	1/1	0.82	-	110,110,110,110	0
87	OHX	A6	2028	7/7	0.23	-	136,136,136,136	7
88	MG	A6	2103	1/1	0.37	-	64,64,64,64	0
87	OHX	A6	1964	7/7	0.15	-	132,132,132,132	7
88	MG	A3	218	1/1	0.27	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A5	3951	1/1	0.26	-	40,40,40,40	0
88	MG	A1	3906	1/1	0.30	-	91,91,91,91	0
88	MG	A3	228	1/1	0.25	-	81,81,81,81	0
87	OHX	A5	3445	7/7	0.16	-	73,73,73,73	0
87	OHX	A2	1932	7/7	0.15	-	117,117,117,117	7
87	OHX	A5	3534	7/7	0.15	-	92,92,92,92	7
88	MG	A1	3978	1/1	0.38	-	73,73,73,73	0
88	MG	A5	4160	1/1	0.14	-	53,53,53,53	0
87	OHX	A5	3754	7/7	0.19	-	147,147,147,147	7
88	MG	A1	4391	1/1	0.62	-	89,89,89,89	0
88	MG	DV	203	1/1	0.20	-	65,65,65,65	0
87	OHX	Bj	103	7/7	0.36	-	138,138,138,138	7
88	MG	A1	3993	1/1	0.29	-	52,52,52,52	0
87	OHX	A3	210	7/7	0.16	-	175,175,175,175	7
87	OHX	A1	3608	7/7	0.16	-	160,160,160,160	7
88	MG	A5	4305	1/1	0.48	-	88,88,88,88	0
88	MG	A5	4342	1/1	0.16	-	50,50,50,50	0
87	OHX	A5	3746	7/7	0.20	-	151,151,151,151	7
88	MG	A5	4028	1/1	0.42	-	47,47,47,47	0
88	MG	A2	2101	1/1	0.11	-	59,59,59,59	0
87	OHX	AL	201	7/7	0.16	-	119,119,119,119	7
88	MG	A1	4126	1/1	0.23	-	84,84,84,84	0
87	OHX	A6	2076	7/7	0.21	-	90,90,90,90	7
87	OHX	Bj	102	7/7	0.18	-	102,102,102,102	7
88	MG	A5	4140	1/1	0.09	-	56,56,56,56	0
88	MG	A6	2290	1/1	0.19	-	82,82,82,82	0
88	MG	A1	4411	1/1	0.15	-	94,94,94,94	0
87	OHX	A1	3759	7/7	0.39	-	149,149,149,149	7
87	OHX	A2	2038	7/7	0.12	-	195,195,195,195	7
88	MG	A1	4403	1/1	0.15	-	71,71,71,71	0
88	MG	A6	2197	1/1	0.17	-	74,74,74,74	0
88	MG	A6	2276	1/1	0.40	-	105,105,105,105	0
87	OHX	A6	1927	7/7	0.15	-	129,129,129,129	0
87	OHX	A2	2063	7/7	0.13	-	183,183,183,183	7
88	MG	A1	4178	1/1	0.16	-	70,70,70,70	0
88	MG	A5	4178	1/1	0.25	-	83,83,83,83	0
88	MG	BB	406	1/1	0.53	-	59,59,59,59	0
88	MG	A2	2234	1/1	0.23	-	94,94,94,94	0
88	MG	A6	2156	1/1	0.38	-	62,62,62,62	0
87	OHX	A5	3663	7/7	0.21	-	136,136,136,136	7
88	MG	A5	3856	1/1	0.35	-	54,54,54,54	0
87	OHX	A5	3805	7/7	0.15	-	172,172,172,172	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A5	4100	1/1	0.28	-	86,86,86,86	0
87	OHX	A1	3675	7/7	0.12	-	169,169,169,169	7
87	OHX	A6	1939	7/7	0.15	-	134,134,134,134	0
88	MG	A5	3824	1/1	0.29	-	37,37,37,37	0
88	MG	CI	302	1/1	0.25	-	63,63,63,63	0
88	MG	A6	2154	1/1	0.33	-	56,56,56,56	0
87	OHX	A5	3548	7/7	0.15	-	134,134,134,134	7
87	OHX	A5	3437	7/7	0.16	-	83,83,83,83	0
88	MG	A5	3858	1/1	0.32	-	43,43,43,43	0
88	MG	DO	202	1/1	0.47	-	61,61,61,61	0
87	OHX	A1	3663	7/7	0.22	-	126,126,126,126	7
88	MG	A5	4198	1/1	0.17	-	58,58,58,58	0
87	OHX	CP	202	7/7	0.56	-	221,221,221,221	7
88	MG	A1	4144	1/1	0.64	-	82,82,82,82	0
87	OHX	A1	3772	7/7	0.25	-	171,171,171,171	7
87	OHX	A1	3574	7/7	0.25	-	189,189,189,189	7
87	OHX	A5	3647	7/7	0.11	-	204,204,204,204	7
88	MG	A5	4127	1/1	0.28	-	68,68,68,68	0
87	OHX	A1	3585	7/7	0.12	-	122,122,122,122	7
88	MG	A5	3869	1/1	0.36	-	58,58,58,58	0
87	OHX	A2	1943	7/7	0.19	-	123,123,123,123	7
87	OHX	BD	301	7/7	0.17	-	138,138,138,138	7
88	MG	A2	2227	1/1	0.17	-	106,106,106,106	0
88	MG	BB	404	1/1	0.20	-	57,57,57,57	0
88	MG	A2	2163	1/1	0.17	-	80,80,80,80	0
88	MG	CE	301	1/1	0.16	-	57,57,57,57	0
87	OHX	A1	3607	7/7	0.14	-	204,204,204,204	7
88	MG	A5	4519	1/1	0.09	-	63,63,63,63	0
87	OHX	A6	1997	7/7	0.16	-	125,125,125,125	7
87	OHX	A1	3618	7/7	0.12	-	158,158,158,158	7
88	MG	A2	2221	1/1	0.37	-	83,83,83,83	0
87	OHX	A6	2053	7/7	0.17	-	123,123,123,123	7
88	MG	A1	4085	1/1	0.15	-	35,35,35,35	0
88	MG	A2	2246	1/1	0.14	-	100,100,100,100	0
88	MG	A1	4233	1/1	0.23	-	79,79,79,79	0
87	OHX	A1	3448	7/7	0.16	-	85,85,85,85	7
88	MG	A1	4213	1/1	0.20	-	79,79,79,79	0
88	MG	A1	4115	1/1	0.27	-	62,62,62,62	0
87	OHX	A8	206	7/7	0.17	-	136,136,136,136	7
87	OHX	A1	3553	7/7	0.19	-	110,110,110,110	7
87	OHX	A1	3719	7/7	0.17	-	154,154,154,154	7
87	OHX	A1	3594	7/7	0.12	-	144,144,144,144	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A6	2211	1/1	0.12	-	86,86,86,86	0
88	MG	A1	3963	1/1	0.23	-	56,56,56,56	0
88	MG	A5	4465	1/1	0.29	-	62,62,62,62	0
88	MG	A5	3850	1/1	0.32	-	55,55,55,55	0
87	OHX	A5	3734	7/7	0.27	-	208,208,208,208	7
87	OHX	A2	1980	7/7	0.13	-	152,152,152,152	7
88	MG	A5	4326	1/1	0.17	-	75,75,75,75	0
88	MG	A5	4163	1/1	0.18	-	58,58,58,58	0
87	OHX	BT	201	7/7	0.18	-	78,78,78,78	0
88	MG	A5	3901	1/1	0.25	-	85,85,85,85	0
89	ZN	Af	202	1/1	0.11	-	113,113,113,113	0
87	OHX	A1	3710	7/7	0.15	-	122,122,122,122	7
87	OHX	A3	207	7/7	0.14	-	167,167,167,167	7
88	MG	A5	3978	1/1	0.27	-	29,29,29,29	0
87	OHX	A1	3703	7/7	0.17	-	93,93,93,93	7
88	MG	A5	4338	1/1	0.27	-	93,93,93,93	0
87	OHX	A4	201	7/7	0.23	-	77,77,77,77	0
87	OHX	A1	3771	7/7	0.25	-	174,174,174,174	7
88	MG	A1	4429	1/1	0.27	-	54,54,54,54	0
88	MG	A2	2160	1/1	0.26	-	66,66,66,66	0
88	MG	A5	3888	1/1	0.23	-	64,64,64,64	0
87	OHX	A1	3668	7/7	0.15	-	151,151,151,151	7
88	MG	A1	3826	1/1	0.17	-	51,51,51,51	0
87	OHX	A1	3559	7/7	0.15	-	116,116,116,116	7
88	MG	A1	4248	1/1	0.60	-	78,78,78,78	0
88	MG	A7	226	1/1	0.15	-	74,74,74,74	0
87	OHX	A1	3491	7/7	0.16	-	90,90,90,90	7
88	MG	A1	3894	1/1	0.32	-	43,43,43,43	0
87	OHX	A5	3658	7/7	0.28	-	141,141,141,141	7
88	MG	A2	2131	1/1	0.20	-	65,65,65,65	0
87	OHX	A6	1958	7/7	0.14	-	133,133,133,133	7
87	OHX	Do	201	7/7	0.18	-	89,89,89,89	7
88	MG	BO	207	1/1	0.77	-	56,56,56,56	0
88	MG	A1	3896	1/1	0.25	-	40,40,40,40	0
88	MG	A1	4443	1/1	0.32	-	65,65,65,65	0
87	OHX	A6	2016	7/7	0.12	-	124,124,124,124	7
88	MG	A6	2145	1/1	0.26	-	46,46,46,46	0
88	MG	A5	4351	1/1	0.29	-	85,85,85,85	0
87	OHX	A5	3778	7/7	0.18	-	153,153,153,153	7
88	MG	DA	304	1/1	0.68	-	69,69,69,69	0
87	OHX	A1	3427	7/7	0.17	-	86,86,86,86	0
88	MG	A5	3411	1/1	0.20	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	3838	1/1	0.24	-	67,67,67,67	0
87	OHX	A5	3675	7/7	0.17	-	132,132,132,132	7
88	MG	A5	4037	1/1	0.33	-	67,67,67,67	0
87	OHX	A3	212	7/7	0.29	-	159,159,159,159	7
88	MG	A5	3990	1/1	0.45	-	68,68,68,68	0
87	OHX	A6	2078	7/7	0.13	-	185,185,185,185	7
87	OHX	A1	3532	7/7	0.18	-	87,87,87,87	7
87	OHX	A1	3788	7/7	0.58	-	232,232,232,232	7
87	OHX	A5	3798	7/7	0.25	-	202,202,202,202	7
88	MG	A5	4267	1/1	0.25	-	88,88,88,88	0
88	MG	A2	2257	1/1	0.32	-	75,75,75,75	0
88	MG	A5	4439	1/1	0.07	-	56,56,56,56	0
88	MG	A1	4373	1/1	0.45	-	56,56,56,56	0
88	MG	A6	2260	1/1	0.21	-	62,62,62,62	0
87	OHX	A5	3477	7/7	0.14	-	108,108,108,108	7
88	MG	A6	2312	1/1	0.34	-	85,85,85,85	0
87	OHX	A2	1970	7/7	0.12	-	138,138,138,138	7
88	MG	A5	3941	1/1	0.27	-	51,51,51,51	0
87	OHX	A5	3414	7/7	0.25	-	69,69,69,69	0
88	MG	A5	4551	1/1	0.24	-	62,62,62,62	0
88	MG	DS	204	1/1	0.56	-	63,63,63,63	0
88	MG	A1	3884	1/1	0.31	-	64,64,64,64	0
87	OHX	A1	3635	7/7	0.26	-	84,84,84,84	7
87	OHX	A1	3780	7/7	0.20	-	136,136,136,136	7
87	OHX	A1	3725	7/7	0.20	-	191,191,191,191	7
87	OHX	A1	3647	7/7	0.14	-	129,129,129,129	7
87	OHX	A6	2026	7/7	0.14	-	176,176,176,176	7
87	OHX	A5	3499	7/7	0.18	-	84,84,84,84	7
88	MG	A1	3903	1/1	0.29	-	85,85,85,85	0
88	MG	BI	307	1/1	1.78	-	81,81,81,81	0
87	OHX	A1	3455	7/7	0.15	-	100,100,100,100	0
88	MG	A6	2231	1/1	0.24	-	69,69,69,69	0
88	MG	A1	3886	1/1	0.34	-	72,72,72,72	0
87	OHX	A1	3640	7/7	0.14	-	153,153,153,153	7
87	OHX	A5	3501	7/7	0.15	-	106,106,106,106	7
88	MG	A1	4344	1/1	0.17	-	88,88,88,88	0
87	OHX	A6	2015	7/7	0.21	-	159,159,159,159	7
88	MG	A1	4305	1/1	0.24	-	65,65,65,65	0
88	MG	A1	4030	1/1	0.17	-	37,37,37,37	0
88	MG	A1	4349	1/1	0.26	-	119,119,119,119	0
87	OHX	A1	3734	7/7	0.23	-	190,190,190,190	7
88	MG	A6	2252	1/1	0.23	-	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A5	3875	1/1	0.36	-	78,78,78,78	0
88	MG	A1	4093	1/1	0.20	-	55,55,55,55	0
87	OHX	A1	3508	7/7	0.17	-	93,93,93,93	7
87	OHX	A5	3679	7/7	0.14	-	174,174,174,174	7
88	MG	A5	4442	1/1	0.45	-	76,76,76,76	0
88	MG	BL	204	1/1	0.61	-	72,72,72,72	0
88	MG	DP	207	1/1	0.84	-	64,64,64,64	0
88	MG	A5	4207	1/1	0.34	-	102,102,102,102	0
88	MG	A1	4182	1/1	0.17	-	81,81,81,81	0
87	OHX	A2	2069	7/7	0.36	-	191,191,191,191	7
87	OHX	BP	201	7/7	0.33	-	115,115,115,115	7
88	MG	A5	4110	1/1	0.19	-	63,63,63,63	0
88	MG	A5	4365	1/1	0.18	-	80,80,80,80	0
87	OHX	A1	3754	7/7	0.18	-	159,159,159,159	7
88	MG	Bf	202	1/1	0.44	-	69,69,69,69	0
88	MG	A5	4516	1/1	0.69	-	74,74,74,74	0
88	MG	A5	4540	1/1	0.20	-	94,94,94,94	0
88	MG	A1	3867	1/1	0.31	-	61,61,61,61	0
88	MG	A1	4312	1/1	0.57	-	60,60,60,60	0
88	MG	A5	4272	1/1	0.11	-	69,69,69,69	0
88	MG	A5	4300	1/1	0.39	-	51,51,51,51	0
87	OHX	A5	3513	7/7	0.17	-	115,115,115,115	7
88	MG	A2	2129	1/1	0.32	-	59,59,59,59	0
88	MG	A5	4090	1/1	0.35	-	45,45,45,45	0
87	OHX	A1	3499	7/7	0.16	-	83,83,83,83	7
88	MG	A1	4291	1/1	0.16	-	112,112,112,112	0
88	MG	A1	4313	1/1	0.20	-	105,105,105,105	0
87	OHX	A1	3430	7/7	0.19	-	93,93,93,93	0
88	MG	A5	3952	1/1	0.42	-	43,43,43,43	0
87	OHX	A1	3467	7/7	0.15	-	91,91,91,91	7
88	MG	A5	4406	1/1	0.40	-	75,75,75,75	0
88	MG	A2	2114	1/1	0.38	-	84,84,84,84	0
88	MG	A1	4153	1/1	0.26	-	96,96,96,96	0
88	MG	Ad	103	1/1	0.16	-	67,67,67,67	0
88	MG	A2	2188	1/1	0.20	-	82,82,82,82	0
88	MG	A5	4388	1/1	0.35	-	47,47,47,47	0
88	MG	A6	2186	1/1	0.59	-	104,104,104,104	0
88	MG	A5	4070	1/1	0.30	-	56,56,56,56	0
88	MG	A5	4559	1/1	0.21	-	74,74,74,74	0
87	OHX	A1	3403	7/7	0.13	-	169,169,169,169	7
88	MG	A1	3881	1/1	0.20	-	39,39,39,39	0
88	MG	A1	3973	1/1	0.35	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
88	MG	A5	3985	1/1	0.44	-	51,51,51,51	0
88	MG	A1	4371	1/1	0.44	-	63,63,63,63	0
88	MG	A1	4044	1/1	0.26	-	44,44,44,44	0
88	MG	A5	4129	1/1	0.54	-	94,94,94,94	0
87	OHX	A5	3756	7/7	0.19	-	158,158,158,158	7
88	MG	A5	4376	1/1	0.51	-	67,67,67,67	0
88	MG	A1	4137	1/1	0.28	-	84,84,84,84	0
87	OHX	A5	3720	7/7	0.13	-	101,101,101,101	7
87	OHX	A5	3689	7/7	0.21	-	134,134,134,134	7
88	MG	A5	3902	1/1	0.14	-	31,31,31,31	0
87	OHX	A5	3630	7/7	0.19	-	128,128,128,128	7
88	MG	A1	4226	1/1	0.61	-	63,63,63,63	0
88	MG	A1	4088	1/1	0.28	-	90,90,90,90	0
88	MG	A5	4416	1/1	0.49	-	48,48,48,48	0
88	MG	A1	4507	1/1	0.20	-	90,90,90,90	0
88	MG	BI	306	1/1	0.15	-	32,32,32,32	0
88	MG	BP	205	1/1	0.21	-	53,53,53,53	0
88	MG	A6	2210	1/1	0.20	-	72,72,72,72	0
88	MG	BO	208	1/1	0.19	-	75,75,75,75	0
88	MG	A6	2220	1/1	0.17	-	91,91,91,91	0
87	OHX	A1	3606	7/7	0.15	-	132,132,132,132	7
88	MG	A5	4371	1/1	0.28	-	90,90,90,90	0
88	MG	A1	3947	1/1	0.41	-	42,42,42,42	0
87	OHX	A2	1977	7/7	0.10	-	174,174,174,174	7
88	MG	A5	4222	1/1	0.27	-	75,75,75,75	0
88	MG	A1	3874	1/1	0.31	-	60,60,60,60	0
88	MG	AL	202	1/1	0.89	-	78,78,78,78	0
88	MG	DH	203	1/1	0.45	-	72,72,72,72	0
88	MG	A5	4386	1/1	0.22	-	65,65,65,65	0
88	MG	A1	4149	1/1	0.14	-	74,74,74,74	0
88	MG	A5	3942	1/1	0.33	-	38,38,38,38	0
88	MG	A1	3849	1/1	0.35	-	56,56,56,56	0
87	OHX	A3	204	7/7	0.15	-	125,125,125,125	7
87	OHX	A1	3685	7/7	0.12	-	150,150,150,150	7
88	MG	A6	2238	1/1	0.19	-	73,73,73,73	0
88	MG	A1	4038	1/1	0.24	-	89,89,89,89	0
88	MG	A1	4480	1/1	0.64	-	91,91,91,91	0
88	MG	A5	4419	1/1	0.23	-	65,65,65,65	0
88	MG	BL	203	1/1	0.20	-	61,61,61,61	0
88	MG	BP	206	1/1	0.16	-	86,86,86,86	0
87	OHX	A5	3629	7/7	0.22	-	100,100,100,100	7
88	MG	A5	4131	1/1	0.20	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A6	2267	1/1	0.18	-	72,72,72,72	0
88	MG	Bg	201	1/1	0.17	-	63,63,63,63	0
88	MG	A1	4260	1/1	0.20	-	75,75,75,75	0
87	OHX	A5	3823	7/7	0.11	-	225,225,225,225	7
88	MG	A2	2219	1/1	0.20	-	93,93,93,93	0
88	MG	A6	2240	1/1	0.17	-	95,95,95,95	0
87	OHX	A2	1916	7/7	0.16	-	110,110,110,110	7
88	MG	A2	2093	1/1	0.23	-	47,47,47,47	0
88	MG	A5	3911	1/1	0.13	-	82,82,82,82	0
88	MG	A1	3936	1/1	0.30	-	34,34,34,34	0
88	MG	A1	4028	1/1	0.37	-	28,28,28,28	0
87	OHX	A6	2075	7/7	0.14	-	194,194,194,194	7
88	MG	A5	4547	1/1	0.58	-	88,88,88,88	0
88	MG	A2	2112	1/1	0.39	-	95,95,95,95	0
87	OHX	A6	1931	7/7	0.17	-	84,84,84,84	7
88	MG	A1	4197	1/1	0.18	-	74,74,74,74	0
87	OHX	A6	1901	7/7	0.22	-	78,78,78,78	0
87	OHX	A2	2050	7/7	0.16	-	181,181,181,181	7
88	MG	A2	2244	1/1	0.14	-	99,99,99,99	0
87	OHX	A1	3612	7/7	0.14	-	146,146,146,146	7
88	MG	A1	4413	1/1	0.23	-	106,106,106,106	0
88	MG	DB	407	1/1	0.68	-	72,72,72,72	0
88	MG	A5	4095	1/1	0.25	-	79,79,79,79	0
88	MG	A6	2255	1/1	0.32	-	81,81,81,81	0
87	OHX	A1	3662	7/7	0.26	-	119,119,119,119	7
88	MG	A6	2298	1/1	0.12	-	77,77,77,77	0
87	OHX	A2	1945	7/7	0.15	-	140,140,140,140	7
87	OHX	A1	3671	7/7	0.18	-	96,96,96,96	7
88	MG	A6	2324	1/1	0.22	-	74,74,74,74	0
88	MG	A6	2113	1/1	0.24	-	48,48,48,48	0
88	MG	A5	4513	1/1	0.28	-	53,53,53,53	0
89	ZN	Do	203	1/1	0.15	-	181,181,181,181	0
87	OHX	CJ	201	7/7	0.22	-	105,105,105,105	7
88	MG	A5	4298	1/1	0.09	-	106,106,106,106	0
88	MG	A5	4202	1/1	0.25	-	45,45,45,45	0
88	MG	A1	4224	1/1	0.18	-	72,72,72,72	0
87	OHX	A1	3672	7/7	0.16	-	99,99,99,99	7
88	MG	A1	4112	1/1	0.18	-	58,58,58,58	0
87	OHX	A1	3500	7/7	0.17	-	87,87,87,87	7
88	MG	A1	4118	1/1	0.16	-	74,74,74,74	0
88	MG	BI	308	1/1	0.14	-	57,57,57,57	0
88	MG	A5	4259	1/1	0.27	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	4339	1/1	0.61	-	97,97,97,97	0
88	MG	A5	4204	1/1	0.11	-	56,56,56,56	0
88	MG	DY	202	1/1	0.19	-	55,55,55,55	0
87	OHX	A2	2013	7/7	0.16	-	116,116,116,116	7
88	MG	A2	2139	1/1	0.22	-	81,81,81,81	0
88	MG	A5	4009	1/1	0.36	-	45,45,45,45	0
88	MG	A5	4229	1/1	0.20	-	81,81,81,81	0
88	MG	DO	206	1/1	0.56	-	55,55,55,55	0
88	MG	A5	3947	1/1	0.17	-	40,40,40,40	0
88	MG	A1	4104	1/1	0.18	-	65,65,65,65	0
88	MG	A5	4079	1/1	0.22	-	67,67,67,67	0
88	MG	A5	4483	1/1	0.39	-	112,112,112,112	0
88	MG	A1	3958	1/1	0.29	-	45,45,45,45	0
88	MG	A5	4294	1/1	0.22	-	62,62,62,62	0
88	MG	A5	4478	1/1	0.30	-	81,81,81,81	0
88	MG	A5	4337	1/1	0.42	-	70,70,70,70	0
88	MG	A1	4211	1/1	0.30	-	102,102,102,102	0
87	OHX	A5	3672	7/7	0.19	-	142,142,142,142	7
88	MG	BP	212	1/1	0.27	-	93,93,93,93	0
88	MG	A2	2158	1/1	0.26	-	71,71,71,71	0
88	MG	A5	4010	1/1	0.43	-	50,50,50,50	0
88	MG	A6	2132	1/1	0.22	-	81,81,81,81	0
88	MG	A1	3950	1/1	0.18	-	48,48,48,48	0
87	OHX	A1	3571	7/7	0.14	-	119,119,119,119	7
87	OHX	A2	2066	7/7	0.19	-	164,164,164,164	7
88	MG	A2	2127	1/1	0.32	-	49,49,49,49	0
88	MG	A5	4332	1/1	0.09	-	73,73,73,73	0
87	OHX	A5	3435	7/7	0.15	-	70,70,70,70	0
88	MG	A5	4325	1/1	0.65	-	57,57,57,57	0
88	MG	A1	4377	1/1	0.53	-	54,54,54,54	0
88	MG	A1	4008	1/1	0.33	-	36,36,36,36	0
88	MG	A6	2257	1/1	0.20	-	65,65,65,65	0
88	MG	A5	4424	1/1	0.43	-	86,86,86,86	0
88	MG	A1	4439	1/1	0.27	-	88,88,88,88	0
87	OHX	A2	2026	7/7	0.14	-	140,140,140,140	7
88	MG	A5	4266	1/1	0.32	-	72,72,72,72	0
88	MG	A5	4155	1/1	0.33	-	95,95,95,95	0
88	MG	A5	4366	1/1	0.31	-	65,65,65,65	0
88	MG	A5	4221	1/1	0.35	-	88,88,88,88	0
88	MG	A1	4048	1/1	0.20	-	67,67,67,67	0
88	MG	A6	2222	1/1	0.23	-	86,86,86,86	0
87	OHX	A1	3579	7/7	0.18	-	97,97,97,97	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	4111	1/1	0.25	-	65,65,65,65	0
87	OHX	A2	2053	7/7	0.16	-	173,173,173,173	7
88	MG	A1	4084	1/1	0.20	-	67,67,67,67	0
87	OHX	BI	301	7/7	0.18	-	94,94,94,94	7
87	OHX	A2	2060	7/7	0.26	-	168,168,168,168	7
87	OHX	A1	3740	7/7	0.24	-	107,107,107,107	7
88	MG	A5	4301	1/1	0.08	-	71,71,71,71	0
87	OHX	A5	3775	7/7	0.19	-	152,152,152,152	7
87	OHX	A5	3632	7/7	0.17	-	106,106,106,106	7
88	MG	A1	4374	1/1	0.85	-	60,60,60,60	0
87	OHX	A1	3428	7/7	0.18	-	87,87,87,87	0
87	OHX	A2	2018	7/7	0.15	-	176,176,176,176	7
88	MG	BA	306	1/1	0.25	-	74,74,74,74	0
88	MG	A5	4398	1/1	0.15	-	54,54,54,54	0
88	MG	A1	3897	1/1	0.16	-	75,75,75,75	0
87	OHX	A2	1927	7/7	0.15	-	115,115,115,115	7
88	MG	A5	3855	1/1	0.37	-	55,55,55,55	0
87	OHX	A5	3581	7/7	0.14	-	148,148,148,148	7
88	MG	A6	2181	1/1	0.28	-	77,77,77,77	0
88	MG	A6	2313	1/1	0.86	-	78,78,78,78	0
88	MG	A5	4355	1/1	0.20	-	66,66,66,66	0
88	MG	A1	3982	1/1	0.39	-	43,43,43,43	0
88	MG	A6	2178	1/1	0.24	-	71,71,71,71	0
88	MG	A1	4346	1/1	0.18	-	53,53,53,53	0
87	OHX	A5	3508	7/7	0.14	-	119,119,119,119	7
88	MG	A7	217	1/1	0.36	-	55,55,55,55	0
87	OHX	A5	3719	7/7	0.20	-	180,180,180,180	7
88	MG	A7	237	1/1	0.32	-	69,69,69,69	0
88	MG	DF	304	1/1	0.44	-	57,57,57,57	0
87	OHX	A5	3654	7/7	0.15	-	116,116,116,116	7
87	OHX	A5	3710	7/7	0.14	-	132,132,132,132	7
87	OHX	A1	3438	7/7	0.16	-	91,91,91,91	7
88	MG	A5	4315	1/1	0.17	-	106,106,106,106	0
87	OHX	A6	2050	7/7	0.14	-	206,206,206,206	7
88	MG	A3	219	1/1	0.34	-	40,40,40,40	0
88	MG	A5	4133	1/1	0.18	-	54,54,54,54	0
87	OHX	A1	3409	7/7	0.23	-	70,70,70,70	0
88	MG	A1	3873	1/1	0.39	-	62,62,62,62	0
88	MG	A1	3853	1/1	0.09	-	43,43,43,43	0
88	MG	A6	2162	1/1	0.53	-	63,63,63,63	0
