



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2017 – 09:37 PM EST

PDB ID : 4V7R  
Title : Yeast 80S ribosome.  
Authors : Ben-Shem, A.; Jenner, L.; Yusupova, G.; Yusupov, M.  
Deposited on : unknown  
Resolution : 4.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

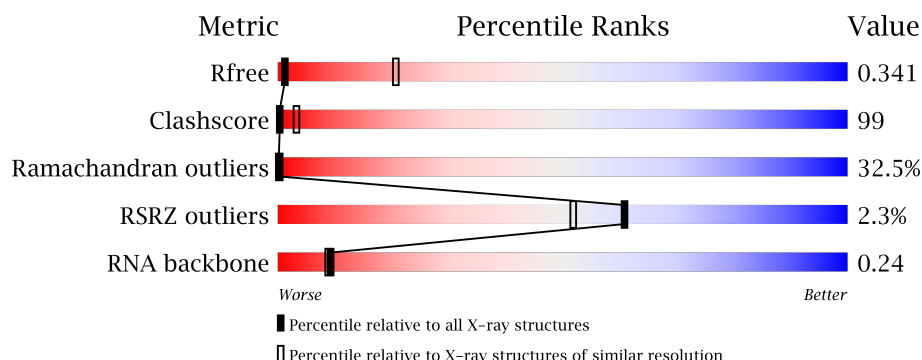
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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.



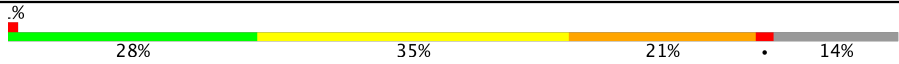

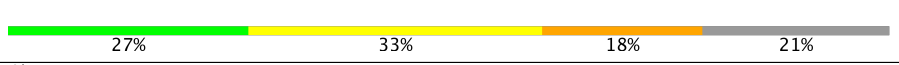

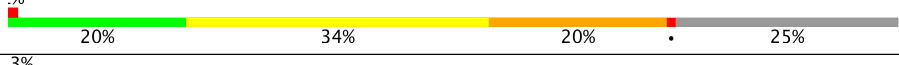
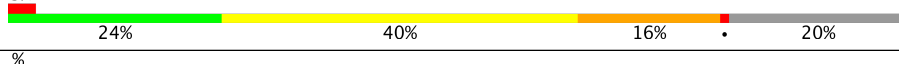
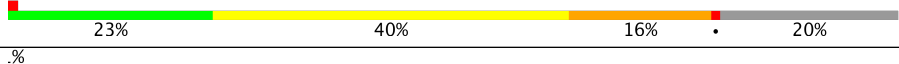


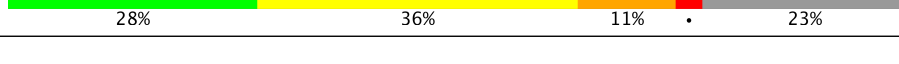
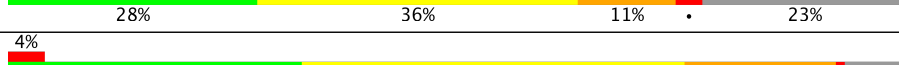
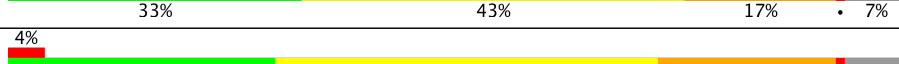
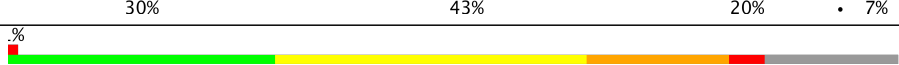
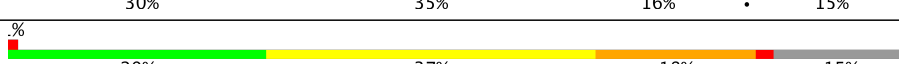
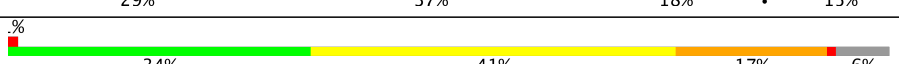
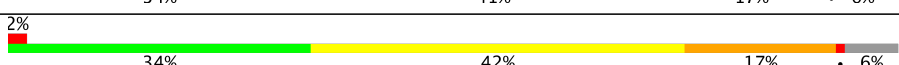

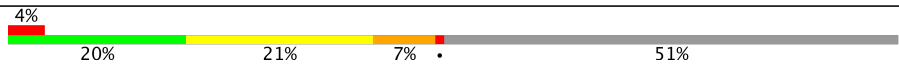
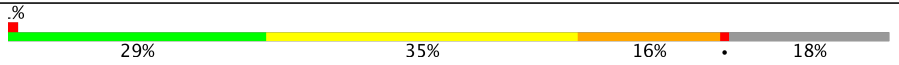
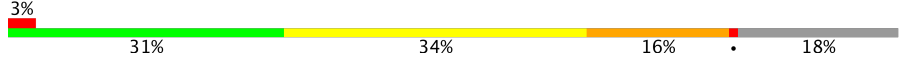

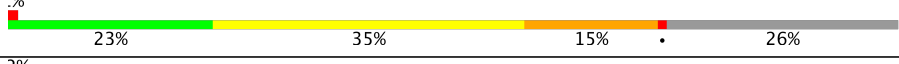
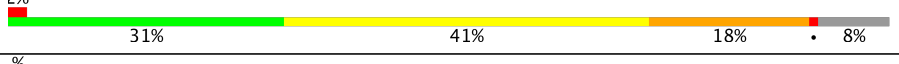
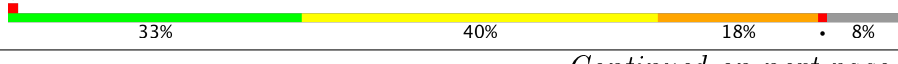

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1088 (4.40-3.60)
Clashscore	112137	1187 (4.40-3.60)
Ramachandran outliers	110173	1139 (4.40-3.60)
RSRZ outliers	101464	1099 (4.40-3.60)
RNA backbone	2435	1026 (5.04-2.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A1	1800	
1	C1	1800	
2	AA	252	
2	CA	252	
3	AB	254	


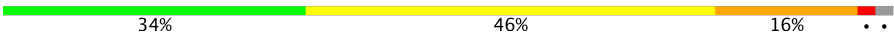
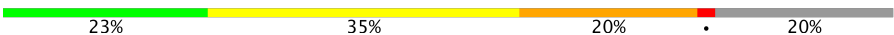



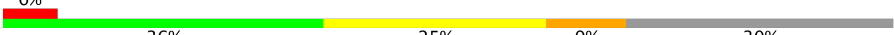
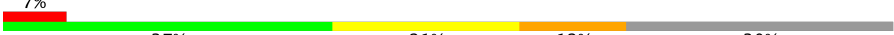