87	OHX	A6	2039	7/7	0.16	-	168,168,168,168	7
87	OHX	A1	3416	7/7	0.19	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	A2	1946	7/7	0.15	-	156,156,156,156	7
88	MG	A2	2106	1/1	0.36	-	57,57,57,57	0
87	OHX	A2	2002	7/7	0.11	-	169,169,169,169	7
88	MG	A2	2122	1/1	0.24	-	74,74,74,74	0
88	MG	A6	2118	1/1	0.30	-	57,57,57,57	0
87	OHX	A1	3588	7/7	0.17	-	104,104,104,104	7
88	MG	A1	4319	1/1	0.27	-	76,76,76,76	0
88	MG	A1	4136	1/1	0.22	-	53,53,53,53	0
88	MG	A1	4502	1/1	0.26	-	93,93,93,93	0
87	OHX	A5	3449	7/7	0.17	-	85,85,85,85	7
88	MG	A1	4261	1/1	0.23	-	79,79,79,79	0
88	MG	A1	3855	1/1	0.20	-	40,40,40,40	0
87	OHX	A6	1935	7/7	0.15	-	102,102,102,102	7
87	OHX	A1	3637	7/7	0.11	-	146,146,146,146	7
88	MG	DQ	202	1/1	0.16	-	88,88,88,88	0
88	MG	A5	4112	1/1	0.24	-	65,65,65,65	0
88	MG	A5	3898	1/1	0.17	-	44,44,44,44	0
88	MG	CF	302	1/1	0.26	-	73,73,73,73	0
88	MG	A2	2212	1/1	0.32	-	100,100,100,100	0
88	MG	A6	2200	1/1	0.24	-	82,82,82,82	0
88	MG	A5	4086	1/1	0.26	-	59,59,59,59	0
87	OHX	A2	1982	7/7	0.17	-	125,125,125,125	7
88	MG	A6	2327	1/1	0.11	-	108,108,108,108	0
88	MG	A5	4117	1/1	0.08	-	49,49,49,49	0
88	MG	A6	2316	1/1	0.45	-	112,112,112,112	0
88	MG	A5	3930	1/1	0.19	-	29,29,29,29	0
88	MG	A5	4295	1/1	0.22	-	61,61,61,61	0
87	OHX	CG	301	7/7	0.12	-	147,147,147,147	7
88	MG	A1	4119	1/1	0.17	-	78,78,78,78	0
88	MG	AS	201	1/1	0.12	-	105,105,105,105	0
88	MG	A1	3862	1/1	0.24	-	76,76,76,76	0
87	OHX	A6	2072	7/7	0.26	-	133,133,133,133	7
87	OHX	A6	1948	7/7	0.14	-	114,114,114,114	7
88	MG	A5	4531	1/1	0.24	-	65,65,65,65	0
88	MG	A5	3958	1/1	0.27	-	64,64,64,64	0
88	MG	A1	4222	1/1	0.22	-	73,73,73,73	0
88	MG	A1	4095	1/1	0.26	-	56,56,56,56	0
87	OHX	A5	3564	7/7	0.12	-	143,143,143,143	7
87	OHX	A5	3651	7/7	0.22	-	137,137,137,137	7
87	OHX	A5	3789	7/7	0.22	-	165,165,165,165	7
87	OHX	DR	201	7/7	0.16	-	171,171,171,171	7
87	OHX	A1	3613	7/7	0.19	-	98,98,98,98	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A2	2259	1/1	0.47	-	63,63,63,63	0
87	OHX	A1	3623	7/7	0.19	-	147,147,147,147	7
88	MG	A1	4478	1/1	0.27	-	100,100,100,100	0
88	MG	A1	3953	1/1	0.34	-	43,43,43,43	0
88	MG	A5	4340	1/1	0.61	-	61,61,61,61	0
88	MG	A1	3933	1/1	0.46	-	53,53,53,53	0
88	MG	A1	4067	1/1	0.15	-	66,66,66,66	0
88	MG	A6	2221	1/1	0.39	-	69,69,69,69	0
88	MG	A6	2198	1/1	0.13	-	49,49,49,49	0
87	OHX	A1	3698	7/7	0.15	-	105,105,105,105	7
87	OHX	A1	3632	7/7	0.09	-	170,170,170,170	7
87	OHX	A6	2009	7/7	0.17	-	136,136,136,136	7
87	OHX	A5	3697	7/7	0.13	-	167,167,167,167	7
88	MG	A5	3970	1/1	0.50	-	60,60,60,60	0
88	MG	A5	4296	1/1	0.29	-	54,54,54,54	0
87	OHX	A1	3702	7/7	0.18	-	141,141,141,141	7
87	OHX	A1	3707	7/7	0.18	-	135,135,135,135	7
87	OHX	A1	3434	7/7	0.14	-	72,72,72,72	7
88	MG	A1	4031	1/1	0.23	-	32,32,32,32	0
88	MG	A1	3925	1/1	0.21	-	40,40,40,40	0
87	OHX	A2	1960	7/7	0.12	-	173,173,173,173	7
87	OHX	A1	3481	7/7	0.15	-	97,97,97,97	7
87	OHX	A1	3745	7/7	0.26	-	178,178,178,178	7
87	OHX	A5	3462	7/7	0.17	-	102,102,102,102	0
88	MG	A1	4475	1/1	0.77	-	64,64,64,64	0
88	MG	A5	4484	1/1	0.76	-	89,89,89,89	0
88	MG	A5	4203	1/1	0.26	-	82,82,82,82	0
87	OHX	Df	201	7/7	0.16	-	99,99,99,99	7
88	MG	A1	3858	1/1	0.34	-	64,64,64,64	0
88	MG	A5	4528	1/1	0.27	-	97,97,97,97	0
88	MG	A1	4168	1/1	0.13	-	44,44,44,44	0
88	MG	A2	2170	1/1	0.35	-	88,88,88,88	0
88	MG	A1	3945	1/1	0.34	-	50,50,50,50	0
88	MG	A5	4089	1/1	0.15	-	81,81,81,81	0
88	MG	A6	2160	1/1	0.41	-	45,45,45,45	0
88	MG	DF	303	1/1	0.28	-	73,73,73,73	0
87	OHX	A1	3812	7/7	0.47	-	187,187,187,187	7
88	MG	A5	3916	1/1	0.27	-	49,49,49,49	0
88	MG	A5	4190	1/1	0.48	-	58,58,58,58	0
87	OHX	A5	3421	7/7	0.21	-	81,81,81,81	0
87	OHX	A5	3638	7/7	0.16	-	135,135,135,135	7
87	OHX	A4	212	7/7	0.21	-	118,118,118,118	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A5	3582	7/7	0.17	-	95,95,95,95	7
87	OHX	A2	1978	7/7	0.17	-	108,108,108,108	7
88	MG	A5	3975	1/1	0.43	-	41,41,41,41	0
88	MG	A5	4034	1/1	0.17	-	46,46,46,46	0
87	OHX	A5	3530	7/7	0.14	-	105,105,105,105	7
87	OHX	A5	3782	7/7	0.26	-	169,169,169,169	7
88	MG	A2	2130	1/1	0.11	-	56,56,56,56	0
87	OHX	A1	3747	7/7	0.28	-	118,118,118,118	7
88	MG	A5	4550	1/1	0.92	-	83,83,83,83	0
87	OHX	A1	3611	7/7	0.14	-	96,96,96,96	7
88	MG	BL	205	1/1	0.41	-	62,62,62,62	0
87	OHX	A1	3541	7/7	0.19	-	109,109,109,109	7
87	OHX	A5	3542	7/7	0.18	-	103,103,103,103	7
87	OHX	A2	2079	7/7	0.19	-	157,157,157,157	7
88	MG	A1	4236	1/1	0.28	-	73,73,73,73	0
88	MG	A1	3869	1/1	0.25	-	69,69,69,69	0
87	OHX	A1	3656	7/7	0.16	-	114,114,114,114	7
87	OHX	A5	3522	7/7	0.15	-	123,123,123,123	7
88	MG	A1	3975	1/1	0.31	-	67,67,67,67	0
87	OHX	A5	3755	7/7	0.17	-	174,174,174,174	7
87	OHX	A1	3479	7/7	0.17	-	117,117,117,117	7
87	OHX	A1	3757	7/7	0.21	-	73,73,73,73	7
88	MG	A1	4102	1/1	0.10	-	61,61,61,61	0
88	MG	A5	3893	1/1	0.29	-	73,73,73,73	0
87	OHX	A2	1976	7/7	0.15	-	139,139,139,139	7
87	OHX	A5	3612	7/7	0.16	-	147,147,147,147	7
88	MG	A6	2217	1/1	0.55	-	87,87,87,87	0
87	OHX	A5	3618	7/7	0.19	-	101,101,101,101	7
87	OHX	A5	3418	7/7	0.24	-	77,77,77,77	0
88	MG	A5	4047	1/1	0.21	-	57,57,57,57	0
87	OHX	A5	3645	7/7	0.17	-	141,141,141,141	7
87	OHX	A7	202	7/7	0.19	-	81,81,81,81	7
87	OHX	A5	3705	7/7	0.15	-	152,152,152,152	7
88	MG	Dg	203	1/1	1.22	-	88,88,88,88	0
88	MG	A6	2165	1/1	0.38	-	51,51,51,51	0
88	MG	A5	4576	1/1	0.32	-	77,77,77,77	0
88	MG	A1	4474	1/1	0.27	-	72,72,72,72	0
87	OHX	A1	3649	7/7	0.14	-	167,167,167,167	7
89	ZN	Bj	111	1/1	0.15	-	44,44,44,44	0
88	MG	A5	4287	1/1	0.23	-	101,101,101,101	0
87	OHX	A1	3718	7/7	0.17	-	94,94,94,94	7
87	OHX	A5	3567	7/7	0.16	-	106,106,106,106	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	3937	1/1	0.36	-	40,40,40,40	0
88	MG	A1	3923	1/1	0.23	-	44,44,44,44	0
88	MG	A5	3854	1/1	0.29	-	74,74,74,74	0
88	MG	A1	4058	1/1	0.28	-	97,97,97,97	0
88	MG	A1	4385	1/1	0.67	-	65,65,65,65	0
87	OHX	A6	1976	7/7	0.23	-	105,105,105,105	7
88	MG	A2	2121	1/1	0.41	-	61,61,61,61	0
87	OHX	A1	3742	7/7	0.26	-	140,140,140,140	7
87	OHX	A6	2086	7/7	0.67	-	215,215,215,215	7
88	MG	DO	209	1/1	0.61	-	62,62,62,62	0
87	OHX	A1	3587	7/7	0.12	-	147,147,147,147	7
88	MG	A5	4530	1/1	0.36	-	113,113,113,113	0
87	OHX	A2	2040	7/7	0.11	-	171,171,171,171	7
88	MG	A1	4327	1/1	0.12	-	108,108,108,108	0
88	MG	BC	403	1/1	0.40	-	72,72,72,72	0
87	OHX	A5	3606	7/7	0.14	-	130,130,130,130	7
88	MG	A1	4077	1/1	0.33	-	77,77,77,77	0
88	MG	A5	3890	1/1	0.38	-	82,82,82,82	0
88	MG	A1	4351	1/1	0.12	-	97,97,97,97	0
88	MG	A1	4471	1/1	0.14	-	88,88,88,88	0
87	OHX	A6	2030	7/7	0.10	-	170,170,170,170	7
87	OHX	A5	3752	7/7	0.23	-	127,127,127,127	7
88	MG	A6	2137	1/1	0.33	-	71,71,71,71	0
88	MG	A5	3908	1/1	0.27	-	37,37,37,37	0
87	OHX	A8	208	7/7	0.16	-	115,115,115,115	7
87	OHX	A1	3568	7/7	0.13	-	133,133,133,133	7
87	OHX	A6	1905	7/7	0.18	-	88,88,88,88	0
88	MG	CL	203	1/1	0.18	-	61,61,61,61	0
88	MG	A6	2234	1/1	0.18	-	92,92,92,92	0
88	MG	A1	4329	1/1	0.35	-	85,85,85,85	0
87	OHX	A5	3519	7/7	0.17	-	78,78,78,78	7
88	MG	A5	4370	1/1	0.18	-	59,59,59,59	0
88	MG	A1	4430	1/1	0.28	-	67,67,67,67	0
88	MG	A1	4017	1/1	0.37	-	48,48,48,48	0
87	OHX	A8	204	7/7	0.17	-	101,101,101,101	7
87	OHX	A6	2006	7/7	0.17	-	87,87,87,87	7
87	OHX	A6	1920	7/7	0.16	-	87,87,87,87	7
88	MG	A5	3955	1/1	0.33	-	62,62,62,62	0
87	OHX	A2	2030	7/7	0.26	-	155,155,155,155	7
88	MG	A5	3923	1/1	0.18	-	68,68,68,68	0
87	OHX	A1	3475	7/7	0.18	-	98,98,98,98	7
88	MG	Ad	104	1/1	0.15	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	A1	3495	7/7	0.16	-	101,101,101,101	7
88	MG	A2	2145	1/1	0.25	-	71,71,71,71	0
88	MG	BT	202	1/1	0.35	-	89,89,89,89	0
88	MG	A2	2231	1/1	0.29	-	75,75,75,75	0
88	MG	DV	204	1/1	0.99	-	83,83,83,83	0
88	MG	A6	2318	1/1	0.20	-	68,68,68,68	0
88	MG	A1	4170	1/1	0.14	-	50,50,50,50	0
88	MG	A2	2183	1/1	0.24	-	49,49,49,49	0
87	OHX	A1	3720	7/7	0.18	-	139,139,139,139	7
87	OHX	A6	2048	7/7	0.20	-	169,169,169,169	7
87	OHX	A6	1912	7/7	0.16	-	96,96,96,96	0
88	MG	A6	2136	1/1	0.27	-	48,48,48,48	0
88	MG	A1	4072	1/1	0.23	-	73,73,73,73	0
87	OHX	A2	2027	7/7	0.15	-	166,166,166,166	7
88	MG	A2	2209	1/1	0.40	-	96,96,96,96	0
88	MG	BA	304	1/1	0.17	-	62,62,62,62	0
87	OHX	A5	3565	7/7	0.17	-	105,105,105,105	7
88	MG	A5	4307	1/1	0.09	-	78,78,78,78	0
88	MG	A1	4163	1/1	0.36	-	81,81,81,81	0
87	OHX	BP	202	7/7	0.11	-	139,139,139,139	7
88	MG	A4	232	1/1	0.18	-	74,74,74,74	0
88	MG	A5	4201	1/1	0.10	-	49,49,49,49	0
87	OHX	DV	201	7/7	0.14	-	126,126,126,126	7
87	OHX	A2	2006	7/7	0.13	-	162,162,162,162	7
88	MG	A5	4008	1/1	0.34	-	42,42,42,42	0
87	OHX	A6	1959	7/7	0.18	-	107,107,107,107	7
88	MG	A1	3878	1/1	0.30	-	45,45,45,45	0
88	MG	A1	4158	1/1	0.23	-	87,87,87,87	0
88	MG	A5	4109	1/1	0.26	-	88,88,88,88	0
87	OHX	A5	3563	7/7	0.17	-	98,98,98,98	7
88	MG	A8	230	1/1	0.34	-	68,68,68,68	0
88	MG	A1	4202	1/1	0.21	-	67,67,67,67	0
88	MG	A2	2149	1/1	0.28	-	83,83,83,83	0
87	OHX	A1	3542	7/7	0.17	-	159,159,159,159	7
88	MG	A1	4024	1/1	0.38	-	40,40,40,40	0
88	MG	A2	2105	1/1	0.27	-	55,55,55,55	0
87	OHX	A6	1936	7/7	0.16	-	100,100,100,100	7
87	OHX	A5	3811	7/7	0.30	-	214,214,214,214	7
88	MG	A5	4130	1/1	0.22	-	49,49,49,49	0
88	MG	A1	4164	1/1	0.27	-	78,78,78,78	0
87	OHX	A8	213	7/7	0.17	-	146,146,146,146	7
87	OHX	A6	2040	7/7	0.20	-	87,87,87,87	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	4486	1/1	0.28	-	55,55,55,55	0
88	MG	A1	4006	1/1	0.36	-	42,42,42,42	0
88	MG	A1	4244	1/1	0.24	-	52,52,52,52	0
88	MG	BP	204	1/1	0.34	-	51,51,51,51	0
87	OHX	A5	3813	7/7	0.19	-	191,191,191,191	7
88	MG	A5	4176	1/1	0.18	-	89,89,89,89	0
88	MG	A5	4038	1/1	0.18	-	42,42,42,42	0
87	OHX	A1	3667	7/7	0.24	-	92,92,92,92	7
87	OHX	A2	2035	7/7	0.17	-	120,120,120,120	7
87	OHX	A6	2018	7/7	0.16	-	153,153,153,153	7
88	MG	A1	4173	1/1	0.13	-	45,45,45,45	0
88	MG	A5	4320	1/1	0.18	-	117,117,117,117	0
87	OHX	A1	3631	7/7	0.13	-	141,141,141,141	7
88	MG	A5	3935	1/1	0.30	-	51,51,51,51	0
87	OHX	A4	209	7/7	0.12	-	153,153,153,153	7
87	OHX	A6	2020	7/7	0.18	-	88,88,88,88	7
88	MG	A1	4208	1/1	0.55	-	58,58,58,58	0
87	OHX	A2	2064	7/7	0.23	-	169,169,169,169	7
88	MG	A2	2198	1/1	0.19	-	80,80,80,80	0
88	MG	A2	2196	1/1	0.27	-	131,131,131,131	0
88	MG	A1	4448	1/1	0.25	-	66,66,66,66	0
88	MG	Dj	101	1/1	0.21	-	38,38,38,38	0
88	MG	A1	4428	1/1	0.62	-	58,58,58,58	0
88	MG	A1	4034	1/1	0.17	-	46,46,46,46	0
88	MG	A1	4278	1/1	0.23	-	67,67,67,67	0
88	MG	A5	4164	1/1	0.11	-	87,87,87,87	0
87	OHX	A1	3597	7/7	0.17	-	123,123,123,123	7
87	OHX	A5	3448	7/7	0.17	-	93,93,93,93	0
88	MG	A1	3924	1/1	0.28	-	57,57,57,57	0
88	MG	A6	2192	1/1	0.31	-	81,81,81,81	0
87	OHX	A1	3717	7/7	0.16	-	141,141,141,141	7
88	MG	A5	4252	1/1	0.22	-	68,68,68,68	0
88	MG	A5	4063	1/1	0.23	-	52,52,52,52	0
87	OHX	A5	3429	7/7	0.21	-	84,84,84,84	0
87	OHX	A1	3625	7/7	0.18	-	92,92,92,92	7
88	MG	A1	4263	1/1	1.04	-	71,71,71,71	0
88	MG	A1	3967	1/1	0.38	-	40,40,40,40	0
88	MG	A5	3921	1/1	0.23	-	82,82,82,82	0
87	OHX	A1	3799	7/7	0.14	-	165,165,165,165	7
87	OHX	A2	1920	7/7	0.16	-	115,115,115,115	7
88	MG	A2	2150	1/1	0.17	-	102,102,102,102	0
87	OHX	A2	2020	7/7	0.17	-	118,118,118,118	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A5	3524	7/7	0.17	-	92,92,92,92	7
88	MG	A1	3865	1/1	0.09	-	31,31,31,31	0
88	MG	A5	4058	1/1	0.21	-	59,59,59,59	0
88	MG	A5	4330	1/1	0.18	-	86,86,86,86	0
88	MG	A1	4272	1/1	0.19	-	53,53,53,53	0
88	MG	A2	2175	1/1	0.33	-	68,68,68,68	0
88	MG	A1	4042	1/1	0.29	-	68,68,68,68	0
87	OHX	A6	2042	7/7	0.17	-	169,169,169,169	7
87	OHX	A5	3498	7/7	0.17	-	89,89,89,89	7
88	MG	A5	4248	1/1	0.22	-	99,99,99,99	0
87	OHX	A1	3687	7/7	0.33	-	182,182,182,182	7
87	OHX	A3	202	7/7	0.14	-	103,103,103,103	7
88	MG	A7	220	1/1	0.23	-	61,61,61,61	0
88	MG	A5	4422	1/1	0.38	-	52,52,52,52	0
87	OHX	A5	3419	7/7	0.21	-	79,79,79,79	0
87	OHX	A1	3730	7/7	0.19	-	135,135,135,135	7
88	MG	A1	4201	1/1	0.37	-	65,65,65,65	0
88	MG	A5	3928	1/1	0.35	-	90,90,90,90	0
88	MG	A5	4045	1/1	0.31	-	63,63,63,63	0
88	MG	A5	4494	1/1	0.35	-	111,111,111,111	0
88	MG	A5	4143	1/1	0.14	-	70,70,70,70	0
87	OHX	A2	2043	7/7	0.10	-	192,192,192,192	7
88	MG	A5	4182	1/1	0.24	-	66,66,66,66	0
88	MG	A5	4512	1/1	0.24	-	56,56,56,56	0
88	MG	A1	3915	1/1	0.24	-	32,32,32,32	0
88	MG	A1	3988	1/1	0.30	-	67,67,67,67	0
87	OHX	A5	3655	7/7	0.19	-	124,124,124,124	7
88	MG	A5	4569	1/1	0.77	-	103,103,103,103	0
88	MG	A5	4199	1/1	0.35	-	70,70,70,70	0
87	OHX	A5	3404	7/7	0.20	-	111,111,111,111	7
87	OHX	A6	2059	7/7	0.13	-	153,153,153,153	7
88	MG	A1	3914	1/1	0.22	-	73,73,73,73	0
87	OHX	A5	3489	7/7	0.17	-	88,88,88,88	7
88	MG	A5	4012	1/1	0.39	-	43,43,43,43	0
87	OHX	A5	3743	7/7	0.23	-	167,167,167,167	7
87	OHX	A5	3671	7/7	0.17	-	171,171,171,171	7
88	MG	A1	4097	1/1	0.28	-	73,73,73,73	0
87	OHX	A5	3804	7/7	0.13	-	162,162,162,162	7
88	MG	A1	3851	1/1	0.25	-	53,53,53,53	0
88	MG	A2	2201	1/1	0.16	-	96,96,96,96	0
87	OHX	A1	3615	7/7	0.15	-	139,139,139,139	7
88	MG	A5	4421	1/1	0.37	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	3887	1/1	0.20	-	54,54,54,54	0
88	MG	A6	2261	1/1	0.27	-	76,76,76,76	0
88	MG	A1	4237	1/1	0.15	-	46,46,46,46	0
88	MG	A1	3871	1/1	0.27	-	48,48,48,48	0
88	MG	A6	2284	1/1	0.33	-	107,107,107,107	0
87	OHX	A5	3570	7/7	0.20	-	97,97,97,97	7
88	MG	A5	4401	1/1	0.20	-	64,64,64,64	0
88	MG	AP	202	1/1	0.25	-	88,88,88,88	0
87	OHX	A1	3577	7/7	0.15	-	122,122,122,122	7
87	OHX	A1	3581	7/7	0.19	-	73,73,73,73	7
88	MG	A4	242	1/1	0.19	-	81,81,81,81	0
87	OHX	A5	3807	7/7	0.18	-	107,107,107,107	7
88	MG	A5	3936	1/1	0.41	-	62,62,62,62	0
88	MG	DH	202	1/1	0.50	-	73,73,73,73	0
88	MG	CX	201	1/1	0.27	-	68,68,68,68	0
87	OHX	A5	3688	7/7	0.16	-	212,212,212,212	7
87	OHX	A8	220	7/7	0.21	-	111,111,111,111	7
87	OHX	A2	2049	7/7	0.13	-	140,140,140,140	7
88	MG	A5	4485	1/1	0.47	-	77,77,77,77	0
87	OHX	CL	201	7/7	0.14	-	134,134,134,134	7
88	MG	A4	235	1/1	0.14	-	119,119,119,119	0
87	OHX	A5	3480	7/7	0.15	-	101,101,101,101	7
88	MG	BJ	201	1/1	0.16	-	81,81,81,81	0
88	MG	A5	4408	1/1	0.29	-	65,65,65,65	0
88	MG	A1	4328	1/1	1.00	-	76,76,76,76	0
88	MG	A6	2193	1/1	0.13	-	75,75,75,75	0
87	OHX	A1	3412	7/7	0.23	-	76,76,76,76	0
87	OHX	A5	3684	7/7	0.18	-	122,122,122,122	7
88	MG	A5	4537	1/1	0.12	-	83,83,83,83	0
87	OHX	A1	3437	7/7	0.19	-	74,74,74,74	7
87	OHX	A5	3810	7/7	0.47	-	199,199,199,199	7
87	OHX	A1	3785	7/7	0.35	-	183,183,183,183	7
88	MG	BC	404	1/1	1.00	-	67,67,67,67	0
87	OHX	A5	3544	7/7	0.18	-	97,97,97,97	7
88	MG	A5	4185	1/1	0.52	-	49,49,49,49	0
88	MG	A1	4125	1/1	0.18	-	56,56,56,56	0
88	MG	A1	4323	1/1	0.12	-	92,92,92,92	0
88	MG	A1	4487	1/1	0.20	-	80,80,80,80	0
87	OHX	A1	3680	7/7	0.22	-	127,127,127,127	7
88	MG	A7	218	1/1	0.41	-	43,43,43,43	0
88	MG	A1	3951	1/1	0.43	-	46,46,46,46	0
87	OHX	DC	401	7/7	0.14	-	148,148,148,148	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A5	4066	1/1	0.23	-	73,73,73,73	0
88	MG	A6	2319	1/1	0.17	-	64,64,64,64	0
87	OHX	A2	1949	7/7	0.14	-	135,135,135,135	7
88	MG	A6	2120	1/1	0.39	-	51,51,51,51	0
87	OHX	A6	1969	7/7	0.18	-	90,90,90,90	7
88	MG	A1	4415	1/1	0.54	-	85,85,85,85	0
87	OHX	A6	1911	7/7	0.19	-	100,100,100,100	0
88	MG	CL	202	1/1	0.24	-	82,82,82,82	0
88	MG	BO	204	1/1	0.35	-	53,53,53,53	0
88	MG	BS	201	1/1	0.48	-	64,64,64,64	0
88	MG	A1	4019	1/1	0.40	-	42,42,42,42	0
88	MG	A6	2139	1/1	0.34	-	72,72,72,72	0
87	OHX	A5	3591	7/7	0.21	-	209,209,209,209	7
88	MG	A5	3995	1/1	0.41	-	53,53,53,53	0
88	MG	A1	3841	1/1	0.19	-	47,47,47,47	0
88	MG	A5	4118	1/1	0.27	-	57,57,57,57	0
88	MG	A5	4575	1/1	0.32	-	68,68,68,68	0
88	MG	BN	304	1/1	0.27	-	80,80,80,80	0
87	OHX	A5	3790	7/7	0.18	-	157,157,157,157	7
88	MG	A1	4342	1/1	0.18	-	79,79,79,79	0
87	OHX	A1	3624	7/7	0.20	-	137,137,137,137	7
87	OHX	A1	3489	7/7	0.17	-	90,90,90,90	7
88	MG	A5	4348	1/1	0.35	-	58,58,58,58	0
88	MG	A1	3984	1/1	0.35	-	51,51,51,51	0
88	MG	A2	2125	1/1	0.45	-	61,61,61,61	0
88	MG	DN	301	1/1	0.17	-	77,77,77,77	0
87	OHX	Bb	101	7/7	0.18	-	77,77,77,77	0
87	OHX	A1	3583	7/7	0.15	-	147,147,147,147	7
88	MG	A7	232	1/1	0.17	-	91,91,91,91	0
88	MG	AB	302	1/1	0.15	-	63,63,63,63	0
88	MG	A5	4232	1/1	0.53	-	53,53,53,53	0
88	MG	BQ	204	1/1	1.43	-	99,99,99,99	0
88	MG	A6	2190	1/1	0.13	-	74,74,74,74	0
87	OHX	A6	1955	7/7	0.13	-	153,153,153,153	7
88	MG	A1	4264	1/1	0.21	-	65,65,65,65	0
88	MG	A5	4415	1/1	0.20	-	75,75,75,75	0
88	MG	A4	229	1/1	0.14	-	54,54,54,54	0
88	MG	A5	4379	1/1	0.31	-	45,45,45,45	0
87	OHX	A5	3447	7/7	0.21	-	107,107,107,107	0
87	OHX	A1	3660	7/7	0.24	-	137,137,137,137	7
88	MG	A5	3906	1/1	0.29	-	56,56,56,56	0