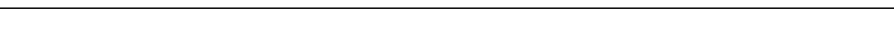
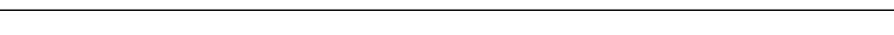
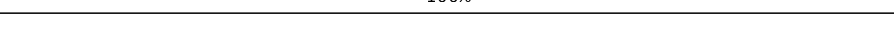
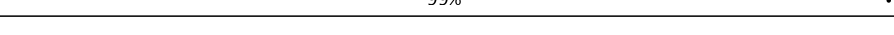
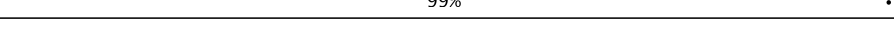
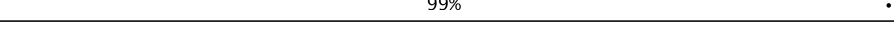
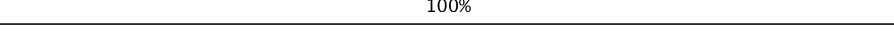
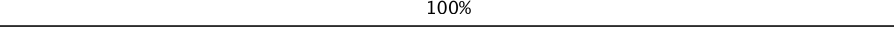
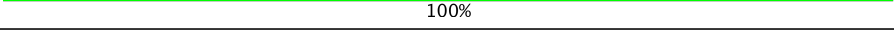
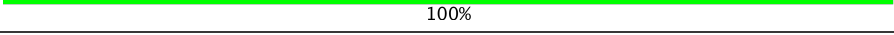
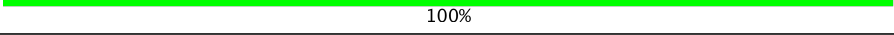
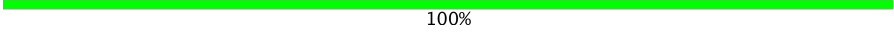
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Mol	Chain	Length	Quality of chain
3	CB	254	
4	AC	240	
4	CC	240	
5	AD	225	
5	CD	225	
6	AE	197	
6	CE	197	
7	AF	156	
7	CF	156	
8	AG	151	
8	CG	151	
9	AH	137	
9	CH	137	
10	AI	142	
10	CI	142	
11	AJ	143	
11	CJ	143	
12	AK	136	
12	CK	136	
13	AL	146	
13	CL	146	
14	AM	144	
14	CM	144	
15	AN	121	
15	CN	121	

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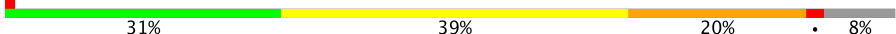
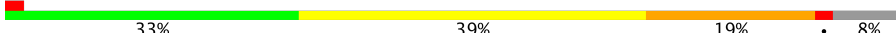

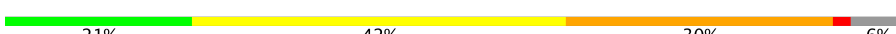
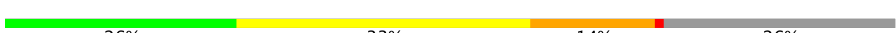




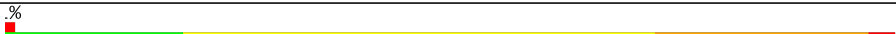





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Mol	Chain	Length	Quality of chain
16	AO	130	
16	CO	130	
17	AP	145	
17	CP	145	
18	AQ	108	
18	CQ	108	
19	AR	67	
19	CR	67	
20	AS	56	
20	CS	56	
21	AT	319	
21	CT	319	
22	Aa	20	
22	Bo	20	
22	Ca	20	
23	Ab	105	
23	Cb	105	
24	Ac	93	
24	Cc	93	
25	Ad	35	
25	Cd	35	
26	Ae	21	
26	Bj	21	
26	Dj	21	
27	Af	11	

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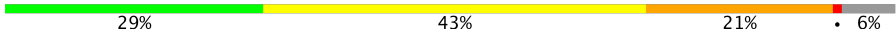
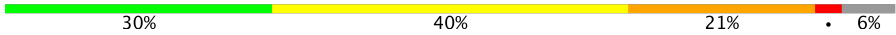
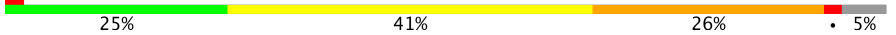
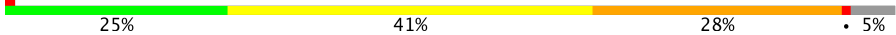
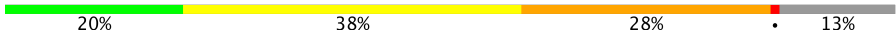
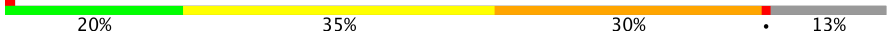
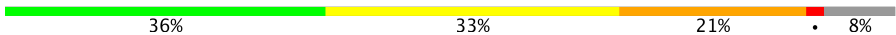
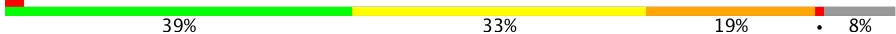
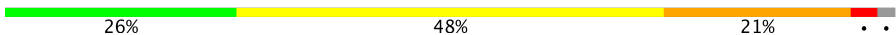
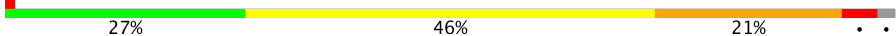
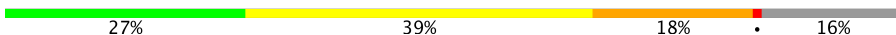
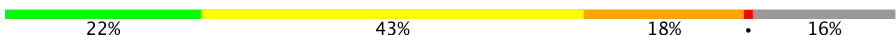
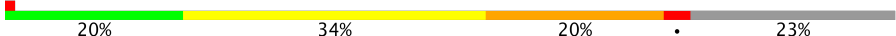













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Mol	Chain	Length	Quality of chain
28	Ah	41	 100%
28	Ch	41	 100%
29	B1	3396	 2% 28% 45% 19% 6%
29	D1	3396	 3% 30% 44% 17% 6%
30	B2	121	 35% 45% 21%
30	D2	121	 33% 44% 22%
31	B3	158	 4% 39% 47% 11%
31	D3	158	 41% 50% 6%
32	BA	217	 15% 53% 36% 8% 2%
32	DA	217	 19% 59% 32% 7% 1%
33	BB	254	 31% 39% 20% 8% 2%
33	DB	254	 2% 33% 39% 19% 8%
34	BC	387	 22% 42% 28% 6% 2%
34	DC	387	 21% 42% 30% 6% 1%
35	BD	362	 26% 33% 14% 26% 1%
35	DD	362	 26% 33% 14% 26% 1%
36	BE	297	 25% 48% 22% 3% 2%
36	DE	297	 26% 47% 22% 3% 2%
37	BF	176	 23% 48% 27% 2% 1%
37	DF	176	 20% 53% 24% 3% 1%
38	BG	244	 31% 36% 19% 12% 1%
38	DG	244	 31% 35% 20% 12% 1%
39	BH	256	 2% 26% 29% 13% 32%
39	DH	256	 2% 30% 25% 12% 32%
40	BI	191	 38% 40% 21% 1% 1%

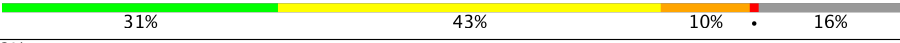

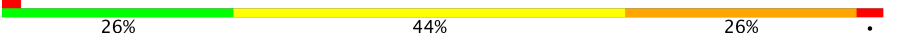
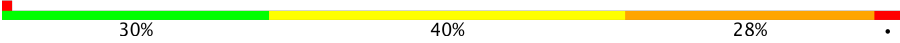


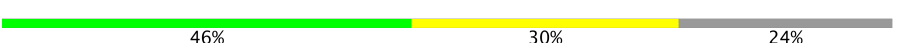
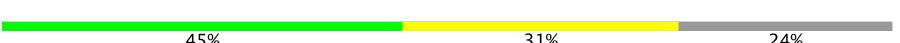



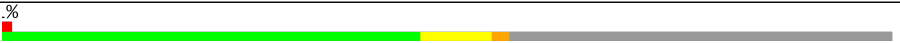
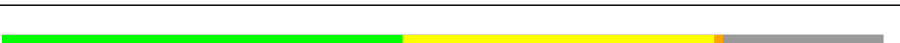
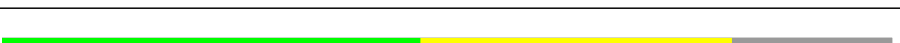