87	OHX	A1	3450	7/7	0.17	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	Da	204	1/1	0.47	-	52,52,52,52	0
87	OHX	A5	3598	7/7	0.12	-	143,143,143,143	7
88	MG	A5	3973	1/1	0.36	-	38,38,38,38	0
87	OHX	A1	3561	7/7	0.18	-	110,110,110,110	7
88	MG	A4	225	1/1	0.33	-	65,65,65,65	0
88	MG	A5	4013	1/1	0.31	-	44,44,44,44	0
88	MG	A2	2164	1/1	0.18	-	74,74,74,74	0
87	OHX	A5	3626	7/7	0.17	-	147,147,147,147	7
88	MG	A5	4353	1/1	0.57	-	71,71,71,71	0
87	OHX	A5	3471	7/7	0.15	-	90,90,90,90	7
88	MG	A5	4479	1/1	0.33	-	64,64,64,64	0
87	OHX	A5	3503	7/7	0.17	-	97,97,97,97	7
88	MG	A1	4289	1/1	0.21	-	74,74,74,74	0
87	OHX	A5	3795	7/7	0.23	-	117,117,117,117	7
87	OHX	A5	3518	7/7	0.17	-	159,159,159,159	7
88	MG	A1	4394	1/1	0.50	-	58,58,58,58	0
88	MG	A2	2252	1/1	0.19	-	89,89,89,89	0
88	MG	A1	3956	1/1	0.34	-	45,45,45,45	0
88	MG	A2	2162	1/1	0.46	-	84,84,84,84	0
87	OHX	BB	402	7/7	0.23	-	173,173,173,173	7
88	MG	A5	4039	1/1	0.35	-	63,63,63,63	0
88	MG	A5	4271	1/1	0.47	-	68,68,68,68	0
88	MG	A1	4340	1/1	0.55	-	96,96,96,96	0
88	MG	A1	3918	1/1	0.35	-	83,83,83,83	0
88	MG	A5	4497	1/1	0.26	-	76,76,76,76	0
88	MG	A5	3410	1/1	0.23	-	61,61,61,61	0
88	MG	A7	233	1/1	0.26	-	60,60,60,60	0
87	OHX	A5	3700	7/7	0.30	-	146,146,146,146	7
88	MG	A5	4507	1/1	0.69	-	92,92,92,92	0
87	OHX	DB	402	7/7	0.18	-	145,145,145,145	7
87	OHX	A4	203	7/7	0.17	-	93,93,93,93	7
87	OHX	A3	205	7/7	0.15	-	113,113,113,113	7
88	MG	A6	2289	1/1	0.20	-	96,96,96,96	0
87	OHX	A6	2064	7/7	0.10	-	164,164,164,164	7
88	MG	A5	3900	1/1	0.23	-	63,63,63,63	0
88	MG	A6	2335	1/1	0.56	-	84,84,84,84	0
88	MG	A8	223	1/1	0.33	-	50,50,50,50	0
88	MG	A2	2108	1/1	0.15	-	56,56,56,56	0
87	OHX	A5	3643	7/7	0.12	-	150,150,150,150	7
87	OHX	A5	3796	7/7	0.21	-	176,176,176,176	7
88	MG	A1	4493	1/1	0.29	-	66,66,66,66	0
88	MG	A7	222	1/1	0.31	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A5	4345	1/1	0.64	-	77,77,77,77	0
88	MG	A6	2167	1/1	0.27	-	46,46,46,46	0
88	MG	A1	4062	1/1	0.30	-	72,72,72,72	0
88	MG	A2	2094	1/1	0.40	-	68,68,68,68	0
88	MG	A2	2229	1/1	0.11	-	60,60,60,60	0
87	OHX	A2	2061	7/7	0.23	-	142,142,142,142	7
88	MG	Da	203	1/1	0.18	-	54,54,54,54	0
87	OHX	A5	3669	7/7	0.23	-	109,109,109,109	7
88	MG	A2	2088	1/1	0.30	-	59,59,59,59	0
87	OHX	A7	201	7/7	0.19	-	107,107,107,107	0
88	MG	A5	4546	1/1	0.28	-	66,66,66,66	0
87	OHX	A6	1930	7/7	0.15	-	120,120,120,120	7
87	OHX	A5	3521	7/7	0.18	-	150,150,150,150	7
87	OHX	A1	3609	7/7	0.18	-	122,122,122,122	7
88	MG	A1	4392	1/1	0.86	-	86,86,86,86	0
87	OHX	A6	1995	7/7	0.08	-	143,143,143,143	7
88	MG	A1	4206	1/1	0.20	-	55,55,55,55	0
88	MG	A1	4060	1/1	0.19	-	67,67,67,67	0
87	OHX	A2	1913	7/7	0.16	-	129,129,129,129	0
88	MG	A5	4404	1/1	0.58	-	54,54,54,54	0
87	OHX	A5	3467	7/7	0.18	-	104,104,104,104	7
88	MG	A5	4247	1/1	0.15	-	64,64,64,64	0
88	MG	A1	4145	1/1	0.18	-	54,54,54,54	0
88	MG	A1	4230	1/1	0.39	-	91,91,91,91	0
88	MG	A1	4180	1/1	0.66	-	79,79,79,79	0
87	OHX	A1	3410	7/7	0.22	-	68,68,68,68	0
88	MG	A2	2190	1/1	0.20	-	82,82,82,82	0
88	MG	DC	405	1/1	0.46	-	72,72,72,72	0
88	MG	A1	3885	1/1	0.26	-	61,61,61,61	0
87	OHX	A5	3483	7/7	0.15	-	103,103,103,103	7
88	MG	A5	4132	1/1	0.28	-	66,66,66,66	0
87	OHX	A1	3569	7/7	0.16	-	144,144,144,144	7
87	OHX	A1	3582	7/7	0.18	-	92,92,92,92	7
88	MG	A1	4069	1/1	0.21	-	69,69,69,69	0
87	OHX	A5	3430	7/7	0.17	-	80,80,80,80	0
88	MG	A7	239	1/1	0.14	-	71,71,71,71	0
87	OHX	A6	2008	7/7	0.14	-	176,176,176,176	7
88	MG	A5	3843	1/1	0.24	-	50,50,50,50	0
87	OHX	A1	3644	7/7	0.13	-	139,139,139,139	7
87	OHX	A2	2052	7/7	0.21	-	117,117,117,117	7
88	MG	A5	3866	1/1	0.24	-	51,51,51,51	0
87	OHX	DI	301	7/7	0.18	-	118,118,118,118	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A5	3966	1/1	0.38	-	56,56,56,56	0
88	MG	Ba	202	1/1	0.39	-	63,63,63,63	0
88	MG	A5	4191	1/1	0.23	-	99,99,99,99	0
88	MG	A1	3922	1/1	0.39	-	107,107,107,107	0
88	MG	AL	203	1/1	0.67	-	80,80,80,80	0
88	MG	A5	4240	1/1	0.66	-	77,77,77,77	0
88	MG	A5	4276	1/1	0.20	-	60,60,60,60	0
88	MG	A5	4541	1/1	0.39	-	107,107,107,107	0
88	MG	DC	406	1/1	0.26	-	111,111,111,111	0
87	OHX	A5	3426	7/7	0.17	-	67,67,67,67	0
88	MG	A6	2140	1/1	0.24	-	61,61,61,61	0
87	OHX	A6	2023	7/7	0.18	-	177,177,177,177	7
88	MG	A1	3843	1/1	0.24	-	46,46,46,46	0
88	MG	A6	2301	1/1	0.49	-	116,116,116,116	0
87	OHX	A6	1954	7/7	0.12	-	141,141,141,141	7
88	MG	A5	4274	1/1	0.10	-	51,51,51,51	0
87	OHX	A1	3638	7/7	0.15	-	141,141,141,141	7
88	MG	A5	3957	1/1	0.42	-	43,43,43,43	0
87	OHX	A5	3695	7/7	0.17	-	158,158,158,158	7
88	MG	A5	3937	1/1	0.31	-	69,69,69,69	0
87	OHX	A1	3511	7/7	0.17	-	154,154,154,154	0
88	MG	A5	3980	1/1	0.33	-	58,58,58,58	0
88	MG	A3	227	1/1	0.54	-	59,59,59,59	0
87	OHX	A1	3749	7/7	0.15	-	177,177,177,177	7
87	OHX	A5	3714	7/7	0.17	-	126,126,126,126	7
88	MG	A6	2133	1/1	0.26	-	65,65,65,65	0
87	OHX	A5	3706	7/7	0.15	-	139,139,139,139	7
87	OHX	A5	3546	7/7	0.14	-	132,132,132,132	7
87	OHX	A5	3659	7/7	0.21	-	106,106,106,106	7
87	OHX	A5	3781	7/7	0.14	-	199,199,199,199	7
88	MG	A5	3976	1/1	0.22	-	43,43,43,43	0
88	MG	A1	4020	1/1	0.33	-	52,52,52,52	0
88	MG	A5	4535	1/1	0.14	-	68,68,68,68	0
88	MG	A1	4240	1/1	0.18	-	59,59,59,59	0
88	MG	A5	4397	1/1	0.17	-	101,101,101,101	0
88	MG	A1	4406	1/1	0.39	-	69,69,69,69	0
87	OHX	A5	3783	7/7	0.21	-	154,154,154,154	7
87	OHX	A1	3539	7/7	0.18	-	103,103,103,103	7
88	MG	A6	2106	1/1	0.29	-	64,64,64,64	0
88	MG	A5	4472	1/1	0.34	-	75,75,75,75	0
88	MG	A5	3845	1/1	0.29	-	51,51,51,51	0
87	OHX	A6	2067	7/7	0.22	-	136,136,136,136	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	3957	1/1	0.46	-	50,50,50,50	0
87	OHX	A5	3562	7/7	0.18	-	104,104,104,104	7
88	MG	A5	4080	1/1	0.33	-	71,71,71,71	0
87	OHX	A5	3691	7/7	0.18	-	155,155,155,155	7
87	OHX	Bf	201	7/7	0.18	-	85,85,85,85	7
88	MG	A6	2205	1/1	0.28	-	72,72,72,72	0
87	OHX	A1	3420	7/7	0.17	-	69,69,69,69	0
88	MG	A5	3943	1/1	0.39	-	38,38,38,38	0
88	MG	A5	3981	1/1	0.41	-	79,79,79,79	0
87	OHX	A5	3690	7/7	0.17	-	130,130,130,130	7
87	OHX	A8	203	7/7	0.13	-	111,111,111,111	7
88	MG	A5	4196	1/1	0.11	-	66,66,66,66	0
87	OHX	A2	1917	7/7	0.14	-	111,111,111,111	7
88	MG	A5	4525	1/1	0.58	-	66,66,66,66	0
88	MG	A1	3962	1/1	0.38	-	61,61,61,61	0
88	MG	A6	2241	1/1	0.60	-	112,112,112,112	0
87	OHX	A2	2033	7/7	0.18	-	97,97,97,97	7
87	OHX	A2	2076	7/7	0.14	-	185,185,185,185	7
87	OHX	A1	3695	7/7	0.12	-	163,163,163,163	7
87	OHX	A5	3539	7/7	0.17	-	125,125,125,125	7
88	MG	A5	4257	1/1	0.25	-	70,70,70,70	0
88	MG	A5	4096	1/1	0.36	-	72,72,72,72	0
88	MG	Df	205	1/1	0.30	-	76,76,76,76	0
87	OHX	A6	1940	7/7	0.14	-	129,129,129,129	7
88	MG	BL	201	1/1	0.20	-	51,51,51,51	0
88	MG	A1	3954	1/1	0.25	-	45,45,45,45	0
87	OHX	A1	3684	7/7	0.14	-	143,143,143,143	7
87	OHX	A1	3775	7/7	0.20	-	69,69,69,69	7
88	MG	A6	2111	1/1	0.14	-	51,51,51,51	0
87	OHX	A2	2036	7/7	0.20	-	162,162,162,162	7
87	OHX	A1	3417	7/7	0.22	-	82,82,82,82	0
88	MG	A5	4094	1/1	0.24	-	69,69,69,69	0
88	MG	A5	4270	1/1	0.24	-	57,57,57,57	0
87	OHX	A6	1996	7/7	0.14	-	148,148,148,148	7
87	OHX	A5	3405	7/7	0.25	-	118,118,118,118	7
88	MG	A5	3842	1/1	0.05	-	34,34,34,34	0
87	OHX	A1	3580	7/7	0.14	-	149,149,149,149	7
87	OHX	A1	3696	7/7	0.20	-	143,143,143,143	7
87	OHX	A5	3526	7/7	0.17	-	85,85,85,85	7
88	MG	A1	4359	1/1	0.25	-	70,70,70,70	0
88	MG	A2	2254	1/1	0.20	-	61,61,61,61	0
88	MG	A6	2163	1/1	0.33	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A2	1925	7/7	0.11	-	138,138,138,138	0
87	OHX	A1	3463	7/7	0.13	-	110,110,110,110	7
87	OHX	A1	3813	7/7	0.18	-	201,201,201,201	7
87	OHX	A1	3512	7/7	0.41	-	197,197,197,197	7
87	OHX	A5	3625	7/7	0.16	-	117,117,117,117	7
88	MG	A5	3961	1/1	0.25	-	55,55,55,55	0
88	MG	A6	2270	1/1	0.37	-	90,90,90,90	0
88	MG	A1	4308	1/1	0.55	-	59,59,59,59	0
88	MG	A4	222	1/1	0.34	-	43,43,43,43	0
88	MG	A1	3935	1/1	0.41	-	59,59,59,59	0
87	OHX	A1	3562	7/7	0.18	-	143,143,143,143	7
88	MG	A1	4166	1/1	0.26	-	74,74,74,74	0
88	MG	CB	302	1/1	0.16	-	93,93,93,93	0
88	MG	A5	4414	1/1	0.93	-	101,101,101,101	0
88	MG	A5	4515	1/1	0.38	-	109,109,109,109	0
88	MG	A2	2251	1/1	0.24	-	77,77,77,77	0
88	MG	A1	4317	1/1	0.26	-	92,92,92,92	0
88	MG	A2	2119	1/1	0.26	-	67,67,67,67	0
87	OHX	A1	3543	7/7	0.13	-	137,137,137,137	7
88	MG	A3	221	1/1	0.14	-	69,69,69,69	0
88	MG	A1	4047	1/1	0.27	-	98,98,98,98	0
88	MG	A5	3885	1/1	0.17	-	58,58,58,58	0
87	OHX	A5	3434	7/7	0.17	-	85,85,85,85	0
87	OHX	A5	3574	7/7	0.15	-	154,154,154,154	7
87	OHX	A5	3456	7/7	0.17	-	85,85,85,85	7
88	MG	A6	2274	1/1	0.14	-	95,95,95,95	0
88	MG	BP	207	1/1	0.26	-	65,65,65,65	0
87	OHX	A5	3736	7/7	0.24	-	143,143,143,143	7
88	MG	A5	4543	1/1	0.16	-	78,78,78,78	0
87	OHX	A6	1960	7/7	0.14	-	120,120,120,120	7
87	OHX	A2	1936	7/7	0.18	-	112,112,112,112	7
88	MG	A4	221	1/1	0.24	-	43,43,43,43	0
88	MG	A5	4450	1/1	0.28	-	73,73,73,73	0
89	ZN	Ca	202	1/1	0.12	-	73,73,73,73	0
88	MG	A1	3830	1/1	0.28	-	60,60,60,60	0
88	MG	A5	4420	1/1	0.23	-	93,93,93,93	0
88	MG	A6	2338	1/1	0.35	-	80,80,80,80	0
88	MG	A5	3829	1/1	0.18	-	35,35,35,35	0
88	MG	A5	3938	1/1	0.29	-	45,45,45,45	0
87	OHX	A1	3803	7/7	0.17	-	196,196,196,196	7
87	OHX	A5	3475	7/7	0.14	-	95,95,95,95	7
88	MG	A1	4051	1/1	0.25	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A6	1968	7/7	0.13	-	101,101,101,101	7
87	OHX	A6	2022	7/7	0.13	-	145,145,145,145	7
87	OHX	A5	3819	7/7	0.47	-	238,238,238,238	7
87	OHX	A2	1942	7/7	0.15	-	113,113,113,113	7
88	MG	Aa	201	1/1	0.49	-	82,82,82,82	0
88	MG	A6	2320	1/1	1.46	-	117,117,117,117	0
88	MG	A1	4154	1/1	0.18	-	91,91,91,91	0
87	OHX	A1	3497	7/7	0.23	-	100,100,100,100	7
88	MG	A5	4020	1/1	0.42	-	33,33,33,33	0
88	MG	A1	3952	1/1	0.34	-	89,89,89,89	0
88	MG	BL	202	1/1	0.26	-	78,78,78,78	0
88	MG	A5	4475	1/1	0.67	-	127,127,127,127	0
88	MG	A1	4315	1/1	0.59	-	62,62,62,62	0
87	OHX	DQ	201	7/7	0.21	-	147,147,147,147	7
88	MG	A6	2123	1/1	0.31	-	51,51,51,51	0
88	MG	A5	3954	1/1	0.37	-	46,46,46,46	0
88	MG	A2	2152	1/1	0.20	-	88,88,88,88	0
88	MG	A1	4425	1/1	0.13	-	106,106,106,106	0
87	OHX	A6	2083	7/7	0.49	-	214,214,214,214	7
88	MG	BO	209	1/1	1.27	-	95,95,95,95	0
88	MG	A1	4499	1/1	0.22	-	65,65,65,65	0
87	OHX	A1	3534	7/7	0.16	-	106,106,106,106	7
88	MG	Dp	103	1/1	0.21	-	72,72,72,72	0
87	OHX	A1	3424	7/7	0.17	-	81,81,81,81	0
87	OHX	A5	3610	7/7	0.13	-	161,161,161,161	7
88	MG	A1	4181	1/1	0.28	-	61,61,61,61	0
88	MG	A1	4131	1/1	0.14	-	75,75,75,75	0
88	MG	A1	3946	1/1	0.35	-	41,41,41,41	0
88	MG	A6	2295	1/1	0.14	-	79,79,79,79	0
88	MG	A1	3960	1/1	0.22	-	54,54,54,54	0
88	MG	A1	4341	1/1	0.21	-	118,118,118,118	0
88	MG	A2	2176	1/1	0.34	-	64,64,64,64	0
88	MG	A6	2294	1/1	0.12	-	54,54,54,54	0
87	OHX	A1	3423	7/7	0.15	-	75,75,75,75	0
88	MG	DB	414	1/1	0.92	-	76,76,76,76	0
88	MG	A6	2128	1/1	0.38	-	81,81,81,81	0
88	MG	BV	205	1/1	0.68	-	68,68,68,68	0
88	MG	A5	4242	1/1	0.53	-	65,65,65,65	0
89	ZN	Aa	202	1/1	0.10	-	92,92,92,92	0
87	OHX	A5	3517	7/7	0.18	-	80,80,80,80	7
88	MG	A5	4049	1/1	0.29	-	70,70,70,70	0
88	MG	A1	4183	1/1	0.16	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A1	3506	7/7	0.17	-	103,103,103,103	7
88	MG	A7	235	1/1	0.33	-	74,74,74,74	0
88	MG	A5	4206	1/1	0.27	-	110,110,110,110	0
88	MG	A5	3860	1/1	0.31	-	66,66,66,66	0
87	OHX	A5	3406	7/7	0.11	-	170,170,170,170	7
87	OHX	A6	2097	7/7	0.20	-	181,181,181,181	7
88	MG	A6	2246	1/1	0.38	-	78,78,78,78	0
87	OHX	A2	2062	7/7	0.16	-	196,196,196,196	7
88	MG	A1	4235	1/1	0.25	-	62,62,62,62	0
87	OHX	A6	1942	7/7	0.16	-	114,114,114,114	7
88	MG	A1	4218	1/1	0.19	-	69,69,69,69	0
87	OHX	A6	1903	7/7	0.21	-	84,84,84,84	0
88	MG	A1	3983	1/1	0.12	-	65,65,65,65	0
88	MG	A5	4184	1/1	0.27	-	55,55,55,55	0
88	MG	DF	301	1/1	0.16	-	75,75,75,75	0
88	MG	A5	4444	1/1	0.35	-	66,66,66,66	0
87	OHX	A5	3793	7/7	0.19	-	158,158,158,158	7
88	MG	A2	2240	1/1	0.39	-	97,97,97,97	0
87	OHX	A5	3556	7/7	0.16	-	111,111,111,111	7
88	MG	A2	2194	1/1	0.36	-	113,113,113,113	0
87	OHX	A1	3560	7/7	0.15	-	116,116,116,116	7
88	MG	Df	203	1/1	0.25	-	93,93,93,93	0
88	MG	A1	4242	1/1	0.18	-	84,84,84,84	0
88	MG	A6	2339	1/1	0.18	-	64,64,64,64	0
88	MG	A1	4050	1/1	0.19	-	63,63,63,63	0
88	MG	A1	4082	1/1	0.17	-	73,73,73,73	0
88	MG	A1	4156	1/1	0.24	-	75,75,75,75	0
87	OHX	A5	3441	7/7	0.22	-	96,96,96,96	0
87	OHX	A6	2002	7/7	0.17	-	96,96,96,96	7
88	MG	A5	4099	1/1	0.30	-	93,93,93,93	0
88	MG	A1	3938	1/1	0.24	-	48,48,48,48	0
88	MG	BA	305	1/1	0.43	-	61,61,61,61	0
88	MG	A6	2124	1/1	0.17	-	55,55,55,55	0
88	MG	A1	4434	1/1	0.80	-	55,55,55,55	0
88	MG	A6	2157	1/1	0.42	-	70,70,70,70	0
88	MG	A5	4165	1/1	0.10	-	73,73,73,73	0
87	OHX	A6	1961	7/7	0.20	-	132,132,132,132	7
88	MG	A4	233	1/1	0.16	-	57,57,57,57	0
88	MG	A5	3877	1/1	0.27	-	60,60,60,60	0
88	MG	BA	302	1/1	0.26	-	63,63,63,63	0
88	MG	DP	205	1/1	0.16	-	56,56,56,56	0
88	MG	A5	3940	1/1	0.41	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A5	4285	1/1	0.34	-	68,68,68,68	0
88	MG	A1	4423	1/1	0.39	-	85,85,85,85	0
87	OHX	A5	3585	7/7	0.19	-	163,163,163,163	7
88	MG	A6	2253	1/1	0.33	-	85,85,85,85	0
88	MG	A3	231	1/1	0.28	-	92,92,92,92	0
87	OHX	A2	1968	7/7	0.16	-	134,134,134,134	7
88	MG	A1	4322	1/1	0.27	-	74,74,74,74	0
88	MG	A5	4030	1/1	0.45	-	39,39,39,39	0
88	MG	A6	2129	1/1	0.27	-	66,66,66,66	0
88	MG	A2	2155	1/1	0.28	-	86,86,86,86	0
87	OHX	A1	3460	7/7	0.16	-	111,111,111,111	0
88	MG	A5	4453	1/1	0.42	-	66,66,66,66	0
88	MG	A5	3903	1/1	0.26	-	34,34,34,34	0
87	OHX	A1	3584	7/7	0.16	-	88,88,88,88	7
88	MG	A5	4018	1/1	0.40	-	40,40,40,40	0
88	MG	A2	2203	1/1	0.21	-	68,68,68,68	0
88	MG	A5	4057	1/1	0.31	-	82,82,82,82	0
87	OHX	A5	3631	7/7	0.20	-	89,89,89,89	7
88	MG	A5	4189	1/1	0.32	-	96,96,96,96	0
87	OHX	A6	2077	7/7	0.16	-	197,197,197,197	7
88	MG	A1	4485	1/1	0.18	-	93,93,93,93	0
87	OHX	A5	3664	7/7	0.21	-	106,106,106,106	7
88	MG	A1	4489	1/1	0.33	-	94,94,94,94	0
88	MG	A5	4343	1/1	0.51	-	56,56,56,56	0
87	OHX	A5	3676	7/7	0.15	-	155,155,155,155	7
88	MG	A1	4449	1/1	0.13	-	98,98,98,98	0
87	OHX	A5	3476	7/7	0.15	-	103,103,103,103	7
88	MG	A1	3856	1/1	0.27	-	38,38,38,38	0
88	MG	A6	2306	1/1	0.13	-	103,103,103,103	0
88	MG	A5	4033	1/1	0.10	-	31,31,31,31	0
88	MG	A5	4451	1/1	0.31	-	80,80,80,80	0
87	OHX	A2	1919	7/7	0.15	-	106,106,106,106	7
88	MG	A1	4336	1/1	0.12	-	80,80,80,80	0
87	OHX	A2	2083	7/7	0.51	-	185,185,185,185	7
87	OHX	A6	2095	7/7	0.41	-	213,213,213,213	7
87	OHX	A2	2073	7/7	0.19	-	147,147,147,147	7
87	OHX	A5	3525	7/7	0.15	-	112,112,112,112	7
87	OHX	A5	3439	7/7	0.16	-	81,81,81,81	0
88	MG	A5	3915	1/1	0.24	-	78,78,78,78	0
88	MG	A1	4375	1/1	0.22	-	51,51,51,51	0
87	OHX	A2	1957	7/7	0.15	-	101,101,101,101	7
88	MG	A2	2230	1/1	0.14	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A5	4463	1/1	0.08	-	89,89,89,89	0
87	OHX	A1	3636	7/7	0.14	-	148,148,148,148	7
87	OHX	A1	3791	7/7	0.17	-	149,149,149,149	7
87	OHX	A1	3554	7/7	0.17	-	159,159,159,159	7
88	MG	CL	204	1/1	0.47	-	83,83,83,83	0
88	MG	A5	4219	1/1	0.30	-	74,74,74,74	0
87	OHX	A1	3619	7/7	0.24	-	128,128,128,128	7
87	OHX	A1	3746	7/7	0.28	-	142,142,142,142	7
88	MG	A5	3917	1/1	0.25	-	44,44,44,44	0
87	OHX	A6	2088	7/7	0.23	-	160,160,160,160	7
87	OHX	DA	302	7/7	0.28	-	157,157,157,157	7
88	MG	A5	3963	1/1	0.34	-	44,44,44,44	0
88	MG	A6	2171	1/1	0.19	-	77,77,77,77	0
88	MG	A6	2275	1/1	0.15	-	63,63,63,63	0
88	MG	A5	4350	1/1	0.81	-	58,58,58,58	0
88	MG	A1	4262	1/1	0.17	-	70,70,70,70	0
88	MG	A5	4101	1/1	0.14	-	64,64,64,64	0
87	OHX	A6	1962	7/7	0.15	-	126,126,126,126	7
87	OHX	A2	2070	7/7	0.14	-	202,202,202,202	7
87	OHX	A5	3547	7/7	0.22	-	104,104,104,104	7
87	OHX	A5	3771	7/7	0.22	-	176,176,176,176	7
87	OHX	A5	3485	7/7	0.15	-	85,85,85,85	7
87	OHX	A2	2084	7/7	0.18	-	183,183,183,183	7
88	MG	A5	4375	1/1	0.48	-	65,65,65,65	0
88	MG	A1	4171	1/1	0.17	-	79,79,79,79	0
88	MG	A4	248	1/1	0.38	-	114,114,114,114	0
87	OHX	A6	1990	7/7	0.17	-	177,177,177,177	7
87	OHX	A5	3633	7/7	0.22	-	126,126,126,126	7
87	OHX	A2	2058	7/7	0.21	-	201,201,201,201	7
88	MG	A6	2271	1/1	0.17	-	95,95,95,95	0
87	OHX	A1	3792	7/7	0.44	-	213,213,213,213	7
88	MG	A5	3986	1/1	0.23	-	53,53,53,53	0
87	OHX	A1	3688	7/7	0.12	-	181,181,181,181	7
87	OHX	A2	1939	7/7	0.14	-	144,144,144,144	7
88	MG	A2	2173	1/1	0.12	-	82,82,82,82	0
88	MG	Bm	201	1/1	0.51	-	68,68,68,68	0
88	MG	A1	4219	1/1	0.16	-	85,85,85,85	0
87	OHX	A6	1966	7/7	0.17	-	92,92,92,92	7
88	MG	A5	4061	1/1	0.20	-	83,83,83,83	0
88	MG	A2	2135	1/1	0.11	-	54,54,54,54	0
87	OHX	A5	3440	7/7	0.18	-	63,63,63,63	7