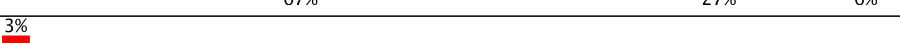
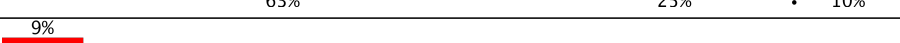



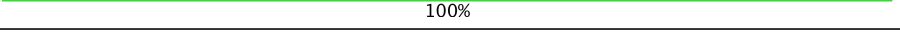
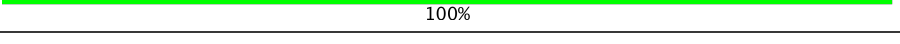
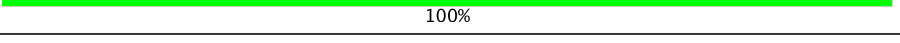
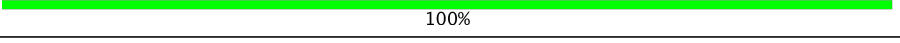
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Mol	Chain	Length	Quality of chain
40	DI	191	
41	BJ	221	
41	DJ	221	
42	BK	174	
42	DK	174	
43	BN	138	
43	DN	138	
44	BO	204	
44	DO	204	
45	BP	199	
45	DP	199	
46	BQ	184	
46	DQ	184	
47	BR	186	
47	DR	186	
48	BS	189	
48	DS	189	
49	BT	160	
49	DT	160	
50	BU	137	
50	DU	137	
51	BV	155	
51	DV	155	
52	BW	142	
52	DW	142	








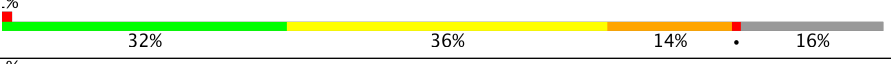

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Mol	Chain	Length	Quality of chain
53	BX	127	
53	DX	127	
54	BY	149	
54	DY	149	
55	BZ	105	
55	DZ	105	
56	Ba	113	
56	Da	113	
57	Bb	130	
57	Db	130	
58	Bc	120	
58	Dc	120	
59	Bd	88	
59	Dd	88	
60	Be	51	
60	De	51	
61	Bf	106	
61	Df	106	
62	Bg	92	
62	Dg	92	
63	Bh	44	
63	Dh	44	
64	Bi	12	
64	Di	12	
65	Bk	16	