87	OHX	A2	1924	7/7	0.15	-	111,111,111,111	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	Ad	101	7/7	0.16	-	130,130,130,130	7
88	MG	A6	2224	1/1	0.10	-	47,47,47,47	0
88	MG	A1	4398	1/1	0.18	-	49,49,49,49	0
87	OHX	CN	201	7/7	0.20	-	174,174,174,174	7
87	OHX	A6	1909	7/7	0.17	-	84,84,84,84	0
88	MG	A5	4423	1/1	0.30	-	82,82,82,82	0
87	OHX	A1	3755	7/7	0.31	-	135,135,135,135	7
88	MG	A5	4000	1/1	0.40	-	53,53,53,53	0
89	ZN	Bo	205	1/1	0.14	-	209,209,209,209	0
88	MG	A2	2181	1/1	0.15	-	79,79,79,79	0
87	OHX	A1	3641	7/7	0.18	-	137,137,137,137	7
87	OHX	A6	2098	7/7	0.23	-	144,144,144,144	7
87	OHX	A6	1929	7/7	0.15	-	128,128,128,128	0
87	OHX	A5	3750	7/7	0.17	-	199,199,199,199	7
88	MG	A5	4286	1/1	0.24	-	58,58,58,58	0
88	MG	Do	202	1/1	0.40	-	50,50,50,50	0
87	OHX	A8	205	7/7	0.12	-	107,107,107,107	7
87	OHX	A4	208	7/7	0.19	-	90,90,90,90	7
87	OHX	A1	3806	7/7	0.23	-	198,198,198,198	7
88	MG	A6	2330	1/1	0.30	-	80,80,80,80	0
87	OHX	A5	3608	7/7	0.12	-	125,125,125,125	7
88	MG	A5	4522	1/1	0.14	-	73,73,73,73	0
87	OHX	A5	3472	7/7	0.21	-	105,105,105,105	0
88	MG	A1	4018	1/1	0.41	-	38,38,38,38	0
88	MG	A1	4016	1/1	0.34	-	40,40,40,40	0
87	OHX	A2	1910	7/7	0.15	-	104,104,104,104	0
87	OHX	A1	3622	7/7	0.18	-	112,112,112,112	7
88	MG	A5	3834	1/1	0.39	-	59,59,59,59	0
88	MG	A5	3969	1/1	0.36	-	37,37,37,37	0
88	MG	A5	3884	1/1	0.27	-	54,54,54,54	0
88	MG	A6	2153	1/1	0.38	-	54,54,54,54	0
88	MG	A1	4081	1/1	0.14	-	56,56,56,56	0
87	OHX	A5	3753	7/7	0.11	-	207,207,207,207	7
87	OHX	A1	3510	7/7	0.19	-	92,92,92,92	7
88	MG	A5	4335	1/1	0.39	-	94,94,94,94	0
87	OHX	A1	3802	7/7	0.33	-	146,146,146,146	7
88	MG	A2	2213	1/1	0.20	-	107,107,107,107	0
88	MG	A1	3837	1/1	0.29	-	68,68,68,68	0
88	MG	A5	4048	1/1	0.10	-	34,34,34,34	0
88	MG	A5	4458	1/1	0.40	-	76,76,76,76	0
87	OHX	A5	3701	7/7	0.18	-	57,57,57,57	7
87	OHX	A2	1997	7/7	0.23	-	121,121,121,121	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	DO	203	1/1	0.26	-	58,58,58,58	0
87	OHX	A1	3545	7/7	0.16	-	78,78,78,78	7
88	MG	BR	204	1/1	0.30	-	67,67,67,67	0
88	MG	A1	4232	1/1	0.41	-	75,75,75,75	0
87	OHX	A5	3667	7/7	0.23	-	100,100,100,100	7
88	MG	A1	3860	1/1	0.28	-	59,59,59,59	0
88	MG	A2	2186	1/1	0.28	-	76,76,76,76	0
87	OHX	BO	201	7/7	0.16	-	97,97,97,97	7
88	MG	A6	2195	1/1	0.31	-	93,93,93,93	0
87	OHX	A5	3656	7/7	0.18	-	169,169,169,169	7
88	MG	A1	4281	1/1	0.20	-	74,74,74,74	0
87	OHX	A2	1929	7/7	0.15	-	90,90,90,90	7
88	MG	A4	226	1/1	0.28	-	70,70,70,70	0
88	MG	A5	4303	1/1	0.31	-	57,57,57,57	0
88	MG	A6	2150	1/1	0.41	-	48,48,48,48	0
87	OHX	A5	3473	7/7	0.17	-	82,82,82,82	7
87	OHX	A1	3593	7/7	0.16	-	113,113,113,113	7
88	MG	A5	4171	1/1	0.29	-	108,108,108,108	0
87	OHX	A1	3787	7/7	0.15	-	173,173,173,173	7
88	MG	A5	3408	1/1	0.53	-	63,63,63,63	0
87	OHX	A5	3732	7/7	0.27	-	209,209,209,209	7
88	MG	CZ	201	1/1	0.19	-	74,74,74,74	0
88	MG	A5	4563	1/1	0.31	-	89,89,89,89	0
87	OHX	A5	3538	7/7	0.16	-	104,104,104,104	7
88	MG	A1	4464	1/1	0.25	-	63,63,63,63	0
88	MG	A1	3889	1/1	0.45	-	74,74,74,74	0
88	MG	A5	4209	1/1	0.24	-	53,53,53,53	0
88	MG	A1	4482	1/1	0.17	-	129,129,129,129	0
88	MG	A2	2134	1/1	0.17	-	74,74,74,74	0
88	MG	A6	2218	1/1	0.15	-	53,53,53,53	0
88	MG	A2	2172	1/1	0.18	-	69,69,69,69	0
87	OHX	A6	2096	7/7	0.17	-	156,156,156,156	7
87	OHX	A5	3596	7/7	0.19	-	84,84,84,84	7
88	MG	A1	4438	1/1	0.33	-	82,82,82,82	0
88	MG	A5	4524	1/1	0.20	-	85,85,85,85	0
88	MG	DT	202	1/1	1.08	-	89,89,89,89	0
87	OHX	A1	3721	7/7	0.16	-	153,153,153,153	7
87	OHX	A1	3694	7/7	0.18	-	131,131,131,131	7
87	OHX	A1	3776	7/7	0.28	-	123,123,123,123	7
87	OHX	A2	2021	7/7	0.21	-	158,158,158,158	7
88	MG	A5	4217	1/1	0.34	-	83,83,83,83	0
88	MG	A5	4378	1/1	0.98	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A5	4255	1/1	0.19	-	72,72,72,72	0
88	MG	BB	403	1/1	0.24	-	53,53,53,53	0
87	OHX	A1	3778	7/7	0.30	-	150,150,150,150	7
87	OHX	A1	3766	7/7	0.35	-	135,135,135,135	7
88	MG	A6	2249	1/1	0.18	-	71,71,71,71	0
88	MG	A5	4399	1/1	0.17	-	64,64,64,64	0
87	OHX	A1	3774	7/7	0.17	-	206,206,206,206	7
88	MG	A1	4117	1/1	0.20	-	80,80,80,80	0
87	OHX	A5	3779	7/7	0.32	-	167,167,167,167	7
88	MG	BI	305	1/1	0.28	-	84,84,84,84	0
88	MG	A6	2152	1/1	0.44	-	64,64,64,64	0
88	MG	BB	405	1/1	0.50	-	51,51,51,51	0
88	MG	A2	2239	1/1	0.24	-	92,92,92,92	0
87	OHX	A6	2082	7/7	0.21	-	180,180,180,180	7
87	OHX	A4	215	7/7	0.18	-	175,175,175,175	7
87	OHX	A1	3470	7/7	0.15	-	96,96,96,96	7
88	MG	A1	4368	1/1	0.73	-	80,80,80,80	0
88	MG	A5	4159	1/1	0.23	-	64,64,64,64	0
87	OHX	A2	2077	7/7	0.27	-	206,206,206,206	7
87	OHX	A6	1975	7/7	0.15	-	106,106,106,106	7
88	MG	A5	4367	1/1	0.53	-	74,74,74,74	0
88	MG	A1	4274	1/1	0.35	-	87,87,87,87	0
87	OHX	A1	3697	7/7	0.20	-	182,182,182,182	7
88	MG	A5	4142	1/1	0.19	-	91,91,91,91	0
88	MG	A5	3847	1/1	0.30	-	61,61,61,61	0
87	OHX	Ag	401	7/7	0.12	-	167,167,167,167	7
88	MG	A1	4061	1/1	0.27	-	35,35,35,35	0
88	MG	A6	2226	1/1	0.15	-	68,68,68,68	0
87	OHX	A6	2010	7/7	0.12	-	181,181,181,181	7
88	MG	A5	3948	1/1	0.29	-	28,28,28,28	0
87	OHX	A6	2060	7/7	0.23	-	165,165,165,165	7
88	MG	A6	2108	1/1	0.27	-	52,52,52,52	0
87	OHX	A1	3503	7/7	0.15	-	111,111,111,111	7
88	MG	A8	225	1/1	0.29	-	58,58,58,58	0
87	OHX	A6	2093	7/7	0.20	-	149,149,149,149	7
88	MG	A5	4214	1/1	0.26	-	66,66,66,66	0
88	MG	A2	2235	1/1	0.19	-	80,80,80,80	0
87	OHX	A4	207	7/7	0.14	-	129,129,129,129	7
87	OHX	A5	3624	7/7	0.23	-	82,82,82,82	7
88	MG	A5	3934	1/1	0.21	-	61,61,61,61	0
87	OHX	A6	1902	7/7	0.23	-	90,90,90,90	0
87	OHX	A6	1983	7/7	0.13	-	133,133,133,133	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A5	4102	1/1	0.42	-	71,71,71,71	0
88	MG	BO	203	1/1	0.52	-	74,74,74,74	0
88	MG	A1	4488	1/1	0.21	-	73,73,73,73	0
88	MG	A1	4354	1/1	0.19	-	61,61,61,61	0
88	MG	CF	301	1/1	0.33	-	87,87,87,87	0
87	OHX	A6	2005	7/7	0.15	-	145,145,145,145	7
88	MG	A6	2112	1/1	0.31	-	64,64,64,64	0
88	MG	A1	3974	1/1	0.22	-	35,35,35,35	0
87	OHX	A6	2013	7/7	0.19	-	180,180,180,180	7
87	OHX	A6	2038	7/7	0.15	-	169,169,169,169	7
88	MG	CP	203	1/1	0.85	-	63,63,63,63	0
87	OHX	BI	303	7/7	0.43	-	215,215,215,215	7
88	MG	A5	4578	1/1	0.20	-	74,74,74,74	0
87	OHX	A5	3438	7/7	0.20	-	91,91,91,91	0
88	MG	A1	4290	1/1	0.20	-	69,69,69,69	0
88	MG	DP	206	1/1	0.66	-	55,55,55,55	0
88	MG	A5	3878	1/1	0.24	-	56,56,56,56	0
88	MG	A1	4015	1/1	0.39	-	63,63,63,63	0
88	MG	A6	2219	1/1	0.16	-	50,50,50,50	0
88	MG	A5	4361	1/1	0.23	-	92,92,92,92	0
87	OHX	A1	3476	7/7	0.20	-	129,129,129,129	0
87	OHX	A5	3786	7/7	0.31	-	238,238,238,238	7
88	MG	A4	217	1/1	0.33	-	69,69,69,69	0
88	MG	A2	2174	1/1	0.16	-	53,53,53,53	0
88	MG	A5	4042	1/1	0.28	-	75,75,75,75	0
87	OHX	DH	201	7/7	0.12	-	142,142,142,142	7
87	OHX	A1	3485	7/7	0.15	-	113,113,113,113	7
88	MG	A1	4160	1/1	0.19	-	70,70,70,70	0
88	MG	A5	4001	1/1	0.41	-	48,48,48,48	0
88	MG	A5	4004	1/1	0.33	-	55,55,55,55	0
87	OHX	A5	3708	7/7	0.15	-	141,141,141,141	7
88	MG	A1	4187	1/1	0.62	-	90,90,90,90	0
88	MG	A2	2237	1/1	0.15	-	90,90,90,90	0
87	OHX	A5	3817	7/7	0.17	-	205,205,205,205	7
87	OHX	A2	2011	7/7	0.13	-	154,154,154,154	7
87	OHX	A2	1965	7/7	0.18	-	138,138,138,138	7
87	OHX	A1	3784	7/7	0.16	-	169,169,169,169	7
88	MG	A5	4341	1/1	0.34	-	96,96,96,96	0
88	MG	A5	4060	1/1	0.33	-	57,57,57,57	0
87	OHX	A1	3816	7/7	0.10	-	150,150,150,150	7
88	MG	A5	4239	1/1	0.21	-	44,44,44,44	0
88	MG	A1	4432	1/1	0.59	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A2	1928	7/7	0.14	-	126,126,126,126	7
88	MG	DD	302	1/1	0.18	-	66,66,66,66	0
88	MG	A4	223	1/1	0.40	-	44,44,44,44	0
87	OHX	A5	3531	7/7	0.17	-	106,106,106,106	7
88	MG	BP	209	1/1	0.19	-	59,59,59,59	0
87	OHX	A2	2034	7/7	0.13	-	173,173,173,173	7
88	MG	A1	4418	1/1	0.39	-	48,48,48,48	0
88	MG	BV	203	1/1	0.31	-	63,63,63,63	0
88	MG	A1	3948	1/1	0.40	-	55,55,55,55	0
88	MG	A5	4073	1/1	0.30	-	66,66,66,66	0
88	MG	A5	4173	1/1	0.23	-	67,67,67,67	0
87	OHX	A5	3739	7/7	0.19	-	105,105,105,105	7
87	OHX	A2	2019	7/7	0.14	-	174,174,174,174	7
88	MG	A1	4277	1/1	0.60	-	89,89,89,89	0
88	MG	A5	3826	1/1	0.45	-	63,63,63,63	0
87	OHX	A1	3634	7/7	0.14	-	133,133,133,133	7
88	MG	A3	217	1/1	0.38	-	56,56,56,56	0
87	OHX	A1	3728	7/7	0.15	-	203,203,203,203	7
88	MG	A2	2128	1/1	0.40	-	62,62,62,62	0
88	MG	A8	238	1/1	0.30	-	93,93,93,93	0
88	MG	A1	4431	1/1	0.28	-	59,59,59,59	0
88	MG	A5	4104	1/1	0.23	-	52,52,52,52	0
87	OHX	A5	3452	7/7	0.18	-	86,86,86,86	7
88	MG	A1	4295	1/1	0.18	-	62,62,62,62	0
87	OHX	A2	1958	7/7	0.13	-	139,139,139,139	7
88	MG	A1	4357	1/1	0.19	-	89,89,89,89	0
88	MG	A5	4334	1/1	0.11	-	109,109,109,109	0
88	MG	A1	4210	1/1	0.39	-	44,44,44,44	0
87	OHX	A5	3803	7/7	0.20	-	107,107,107,107	7
87	OHX	A1	3603	7/7	0.14	-	136,136,136,136	7
88	MG	A2	2189	1/1	0.23	-	55,55,55,55	0
87	OHX	A1	3436	7/7	0.15	-	69,69,69,69	7
88	MG	A5	3861	1/1	0.20	-	65,65,65,65	0
87	OHX	A6	1938	7/7	0.17	-	96,96,96,96	7
88	MG	A5	4098	1/1	0.13	-	55,55,55,55	0
88	MG	A1	4225	1/1	0.17	-	67,67,67,67	0
88	MG	A5	3918	1/1	0.26	-	79,79,79,79	0
87	OHX	A7	211	7/7	0.19	-	117,117,117,117	7
88	MG	A5	4181	1/1	0.27	-	80,80,80,80	0
87	OHX	A6	1988	7/7	0.20	-	138,138,138,138	7
88	MG	A2	2248	1/1	0.14	-	69,69,69,69	0
88	MG	A1	3926	1/1	0.29	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A1	3505	7/7	0.15	-	124,124,124,124	7
88	MG	A1	3880	1/1	0.31	-	42,42,42,42	0
88	MG	A1	4259	1/1	0.21	-	102,102,102,102	0
88	MG	A2	2107	1/1	0.43	-	66,66,66,66	0
88	MG	A5	4555	1/1	0.47	-	63,63,63,63	0
88	MG	A5	4380	1/1	0.56	-	89,89,89,89	0
88	MG	A5	4553	1/1	1.00	-	73,73,73,73	0
87	OHX	A5	3722	7/7	0.13	-	164,164,164,164	7
88	MG	A5	4278	1/1	0.57	-	82,82,82,82	0
88	MG	Ch	302	1/1	0.17	-	53,53,53,53	0
88	MG	A6	2317	1/1	0.72	-	82,82,82,82	0
88	MG	A2	2159	1/1	0.28	-	88,88,88,88	0
88	MG	A1	4140	1/1	0.28	-	56,56,56,56	0
88	MG	A2	2205	1/1	0.13	-	83,83,83,83	0
87	OHX	A6	2011	7/7	0.16	-	120,120,120,120	7
88	MG	A6	2287	1/1	0.95	-	96,96,96,96	0
89	ZN	Cf	501	1/1	0.14	-	152,152,152,152	0
87	OHX	A5	3488	7/7	0.17	-	125,125,125,125	0
87	OHX	A2	2012	7/7	0.14	-	180,180,180,180	7
88	MG	A1	4142	1/1	0.27	-	68,68,68,68	0
88	MG	A1	4124	1/1	0.20	-	53,53,53,53	0
87	OHX	A5	3650	7/7	0.17	-	133,133,133,133	7
87	OHX	A6	2046	7/7	0.19	-	204,204,204,204	7
87	OHX	A6	2032	7/7	0.14	-	143,143,143,143	7
88	MG	A5	4299	1/1	0.23	-	80,80,80,80	0
88	MG	A1	4426	1/1	0.62	-	82,82,82,82	0
88	MG	A1	4110	1/1	0.16	-	71,71,71,71	0
88	MG	A5	4357	1/1	0.49	-	75,75,75,75	0
88	MG	A1	4075	1/1	0.21	-	62,62,62,62	0
88	MG	A1	4147	1/1	0.27	-	73,73,73,73	0
88	MG	A2	2140	1/1	0.35	-	69,69,69,69	0
87	OHX	A5	3699	7/7	0.22	-	107,107,107,107	7
88	MG	A5	4275	1/1	0.33	-	63,63,63,63	0
88	MG	A1	4098	1/1	0.19	-	54,54,54,54	0
88	MG	A5	3971	1/1	0.34	-	53,53,53,53	0
87	OHX	A6	1913	7/7	0.15	-	91,91,91,91	0
87	OHX	A1	3402	7/7	0.17	-	130,130,130,130	7
88	MG	DO	205	1/1	0.48	-	52,52,52,52	0
88	MG	A6	2227	1/1	0.23	-	67,67,67,67	0
88	MG	A2	2144	1/1	0.29	-	57,57,57,57	0
87	OHX	A6	1953	7/7	0.10	-	136,136,136,136	7
88	MG	A1	4367	1/1	0.12	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	4133	1/1	0.23	-	91,91,91,91	0
88	MG	A1	4270	1/1	0.33	-	57,57,57,57	0
87	OHX	A3	209	7/7	0.16	-	180,180,180,180	7
88	MG	A1	4345	1/1	0.14	-	73,73,73,73	0
88	MG	A5	3991	1/1	0.31	-	46,46,46,46	0
88	MG	A5	4002	1/1	0.33	-	40,40,40,40	0
88	MG	A1	4321	1/1	0.15	-	88,88,88,88	0
87	OHX	A5	3800	7/7	0.21	-	203,203,203,203	7
88	MG	A6	2225	1/1	0.21	-	59,59,59,59	0
88	MG	A1	4099	1/1	0.22	-	71,71,71,71	0
88	MG	A2	2238	1/1	0.32	-	92,92,92,92	0
87	OHX	A1	3658	7/7	0.17	-	118,118,118,118	7
88	MG	A5	3841	1/1	0.35	-	44,44,44,44	0
88	MG	A5	4007	1/1	0.37	-	47,47,47,47	0
88	MG	A5	4477	1/1	0.28	-	66,66,66,66	0
88	MG	A2	2226	1/1	0.27	-	87,87,87,87	0
87	OHX	A6	1924	7/7	0.15	-	83,83,83,83	7
88	MG	A1	4389	1/1	0.43	-	46,46,46,46	0
88	MG	A6	2329	1/1	0.93	-	138,138,138,138	0
87	OHX	A5	3740	7/7	0.17	-	155,155,155,155	7
88	MG	A5	3880	1/1	0.28	-	45,45,45,45	0
88	MG	A1	4462	1/1	0.33	-	71,71,71,71	0
87	OHX	A5	3733	7/7	0.19	-	162,162,162,162	7
88	MG	A6	2304	1/1	0.11	-	81,81,81,81	0
88	MG	A5	4492	1/1	0.36	-	73,73,73,73	0
88	MG	A7	225	1/1	0.37	-	45,45,45,45	0
87	OHX	A1	3477	7/7	0.18	-	83,83,83,83	7
88	MG	A3	225	1/1	0.36	-	61,61,61,61	0
87	OHX	A1	3513	7/7	0.15	-	101,101,101,101	7
88	MG	Be	202	1/1	0.48	-	67,67,67,67	0
88	MG	A1	4190	1/1	0.26	-	98,98,98,98	0
88	MG	A1	4407	1/1	0.44	-	113,113,113,113	0
87	OHX	A5	3808	7/7	0.31	-	182,182,182,182	7
88	MG	A1	4121	1/1	0.11	-	74,74,74,74	0
87	OHX	A5	3458	7/7	0.16	-	91,91,91,91	0
88	MG	DC	404	1/1	0.27	-	70,70,70,70	0
87	OHX	A1	3507	7/7	0.16	-	75,75,75,75	7
87	OHX	A1	3454	7/7	0.17	-	106,106,106,106	7
88	MG	Ch	301	1/1	0.15	-	44,44,44,44	0
87	OHX	A6	1937	7/7	0.16	-	96,96,96,96	7
88	MG	A5	4289	1/1	0.29	-	112,112,112,112	0
88	MG	A2	2236	1/1	0.08	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A1	3706	7/7	0.14	-	135,135,135,135	7
88	MG	A1	3912	1/1	0.46	-	84,84,84,84	0
87	OHX	A1	3797	7/7	0.16	-	171,171,171,171	7
87	OHX	A1	3488	7/7	0.17	-	109,109,109,109	7
88	MG	B0	203	1/1	0.30	-	79,79,79,79	0
87	OHX	A5	3611	7/7	0.23	-	115,115,115,115	7
87	OHX	A1	3591	7/7	0.15	-	95,95,95,95	7
88	MG	A5	4579	1/1	0.59	-	57,57,57,57	0
88	MG	A1	4296	1/1	0.32	-	94,94,94,94	0
87	OHX	A5	3460	7/7	0.16	-	80,80,80,80	7
88	MG	A2	2166	1/1	0.32	-	90,90,90,90	0
88	MG	BD	302	1/1	0.19	-	79,79,79,79	0
87	OHX	A6	2017	7/7	0.19	-	132,132,132,132	7
88	MG	A5	3972	1/1	0.29	-	55,55,55,55	0
87	OHX	A6	2019	7/7	0.15	-	127,127,127,127	7
88	MG	Bj	110	1/1	0.54	-	94,94,94,94	0
88	MG	A1	4409	1/1	0.73	-	58,58,58,58	0
87	OHX	A8	212	7/7	0.15	-	172,172,172,172	7
87	OHX	A5	3468	7/7	0.16	-	75,75,75,75	7
87	OHX	A1	3469	7/7	0.16	-	122,122,122,122	0
87	OHX	A1	3514	7/7	0.18	-	99,99,99,99	7
88	MG	A6	2204	1/1	0.16	-	70,70,70,70	0
88	MG	A1	4012	1/1	0.33	-	41,41,41,41	0
88	MG	A4	244	1/1	0.20	-	61,61,61,61	0
88	MG	A6	2199	1/1	0.21	-	62,62,62,62	0
87	OHX	A1	3769	7/7	0.14	-	142,142,142,142	7
88	MG	A5	4468	1/1	0.62	-	73,73,73,73	0
88	MG	A5	4318	1/1	0.16	-	83,83,83,83	0
88	MG	A1	4040	1/1	0.10	-	40,40,40,40	0
87	OHX	A1	3493	7/7	0.15	-	148,148,148,148	0
87	OHX	A1	3650	7/7	0.24	-	120,120,120,120	7
88	MG	BO	202	1/1	0.20	-	77,77,77,77	0
88	MG	A6	2262	1/1	0.42	-	101,101,101,101	0
87	OHX	A1	3773	7/7	0.27	-	159,159,159,159	7
87	OHX	A2	1959	7/7	0.13	-	147,147,147,147	7
88	MG	A5	4428	1/1	0.11	-	75,75,75,75	0
87	OHX	A8	218	7/7	0.38	-	221,221,221,221	7
88	MG	BN	305	1/1	0.98	-	56,56,56,56	0
88	MG	DC	403	1/1	0.35	-	65,65,65,65	0
87	OHX	A1	3722	7/7	0.21	-	150,150,150,150	7
88	MG	A1	3847	1/1	0.13	-	74,74,74,74	0
88	MG	A4	240	1/1	0.24	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A1	3575	7/7	0.13	-	120,120,120,120	7
88	MG	A1	4179	1/1	0.33	-	69,69,69,69	0
88	MG	A2	2118	1/1	0.32	-	47,47,47,47	0
87	OHX	A5	3470	7/7	0.13	-	118,118,118,118	0
87	OHX	A2	1966	7/7	0.19	-	101,101,101,101	7
88	MG	A6	2180	1/1	0.27	-	87,87,87,87	0
88	MG	AI	303	1/1	0.53	-	73,73,73,73	0
88	MG	A5	3832	1/1	0.14	-	35,35,35,35	0
87	OHX	A5	3482	7/7	0.19	-	85,85,85,85	7
88	MG	A6	2334	1/1	0.27	-	72,72,72,72	0
87	OHX	A6	1925	7/7	0.13	-	112,112,112,112	7
88	MG	A1	4209	1/1	0.13	-	76,76,76,76	0
88	MG	A6	2273	1/1	0.23	-	90,90,90,90	0
88	MG	A1	3908	1/1	0.16	-	64,64,64,64	0
88	MG	A1	4054	1/1	0.33	-	65,65,65,65	0
87	OHX	A5	3723	7/7	0.16	-	180,180,180,180	7
87	OHX	A1	3524	7/7	0.18	-	139,139,139,139	7
88	MG	A2	2185	1/1	0.12	-	72,72,72,72	0
88	MG	A6	2215	1/1	0.14	-	56,56,56,56	0
87	OHX	A5	3682	7/7	0.14	-	110,110,110,110	7
87	OHX	A2	1952	7/7	0.13	-	127,127,127,127	7
88	MG	A5	4139	1/1	0.18	-	99,99,99,99	0
87	OHX	Cg	401	7/7	0.12	-	182,182,182,182	7
87	OHX	A1	3628	7/7	0.15	-	154,154,154,154	7
87	OHX	A5	3540	7/7	0.17	-	119,119,119,119	7
87	OHX	A1	3536	7/7	0.14	-	136,136,136,136	7
88	MG	A5	3892	1/1	0.21	-	45,45,45,45	0
88	MG	A5	4120	1/1	0.30	-	49,49,49,49	0
87	OHX	A6	1957	7/7	0.14	-	144,144,144,144	7
88	MG	A2	2151	1/1	0.07	-	49,49,49,49	0
88	MG	A1	4500	1/1	0.24	-	106,106,106,106	0
88	MG	A2	2100	1/1	0.24	-	67,67,67,67	0
88	MG	A1	3824	1/1	0.24	-	65,65,65,65	0
87	OHX	A1	3794	7/7	0.25	-	150,150,150,150	7
88	MG	A6	2332	1/1	0.31	-	80,80,80,80	0
88	MG	A6	2322	1/1	0.30	-	77,77,77,77	0
88	MG	BN	307	1/1	0.59	-	58,58,58,58	0
87	OHX	A5	3685	7/7	0.23	-	141,141,141,141	7
88	MG	DB	410	1/1	0.45	-	54,54,54,54	0
88	MG	A5	4067	1/1	0.25	-	61,61,61,61	0
87	OHX	A1	3655	7/7	0.20	-	150,150,150,150	7
87	OHX	A5	3749	7/7	0.11	-	178,178,178,178	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	4481	1/1	0.24	-	97,97,97,97	0
88	MG	A1	4026	1/1	0.37	-	42,42,42,42	0
87	OHX	A2	1973	7/7	0.18	-	136,136,136,136	7
88	MG	A5	4249	1/1	0.40	-	40,40,40,40	0
88	MG	A1	4094	1/1	0.21	-	34,34,34,34	0
87	OHX	A1	3620	7/7	0.15	-	139,139,139,139	7
88	MG	A5	4565	1/1	0.15	-	87,87,87,87	0
88	MG	A3	230	1/1	0.45	-	85,85,85,85	0
88	MG	Dm	201	1/1	0.23	-	75,75,75,75	0
88	MG	A1	4174	1/1	0.18	-	57,57,57,57	0
88	MG	A5	4169	1/1	0.17	-	90,90,90,90	0
88	MG	A5	4152	1/1	0.18	-	79,79,79,79	0
87	OHX	A2	1971	7/7	0.12	-	110,110,110,110	7
87	OHX	A6	2087	7/7	0.21	-	205,205,205,205	7
88	MG	A2	2204	1/1	0.94	-	109,109,109,109	0
88	MG	A1	4271	1/1	0.20	-	58,58,58,58	0
88	MG	A5	4302	1/1	0.20	-	72,72,72,72	0
88	MG	A2	2168	1/1	0.20	-	78,78,78,78	0
88	MG	Ad	102	1/1	0.11	-	89,89,89,89	0
88	MG	A5	4022	1/1	0.41	-	52,52,52,52	0
88	MG	A1	4365	1/1	0.21	-	66,66,66,66	0
87	OHX	A6	1916	7/7	0.18	-	87,87,87,87	7
87	OHX	A2	2085	7/7	0.35	-	200,200,200,200	7
88	MG	A5	4526	1/1	0.21	-	83,83,83,83	0
87	OHX	A5	3537	7/7	0.12	-	115,115,115,115	7
88	MG	A5	4435	1/1	0.17	-	87,87,87,87	0
88	MG	A5	3909	1/1	0.38	-	70,70,70,70	0
87	OHX	A6	1907	7/7	0.19	-	91,91,91,91	0
88	MG	A5	4011	1/1	0.29	-	54,54,54,54	0
88	MG	A1	4041	1/1	0.17	-	70,70,70,70	0
88	MG	A5	3865	1/1	0.28	-	37,37,37,37	0
87	OHX	A1	3522	7/7	0.19	-	79,79,79,79	7
88	MG	A6	2258	1/1	0.20	-	71,71,71,71	0
88	MG	A5	4407	1/1	0.12	-	95,95,95,95	0
87	OHX	A5	3622	7/7	0.17	-	136,136,136,136	7
88	MG	A6	2266	1/1	0.45	-	106,106,106,106	0
88	MG	A1	4362	1/1	0.25	-	85,85,85,85	0
87	OHX	A6	1941	7/7	0.16	-	112,112,112,112	7
88	MG	A1	4422	1/1	0.21	-	68,68,68,68	0
87	OHX	A1	3804	7/7	0.29	-	152,152,152,152	7
87	OHX	A6	1978	7/7	0.16	-	146,146,146,146	7
88	MG	DB	411	1/1	1.00	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A1	3520	7/7	0.16	-	129,129,129,129	7
88	MG	A1	4402	1/1	0.16	-	65,65,65,65	0
87	OHX	A1	3602	7/7	0.18	-	99,99,99,99	7
88	MG	Bo	204	1/1	0.14	-	76,76,76,76	0
87	OHX	A1	3433	7/7	0.17	-	85,85,85,85	0
87	OHX	A5	3551	7/7	0.15	-	142,142,142,142	7
88	MG	A1	4470	1/1	0.17	-	97,97,97,97	0
88	MG	A6	2177	1/1	0.21	-	79,79,79,79	0
88	MG	A1	4441	1/1	0.59	-	61,61,61,61	0
88	MG	A5	4382	1/1	0.40	-	99,99,99,99	0
88	MG	A5	4141	1/1	0.09	-	66,66,66,66	0
88	MG	A5	4050	1/1	0.20	-	39,39,39,39	0
87	OHX	A5	3816	7/7	0.24	-	195,195,195,195	7
88	MG	DB	408	1/1	0.21	-	67,67,67,67	0
87	OHX	A5	3568	7/7	0.17	-	103,103,103,103	7
87	OHX	A5	3424	7/7	0.23	-	86,86,86,86	0
87	OHX	A1	3555	7/7	0.15	-	125,125,125,125	7
87	OHX	A1	3737	7/7	0.15	-	183,183,183,183	7
88	MG	A1	3842	1/1	0.41	-	77,77,77,77	0
88	MG	A5	4493	1/1	0.22	-	76,76,76,76	0
88	MG	A5	4177	1/1	0.32	-	65,65,65,65	0
88	MG	CQ	201	1/1	0.14	-	75,75,75,75	0
87	OHX	A5	3791	7/7	0.16	-	175,175,175,175	7
88	MG	A5	4502	1/1	0.23	-	84,84,84,84	0
88	MG	A5	4150	1/1	0.47	-	68,68,68,68	0
88	MG	A1	3964	1/1	0.40	-	50,50,50,50	0
88	MG	A5	4505	1/1	1.44	-	71,71,71,71	0
88	MG	A1	3836	1/1	0.32	-	48,48,48,48	0
87	OHX	A1	3801	7/7	0.27	-	125,125,125,125	7
87	OHX	A1	3590	7/7	0.12	-	135,135,135,135	7
88	MG	A5	4489	1/1	0.23	-	82,82,82,82	0
88	MG	A5	3953	1/1	0.44	-	69,69,69,69	0
87	OHX	A1	3566	7/7	0.17	-	122,122,122,122	7
87	OHX	A2	1933	7/7	0.15	-	109,109,109,109	7
88	MG	A1	4196	1/1	0.21	-	71,71,71,71	0
88	MG	A5	4542	1/1	0.85	-	59,59,59,59	0
88	MG	AN	202	1/1	0.15	-	63,63,63,63	0
88	MG	A6	2212	1/1	0.12	-	91,91,91,91	0
87	OHX	A1	3599	7/7	0.23	-	196,196,196,196	7
88	MG	A6	2286	1/1	0.27	-	75,75,75,75	0
87	OHX	A5	3514	7/7	0.19	-	90,90,90,90	7
88	MG	A5	4496	1/1	0.21	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	4252	1/1	0.35	-	121,121,121,121	0
87	OHX	A5	3674	7/7	0.20	-	100,100,100,100	7
88	MG	DS	203	1/1	0.33	-	65,65,65,65	0
88	MG	A5	4231	1/1	0.20	-	105,105,105,105	0
88	MG	A6	2184	1/1	0.13	-	67,67,67,67	0
88	MG	A5	4194	1/1	0.29	-	88,88,88,88	0
88	MG	A6	2314	1/1	1.61	-	112,112,112,112	0
88	MG	A1	3406	1/1	0.19	-	67,67,67,67	0
87	OHX	A1	3665	7/7	0.22	-	104,104,104,104	7
88	MG	A5	4234	1/1	0.12	-	67,67,67,67	0
88	MG	A4	237	1/1	0.23	-	94,94,94,94	0
88	MG	A5	4557	1/1	0.27	-	69,69,69,69	0
87	OHX	A5	3510	7/7	0.18	-	90,90,90,90	7
88	MG	A1	4113	1/1	0.36	-	70,70,70,70	0
88	MG	A1	4043	1/1	0.30	-	62,62,62,62	0
87	OHX	A1	3558	7/7	0.15	-	139,139,139,139	7
88	MG	A1	3868	1/1	0.23	-	55,55,55,55	0
88	MG	A6	2263	1/1	0.22	-	89,89,89,89	0
87	OHX	DM	201	7/7	0.23	-	208,208,208,208	7
87	OHX	BI	302	7/7	0.26	-	177,177,177,177	7
88	MG	A1	3823	1/1	0.28	-	60,60,60,60	0
88	MG	A6	2201	1/1	0.24	-	72,72,72,72	0
88	MG	A2	2120	1/1	0.34	-	73,73,73,73	0
88	MG	A2	2143	1/1	0.25	-	82,82,82,82	0
88	MG	A1	4326	1/1	0.98	-	80,80,80,80	0
88	MG	A2	2156	1/1	0.28	-	70,70,70,70	0
87	OHX	A2	1972	7/7	0.13	-	138,138,138,138	7
88	MG	A5	3977	1/1	0.33	-	69,69,69,69	0
88	MG	A1	4176	1/1	0.07	-	84,84,84,84	0
87	OHX	A5	3662	7/7	0.20	-	148,148,148,148	7
88	MG	A5	4360	1/1	0.22	-	85,85,85,85	0
87	OHX	A1	3589	7/7	0.19	-	97,97,97,97	7
87	OHX	A4	214	7/7	0.14	-	167,167,167,167	7
88	MG	DP	204	1/1	0.22	-	78,78,78,78	0
88	MG	A1	4427	1/1	0.23	-	77,77,77,77	0
88	MG	A5	3830	1/1	0.24	-	39,39,39,39	0
87	OHX	A1	3592	7/7	0.15	-	108,108,108,108	7
88	MG	A5	4564	1/1	0.22	-	79,79,79,79	0
88	MG	A4	224	1/1	0.18	-	30,30,30,30	0
88	MG	A4	220	1/1	0.40	-	70,70,70,70	0
87	OHX	A5	3680	7/7	0.24	-	134,134,134,134	7
89	ZN	Dj	105	1/1	0.14	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	DO	208	1/1	0.41	-	77,77,77,77	0
87	OHX	A1	3639	7/7	0.18	-	145,145,145,145	7
88	MG	A1	3839	1/1	0.29	-	64,64,64,64	0
88	MG	A1	3870	1/1	0.38	-	57,57,57,57	0
87	OHX	A5	3657	7/7	0.23	-	83,83,83,83	7
88	MG	A5	4538	1/1	0.30	-	67,67,67,67	0
87	OHX	A1	3699	7/7	0.18	-	107,107,107,107	7
88	MG	A1	4436	1/1	0.10	-	115,115,115,115	0
88	MG	A5	4076	1/1	0.28	-	64,64,64,64	0
88	MG	A1	4335	1/1	0.38	-	86,86,86,86	0
87	OHX	A1	3518	7/7	0.15	-	140,140,140,140	7
88	MG	A1	4089	1/1	0.15	-	89,89,89,89	0
87	OHX	A1	3711	7/7	0.16	-	155,155,155,155	7
88	MG	A5	4083	1/1	0.22	-	70,70,70,70	0
88	MG	A1	3917	1/1	0.19	-	31,31,31,31	0
87	OHX	A6	2041	7/7	0.22	-	145,145,145,145	7
87	OHX	A1	3407	7/7	0.22	-	138,138,138,138	7
87	OHX	A5	3490	7/7	0.14	-	113,113,113,113	7
87	OHX	A2	1944	7/7	0.15	-	109,109,109,109	7
88	MG	A5	4509	1/1	0.62	-	134,134,134,134	0
88	MG	A1	4292	1/1	0.20	-	67,67,67,67	0
88	MG	A1	3822	1/1	0.22	-	50,50,50,50	0
87	OHX	A8	211	7/7	0.22	-	135,135,135,135	7
88	MG	A1	4200	1/1	0.18	-	71,71,71,71	0
88	MG	A5	4052	1/1	0.21	-	46,46,46,46	0
88	MG	A2	2211	1/1	0.59	-	94,94,94,94	0
87	OHX	A2	2029	7/7	0.30	-	150,150,150,150	7
87	OHX	A1	3549	7/7	0.23	-	139,139,139,139	7
88	MG	AE	301	1/1	0.62	-	88,88,88,88	0
88	MG	A5	3927	1/1	0.22	-	49,49,49,49	0
87	OHX	A6	2080	7/7	0.25	-	167,167,167,167	7
88	MG	A1	3845	1/1	0.17	-	70,70,70,70	0
88	MG	A1	4129	1/1	0.19	-	75,75,75,75	0
88	MG	A2	2242	1/1	0.17	-	105,105,105,105	0
88	MG	A6	2216	1/1	0.13	-	64,64,64,64	0
87	OHX	A5	3768	7/7	0.63	-	198,198,198,198	7
87	OHX	A5	3767	7/7	0.15	-	185,185,185,185	7
87	OHX	A5	3600	7/7	0.11	-	133,133,133,133	7
87	OHX	A5	3735	7/7	0.22	-	149,149,149,149	7
88	MG	A1	3850	1/1	0.37	-	64,64,64,64	0
87	OHX	A6	2091	7/7	0.21	-	165,165,165,165	7
88	MG	A5	3987	1/1	0.40	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	4286	1/1	0.56	-	57,57,57,57	0
88	MG	A1	4458	1/1	0.78	-	92,92,92,92	0
88	MG	A1	3901	1/1	0.28	-	74,74,74,74	0
88	MG	A8	229	1/1	0.17	-	95,95,95,95	0
88	MG	A5	4562	1/1	0.24	-	69,69,69,69	0
87	OHX	A1	3521	7/7	0.19	-	84,84,84,84	7
87	OHX	A1	3595	7/7	0.17	-	120,120,120,120	7
87	OHX	A5	3420	7/7	0.21	-	74,74,74,74	0
88	MG	A1	4468	1/1	0.96	-	79,79,79,79	0
88	MG	A5	4506	1/1	0.24	-	80,80,80,80	0
88	MG	A1	4251	1/1	0.21	-	71,71,71,71	0
87	OHX	A5	3678	7/7	0.20	-	111,111,111,111	7
88	MG	A6	2291	1/1	0.60	-	100,100,100,100	0
87	OHX	A6	2054	7/7	0.30	-	169,169,169,169	7
88	MG	A5	4187	1/1	0.29	-	78,78,78,78	0
88	MG	A5	4392	1/1	0.19	-	64,64,64,64	0
88	MG	A5	4235	1/1	0.24	-	75,75,75,75	0
88	MG	A4	227	1/1	0.09	-	53,53,53,53	0
88	MG	BV	201	1/1	0.27	-	95,95,95,95	0
87	OHX	A6	1932	7/7	0.15	-	109,109,109,109	7
88	MG	A6	2268	1/1	0.29	-	68,68,68,68	0
88	MG	A1	4155	1/1	0.56	-	88,88,88,88	0
88	MG	A5	3931	1/1	0.30	-	35,35,35,35	0
88	MG	A1	4495	1/1	0.35	-	109,109,109,109	0
88	MG	A5	3853	1/1	0.24	-	67,67,67,67	0
87	OHX	A1	3471	7/7	0.16	-	107,107,107,107	7
88	MG	A1	4086	1/1	0.42	-	58,58,58,58	0
88	MG	A5	4003	1/1	0.33	-	46,46,46,46	0
88	MG	A1	3972	1/1	0.42	-	45,45,45,45	0
88	MG	A5	4570	1/1	0.55	-	76,76,76,76	0
87	OHX	A6	1998	7/7	0.13	-	147,147,147,147	7
88	MG	A6	2117	1/1	0.30	-	64,64,64,64	0
87	OHX	A6	2036	7/7	0.18	-	122,122,122,122	7
88	MG	A5	4043	1/1	0.28	-	35,35,35,35	0
87	OHX	A5	3493	7/7	0.18	-	102,102,102,102	7
88	MG	A5	4124	1/1	0.17	-	78,78,78,78	0
88	MG	A1	4273	1/1	0.38	-	85,85,85,85	0
87	OHX	A5	3660	7/7	0.19	-	108,108,108,108	7
88	MG	A5	4347	1/1	0.21	-	78,78,78,78	0
88	MG	A8	233	1/1	0.27	-	78,78,78,78	0
88	MG	A1	3864	1/1	0.17	-	46,46,46,46	0
88	MG	A1	4444	1/1	0.96	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	4437	1/1	0.15	-	60,60,60,60	0
88	MG	A5	4432	1/1	0.28	-	95,95,95,95	0
88	MG	A1	4212	1/1	0.21	-	67,67,67,67	0
88	MG	A5	3919	1/1	0.23	-	66,66,66,66	0
88	MG	A1	4005	1/1	0.33	-	42,42,42,42	0
87	OHX	A5	3478	7/7	0.18	-	76,76,76,76	7
87	OHX	A1	3733	7/7	0.26	-	125,125,125,125	7
88	MG	A1	4021	1/1	0.33	-	54,54,54,54	0
87	OHX	A1	3715	7/7	0.15	-	120,120,120,120	7
87	OHX	A2	2086	7/7	0.45	-	156,156,156,156	7
88	MG	A5	4236	1/1	0.12	-	19,19,19,19	0
87	OHX	A5	3569	7/7	0.15	-	110,110,110,110	7
87	OHX	A2	2031	7/7	0.12	-	140,140,140,140	7
88	MG	Bj	104	1/1	0.16	-	86,86,86,86	0
88	MG	A1	4452	1/1	1.36	-	112,112,112,112	0
88	MG	A2	2214	1/1	0.22	-	75,75,75,75	0
88	MG	A6	2183	1/1	0.26	-	64,64,64,64	0
88	MG	A3	229	1/1	0.28	-	99,99,99,99	0
88	MG	A5	4205	1/1	0.33	-	79,79,79,79	0
88	MG	A5	4328	1/1	0.52	-	72,72,72,72	0
87	OHX	DB	401	7/7	0.17	-	98,98,98,98	7
88	MG	A1	4383	1/1	0.11	-	62,62,62,62	0
88	MG	A1	4002	1/1	0.34	-	37,37,37,37	0
87	OHX	A6	1987	7/7	0.15	-	113,113,113,113	7
88	MG	A5	3851	1/1	0.30	-	45,45,45,45	0
88	MG	A5	3982	1/1	0.21	-	52,52,52,52	0
87	OHX	A2	1905	7/7	0.17	-	88,88,88,88	0
88	MG	A6	2325	1/1	0.53	-	106,106,106,106	0
88	MG	A7	224	1/1	0.15	-	69,69,69,69	0
88	MG	A5	4260	1/1	0.44	-	80,80,80,80	0
88	MG	A5	4433	1/1	0.12	-	83,83,83,83	0
88	MG	A5	4481	1/1	0.58	-	60,60,60,60	0
88	MG	A6	2269	1/1	0.39	-	60,60,60,60	0
87	OHX	A7	203	7/7	0.18	-	105,105,105,105	7
88	MG	A5	4470	1/1	0.12	-	76,76,76,76	0
87	OHX	BI	304	7/7	0.33	-	193,193,193,193	7
87	OHX	A6	1934	7/7	0.19	-	105,105,105,105	7
88	MG	A1	4010	1/1	0.37	-	61,61,61,61	0
88	MG	A6	2293	1/1	0.20	-	78,78,78,78	0
88	MG	A1	4459	1/1	0.39	-	88,88,88,88	0
88	MG	A1	3848	1/1	0.42	-	75,75,75,75	0
87	OHX	A2	1989	7/7	0.15	-	131,131,131,131	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A6	2207	1/1	0.10	-	57,57,57,57	0
88	MG	A5	4344	1/1	0.36	-	66,66,66,66	0
87	OHX	A5	3644	7/7	0.23	-	135,135,135,135	7
87	OHX	A2	1979	7/7	0.19	-	121,121,121,121	7
87	OHX	A6	1956	7/7	0.14	-	130,130,130,130	7
88	MG	A4	243	1/1	0.18	-	48,48,48,48	0
87	OHX	A5	3506	7/7	0.16	-	102,102,102,102	7
88	MG	A5	4032	1/1	0.43	-	41,41,41,41	0
88	MG	A5	4409	1/1	0.29	-	59,59,59,59	0
87	OHX	A5	3636	7/7	0.14	-	111,111,111,111	7
88	MG	A5	4227	1/1	0.21	-	46,46,46,46	0
87	OHX	A1	3736	7/7	0.18	-	174,174,174,174	7
87	OHX	Dh	201	7/7	0.14	-	129,129,129,129	7
87	OHX	BN	301	7/7	0.16	-	116,116,116,116	7
88	MG	A5	3886	1/1	0.28	-	43,43,43,43	0
88	MG	A5	4213	1/1	0.40	-	52,52,52,52	0
88	MG	A5	4304	1/1	0.23	-	66,66,66,66	0
87	OHX	A5	3686	7/7	0.15	-	121,121,121,121	7
87	OHX	A1	3496	7/7	0.17	-	97,97,97,97	7
88	MG	A5	4283	1/1	0.40	-	79,79,79,79	0
88	MG	A1	4152	1/1	0.19	-	34,34,34,34	0
87	OHX	A1	3810	7/7	0.49	-	199,199,199,199	7
88	MG	A5	4385	1/1	0.25	-	74,74,74,74	0
88	MG	A2	2178	1/1	0.23	-	73,73,73,73	0
88	MG	A6	2144	1/1	0.35	-	51,51,51,51	0
87	OHX	Cd	101	7/7	0.14	-	135,135,135,135	7
88	MG	A2	2171	1/1	0.31	-	89,89,89,89	0
88	MG	A1	4467	1/1	0.31	-	68,68,68,68	0
87	OHX	A1	3713	7/7	0.19	-	101,101,101,101	7
88	MG	A1	4229	1/1	0.15	-	89,89,89,89	0
88	MG	A6	2236	1/1	0.19	-	76,76,76,76	0
88	MG	A6	2142	1/1	0.34	-	46,46,46,46	0
88	MG	A1	4027	1/1	0.44	-	65,65,65,65	0
88	MG	A1	3961	1/1	0.31	-	33,33,33,33	0
88	MG	A6	2126	1/1	0.26	-	78,78,78,78	0
87	OHX	A6	1965	7/7	0.14	-	123,123,123,123	7
88	MG	A2	2202	1/1	0.09	-	66,66,66,66	0
88	MG	A1	3966	1/1	0.39	-	60,60,60,60	0
88	MG	A5	4019	1/1	0.46	-	48,48,48,48	0
88	MG	CG	303	1/1	0.30	-	54,54,54,54	0
87	OHX	A5	3597	7/7	0.17	-	95,95,95,95	7
87	OHX	A5	3432	7/7	0.17	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A5	3852	1/1	0.21	-	49,49,49,49	0
88	MG	A1	4207	1/1	0.16	-	85,85,85,85	0
88	MG	A1	4466	1/1	0.18	-	80,80,80,80	0
87	OHX	A6	2004	7/7	0.17	-	105,105,105,105	7
88	MG	DB	413	1/1	0.30	-	101,101,101,101	0
88	MG	A5	4135	1/1	0.36	-	73,73,73,73	0
88	MG	A5	4417	1/1	0.53	-	50,50,50,50	0
87	OHX	A2	2024	7/7	0.18	-	174,174,174,174	7
88	MG	A1	4205	1/1	0.11	-	63,63,63,63	0
88	MG	A8	236	1/1	0.18	-	75,75,75,75	0
88	MG	A1	3905	1/1	0.15	-	19,19,19,19	0
87	OHX	A1	3693	7/7	0.17	-	100,100,100,100	7
88	MG	A6	2131	1/1	0.33	-	46,46,46,46	0
87	OHX	A1	3700	7/7	0.27	-	185,185,185,185	7
87	OHX	A2	2071	7/7	0.21	-	162,162,162,162	7
87	OHX	A1	3604	7/7	0.18	-	254,254,254,254	7
88	MG	A1	4114	1/1	0.31	-	71,71,71,71	0
87	OHX	A6	2071	7/7	0.37	-	160,160,160,160	7
88	MG	A8	228	1/1	0.28	-	86,86,86,86	0
88	MG	A1	4036	1/1	0.30	-	71,71,71,71	0
87	OHX	A6	1914	7/7	0.16	-	111,111,111,111	0
88	MG	A5	4157	1/1	0.17	-	56,56,56,56	0
87	OHX	Dj	104	7/7	0.17	-	105,105,105,105	7
87	OHX	A1	3783	7/7	0.21	-	152,152,152,152	7
87	OHX	A5	3764	7/7	0.22	-	120,120,120,120	7
88	MG	A5	4162	1/1	0.19	-	70,70,70,70	0
88	MG	A5	4471	1/1	0.17	-	61,61,61,61	0
87	OHX	A1	3468	7/7	0.17	-	74,74,74,74	7
88	MG	A1	3989	1/1	0.29	-	42,42,42,42	0
87	OHX	A1	3651	7/7	0.16	-	131,131,131,131	7
87	OHX	A1	3504	7/7	0.17	-	105,105,105,105	7
87	OHX	A1	3464	7/7	0.16	-	88,88,88,88	7
87	OHX	A2	2003	7/7	0.21	-	147,147,147,147	7
88	MG	A5	4566	1/1	0.33	-	74,74,74,74	0
87	OHX	A1	3435	7/7	0.16	-	85,85,85,85	0
88	MG	A1	4106	1/1	0.26	-	69,69,69,69	0
87	OHX	A1	3610	7/7	0.18	-	121,121,121,121	7
88	MG	A6	2310	1/1	0.28	-	89,89,89,89	0
87	OHX	A2	2047	7/7	0.28	-	188,188,188,188	7
88	MG	A5	4161	1/1	0.20	-	51,51,51,51	0
88	MG	A5	4431	1/1	0.33	-	118,118,118,118	0
87	OHX	A7	206	7/7	0.17	-	115,115,115,115	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	4071	1/1	0.20	-	71,71,71,71	0
88	MG	A5	4572	1/1	0.28	-	77,77,77,77	0
88	MG	A5	4071	1/1	0.23	-	79,79,79,79	0
87	OHX	A5	3801	7/7	0.25	-	156,156,156,156	7
88	MG	A1	4416	1/1	0.73	-	57,57,57,57	0
87	OHX	A2	2010	7/7	0.17	-	119,119,119,119	7
87	OHX	A5	3615	7/7	0.18	-	147,147,147,147	7
88	MG	A2	2137	1/1	0.18	-	97,97,97,97	0
88	MG	A5	4473	1/1	0.65	-	94,94,94,94	0
87	OHX	A6	2100	7/7	0.28	-	206,206,206,206	7
87	OHX	A5	3748	7/7	0.24	-	183,183,183,183	7
88	MG	BC	407	1/1	0.41	-	58,58,58,58	0
88	MG	A5	4352	1/1	0.30	-	67,67,67,67	0
88	MG	BV	202	1/1	0.24	-	73,73,73,73	0
88	MG	A1	4380	1/1	0.18	-	95,95,95,95	0
88	MG	A6	2281	1/1	0.36	-	75,75,75,75	0
88	MG	A2	2111	1/1	0.17	-	69,69,69,69	0
87	OHX	A1	3723	7/7	0.20	-	161,161,161,161	7
88	MG	A1	4465	1/1	0.28	-	92,92,92,92	0
88	MG	A1	4334	1/1	0.30	-	104,104,104,104	0
88	MG	A1	4302	1/1	0.43	-	114,114,114,114	0
88	MG	A5	4108	1/1	0.28	-	74,74,74,74	0
88	MG	A5	4246	1/1	0.36	-	38,38,38,38	0
88	MG	A1	4223	1/1	0.29	-	79,79,79,79	0
87	OHX	A1	3748	7/7	0.20	-	163,163,163,163	7
87	OHX	A1	3811	7/7	0.30	-	183,183,183,183	7
88	MG	A1	4065	1/1	0.21	-	47,47,47,47	0
88	MG	A5	4499	1/1	0.33	-	76,76,76,76	0
87	OHX	A8	210	7/7	0.15	-	133,133,133,133	7
88	MG	A1	4300	1/1	0.22	-	76,76,76,76	0
87	OHX	A1	3456	7/7	0.17	-	100,100,100,100	7
88	MG	A6	2321	1/1	0.46	-	93,93,93,93	0
88	MG	A1	3990	1/1	0.43	-	54,54,54,54	0
88	MG	A6	2134	1/1	0.34	-	67,67,67,67	0
88	MG	A6	2187	1/1	0.26	-	64,64,64,64	0
88	MG	A3	226	1/1	0.17	-	69,69,69,69	0
88	MG	A7	223	1/1	0.23	-	69,69,69,69	0
88	MG	A1	4092	1/1	0.28	-	66,66,66,66	0
88	MG	BA	303	1/1	0.22	-	30,30,30,30	0
87	OHX	A5	3595	7/7	0.16	-	125,125,125,125	7
88	MG	A1	4186	1/1	0.16	-	75,75,75,75	0
87	OHX	A5	3806	7/7	0.21	-	120,120,120,120	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	4083	1/1	0.21	-	44,44,44,44	0
87	OHX	A6	2079	7/7	0.14	-	161,161,161,161	7
87	OHX	A5	3641	7/7	0.18	-	127,127,127,127	7