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Mol	Chain	Length	Quality of chain
65	Dk	16	 100%
66	Bl	19	 100%
67	Bm	9	 100%
68	Bn	27	 100%
69	Bp	8	 100%
70	Bq	17	 100%
71	Br	23	 100%
72	DL	165	 % 32% 36% 14% 16%
73	DM	312	 % 14% 18% 9% 58%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
74	OHX	A1	1901	-	-	X	-
74	OHX	A1	1904	-	-	-	X
74	OHX	A1	1905	-	-	-	X
74	OHX	A1	1907	-	-	-	X
74	OHX	A1	1910	-	-	X	-
74	OHX	A1	1913	-	-	X	-
74	OHX	A1	1914	-	-	-	X
74	OHX	A1	1915	-	-	X	-
74	OHX	A1	1916	-	-	X	-
74	OHX	A1	1917	-	-	X	-
74	OHX	A1	1923	-	-	-	X
74	OHX	A1	1925	-	-	-	X
74	OHX	A1	1929	-	-	X	-
74	OHX	A1	1930	-	-	-	X
74	OHX	A1	1931	-	-	X	-
74	OHX	A1	1932	-	-	-	X
74	OHX	A1	1934	-	-	-	X
74	OHX	A1	1935	-	-	X	-
74	OHX	A1	1938	-	-	-	X
74	OHX	A1	1940	-	-	-	X
74	OHX	A1	1943	-	-	X	-
74	OHX	A1	1949	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
74	OHX	A1	1951	-	-	X	X
74	OHX	A1	1952	-	-	-	X
74	OHX	A1	1958	-	-	-	X
74	OHX	A1	1959	-	-	X	X
74	OHX	A1	1965	-	-	-	X
74	OHX	A1	1966	-	-	-	X
74	OHX	A1	1967	-	-	-	X
74	OHX	A1	1969	-	-	-	X
74	OHX	A1	1970	-	-	-	X
74	OHX	A1	1972	-	-	-	X
74	OHX	A1	1975	-	-	X	-
74	OHX	A1	1976	-	-	X	-
74	OHX	A1	1977	-	-	-	X
74	OHX	A1	1978	-	-	-	X
74	OHX	A1	1979	-	-	X	-
74	OHX	A1	1986	-	-	X	-
74	OHX	A1	1988	-	-	-	X
74	OHX	A1	1991	-	-	X	X
74	OHX	A1	1993	-	-	-	X
74	OHX	A1	1999	-	-	-	X
74	OHX	A1	2002	-	-	-	X
74	OHX	AS	101	-	-	X	-
74	OHX	AT	401	-	-	-	X
74	OHX	B1	3401	-	-	-	X
74	OHX	B1	3402	-	-	-	X
74	OHX	B1	3403	-	-	-	X
74	OHX	B1	3423	-	-	-	X
74	OHX	B1	3428	-	-	X	-
74	OHX	B1	3435	-	-	-	X
74	OHX	B1	3438	-	-	X	-
74	OHX	B1	3441	-	-	-	X
74	OHX	B1	3449	-	-	X	-
74	OHX	B1	3450	-	-	X	-
74	OHX	B1	3453	-	-	-	X
74	OHX	B1	3456	-	-	-	X
74	OHX	B1	3459	-	-	X	-
74	OHX	B1	3461	-	-	-	X
74	OHX	B1	3468	-	-	-	X
74	OHX	B1	3469	-	-	-	X
74	OHX	B1	3476	-	-	-	X
74	OHX	B1	3479	-	-	X	X
74	OHX	B1	3484	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
74	OHX	B1	3486	-	-	-	X
74	OHX	B1	3492	-	-	X	-
74	OHX	B1	3495	-	-	-	X
74	OHX	B1	3496	-	-	X	-
74	OHX	B1	3498	-	-	-	X
74	OHX	B1	3501	-	-	-	X
74	OHX	B1	3504	-	-	-	X
74	OHX	B1	3505	-	-	X	-
74	OHX	B1	3506	-	-	-	X
74	OHX	B1	3512	-	-	-	X
74	OHX	B1	3519	-	-	X	-
74	OHX	B1	3520	-	-	-	X
74	OHX	B1	3521	-	-	-	X
74	OHX	B1	3524	-	-	X	X
74	OHX	B1	3525	-	-	-	X
74	OHX	B1	3528	-	-	-	X
74	OHX	B1	3529	-	-	X	-
74	OHX	B1	3530	-	-	-	X
74	OHX	B1	3534	-	-	-	X
74	OHX	B1	3536	-	-	X	X
74	OHX	B1	3537	-	-	X	X