88	MG	A5	4390	1/1	0.20	-	70,70,70,70	0
88	MG	A1	4000	1/1	0.17	-	18,18,18,18	0
87	OHX	A1	3751	7/7	0.12	-	189,189,189,189	7
87	OHX	A6	2037	7/7	0.20	-	138,138,138,138	7
88	MG	A7	236	1/1	0.21	-	102,102,102,102	0
87	OHX	A1	3415	7/7	0.15	-	68,68,68,68	0
87	OHX	A2	1990	7/7	0.14	-	105,105,105,105	7
88	MG	A1	4258	1/1	0.15	-	67,67,67,67	0
88	MG	DA	303	1/1	0.23	-	53,53,53,53	0
88	MG	A1	4198	1/1	0.19	-	79,79,79,79	0
88	MG	A5	4467	1/1	0.13	-	70,70,70,70	0
87	OHX	A1	3492	7/7	0.13	-	98,98,98,98	7
88	MG	A1	3971	1/1	0.33	-	35,35,35,35	0
88	MG	BO	205	1/1	0.75	-	58,58,58,58	0
87	OHX	A2	2009	7/7	0.10	-	144,144,144,144	7
87	OHX	A1	3729	7/7	0.31	-	167,167,167,167	7
88	MG	Ba	204	1/1	0.47	-	74,74,74,74	0
88	MG	A5	3999	1/1	0.26	-	32,32,32,32	0
88	MG	A5	4476	1/1	0.43	-	86,86,86,86	0
88	MG	BC	406	1/1	0.35	-	61,61,61,61	0
88	MG	A1	4148	1/1	0.23	-	94,94,94,94	0
87	OHX	A5	3822	7/7	0.48	-	205,205,205,205	7
87	OHX	A1	3557	7/7	0.16	-	121,121,121,121	7
88	MG	A5	3409	1/1	0.28	-	45,45,45,45	0
87	OHX	A5	3766	7/7	0.11	-	173,173,173,173	7
87	OHX	A1	3627	7/7	0.16	-	130,130,130,130	7
87	OHX	A2	1995	7/7	0.11	-	171,171,171,171	7
88	MG	A1	3898	1/1	0.19	-	64,64,64,64	0
88	MG	A1	4204	1/1	0.17	-	59,59,59,59	0
88	MG	A2	2210	1/1	0.30	-	81,81,81,81	0
88	MG	A6	2283	1/1	0.18	-	75,75,75,75	0
88	MG	A1	4234	1/1	0.34	-	82,82,82,82	0
88	MG	A1	3949	1/1	0.32	-	43,43,43,43	0
88	MG	A1	4363	1/1	0.25	-	46,46,46,46	0
87	OHX	A5	3491	7/7	0.15	-	106,106,106,106	7
88	MG	A1	3825	1/1	0.19	-	47,47,47,47	0
87	OHX	A6	1986	7/7	0.12	-	165,165,165,165	7
87	OHX	A4	206	7/7	0.13	-	104,104,104,104	7
88	MG	A1	3866	1/1	0.10	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	3863	1/1	0.28	-	125,125,125,125	0
88	MG	BR	203	1/1	0.26	-	65,65,65,65	0
88	MG	A5	4327	1/1	0.16	-	94,94,94,94	0
88	MG	A1	3900	1/1	0.18	-	78,78,78,78	0
88	MG	A6	2272	1/1	0.25	-	115,115,115,115	0
87	OHX	A5	3607	7/7	0.21	-	142,142,142,142	7
87	OHX	A8	219	7/7	0.17	-	166,166,166,166	7
88	MG	A1	4241	1/1	0.37	-	74,74,74,74	0
87	OHX	A1	3572	7/7	0.16	-	114,114,114,114	7
87	OHX	A2	2041	7/7	0.14	-	184,184,184,184	7
88	MG	A1	4003	1/1	0.44	-	48,48,48,48	0
87	OHX	A6	2094	7/7	0.20	-	180,180,180,180	7
88	MG	DL	201	1/1	0.80	-	94,94,94,94	0
88	MG	A6	2155	1/1	0.30	-	41,41,41,41	0
88	MG	A1	4472	1/1	0.24	-	86,86,86,86	0
87	OHX	A1	3421	7/7	0.19	-	80,80,80,80	0
88	MG	A5	4529	1/1	0.36	-	91,91,91,91	0
88	MG	A6	2259	1/1	0.58	-	119,119,119,119	0
88	MG	A5	4064	1/1	0.18	-	30,30,30,30	0
88	MG	A1	4356	1/1	0.23	-	65,65,65,65	0
88	MG	A1	4134	1/1	0.34	-	69,69,69,69	0
88	MG	A5	4074	1/1	0.14	-	51,51,51,51	0
88	MG	A5	4134	1/1	0.19	-	84,84,84,84	0
88	MG	A5	4243	1/1	0.22	-	45,45,45,45	0
88	MG	A6	2315	1/1	0.28	-	84,84,84,84	0
88	MG	A1	3919	1/1	0.61	-	138,138,138,138	0
88	MG	A2	2220	1/1	0.10	-	111,111,111,111	0
87	OHX	A1	3429	7/7	0.18	-	87,87,87,87	0
88	MG	A1	4055	1/1	0.18	-	58,58,58,58	0
88	MG	A1	3985	1/1	0.42	-	51,51,51,51	0
87	OHX	A5	3712	7/7	0.20	-	149,149,149,149	7
88	MG	A1	4505	1/1	0.91	-	145,145,145,145	0
88	MG	A5	4053	1/1	0.32	-	65,65,65,65	0
87	OHX	A5	3698	7/7	0.17	-	173,173,173,173	7
88	MG	A5	3871	1/1	0.25	-	56,56,56,56	0
87	OHX	A5	3516	7/7	0.17	-	89,89,89,89	7
88	MG	A4	241	1/1	0.58	-	60,60,60,60	0
87	OHX	A1	3743	7/7	0.30	-	148,148,148,148	7
88	MG	A1	3817	1/1	0.41	-	63,63,63,63	0
88	MG	A1	3872	1/1	0.29	-	37,37,37,37	0
88	MG	A8	222	1/1	0.32	-	47,47,47,47	0
88	MG	Bj	107	1/1	0.42	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A6	2288	1/1	0.37	-	106,106,106,106	0
88	MG	A1	4393	1/1	0.50	-	78,78,78,78	0
87	OHX	A2	1918	7/7	0.16	-	99,99,99,99	7
88	MG	A5	4281	1/1	0.36	-	56,56,56,56	0
88	MG	A5	3997	1/1	0.42	-	43,43,43,43	0
88	MG	A5	4580	1/1	0.15	-	82,82,82,82	0
88	MG	A2	2098	1/1	0.29	-	62,62,62,62	0
88	MG	A5	3899	1/1	0.23	-	73,73,73,73	0
88	MG	A5	4180	1/1	0.28	-	81,81,81,81	0
88	MG	A1	4378	1/1	0.44	-	51,51,51,51	0
87	OHX	A6	1919	7/7	0.14	-	104,104,104,104	7
87	OHX	A2	2065	7/7	0.29	-	166,166,166,166	7
88	MG	A6	2308	1/1	0.43	-	81,81,81,81	0
88	MG	A6	2125	1/1	0.19	-	47,47,47,47	0
87	OHX	A2	2081	7/7	0.14	-	199,199,199,199	7
88	MG	A5	4554	1/1	0.37	-	86,86,86,86	0
88	MG	A5	3896	1/1	0.34	-	67,67,67,67	0
88	MG	A5	3984	1/1	0.43	-	56,56,56,56	0
87	OHX	A2	1923	7/7	0.14	-	110,110,110,110	7
87	OHX	A6	2035	7/7	0.18	-	129,129,129,129	7
88	MG	A1	4460	1/1	0.16	-	67,67,67,67	0
88	MG	A2	2167	1/1	0.29	-	72,72,72,72	0
87	OHX	A2	2032	7/7	0.14	-	200,200,200,200	7
88	MG	A6	2299	1/1	0.61	-	84,84,84,84	0
88	MG	A5	3944	1/1	0.18	-	36,36,36,36	0
87	OHX	BC	401	7/7	0.19	-	130,130,130,130	7
88	MG	A5	4517	1/1	0.44	-	73,73,73,73	0
88	MG	A1	4143	1/1	0.20	-	70,70,70,70	0
87	OHX	A1	3447	7/7	0.19	-	98,98,98,98	0
88	MG	A1	3928	1/1	0.42	-	88,88,88,88	0
88	MG	A1	3911	1/1	0.12	-	58,58,58,58	0
88	MG	A1	3979	1/1	0.41	-	52,52,52,52	0
87	OHX	A6	1908	7/7	0.21	-	101,101,101,101	0
88	MG	A6	2278	1/1	0.56	-	64,64,64,64	0
88	MG	A5	4486	1/1	0.47	-	94,94,94,94	0
87	OHX	A1	3789	7/7	0.32	-	189,189,189,189	7
88	MG	A5	3857	1/1	0.28	-	53,53,53,53	0
87	OHX	A1	3712	7/7	0.38	-	180,180,180,180	7
88	MG	A6	2279	1/1	0.23	-	81,81,81,81	0
88	MG	A1	4103	1/1	0.17	-	74,74,74,74	0
88	MG	B1	4500	1/1	0.44	-	77,77,77,77	0
88	MG	Ba	208	1/1	0.46	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	A1	3516	7/7	0.17	-	86,86,86,86	7
88	MG	De	202	1/1	0.58	-	52,52,52,52	0
87	OHX	A1	3439	7/7	0.17	-	81,81,81,81	7
87	OHX	A5	3809	7/7	0.18	-	91,91,91,91	7
88	MG	A5	4265	1/1	0.77	-	80,80,80,80	0
88	MG	A5	4448	1/1	0.41	-	64,64,64,64	0
88	MG	A5	4581	1/1	0.35	-	97,97,97,97	0
88	MG	DJ	202	1/1	0.28	-	81,81,81,81	0
87	OHX	A1	3442	7/7	0.17	-	95,95,95,95	0
88	MG	A1	4457	1/1	0.21	-	97,97,97,97	0
88	MG	A5	4558	1/1	0.31	-	63,63,63,63	0
88	MG	A2	2247	1/1	0.23	-	86,86,86,86	0
88	MG	A1	4419	1/1	0.28	-	79,79,79,79	0
87	OHX	A5	3640	7/7	0.14	-	147,147,147,147	7
88	MG	A1	4463	1/1	0.21	-	76,76,76,76	0
87	OHX	A6	1993	7/7	0.15	-	129,129,129,129	7
88	MG	A1	4424	1/1	0.19	-	50,50,50,50	0
87	OHX	A8	216	7/7	0.11	-	198,198,198,198	7
87	OHX	A6	1970	7/7	0.13	-	160,160,160,160	7
87	OHX	A1	3515	7/7	0.14	-	115,115,115,115	7
88	MG	A5	4280	1/1	0.57	-	49,49,49,49	0
88	MG	A5	4146	1/1	0.23	-	80,80,80,80	0
87	OHX	A6	1952	7/7	0.13	-	123,123,123,123	7
87	OHX	A5	3646	7/7	0.18	-	135,135,135,135	7
88	MG	A5	4226	1/1	0.31	-	76,76,76,76	0
88	MG	A2	2222	1/1	0.40	-	103,103,103,103	0
88	MG	A2	2191	1/1	0.20	-	91,91,91,91	0
88	MG	A6	2101	1/1	0.29	-	51,51,51,51	0
87	OHX	A6	1933	7/7	0.18	-	104,104,104,104	7
88	MG	Db	102	1/1	0.77	-	70,70,70,70	0
87	OHX	A2	2005	7/7	0.13	-	134,134,134,134	7
87	OHX	A1	3483	7/7	0.18	-	103,103,103,103	7
88	MG	A5	3846	1/1	0.17	-	37,37,37,37	0
87	OHX	A2	1901	7/7	0.20	-	95,95,95,95	0
88	MG	A1	3828	1/1	0.29	-	43,43,43,43	0
87	OHX	CB	301	7/7	0.17	-	162,162,162,162	7
88	MG	A1	3893	1/1	0.17	-	26,26,26,26	0
88	MG	A1	3405	1/1	0.13	-	71,71,71,71	0
87	OHX	A5	3772	7/7	0.55	-	137,137,137,137	7
88	MG	A1	4101	1/1	0.29	-	86,86,86,86	0
88	MG	A6	2147	1/1	0.27	-	44,44,44,44	0
88	MG	A1	4265	1/1	0.29	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A6	1945	7/7	0.13	-	148,148,148,148	0
88	MG	A5	4036	1/1	0.18	-	60,60,60,60	0
88	MG	A2	2141	1/1	0.24	-	68,68,68,68	0
88	MG	A6	2333	1/1	0.67	-	99,99,99,99	0
88	MG	A6	2223	1/1	0.23	-	75,75,75,75	0
88	MG	A2	2208	1/1	0.23	-	109,109,109,109	0
87	OHX	A5	3728	7/7	0.29	-	131,131,131,131	7
87	OHX	A1	3786	7/7	0.25	-	184,184,184,184	7
88	MG	A5	3889	1/1	0.37	-	86,86,86,86	0
88	MG	A5	3945	1/1	0.24	-	56,56,56,56	0
88	MG	A5	4482	1/1	0.38	-	79,79,79,79	0
88	MG	A5	3905	1/1	0.30	-	75,75,75,75	0
88	MG	A1	4189	1/1	0.18	-	59,59,59,59	0
87	OHX	A5	3402	7/7	0.18	-	116,116,116,116	7
88	MG	A5	4466	1/1	0.20	-	79,79,79,79	0
88	MG	A4	216	1/1	0.36	-	64,64,64,64	0
87	OHX	A1	3646	7/7	0.18	-	110,110,110,110	7
88	MG	A6	2285	1/1	0.24	-	74,74,74,74	0
87	OHX	A2	1953	7/7	0.16	-	120,120,120,120	7
88	MG	A6	2119	1/1	0.25	-	70,70,70,70	0
87	OHX	A5	3652	7/7	0.14	-	150,150,150,150	7
88	MG	A4	236	1/1	0.13	-	100,100,100,100	0
87	OHX	A6	2012	7/7	0.11	-	149,149,149,149	7
88	MG	A2	2215	1/1	0.34	-	86,86,86,86	0
88	MG	A2	2091	1/1	0.40	-	81,81,81,81	0
88	MG	Bj	106	1/1	0.30	-	75,75,75,75	0
88	MG	A6	2336	1/1	0.26	-	93,93,93,93	0
88	MG	A5	4279	1/1	0.85	-	63,63,63,63	0
88	MG	A2	2180	1/1	0.09	-	101,101,101,101	0
87	OHX	A2	1969	7/7	0.13	-	144,144,144,144	7
88	MG	A5	4346	1/1	0.20	-	89,89,89,89	0
87	OHX	A2	2000	7/7	0.17	-	140,140,140,140	7
87	OHX	A5	3576	7/7	0.18	-	124,124,124,124	7
87	OHX	A1	3586	7/7	0.16	-	117,117,117,117	7
87	OHX	A8	214	7/7	0.13	-	125,125,125,125	7
87	OHX	A1	3726	7/7	0.21	-	178,178,178,178	7
88	MG	A5	4356	1/1	0.46	-	74,74,74,74	0
87	OHX	A5	3464	7/7	0.16	-	98,98,98,98	7
87	OHX	A5	3593	7/7	0.13	-	134,134,134,134	7
88	MG	A5	3412	1/1	0.56	-	68,68,68,68	0
88	MG	BR	205	1/1	0.51	-	99,99,99,99	0
88	MG	A1	4405	1/1	0.32	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A5	3876	1/1	0.25	-	66,66,66,66	0
88	MG	AX	201	1/1	0.12	-	70,70,70,70	0
88	MG	Dq	401	1/1	0.11	-	81,81,81,81	0
88	MG	A2	2195	1/1	0.18	-	90,90,90,90	0
88	MG	A1	4161	1/1	0.23	-	73,73,73,73	0
88	MG	A1	4498	1/1	0.14	-	60,60,60,60	0
88	MG	A2	2193	1/1	0.23	-	79,79,79,79	0
88	MG	A6	2323	1/1	0.24	-	77,77,77,77	0
87	OHX	A2	1926	7/7	0.13	-	112,112,112,112	7
87	OHX	A2	1996	7/7	0.17	-	113,113,113,113	7
87	OHX	A2	1999	7/7	0.12	-	168,168,168,168	7
87	OHX	A6	1921	7/7	0.17	-	92,92,92,92	7
88	MG	A5	4024	1/1	0.38	-	42,42,42,42	0
88	MG	A1	4306	1/1	0.11	-	68,68,68,68	0
88	MG	BE	201	1/1	0.19	-	55,55,55,55	0
87	OHX	A2	1909	7/7	0.17	-	93,93,93,93	7
88	MG	A5	4166	1/1	0.23	-	57,57,57,57	0
88	MG	Bj	105	1/1	0.71	-	64,64,64,64	0
88	MG	A5	3849	1/1	0.26	-	41,41,41,41	0
88	MG	A7	231	1/1	0.29	-	87,87,87,87	0
87	OHX	DJ	201	7/7	0.13	-	185,185,185,185	7
88	MG	A5	4552	1/1	0.24	-	84,84,84,84	0
88	MG	A5	4245	1/1	0.19	-	66,66,66,66	0
87	OHX	A6	2092	7/7	0.29	-	182,182,182,182	7
88	MG	A5	3828	1/1	0.10	-	34,34,34,34	0
87	OHX	Bo	201	7/7	0.16	-	97,97,97,97	7
87	OHX	A5	3729	7/7	0.18	-	165,165,165,165	7
87	OHX	A8	207	7/7	0.14	-	126,126,126,126	7
87	OHX	A1	3523	7/7	0.16	-	111,111,111,111	7
87	OHX	A5	3603	7/7	0.20	-	107,107,107,107	7
87	OHX	A1	3466	7/7	0.17	-	90,90,90,90	7
88	MG	A2	2169	1/1	0.23	-	105,105,105,105	0
88	MG	A5	4316	1/1	0.22	-	57,57,57,57	0
88	MG	A1	4135	1/1	0.25	-	96,96,96,96	0
88	MG	A6	2232	1/1	0.24	-	77,77,77,77	0
88	MG	A3	223	1/1	0.19	-	75,75,75,75	0
87	OHX	A5	3559	7/7	0.12	-	109,109,109,109	7
87	OHX	A5	3792	7/7	0.35	-	217,217,217,217	7
88	MG	A1	4256	1/1	0.16	-	86,86,86,86	0
87	OHX	A1	3472	7/7	0.16	-	109,109,109,109	7
88	MG	A1	3819	1/1	0.11	-	63,63,63,63	0
87	OHX	A1	3478	7/7	0.16	-	112,112,112,112	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	A5	3774	7/7	0.22	-	148,148,148,148	7
88	MG	A1	4440	1/1	0.52	-	55,55,55,55	0
88	MG	A1	4267	1/1	0.16	-	82,82,82,82	0
88	MG	A5	4290	1/1	0.37	-	47,47,47,47	0
87	OHX	A7	209	7/7	0.18	-	115,115,115,115	7
87	OHX	A2	2068	7/7	0.22	-	177,177,177,177	7
88	MG	A5	4215	1/1	0.24	-	52,52,52,52	0
88	MG	A3	224	1/1	0.22	-	62,62,62,62	0
88	MG	A1	4167	1/1	0.81	-	66,66,66,66	0
87	OHX	A6	2049	7/7	0.14	-	175,175,175,175	7
88	MG	A5	4041	1/1	0.23	-	47,47,47,47	0
88	MG	DB	404	1/1	0.26	-	68,68,68,68	0
87	OHX	A5	3560	7/7	0.19	-	106,106,106,106	7
88	MG	A2	2249	1/1	0.16	-	85,85,85,85	0
87	OHX	A6	2007	7/7	0.11	-	164,164,164,164	7
87	OHX	BB	401	7/7	0.18	-	111,111,111,111	7
87	OHX	A1	3767	7/7	0.14	-	158,158,158,158	7
87	OHX	A5	3773	7/7	0.17	-	141,141,141,141	7
88	MG	A1	4243	1/1	0.52	-	61,61,61,61	0
88	MG	A1	4246	1/1	0.28	-	80,80,80,80	0
88	MG	A6	2235	1/1	0.29	-	77,77,77,77	0
88	MG	A4	228	1/1	0.23	-	70,70,70,70	0
88	MG	A1	4052	1/1	0.16	-	71,71,71,71	0
87	OHX	A2	1975	7/7	0.12	-	141,141,141,141	7
87	OHX	A5	3502	7/7	0.17	-	141,141,141,141	0
87	OHX	DO	201	7/7	0.18	-	93,93,93,93	7
87	OHX	A1	3482	7/7	0.15	-	106,106,106,106	7
87	OHX	A1	3781	7/7	0.21	-	122,122,122,122	7
87	OHX	A5	3583	7/7	0.14	-	137,137,137,137	7
88	MG	A5	4087	1/1	0.23	-	86,86,86,86	0
88	MG	A5	4208	1/1	0.21	-	75,75,75,75	0
87	OHX	A2	2037	7/7	0.34	-	197,197,197,197	7
87	OHX	A1	3653	7/7	0.11	-	153,153,153,153	7
87	OHX	A2	1903	7/7	0.20	-	94,94,94,94	0
88	MG	A2	2154	1/1	0.36	-	74,74,74,74	0
87	OHX	A1	3714	7/7	0.20	-	118,118,118,118	7
88	MG	A3	214	1/1	0.30	-	70,70,70,70	0
87	OHX	A2	1991	7/7	0.11	-	113,113,113,113	7
87	OHX	A8	215	7/7	0.27	-	151,151,151,151	7
87	OHX	A5	3677	7/7	0.15	-	113,113,113,113	7
87	OHX	A4	211	7/7	0.32	-	108,108,108,108	7
87	OHX	A2	2008	7/7	0.15	-	135,135,135,135	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A6	2264	1/1	0.17	-	62,62,62,62	0
88	MG	A1	4400	1/1	0.12	-	70,70,70,70	0
88	MG	A1	4037	1/1	0.21	-	83,83,83,83	0
88	MG	BC	405	1/1	0.46	-	49,49,49,49	0
87	OHX	A1	3814	7/7	0.46	-	221,221,221,221	7
87	OHX	A5	3492	7/7	0.18	-	89,89,89,89	7
88	MG	A5	4174	1/1	0.19	-	75,75,75,75	0
88	MG	A4	246	1/1	0.68	-	91,91,91,91	0
88	MG	A2	2138	1/1	0.12	-	56,56,56,56	0
88	MG	A1	4303	1/1	0.29	-	105,105,105,105	0
87	OHX	A5	3500	7/7	0.17	-	88,88,88,88	7
88	MG	A5	4091	1/1	0.12	-	54,54,54,54	0
87	OHX	A5	3496	7/7	0.16	-	73,73,73,73	7
88	MG	A5	4571	1/1	0.38	-	84,84,84,84	0
87	OHX	A5	3590	7/7	0.16	-	114,114,114,114	7
88	MG	A5	4145	1/1	0.18	-	57,57,57,57	0
87	OHX	A1	3614	7/7	0.18	-	112,112,112,112	7
88	MG	A1	4070	1/1	0.28	-	76,76,76,76	0
88	MG	A2	2089	1/1	0.28	-	49,49,49,49	0
88	MG	A1	4029	1/1	0.16	-	29,29,29,29	0
88	MG	A2	2245	1/1	0.14	-	71,71,71,71	0
88	MG	A1	4250	1/1	0.25	-	56,56,56,56	0
88	MG	A5	3926	1/1	0.28	-	53,53,53,53	0
88	MG	A1	4469	1/1	0.33	-	66,66,66,66	0
88	MG	A1	4279	1/1	0.63	-	54,54,54,54	0
88	MG	A1	4188	1/1	0.32	-	82,82,82,82	0
88	MG	A5	4577	1/1	0.38	-	76,76,76,76	0
88	MG	A6	2209	1/1	0.22	-	79,79,79,79	0
88	MG	A6	2239	1/1	0.20	-	82,82,82,82	0
88	MG	DB	412	1/1	0.36	-	70,70,70,70	0
88	MG	BR	202	1/1	0.19	-	58,58,58,58	0
87	OHX	AN	201	7/7	0.13	-	192,192,192,192	7
87	OHX	A1	3652	7/7	0.22	-	115,115,115,115	7
88	MG	BQ	203	1/1	0.66	-	63,63,63,63	0
87	OHX	A6	1989	7/7	0.15	-	122,122,122,122	7
88	MG	A1	4483	1/1	0.20	-	72,72,72,72	0
87	OHX	A5	3584	7/7	0.20	-	119,119,119,119	7
89	ZN	Ab	101	1/1	0.19	-	327,327,327,327	0
87	OHX	A2	1922	7/7	0.16	-	99,99,99,99	7
88	MG	A5	4393	1/1	0.48	-	97,97,97,97	0
88	MG	A6	2122	1/1	0.27	-	55,55,55,55	0
88	MG	A5	4103	1/1	0.30	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A5	3653	7/7	0.21	-	130,130,130,130	7
87	OHX	A1	3414	7/7	0.22	-	77,77,77,77	0
87	OHX	A6	2056	7/7	0.13	-	178,178,178,178	7
87	OHX	A5	3620	7/7	0.17	-	113,113,113,113	7
88	MG	A8	231	1/1	0.21	-	71,71,71,71	0
87	OHX	A1	3567	7/7	0.15	-	88,88,88,88	7
87	OHX	CI	301	7/7	0.14	-	172,172,172,172	7
88	MG	A1	3944	1/1	0.45	-	45,45,45,45	0
87	OHX	A1	3626	7/7	0.12	-	162,162,162,162	7
87	OHX	A6	2058	7/7	0.27	-	196,196,196,196	7
88	MG	A5	3864	1/1	0.32	-	63,63,63,63	0
87	OHX	A6	1949	7/7	0.15	-	102,102,102,102	7
88	MG	A5	4317	1/1	0.30	-	63,63,63,63	0
88	MG	A5	4264	1/1	0.39	-	103,103,103,103	0
88	MG	A5	4313	1/1	0.30	-	66,66,66,66	0
88	MG	A8	237	1/1	0.22	-	85,85,85,85	0
88	MG	A5	3933	1/1	0.31	-	74,74,74,74	0
88	MG	A5	4568	1/1	0.29	-	64,64,64,64	0
88	MG	A4	245	1/1	0.31	-	90,90,90,90	0
87	OHX	CS	201	7/7	0.16	-	129,129,129,129	7
88	MG	A5	4319	1/1	0.15	-	86,86,86,86	0
88	MG	A5	4188	1/1	0.34	-	78,78,78,78	0
87	OHX	A5	3515	7/7	0.15	-	121,121,121,121	7
88	MG	A7	221	1/1	0.26	-	82,82,82,82	0
88	MG	DW	201	1/1	1.09	-	85,85,85,85	0
88	MG	A5	3836	1/1	0.33	-	66,66,66,66	0
88	MG	A6	2121	1/1	0.37	-	64,64,64,64	0
87	OHX	A2	1930	7/7	0.14	-	120,120,120,120	7
88	MG	A2	2109	1/1	0.37	-	56,56,56,56	0
87	OHX	A2	1935	7/7	0.16	-	120,120,120,120	7
88	MG	A1	4492	1/1	0.21	-	100,100,100,100	0
87	OHX	A2	1904	7/7	0.16	-	99,99,99,99	0
87	OHX	A2	1937	7/7	0.18	-	122,122,122,122	7
88	MG	A5	4055	1/1	0.24	-	81,81,81,81	0
88	MG	A1	4395	1/1	0.17	-	97,97,97,97	0
87	OHX	A1	3768	7/7	0.31	-	137,137,137,137	7
87	OHX	A2	1911	7/7	0.18	-	124,124,124,124	0
87	OHX	A1	3664	7/7	0.15	-	207,207,207,207	7
87	OHX	A8	217	7/7	0.25	-	169,169,169,169	7
88	MG	A5	3974	1/1	0.39	-	40,40,40,40	0
87	OHX	A5	3599	7/7	0.17	-	120,120,120,120	7
87	OHX	A2	2067	7/7	0.21	-	108,108,108,108	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A1	3605	7/7	0.15	-	166,166,166,166	7
88	MG	A5	4331	1/1	0.18	-	104,104,104,104	0
88	MG	A1	3991	1/1	0.37	-	52,52,52,52	0
88	MG	CY	203	1/1	0.23	-	109,109,109,109	0
87	OHX	A1	3731	7/7	0.18	-	119,119,119,119	7
88	MG	A6	2102	1/1	0.24	-	63,63,63,63	0
87	OHX	BA	301	7/7	0.41	-	217,217,217,217	7
87	OHX	A4	210	7/7	0.09	-	131,131,131,131	7
88	MG	A5	4455	1/1	0.43	-	60,60,60,60	0
88	MG	A1	4358	1/1	0.27	-	86,86,86,86	0
88	MG	A5	4396	1/1	0.17	-	71,71,71,71	0
88	MG	A5	4147	1/1	0.11	-	63,63,63,63	0
88	MG	A6	2282	1/1	0.35	-	83,83,83,83	0
87	OHX	A5	3788	7/7	0.23	-	141,141,141,141	7
88	MG	A6	2109	1/1	0.31	-	54,54,54,54	0
88	MG	A6	2175	1/1	0.29	-	62,62,62,62	0
88	MG	A1	4220	1/1	0.22	-	103,103,103,103	0
88	MG	A1	4245	1/1	0.19	-	73,73,73,73	0
88	MG	A1	4435	1/1	0.21	-	105,105,105,105	0
88	MG	BS	202	1/1	0.38	-	84,84,84,84	0
87	OHX	A2	2075	7/7	0.23	-	204,204,204,204	7
87	OHX	A5	3505	7/7	0.14	-	94,94,94,94	7
88	MG	A5	4561	1/1	0.44	-	111,111,111,111	0
87	OHX	A1	3676	7/7	0.18	-	148,148,148,148	7
87	OHX	A1	3679	7/7	0.26	-	114,114,114,114	7
87	OHX	A1	3758	7/7	0.18	-	139,139,139,139	7
87	OHX	A5	3609	7/7	0.14	-	153,153,153,153	7
88	MG	A5	4238	1/1	0.42	-	44,44,44,44	0
88	MG	A1	4287	1/1	0.20	-	61,61,61,61	0
88	MG	A1	4146	1/1	0.31	-	91,91,91,91	0
88	MG	Bo	202	1/1	0.32	-	82,82,82,82	0
88	MG	A1	4203	1/1	0.21	-	69,69,69,69	0
87	OHX	A1	3540	7/7	0.12	-	141,141,141,141	7
88	MG	Dj	103	1/1	1.21	-	65,65,65,65	0
88	MG	A1	3969	1/1	0.34	-	49,49,49,49	0
87	OHX	A1	3570	7/7	0.17	-	100,100,100,100	7
88	MG	A1	4139	1/1	0.10	-	56,56,56,56	0
88	MG	A6	2158	1/1	0.43	-	66,66,66,66	0
88	MG	DP	202	1/1	0.18	-	56,56,56,56	0
87	OHX	A1	3408	7/7	0.25	-	66,66,66,66	0
87	OHX	A1	3724	7/7	0.22	-	144,144,144,144	7
87	OHX	A5	3751	7/7	0.20	-	148,148,148,148	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A1	3550	7/7	0.17	-	130,130,130,130	7
88	MG	A5	3833	1/1	0.31	-	54,54,54,54	0
88	MG	A1	4390	1/1	0.15	-	82,82,82,82	0
88	MG	A5	3891	1/1	0.23	-	50,50,50,50	0
88	MG	A1	3854	1/1	0.21	-	57,57,57,57	0
88	MG	A6	2127	1/1	0.38	-	41,41,41,41	0
88	MG	A1	4053	1/1	0.15	-	76,76,76,76	0
87	OHX	A1	3457	7/7	0.16	-	97,97,97,97	7
87	OHX	A6	1947	7/7	0.15	-	134,134,134,134	7
88	MG	A5	4088	1/1	0.16	-	41,41,41,41	0
88	MG	A1	3852	1/1	0.30	-	70,70,70,70	0
87	OHX	A1	3669	7/7	0.13	-	130,130,130,130	7
88	MG	A6	2305	1/1	0.15	-	76,76,76,76	0
88	MG	A1	3921	1/1	0.25	-	87,87,87,87	0
87	OHX	A6	2033	7/7	0.25	-	133,133,133,133	7
88	MG	A5	4106	1/1	0.26	-	41,41,41,41	0
88	MG	A6	2247	1/1	0.35	-	88,88,88,88	0
87	OHX	A1	3426	7/7	0.18	-	73,73,73,73	0
88	MG	A5	4288	1/1	0.47	-	49,49,49,49	0
87	OHX	A6	2043	7/7	0.19	-	156,156,156,156	7
87	OHX	A6	1928	7/7	0.17	-	73,73,73,73	7
87	OHX	A1	3535	7/7	0.18	-	102,102,102,102	7
88	MG	A5	3993	1/1	0.27	-	25,25,25,25	0
88	MG	A2	2184	1/1	0.09	-	109,109,109,109	0
88	MG	A5	4125	1/1	0.16	-	67,67,67,67	0
88	MG	A7	215	1/1	0.25	-	46,46,46,46	0
87	OHX	A1	3564	7/7	0.22	-	136,136,136,136	7
88	MG	A5	4384	1/1	0.24	-	77,77,77,77	0
87	OHX	A1	3401	7/7	0.15	-	121,121,121,121	7
88	MG	A5	4113	1/1	0.17	-	39,39,39,39	0
87	OHX	A1	3805	7/7	0.35	-	209,209,209,209	7
88	MG	A5	4412	1/1	0.26	-	104,104,104,104	0
88	MG	A6	2176	1/1	0.42	-	67,67,67,67	0
88	MG	A5	4183	1/1	0.10	-	76,76,76,76	0
88	MG	A5	4532	1/1	0.29	-	95,95,95,95	0
88	MG	A1	3916	1/1	0.28	-	73,73,73,73	0
87	OHX	A5	3818	7/7	0.60	-	226,226,226,226	7
87	OHX	A5	3661	7/7	0.17	-	134,134,134,134	7
88	MG	A1	4217	1/1	0.16	-	57,57,57,57	0
87	OHX	A5	3450	7/7	0.16	-	76,76,76,76	7
88	MG	A5	4051	1/1	0.18	-	77,77,77,77	0
87	OHX	A6	2052	7/7	0.14	-	211,211,211,211	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A5	4449	1/1	1.14	-	122,122,122,122	0
87	OHX	A2	1950	7/7	0.12	-	122,122,122,122	7
88	MG	A5	4436	1/1	0.64	-	90,90,90,90	0
87	OHX	A5	3709	7/7	0.12	-	171,171,171,171	7
88	MG	A1	4450	1/1	0.22	-	68,68,68,68	0
88	MG	DD	304	1/1	0.17	-	71,71,71,71	0
87	OHX	A6	1982	7/7	0.16	-	123,123,123,123	7
87	OHX	A2	1998	7/7	0.23	-	135,135,135,135	7
88	MG	Ba	203	1/1	0.22	-	70,70,70,70	0
88	MG	A6	2107	1/1	0.39	-	52,52,52,52	0
88	MG	A1	4404	1/1	0.20	-	80,80,80,80	0
88	MG	A1	4079	1/1	0.27	-	75,75,75,75	0
87	OHX	A6	2073	7/7	0.18	-	186,186,186,186	7
88	MG	A1	3902	1/1	0.23	-	47,47,47,47	0
87	OHX	A2	2051	7/7	0.37	-	209,209,209,209	7
88	MG	A5	4233	1/1	0.21	-	91,91,91,91	0
88	MG	A5	4251	1/1	0.32	-	85,85,85,85	0
87	OHX	A6	2051	7/7	0.19	-	167,167,167,167	7
88	MG	A1	4484	1/1	1.10	-	106,106,106,106	0
87	OHX	A7	210	7/7	0.24	-	114,114,114,114	7
87	OHX	A1	3674	7/7	0.18	-	159,159,159,159	7
87	OHX	CY	201	7/7	0.15	-	121,121,121,121	7
87	OHX	A2	2087	7/7	0.16	-	196,196,196,196	7
88	MG	A5	4218	1/1	0.23	-	57,57,57,57	0
88	MG	A5	4167	1/1	0.20	-	71,71,71,71	0
88	MG	A1	4298	1/1	0.36	-	95,95,95,95	0
88	MG	A5	4122	1/1	0.28	-	52,52,52,52	0
88	MG	A1	4011	1/1	0.23	-	50,50,50,50	0
88	MG	A5	4539	1/1	0.67	-	77,77,77,77	0
88	MG	A5	4511	1/1	0.52	-	68,68,68,68	0
88	MG	A6	2146	1/1	0.25	-	49,49,49,49	0
87	OHX	A2	1988	7/7	0.16	-	189,189,189,189	7
87	OHX	A2	2039	7/7	0.31	-	157,157,157,157	7
87	OHX	A1	3419	7/7	0.18	-	76,76,76,76	0
87	OHX	A1	3633	7/7	0.20	-	101,101,101,101	7
88	MG	A1	4169	1/1	0.25	-	80,80,80,80	0
88	MG	A5	4029	1/1	0.41	-	44,44,44,44	0
88	MG	A5	4277	1/1	0.27	-	85,85,85,85	0
87	OHX	A5	3799	7/7	0.28	-	168,168,168,168	7
88	MG	A1	4397	1/1	0.15	-	80,80,80,80	0
87	OHX	A5	3461	7/7	0.17	-	82,82,82,82	7
88	MG	A5	4172	1/1	0.34	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	A5	3673	7/7	0.18	-	144,144,144,144	7
88	MG	A2	2113	1/1	0.39	-	80,80,80,80	0
87	OHX	A4	202	7/7	0.20	-	80,80,80,80	0
87	OHX	A5	3776	7/7	0.23	-	184,184,184,184	7
87	OHX	A1	3682	7/7	0.12	-	145,145,145,145	7
88	MG	A1	4412	1/1	0.27	-	104,104,104,104	0
87	OHX	CG	302	7/7	0.28	-	197,197,197,197	7
88	MG	A5	4256	1/1	0.51	-	81,81,81,81	0
88	MG	A2	2233	1/1	0.13	-	80,80,80,80	0
87	OHX	A5	3797	7/7	0.18	-	130,130,130,130	7
88	MG	A1	4221	1/1	0.17	-	92,92,92,92	0
87	OHX	A2	2059	7/7	0.09	-	183,183,183,183	7
88	MG	A5	4368	1/1	0.30	-	75,75,75,75	0
88	MG	A5	4460	1/1	0.52	-	74,74,74,74	0
88	MG	A7	230	1/1	0.20	-	61,61,61,61	0
88	MG	A6	2203	1/1	0.23	-	63,63,63,63	0
88	MG	Ba	205	1/1	0.22	-	69,69,69,69	0
88	MG	BC	402	1/1	0.23	-	54,54,54,54	0
88	MG	A6	2149	1/1	0.36	-	49,49,49,49	0
87	OHX	A1	3798	7/7	0.58	-	226,226,226,226	7
88	MG	Bj	109	1/1	0.24	-	122,122,122,122	0
88	MG	A1	4014	1/1	0.41	-	56,56,56,56	0
87	OHX	A5	3780	7/7	0.35	-	211,211,211,211	7
87	OHX	A2	2004	7/7	0.16	-	164,164,164,164	7
88	MG	A2	2177	1/1	0.25	-	83,83,83,83	0
87	OHX	A5	3785	7/7	0.30	-	126,126,126,126	7
88	MG	A1	4138	1/1	0.33	-	62,62,62,62	0
88	MG	A8	224	1/1	0.18	-	67,67,67,67	0
88	MG	A6	2251	1/1	0.43	-	73,73,73,73	0
87	OHX	A1	3413	7/7	0.23	-	75,75,75,75	0
88	MG	A1	4348	1/1	0.14	-	73,73,73,73	0
88	MG	A1	3942	1/1	0.30	-	38,38,38,38	0
88	MG	A5	4311	1/1	0.22	-	78,78,78,78	0
87	OHX	A2	1974	7/7	0.12	-	170,170,170,170	7
87	OHX	A1	3487	7/7	0.17	-	94,94,94,94	7
88	MG	DJ	203	1/1	0.25	-	80,80,80,80	0
87	OHX	A5	3713	7/7	0.17	-	122,122,122,122	7
88	MG	A5	4363	1/1	0.32	-	83,83,83,83	0
88	MG	A1	4501	1/1	0.69	-	103,103,103,103	0
87	OHX	A2	2048	7/7	0.12	-	155,155,155,155	7
87	OHX	A5	3528	7/7	0.15	-	163,163,163,163	0
87	OHX	A1	3565	7/7	0.12	-	127,127,127,127	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	DI	302	7/7	0.20	-	160,160,160,160	7
88	MG	A5	4437	1/1	0.20	-	86,86,86,86	0
88	MG	A2	2206	1/1	0.12	-	78,78,78,78	0
88	MG	A1	4123	1/1	0.29	-	77,77,77,77	0
88	MG	A1	4353	1/1	0.14	-	77,77,77,77	0
88	MG	A5	4005	1/1	0.38	-	31,31,31,31	0
87	OHX	A1	3800	7/7	0.17	-	188,188,188,188	7
88	MG	A5	4097	1/1	0.22	-	37,37,37,37	0
88	MG	A1	3997	1/1	0.32	-	40,40,40,40	0
87	OHX	A1	3648	7/7	0.13	-	102,102,102,102	7
87	OHX	A5	3623	7/7	0.18	-	156,156,156,156	7
87	OHX	A2	2258	7/7	0.16	-	162,162,162,162	7
88	MG	DM	202	1/1	0.20	-	70,70,70,70	0
88	MG	A5	3879	1/1	0.22	-	61,61,61,61	0
88	MG	A6	2303	1/1	0.27	-	60,60,60,60	0
87	OHX	A6	1946	7/7	0.14	-	105,105,105,105	7
87	OHX	A1	3744	7/7	0.36	-	205,205,205,205	7
88	MG	A1	4370	1/1	0.24	-	104,104,104,104	0
88	MG	D1	101	1/1	0.36	-	112,112,112,112	0
87	OHX	A5	3760	7/7	0.10	-	202,202,202,202	7
88	MG	A1	4254	1/1	0.21	-	72,72,72,72	0
87	OHX	A5	3668	7/7	0.15	-	163,163,163,163	7
88	MG	A5	4212	1/1	0.21	-	73,73,73,73	0
87	OHX	A5	3737	7/7	0.17	-	75,75,75,75	7
88	MG	A4	231	1/1	0.27	-	45,45,45,45	0
88	MG	A1	3998	1/1	0.21	-	28,28,28,28	0
87	OHX	A5	3614	7/7	0.17	-	120,120,120,120	7
88	MG	A5	4490	1/1	0.24	-	90,90,90,90	0
88	MG	A1	4479	1/1	0.26	-	74,74,74,74	0
87	OHX	A1	3752	7/7	0.11	-	207,207,207,207	7
87	OHX	A5	3605	7/7	0.22	-	112,112,112,112	7
88	MG	A1	4497	1/1	0.19	-	79,79,79,79	0
88	MG	A6	2161	1/1	0.39	-	55,55,55,55	0
87	OHX	A1	3531	7/7	0.15	-	140,140,140,140	7
88	MG	A1	3970	1/1	0.34	-	69,69,69,69	0
88	MG	A1	4325	1/1	0.26	-	67,67,67,67	0
88	MG	A5	3910	1/1	0.35	-	57,57,57,57	0
87	OHX	A6	1967	7/7	0.16	-	112,112,112,112	7
87	OHX	A6	2029	7/7	0.19	-	141,141,141,141	7
87	OHX	A5	3479	7/7	0.15	-	110,110,110,110	0
87	OHX	A1	3643	7/7	0.15	-	153,153,153,153	7
88	MG	A1	4347	1/1	0.34	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A6	2085	7/7	0.43	-	188,188,188,188	7
88	MG	A6	2307	1/1	0.40	-	94,94,94,94	0
88	MG	A1	3821	1/1	0.42	-	71,71,71,71	0
87	OHX	A1	3756	7/7	0.19	-	158,158,158,158	7
88	MG	A8	239	1/1	0.11	-	93,93,93,93	0
87	OHX	A5	3683	7/7	0.22	-	119,119,119,119	7
88	MG	A1	4504	1/1	0.95	-	98,98,98,98	0
88	MG	DB	403	1/1	0.40	-	36,36,36,36	0
87	OHX	A5	3649	7/7	0.17	-	129,129,129,129	7
88	MG	A6	2166	1/1	0.29	-	64,64,64,64	0
87	OHX	A7	208	7/7	0.17	-	105,105,105,105	7
87	OHX	A5	3769	7/7	0.23	-	169,169,169,169	7
88	MG	A5	4381	1/1	0.25	-	96,96,96,96	0
87	OHX	A5	3648	7/7	0.22	-	111,111,111,111	7
87	OHX	A6	1994	7/7	0.16	-	133,133,133,133	7
88	MG	A1	4297	1/1	0.21	-	94,94,94,94	0
88	MG	A5	4085	1/1	0.25	-	79,79,79,79	0
88	MG	Bj	108	1/1	1.06	-	66,66,66,66	0
88	MG	A5	4548	1/1	0.52	-	74,74,74,74	0
88	MG	A1	4231	1/1	0.44	-	82,82,82,82	0
88	MG	A5	4501	1/1	0.56	-	56,56,56,56	0
87	OHX	A5	3401	7/7	0.17	-	102,102,102,102	0
88	MG	A1	4049	1/1	0.18	-	59,59,59,59	0
88	MG	A8	232	1/1	0.14	-	43,43,43,43	0
88	MG	A5	3922	1/1	0.17	-	54,54,54,54	0
87	OHX	A6	2034	7/7	0.19	-	137,137,137,137	7
87	OHX	A5	3474	7/7	0.17	-	81,81,81,81	7
87	OHX	A6	1944	7/7	0.13	-	115,115,115,115	7
88	MG	A5	4500	1/1	0.18	-	82,82,82,82	0
88	MG	A2	2200	1/1	0.22	-	88,88,88,88	0
87	OHX	A5	3575	7/7	0.20	-	81,81,81,81	7
87	OHX	Bj	101	7/7	0.16	-	100,100,100,100	7
88	MG	A5	4105	1/1	0.30	-	68,68,68,68	0
88	MG	A1	4446	1/1	0.18	-	62,62,62,62	0
87	OHX	A1	3727	7/7	0.28	-	146,146,146,146	7
88	MG	AI	302	1/1	0.24	-	66,66,66,66	0
88	MG	A1	4122	1/1	0.25	-	57,57,57,57	0
88	MG	A5	4297	1/1	0.26	-	56,56,56,56	0
88	MG	A5	4364	1/1	0.18	-	76,76,76,76	0
87	OHX	A5	3573	7/7	0.15	-	107,107,107,107	7
87	OHX	A5	3777	7/7	0.32	-	187,187,187,187	7
87	OHX	A2	2028	7/7	0.33	-	180,180,180,180	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A1	3770	7/7	0.20	-	179,179,179,179	7
88	MG	A4	218	1/1	0.29	-	59,59,59,59	0
88	MG	A1	3980	1/1	0.32	-	38,38,38,38	0
88	MG	A1	4150	1/1	0.47	-	95,95,95,95	0
87	OHX	A2	1947	7/7	0.15	-	157,157,157,157	7
88	MG	A5	4137	1/1	0.22	-	104,104,104,104	0
88	MG	A1	4477	1/1	0.27	-	108,108,108,108	0
87	OHX	A5	3617	7/7	0.10	-	154,154,154,154	7
88	MG	A5	4128	1/1	0.14	-	66,66,66,66	0
88	MG	DT	201	1/1	0.38	-	63,63,63,63	0
88	MG	A1	3857	1/1	0.25	-	53,53,53,53	0
87	OHX	A6	1918	7/7	0.15	-	100,100,100,100	0
87	OHX	A5	3557	7/7	0.15	-	154,154,154,154	7
88	MG	A1	4401	1/1	0.23	-	69,69,69,69	0
87	OHX	A3	201	7/7	0.17	-	109,109,109,109	0
87	OHX	A1	3621	7/7	0.16	-	119,119,119,119	7
87	OHX	A6	2068	7/7	0.49	-	217,217,217,217	7
87	OHX	A2	1914	7/7	0.15	-	92,92,92,92	7
88	MG	A6	2151	1/1	0.47	-	64,64,64,64	0
88	MG	A7	227	1/1	0.70	-	100,100,100,100	0
88	MG	A5	4454	1/1	0.31	-	68,68,68,68	0
87	OHX	A2	1987	7/7	0.15	-	147,147,147,147	7
88	MG	A5	4488	1/1	0.79	-	81,81,81,81	0
87	OHX	A1	3760	7/7	0.15	-	136,136,136,136	7
87	OHX	A2	1902	7/7	0.19	-	102,102,102,102	0
88	MG	BQ	201	1/1	0.38	-	65,65,65,65	0
87	OHX	A8	202	7/7	0.20	-	77,77,77,77	0
87	OHX	A2	2001	7/7	0.17	-	140,140,140,140	7
88	MG	A1	4421	1/1	0.33	-	63,63,63,63	0
88	MG	A5	4200	1/1	0.31	-	70,70,70,70	0
88	MG	DR	202	1/1	0.87	-	67,67,67,67	0
88	MG	BF	4102	1/1	0.37	-	76,76,76,76	0
87	OHX	A1	3815	7/7	0.41	-	183,183,183,183	7
88	MG	A2	2207	1/1	0.23	-	76,76,76,76	0
88	MG	A1	4184	1/1	0.24	-	81,81,81,81	0
88	MG	A5	4474	1/1	0.47	-	44,44,44,44	0
88	MG	A1	4033	1/1	0.27	-	48,48,48,48	0
87	OHX	A5	3727	7/7	0.17	-	167,167,167,167	7
87	OHX	A1	3782	7/7	0.24	-	186,186,186,186	7
88	MG	A1	4214	1/1	0.46	-	55,55,55,55	0
87	OHX	A5	3466	7/7	0.18	-	120,120,120,120	0
87	OHX	A1	3519	7/7	0.15	-	137,137,137,137	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	A6	2031	6/7	0.12	-	195,195,195,195	6
88	MG	A1	3929	1/1	0.31	-	75,75,75,75	0
88	MG	A5	4504	1/1	0.30	-	84,84,84,84	0
88	MG	A1	3833	1/1	0.34	-	49,49,49,49	0
88	MG	A5	4193	1/1	0.27	-	43,43,43,43	0
88	MG	A1	4255	1/1	0.28	-	87,87,87,87	0
88	MG	A1	3820	1/1	0.28	-	47,47,47,47	0
88	MG	A1	4461	1/1	0.07	-	86,86,86,86	0
87	OHX	A5	3694	7/7	0.17	-	127,127,127,127	7
88	MG	Da	202	1/1	0.45	-	84,84,84,84	0
88	MG	A4	247	1/1	0.56	-	56,56,56,56	0
88	MG	A2	2232	1/1	0.22	-	125,125,125,125	0
87	OHX	A5	3578	7/7	0.09	-	159,159,159,159	7
88	MG	A4	249	1/1	0.24	-	75,75,75,75	0
88	MG	A5	4111	1/1	0.22	-	65,65,65,65	0
88	MG	A5	4534	1/1	0.99	-	72,72,72,72	0
89	ZN	Cb	101	1/1	0.50	-	305,305,305,305	0
87	OHX	A1	3741	7/7	0.22	-	151,151,151,151	7
87	OHX	A6	1943	7/7	0.15	-	106,106,106,106	7
88	MG	A1	4120	1/1	0.15	-	26,26,26,26	0
88	MG	A2	2142	1/1	0.34	-	65,65,65,65	0
87	OHX	A1	3716	7/7	0.23	-	113,113,113,113	7
88	MG	A2	2179	1/1	0.29	-	81,81,81,81	0
87	OHX	CY	202	7/7	0.14	-	130,130,130,130	7
87	OHX	A5	3451	7/7	0.16	-	81,81,81,81	7
87	OHX	A7	212	7/7	0.42	-	165,165,165,165	7
87	OHX	A1	3790	7/7	0.17	-	164,164,164,164	7
88	MG	A5	4077	1/1	0.34	-	55,55,55,55	0
88	MG	A1	4080	1/1	0.16	-	60,60,60,60	0
88	MG	A1	4013	1/1	0.30	-	47,47,47,47	0
88	MG	BN	303	1/1	0.69	-	72,72,72,72	0
87	OHX	A5	3577	7/7	0.17	-	128,128,128,128	7
87	OHX	A5	3527	7/7	0.17	-	105,105,105,105	7
87	OHX	A5	3529	7/7	0.18	-	93,93,93,93	7
88	MG	BO	206	1/1	0.61	-	69,69,69,69	0
87	OHX	A5	3687	7/7	0.18	-	109,109,109,109	7
88	MG	A5	4179	1/1	0.21	-	71,71,71,71	0
88	MG	DG	302	1/1	0.36	-	65,65,65,65	0
87	OHX	A1	3432	7/7	0.18	-	90,90,90,90	0
87	OHX	A5	3541	7/7	0.21	-	113,113,113,113	7
88	MG	A1	4194	1/1	0.31	-	96,96,96,96	0
88	MG	A6	2116	1/1	0.27	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	A1	3793	7/7	0.26	-	232,232,232,232	7
87	OHX	A2	1962	7/7	0.14	-	136,136,136,136	7
87	OHX	A1	3796	7/7	0.28	-	174,174,174,174	7
87	OHX	A6	1999	7/7	0.18	-	140,140,140,140	7
88	MG	A5	4495	1/1	0.27	-	88,88,88,88	0
88	MG	A1	3909	1/1	0.41	-	67,67,67,67	0
88	MG	A5	4518	1/1	0.79	-	144,144,144,144	0
87	OHX	A2	1984	7/7	0.16	-	108,108,108,108	7
87	OHX	A5	3742	7/7	0.25	-	143,143,143,143	7
88	MG	A2	2123	1/1	0.40	-	81,81,81,81	0
88	MG	A5	4536	1/1	0.34	-	73,73,73,73	0
88	MG	A5	4170	1/1	0.42	-	69,69,69,69	0
88	MG	A1	4045	1/1	0.15	-	55,55,55,55	0
88	MG	A5	4081	1/1	0.39	-	79,79,79,79	0
88	MG	A1	3844	1/1	0.19	-	48,48,48,48	0
88	MG	A6	2254	1/1	0.12	-	69,69,69,69	0
88	MG	A6	2189	1/1	0.34	-	42,42,42,42	0
88	MG	A1	4382	1/1	0.18	-	81,81,81,81	0
87	OHX	A1	3661	7/7	0.20	-	118,118,118,118	7
88	MG	A1	4269	1/1	0.51	-	87,87,87,87	0
88	MG	A1	4227	1/1	0.20	-	52,52,52,52	0
88	MG	A1	3927	1/1	0.20	-	31,31,31,31	0
87	OHX	A5	3553	7/7	0.19	-	75,75,75,75	7
88	MG	A1	4350	1/1	0.77	-	76,76,76,76	0
88	MG	A1	4330	1/1	0.16	-	82,82,82,82	0
88	MG	A2	2157	1/1	0.31	-	82,82,82,82	0
88	MG	A5	3929	1/1	0.38	-	80,80,80,80	0
87	OHX	A1	3486	7/7	0.14	-	92,92,92,92	7
88	MG	A5	4186	1/1	0.18	-	84,84,84,84	0
88	MG	AJ	201	1/1	0.25	-	82,82,82,82	0
88	MG	A5	4228	1/1	0.29	-	82,82,82,82	0
88	MG	A1	3882	1/1	0.31	-	47,47,47,47	0
88	MG	DM	203	1/1	0.29	-	94,94,94,94	0
87	OHX	A6	2003	7/7	0.17	-	177,177,177,177	7
88	MG	A1	4491	1/1	0.70	-	80,80,80,80	0
88	MG	A6	2159	1/1	0.21	-	33,33,33,33	0
88	MG	A6	2214	1/1	0.24	-	53,53,53,53	0
88	MG	A1	3846	1/1	0.21	-	37,37,37,37	0
88	MG	A5	3996	1/1	0.45	-	46,46,46,46	0
87	OHX	A1	3630	7/7	0.14	-	119,119,119,119	7
88	MG	A5	3967	1/1	0.33	-	57,57,57,57	0
87	OHX	A1	3551	7/7	0.16	-	100,100,100,100	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	A2	2056	7/7	0.21	-	130,130,130,130	7
88	MG	A5	4027	1/1	0.39	-	53,53,53,53	0
87	OHX	A5	3726	7/7	0.14	-	135,135,135,135	7
87	OHX	A1	3809	7/7	0.12	-	192,192,192,192	7
88	MG	A5	3994	1/1	0.33	-	39,39,39,39	0
88	MG	A5	4349	1/1	1.30	-	79,79,79,79	0
87	OHX	A5	3431	7/7	0.17	-	83,83,83,83	0
87	OHX	A1	3458	7/7	0.16	-	111,111,111,111	7
88	MG	A5	4521	1/1	0.60	-	68,68,68,68	0
88	MG	A5	4021	1/1	0.29	-	35,35,35,35	0
88	MG	DS	202	1/1	0.19	-	75,75,75,75	0
87	OHX	A5	3433	7/7	0.17	-	81,81,81,81	0
88	MG	A2	2243	1/1	0.18	-	86,86,86,86	0
87	OHX	A5	3543	7/7	0.18	-	109,109,109,109	7
87	OHX	A5	3428	7/7	0.22	-	88,88,88,88	0
88	MG	DD	307	1/1	0.60	-	77,77,77,77	0
87	OHX	A5	3715	7/7	0.20	-	100,100,100,100	7
88	MG	A5	4387	1/1	0.32	-	93,93,93,93	0
88	MG	A1	4307	1/1	0.19	-	71,71,71,71	0
88	MG	Df	202	1/1	0.31	-	81,81,81,81	0
87	OHX	A1	3563	7/7	0.15	-	131,131,131,131	7
88	MG	A6	2135	1/1	0.20	-	58,58,58,58	0
88	MG	AB	301	1/1	0.26	-	98,98,98,98	0
87	OHX	A1	3441	7/7	0.17	-	93,93,93,93	0
87	OHX	DD	301	7/7	0.25	-	134,134,134,134	7
88	MG	A5	4480	1/1	0.19	-	76,76,76,76	0
87	OHX	A5	3670	7/7	0.19	-	109,109,109,109	7
88	MG	A1	4417	1/1	0.23	-	94,94,94,94	0
87	OHX	A6	1910	7/7	0.15	-	84,84,84,84	0
88	MG	A5	4498	1/1	0.24	-	90,90,90,90	0
87	OHX	A1	3681	7/7	0.17	-	146,146,146,146	7
87	OHX	A2	1915	7/7	0.15	-	109,109,109,109	7
87	OHX	A2	2046	7/7	0.36	-	139,139,139,139	7
88	MG	A1	4091	1/1	0.27	-	65,65,65,65	0
87	OHX	A5	3555	7/7	0.12	-	152,152,152,152	0
88	MG	A6	2182	1/1	0.16	-	63,63,63,63	0
87	OHX	Dg	201	7/7	0.32	-	153,153,153,153	7
88	MG	A6	2115	1/1	0.36	-	47,47,47,47	0
88	MG	A1	4314	1/1	0.17	-	78,78,78,78	0
88	MG	Ba	201	1/1	0.32	-	66,66,66,66	0
87	OHX	A5	3533	7/7	0.14	-	118,118,118,118	7
88	MG	A7	216	1/1	0.39	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	A1	3598	7/7	0.13	-	139,139,139,139	7
88	MG	Ba	207	1/1	0.64	-	89,89,89,89	0
87	OHX	A5	3639	7/7	0.14	-	157,157,157,157	7
88	MG	A5	4054	1/1	0.22	-	71,71,71,71	0
88	MG	A5	4114	1/1	0.21	-	38,38,38,38	0
88	MG	Af	201	1/1	0.15	-	88,88,88,88	0
88	MG	A1	4408	1/1	0.46	-	81,81,81,81	0
88	MG	A2	2124	1/1	0.26	-	79,79,79,79	0
88	MG	A1	4276	1/1	0.25	-	95,95,95,95	0
87	OHX	A6	1971	7/7	0.12	-	108,108,108,108	7
88	MG	A1	4253	1/1	0.20	-	110,110,110,110	0
88	MG	A1	4494	1/1	0.28	-	87,87,87,87	0
88	MG	A3	232	1/1	0.25	-	95,95,95,95	0
88	MG	A2	2217	1/1	0.17	-	117,117,117,117	0
88	MG	A5	4175	1/1	0.19	-	114,114,114,114	0
87	OHX	A2	2022	7/7	0.15	-	138,138,138,138	7
88	MG	Da	201	1/1	0.23	-	54,54,54,54	0
88	MG	A6	2237	1/1	0.18	-	96,96,96,96	0
88	MG	A5	4487	1/1	0.89	-	76,76,76,76	0
88	MG	A4	239	1/1	0.72	-	70,70,70,70	0
87	OHX	A2	2045	7/7	0.12	-	164,164,164,164	7
88	MG	A5	4044	1/1	0.22	-	35,35,35,35	0
87	OHX	A6	1915	7/7	0.16	-	87,87,87,87	7
88	MG	A1	3834	1/1	0.08	-	44,44,44,44	0
88	MG	A1	4420	1/1	0.46	-	73,73,73,73	0
88	MG	A1	4009	1/1	0.41	-	51,51,51,51	0
88	MG	A1	4476	1/1	0.29	-	68,68,68,68	0
87	OHX	A5	3442	7/7	0.16	-	85,85,85,85	0
88	MG	A5	4438	1/1	0.29	-	58,58,58,58	0
88	MG	A1	4035	1/1	0.09	-	59,59,59,59	0
88	MG	A6	2243	1/1	0.23	-	74,74,74,74	0
88	MG	A5	4151	1/1	0.16	-	64,64,64,64	0
88	MG	A5	4527	1/1	0.19	-	78,78,78,78	0
88	MG	A1	3977	1/1	0.27	-	76,76,76,76	0
87	OHX	A5	3730	7/7	0.20	-	97,97,97,97	7
87	OHX	A1	3533	7/7	0.17	-	104,104,104,104	7
87	OHX	A6	1979	7/7	0.16	-	116,116,116,116	7
88	MG	A6	2248	1/1	0.13	-	75,75,75,75	0
88	MG	A2	2218	1/1	0.20	-	63,63,63,63	0
88	MG	A5	4016	1/1	0.28	-	42,42,42,42	0
88	MG	A1	3879	1/1	0.43	-	89,89,89,89	0
87	OHX	A1	3446	7/7	0.17	-	79,79,79,79	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A5	4220	1/1	0.38	-	82,82,82,82	0
87	OHX	A5	3446	7/7	0.18	-	82,82,82,82	0
88	MG	Dn	101	1/1	0.31	-	84,84,84,84	0
87	OHX	De	201	7/7	0.18	-	91,91,91,91	7
87	OHX	A1	3704	7/7	0.14	-	176,176,176,176	7
87	OHX	A3	206	7/7	0.15	-	140,140,140,140	7
88	MG	BP	208	1/1	0.14	-	52,52,52,52	0
88	MG	A1	3939	1/1	0.31	-	32,32,32,32	0
88	MG	A5	3932	1/1	0.30	-	34,34,34,34	0
89	ZN	Dp	104	1/1	0.14	-	79,79,79,79	0
87	OHX	A1	3453	7/7	0.29	-	134,134,134,134	0
88	MG	A5	3946	1/1	0.42	-	41,41,41,41	0
88	MG	A5	3831	1/1	0.16	-	37,37,37,37	0
88	MG	A5	4121	1/1	0.21	-	55,55,55,55	0
87	OHX	A5	3572	7/7	0.17	-	145,145,145,145	7
88	MG	DC	407	1/1	0.85	-	75,75,75,75	0
88	MG	A5	4403	1/1	0.37	-	81,81,81,81	0
87	OHX	A5	3594	7/7	0.16	-	131,131,131,131	7
87	OHX	AI	301	7/7	0.12	-	156,156,156,156	7
88	MG	A5	4126	1/1	0.23	-	100,100,100,100	0
88	MG	A5	4339	1/1	0.17	-	66,66,66,66	0
88	MG	A1	4285	1/1	0.30	-	64,64,64,64	0
87	OHX	A6	1980	7/7	0.16	-	133,133,133,133	7
88	MG	A5	4225	1/1	0.31	-	66,66,66,66	0
87	OHX	A2	1951	7/7	0.13	-	126,126,126,126	7
88	MG	A5	3872	1/1	0.33	-	81,81,81,81	0
88	MG	A5	4153	1/1	0.27	-	83,83,83,83	0
88	MG	A5	4136	1/1	0.19	-	46,46,46,46	0
88	MG	A5	4148	1/1	0.28	-	75,75,75,75	0
88	MG	Cd	102	1/1	0.20	-	75,75,75,75	0
88	MG	A1	3899	1/1	0.22	-	57,57,57,57	0
88	MG	A1	4266	1/1	0.18	-	70,70,70,70	0
88	MG	A5	4026	1/1	0.40	-	53,53,53,53	0
88	MG	A5	4440	1/1	0.43	-	76,76,76,76	0
87	OHX	A2	2017	7/7	0.11	-	186,186,186,186	7
87	OHX	DP	201	7/7	0.24	-	155,155,155,155	7
87	OHX	A5	3759	7/7	0.18	-	80,80,80,80	7
88	MG	A1	4268	1/1	0.19	-	65,65,65,65	0
87	OHX	A1	3683	7/7	0.19	-	159,159,159,159	7
88	MG	A1	4324	1/1	0.20	-	79,79,79,79	0
88	MG	A6	2328	1/1	0.22	-	87,87,87,87	0
88	MG	A6	2326	1/1	0.11	-	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	3829	1/1	0.35	-	55,55,55,55	0
88	MG	A5	4040	1/1	0.19	-	46,46,46,46	0
87	OHX	A5	3407	7/7	0.13	-	196,196,196,196	7
87	OHX	A1	3544	7/7	0.17	-	96,96,96,96	7
88	MG	A5	4391	1/1	0.41	-	57,57,57,57	0
88	MG	A5	4369	1/1	0.52	-	69,69,69,69	0
89	ZN	Ad	105	1/1	0.17	-	83,83,83,83	0
88	MG	BN	302	1/1	0.25	-	44,44,44,44	0
88	MG	A1	4454	1/1	0.34	-	81,81,81,81	0
87	OHX	A5	3744	7/7	0.18	-	140,140,140,140	7
87	OHX	A5	3602	7/7	0.20	-	109,109,109,109	7
87	OHX	A5	3416	7/7	0.21	-	68,68,68,68	0
88	MG	A1	3981	1/1	0.34	-	41,41,41,41	0
87	OHX	A1	3735	7/7	0.20	-	83,83,83,83	7
88	MG	A6	2164	1/1	0.30	-	57,57,57,57	0
88	MG	A1	4193	1/1	0.34	-	72,72,72,72	0
87	OHX	A5	3497	7/7	0.14	-	81,81,81,81	7
87	OHX	A7	213	7/7	0.25	-	181,181,181,181	7
87	OHX	A5	3711	7/7	0.16	-	164,164,164,164	7
87	OHX	A5	3415	7/7	0.23	-	67,67,67,67	0
88	MG	A5	4237	1/1	0.17	-	51,51,51,51	0
87	OHX	A6	2055	7/7	0.23	-	131,131,131,131	7
87	OHX	AP	201	7/7	0.15	-	196,196,196,196	7
87	OHX	A4	204	7/7	0.14	-	122,122,122,122	7
88	MG	A5	4425	1/1	0.25	-	65,65,65,65	0
87	OHX	A5	3731	7/7	0.11	-	138,138,138,138	7
88	MG	A5	4395	1/1	0.64	-	58,58,58,58	0
88	MG	A1	4369	1/1	0.26	-	85,85,85,85	0
88	MG	A5	4197	1/1	0.23	-	84,84,84,84	0
87	OHX	A6	2065	7/7	0.15	-	156,156,156,156	7
88	MG	A5	4321	1/1	0.19	-	77,77,77,77	0
88	MG	A1	3831	1/1	0.35	-	56,56,56,56	0
88	MG	A5	4084	1/1	0.41	-	112,112,112,112	0
88	MG	A5	4293	1/1	0.22	-	76,76,76,76	0
88	MG	A4	230	1/1	0.24	-	71,71,71,71	0
87	OHX	A5	3494	7/7	0.16	-	97,97,97,97	7
87	OHX	A2	1986	7/7	0.15	-	124,124,124,124	7
88	MG	A6	2174	1/1	0.20	-	50,50,50,50	0
88	MG	A5	3868	1/1	0.17	-	44,44,44,44	0
88	MG	A5	3894	1/1	0.33	-	67,67,67,67	0
87	OHX	A1	3657	7/7	0.15	-	166,166,166,166	7
88	MG	DP	203	1/1	0.36	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	4157	1/1	0.21	-	87,87,87,87	0
88	MG	A5	3881	1/1	0.27	-	60,60,60,60	0
88	MG	A1	4283	1/1	0.82	-	91,91,91,91	0
88	MG	A1	4379	1/1	0.19	-	70,70,70,70	0
87	OHX	A1	3422	7/7	0.18	-	78,78,78,78	0
87	OHX	A5	3587	7/7	0.20	-	96,96,96,96	7
88	MG	A5	4359	1/1	0.20	-	86,86,86,86	0
88	MG	A5	4211	1/1	0.29	-	77,77,77,77	0
87	OHX	A5	3666	7/7	0.24	-	127,127,127,127	7
88	MG	Dg	202	1/1	0.12	-	50,50,50,50	0
88	MG	A1	4066	1/1	0.20	-	53,53,53,53	0
88	MG	A7	229	1/1	0.75	-	98,98,98,98	0
88	MG	A5	4514	1/1	1.23	-	98,98,98,98	0
88	MG	A1	3840	1/1	0.32	-	59,59,59,59	0
87	OHX	A1	3462	7/7	0.17	-	91,91,91,91	7
87	OHX	A6	1972	7/7	0.17	-	109,109,109,109	7
88	MG	A2	2110	1/1	0.32	-	57,57,57,57	0
88	MG	A5	4574	1/1	0.29	-	74,74,74,74	0
88	MG	A5	4336	1/1	0.41	-	77,77,77,77	0
87	OHX	A5	3812	7/7	0.12	-	135,135,135,135	7
87	OHX	A1	3795	7/7	0.34	-	195,195,195,195	7
88	MG	A1	4001	1/1	0.28	-	50,50,50,50	0
87	OHX	A5	3637	7/7	0.15	-	178,178,178,178	7
87	OHX	A5	3536	7/7	0.17	-	97,97,97,97	7
87	OHX	A5	3423	7/7	0.18	-	68,68,68,68	0
87	OHX	A6	2063	7/7	0.19	-	176,176,176,176	7
88	MG	A6	2213	1/1	0.09	-	65,65,65,65	0
88	MG	A5	4508	1/1	0.15	-	67,67,67,67	0
88	MG	A1	4105	1/1	0.25	-	84,84,84,84	0
88	MG	A5	4520	1/1	0.28	-	81,81,81,81	0
88	MG	A5	3988	1/1	0.35	-	51,51,51,51	0
88	MG	A5	4358	1/1	0.42	-	54,54,54,54	0
87	OHX	A5	3613	7/7	0.13	-	137,137,137,137	7
88	MG	A5	3962	1/1	0.37	-	41,41,41,41	0
88	MG	A5	4192	1/1	0.32	-	95,95,95,95	0
87	OHX	A1	3750	7/7	0.31	-	118,118,118,118	7
87	OHX	A5	3504	7/7	0.17	-	101,101,101,101	7
88	MG	BG	301	1/1	0.22	-	91,91,91,91	0
87	OHX	A6	2061	7/7	0.26	-	172,172,172,172	7
88	MG	A2	2216	1/1	0.10	-	63,63,63,63	0
88	MG	A5	4441	1/1	0.24	-	61,61,61,61	0
88	MG	A8	201	1/1	0.12	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	3404	1/1	0.29	-	74,74,74,74	0
87	OHX	A5	3413	7/7	0.27	-	71,71,71,71	0
87	OHX	A5	3535	7/7	0.16	-	77,77,77,77	7
88	MG	A5	4377	1/1	0.27	-	85,85,85,85	0
88	MG	A1	4433	1/1	0.54	-	67,67,67,67	0
88	MG	A1	3895	1/1	0.24	-	92,92,92,92	0
88	MG	A1	4442	1/1	0.34	-	91,91,91,91	0
88	MG	A6	2202	1/1	0.30	-	71,71,71,71	0
88	MG	A5	4411	1/1	0.22	-	94,94,94,94	0
88	MG	A1	4078	1/1	0.20	-	80,80,80,80	0
88	MG	A1	4063	1/1	0.24	-	73,73,73,73	0
87	OHX	A5	3545	7/7	0.14	-	133,133,133,133	7
88	MG	A2	2223	1/1	1.34	-	156,156,156,156	0
88	MG	A1	4508	1/1	0.24	-	58,58,58,58	0
87	OHX	A1	3538	7/7	0.18	-	105,105,105,105	7
88	MG	A5	4452	1/1	0.47	-	57,57,57,57	0
87	OHX	A5	3601	7/7	0.16	-	96,96,96,96	7
88	MG	A1	4192	1/1	0.27	-	86,86,86,86	0
88	MG	BP	203	1/1	0.33	-	71,71,71,71	0
88	MG	A2	2241	1/1	0.19	-	108,108,108,108	0
88	MG	A5	4373	1/1	0.20	-	74,74,74,74	0
87	OHX	A1	3739	7/7	0.18	-	185,185,185,185	7
87	OHX	A5	3512	7/7	0.14	-	111,111,111,111	7
88	MG	A5	4309	1/1	0.67	-	64,64,64,64	0
88	MG	DB	405	1/1	0.60	-	62,62,62,62	0
87	OHX	A1	3670	7/7	0.17	-	152,152,152,152	7
88	MG	A5	4216	1/1	0.25	-	80,80,80,80	0
87	OHX	A7	207	7/7	0.16	-	145,145,145,145	7
87	OHX	A5	3554	7/7	0.15	-	130,130,130,130	7
88	MG	A2	2126	1/1	0.34	-	54,54,54,54	0
87	OHX	A3	208	7/7	0.16	-	126,126,126,126	7
88	MG	A5	4556	1/1	0.24	-	73,73,73,73	0
87	OHX	A5	3619	7/7	0.17	-	119,119,119,119	7
87	OHX	A6	1923	7/7	0.16	-	76,76,76,76	7
87	OHX	A5	3696	7/7	0.17	-	167,167,167,167	7
88	MG	A5	4025	1/1	0.31	-	38,38,38,38	0
88	MG	A5	4372	1/1	0.64	-	74,74,74,74	0
87	OHX	A1	3808	7/7	0.21	-	194,194,194,194	7
88	MG	A1	4191	1/1	0.14	-	58,58,58,58	0
88	MG	DO	207	1/1	0.43	-	109,109,109,109	0
88	MG	A5	4046	1/1	0.13	-	39,39,39,39	0
88	MG	A6	2208	1/1	0.11	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A2	2007	7/7	0.16	-	146,146,146,146	7
88	MG	A1	4151	1/1	0.29	-	71,71,71,71	0
88	MG	A5	4250	1/1	0.46	-	110,110,110,110	0
88	MG	DD	306	1/1	0.39	-	77,77,77,77	0
87	OHX	A1	3705	7/7	0.13	-	164,164,164,164	7
88	MG	Ba	206	1/1	0.21	-	61,61,61,61	0
88	MG	A2	2197	1/1	0.17	-	80,80,80,80	0
87	OHX	A1	3459	7/7	0.18	-	86,86,86,86	7
88	MG	A7	238	1/1	0.46	-	95,95,95,95	0
88	MG	A6	2191	1/1	0.30	-	84,84,84,84	0
87	OHX	A2	2016	7/7	0.14	-	156,156,156,156	7
88	MG	A5	3863	1/1	0.32	-	51,51,51,51	0
88	MG	BP	211	1/1	0.64	-	123,123,123,123	0
88	MG	A1	4455	1/1	0.20	-	79,79,79,79	0
88	MG	A5	3965	1/1	0.37	-	64,64,64,64	0
87	OHX	A2	1948	7/7	0.15	-	108,108,108,108	7
88	MG	A5	4282	1/1	0.29	-	52,52,52,52	0
88	MG	A5	4258	1/1	0.29	-	70,70,70,70	0
88	MG	A1	4343	1/1	0.30	-	78,78,78,78	0
88	MG	A5	3844	1/1	0.17	-	59,59,59,59	0
87	OHX	A1	3461	7/7	0.16	-	104,104,104,104	0
87	OHX	A5	3588	7/7	0.18	-	106,106,106,106	7
87	OHX	A5	3815	7/7	0.21	-	221,221,221,221	7
87	OHX	A6	2066	7/7	0.25	-	119,119,119,119	7
88	MG	A1	4128	1/1	0.27	-	63,63,63,63	0
88	MG	A2	2228	1/1	0.13	-	85,85,85,85	0
88	MG	A6	2206	1/1	0.16	-	63,63,63,63	0
87	OHX	A6	2014	7/7	0.14	-	144,144,144,144	7
88	MG	A2	2133	1/1	0.19	-	72,72,72,72	0
88	MG	DB	409	1/1	0.52	-	56,56,56,56	0
88	MG	A2	2099	1/1	0.22	-	53,53,53,53	0
88	MG	A5	4210	1/1	0.23	-	79,79,79,79	0
88	MG	A5	4078	1/1	0.29	-	49,49,49,49	0
87	OHX	A5	3628	7/7	0.16	-	129,129,129,129	7
88	MG	A1	4338	1/1	0.52	-	84,84,84,84	0
87	OHX	AC	301	7/7	0.70	-	213,213,213,213	7
87	OHX	A5	3784	7/7	0.19	-	173,173,173,173	7
88	MG	A2	2104	1/1	0.27	-	63,63,63,63	0
88	MG	DD	308	1/1	0.74	-	70,70,70,70	0
88	MG	A6	2297	1/1	0.65	-	68,68,68,68	0
88	MG	A5	3837	1/1	0.32	-	58,58,58,58	0
88	MG	A1	4333	1/1	0.57	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A5	3484	7/7	0.15	-	99,99,99,99	7
87	OHX	A1	3690	7/7	0.21	-	178,178,178,178	7
88	MG	A1	4386	1/1	0.45	-	78,78,78,78	0
88	MG	A1	3955	1/1	0.39	-	42,42,42,42	0
87	OHX	A2	1940	7/7	0.18	-	100,100,100,100	7
87	OHX	A5	3692	7/7	0.13	-	170,170,170,170	7
87	OHX	A5	3586	7/7	0.15	-	112,112,112,112	7
88	MG	A3	222	1/1	0.16	-	66,66,66,66	0
88	MG	DB	415	1/1	0.23	-	91,91,91,91	0
88	MG	A5	4195	1/1	0.18	-	72,72,72,72	0
88	MG	A5	4434	1/1	0.28	-	72,72,72,72	0
87	OHX	A1	3530	7/7	0.14	-	125,125,125,125	7
88	MG	A5	4023	1/1	0.39	-	44,44,44,44	0
87	OHX	A1	3708	7/7	0.15	-	158,158,158,158	7
87	OHX	A1	3529	7/7	0.20	-	77,77,77,77	7
88	MG	A6	2169	1/1	0.33	-	77,77,77,77	0
88	MG	A1	4073	1/1	0.13	-	57,57,57,57	0
87	OHX	A1	3465	7/7	0.16	-	94,94,94,94	7
88	MG	A5	4402	1/1	0.52	-	91,91,91,91	0
87	OHX	A1	3411	7/7	0.22	-	71,71,71,71	0
87	OHX	A1	3573	7/7	0.16	-	120,120,120,120	7
87	OHX	A5	3454	7/7	0.18	-	103,103,103,103	0
88	MG	A5	3950	1/1	0.44	-	38,38,38,38	0
88	MG	A1	3920	1/1	0.24	-	53,53,53,53	0
88	MG	A1	4108	1/1	0.27	-	60,60,60,60	0
88	MG	A1	4445	1/1	0.30	-	69,69,69,69	0
87	OHX	A2	1954	7/7	0.20	-	162,162,162,162	7
87	OHX	A7	205	7/7	0.18	-	106,106,106,106	7
88	MG	A6	2296	1/1	1.13	-	119,119,119,119	0
87	OHX	A1	3445	7/7	0.16	-	81,81,81,81	0
87	OHX	A5	3403	7/7	0.18	-	171,171,171,171	7
88	MG	CY	204	1/1	0.14	-	56,56,56,56	0
87	OHX	A5	3532	7/7	0.16	-	164,164,164,164	7
87	OHX	A1	3425	7/7	0.18	-	85,85,85,85	0
88	MG	A5	3956	1/1	0.25	-	39,39,39,39	0
88	MG	A2	2115	1/1	0.29	-	78,78,78,78	0
88	MG	A1	4320	1/1	0.24	-	59,59,59,59	0
88	MG	A5	3827	1/1	0.36	-	67,67,67,67	0
87	OHX	A5	3794	7/7	0.20	-	179,179,179,179	7
88	MG	A1	4360	1/1	0.31	-	88,88,88,88	0
87	OHX	DC	402	7/7	0.25	-	145,145,145,145	7
87	OHX	A5	3741	7/7	0.12	-	185,185,185,185	7

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	MG	A1	4007	1/1	0.20	-	29,29,29,29	0
88	MG	A1	3959	1/1	0.42	-	43,43,43,43	0
88	MG	A5	4549	1/1	0.41	-	70,70,70,70	0
88	MG	A2	2136	1/1	0.15	-	70,70,70,70	0
87	OHX	A6	2069	7/7	0.16	-	206,206,206,206	7
87	OHX	A1	3449	7/7	0.17	-	99,99,99,99	0
88	MG	A2	2161	1/1	0.22	-	58,58,58,58	0
87	OHX	A2	2044	7/7	0.14	-	162,162,162,162	7
88	MG	A5	4241	1/1	0.32	-	106,106,106,106	0
87	OHX	A1	3494	7/7	0.15	-	133,133,133,133	0
88	MG	A1	3930	1/1	0.31	-	38,38,38,38	0
87	OHX	A2	1961	7/7	0.15	-	150,150,150,150	7
87	OHX	A6	2000	7/7	0.17	-	128,128,128,128	7
87	OHX	A2	1964	7/7	0.16	-	135,135,135,135	7
88	MG	A6	2250	1/1	0.47	-	96,96,96,96	0
88	MG	A5	4374	1/1	0.36	-	95,95,95,95	0
88	MG	A1	4496	1/1	0.83	-	82,82,82,82	0
88	MG	A5	4154	1/1	0.17	-	54,54,54,54	0
87	OHX	A6	1917	7/7	0.16	-	100,100,100,100	7
88	MG	A1	4130	1/1	0.24	-	69,69,69,69	0
88	MG	A6	2172	1/1	0.28	-	66,66,66,66	0
88	MG	A5	4056	1/1	0.26	-	78,78,78,78	0
88	MG	A5	4253	1/1	0.23	-	75,75,75,75	0
87	OHX	A1	3525	7/7	0.18	-	101,101,101,101	7
88	MG	A1	4447	1/1	0.45	-	104,104,104,104	0
87	OHX	A1	3629	7/7	0.17	-	128,128,128,128	7
87	OHX	A1	3738	7/7	0.26	-	138,138,138,138	7
88	MG	A2	2092	1/1	0.23	-	69,69,69,69	0
88	MG	A6	2300	1/1	0.45	-	56,56,56,56	0
88	MG	A5	3873	1/1	0.33	-	60,60,60,60	0
88	MG	A1	4076	1/1	0.25	-	64,64,64,64	0
88	MG	BQ	202	1/1	0.69	-	80,80,80,80	0
87	OHX	A5	3561	7/7	0.14	-	121,121,121,121	7
88	MG	A5	4418	1/1	0.21	-	91,91,91,91	0
87	OHX	A2	1963	7/7	0.14	-	129,129,129,129	7
87	OHX	A5	3520	7/7	0.16	-	113,113,113,113	7
88	MG	A6	2277	1/1	0.28	-	79,79,79,79	0
88	MG	A5	4119	1/1	0.29	-	65,65,65,65	0
88	MG	A5	4068	1/1	0.18	-	72,72,72,72	0
88	MG	A2	2224	1/1	0.18	-	77,77,77,77	0
87	OHX	A1	3501	7/7	0.16	-	94,94,94,94	7
88	MG	A6	2309	1/1	0.32	-	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	A1	3654	7/7	0.11	-	149,149,149,149	7
88	MG	A5	4410	1/1	0.54	-	66,66,66,66	0
87	OHX	A1	3548	7/7	0.19	-	136,136,136,136	7

6.5 Other polymers ⓘ

There are no such residues in this entry.