74	OHX	B1	3539	-	-	-	X
74	OHX	B1	3542	-	-	-	X
74	OHX	B1	3544	-	-	X	X
74	OHX	B1	3549	-	-	-	X
74	OHX	B1	3551	-	-	-	X
74	OHX	B1	3556	-	-	-	X
74	OHX	B1	3558	-	-	X	-
74	OHX	B1	3560	-	-	-	X
74	OHX	B1	3562	-	-	-	X
74	OHX	B1	3563	-	-	X	X
74	OHX	B1	3566	-	-	-	X
74	OHX	B1	3567	-	-	X	-
74	OHX	B1	3568	-	-	-	X
74	OHX	B1	3571	-	-	-	X
74	OHX	B1	3572	-	-	-	X
74	OHX	B1	3575	-	-	-	X
74	OHX	B1	3577	-	-	-	X
74	OHX	B1	3579	-	-	-	X
74	OHX	B1	3580	-	-	-	X
74	OHX	B1	3581	-	-	X	X
74	OHX	B1	3582	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
74	OHX	B1	3583	-	-	-	X
74	OHX	B1	3587	-	-	X	-
74	OHX	B1	3589	-	-	-	X
74	OHX	B1	3594	-	-	-	X
74	OHX	B1	3595	-	-	-	X
74	OHX	B1	3599	-	-	X	X
74	OHX	B1	3604	-	-	-	X
74	OHX	B1	3605	-	-	X	-
74	OHX	B1	3608	-	-	-	X
74	OHX	B1	3611	-	-	-	X
74	OHX	B1	3615	-	-	-	X
74	OHX	B1	3616	-	-	X	X
74	OHX	B1	3617	-	-	X	-
74	OHX	B1	3619	-	-	X	-
74	OHX	B1	3620	-	-	X	-
74	OHX	B2	201	-	-	X	-
74	OHX	B2	203	-	-	-	X
74	OHX	B3	206	-	-	X	-
74	OHX	B3	209	-	-	-	X
74	OHX	B3	210	-	-	-	X
74	OHX	C1	1903	-	-	-	X
74	OHX	C1	1912	-	-	X	-
74	OHX	C1	1916	-	-	X	-
74	OHX	C1	1917	-	-	X	-
74	OHX	C1	1919	-	-	-	X
74	OHX	C1	1924	-	-	X	-
74	OHX	C1	1928	-	-	X	-
74	OHX	C1	1929	-	-	-	X
74	OHX	C1	1930	-	-	X	-
74	OHX	C1	1933	-	-	X	-
74	OHX	C1	1940	-	-	-	X
74	OHX	C1	1947	-	-	-	X
74	OHX	C1	1955	-	-	X	-
74	OHX	C1	1958	-	-	-	X
74	OHX	C1	1963	-	-	-	X
74	OHX	C1	1964	-	-	X	-
74	OHX	C1	1967	-	-	-	X
74	OHX	C1	1970	-	-	X	-
74	OHX	C1	1972	-	-	-	X
74	OHX	C1	1973	-	-	-	X
74	OHX	C1	1974	-	-	-	X
74	OHX	C1	1975	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
74	OHX	C1	1979	-	-	-	X
74	OHX	C1	1983	-	-	X	-
74	OHX	C1	1986	-	-	-	X
74	OHX	C1	1992	-	-	-	X
74	OHX	C1	1993	-	-	-	X
74	OHX	C1	1995	-	-	-	X
74	OHX	C1	1997	-	-	-	X
74	OHX	C1	1998	-	-	-	X
74	OHX	C1	2000	-	-	-	X
74	OHX	C1	2001	-	-	X	-
74	OHX	CS	101	-	-	X	-
74	OHX	D1	3401	-	-	-	X
74	OHX	D1	3402	-	-	-	X
74	OHX	D1	3405	-	-	-	X
74	OHX	D1	3408	-	-	X	-
74	OHX	D1	3409	-	-	-	X
74	OHX	D1	3410	-	-	-	X
74	OHX	D1	3413	-	-	-	X
74	OHX	D1	3415	-	-	X	-
74	OHX	D1	3430	-	-	X	-
74	OHX	D1	3431	-	-	X	-
74	OHX	D1	3435	-	-	-	X
74	OHX	D1	3437	-	-	-	X
74	OHX	D1	3439	-	-	-	X
74	OHX	D1	3442	-	-	X	-
74	OHX	D1	3446	-	-	X	-
74	OHX	D1	3452	-	-	X	-
74	OHX	D1	3459	-	-	-	X
74	OHX	D1	3463	-	-	X	-
74	OHX	D1	3471	-	-	X	-
74	OHX	D1	3473	-	-	X	-
74	OHX	D1	3475	-	-	-	X
74	OHX	D1	3476	-	-	-	X
74	OHX	D1	3477	-	-	X	-
74	OHX	D1	3479	-	-	-	X
74	OHX	D1	3480	-	-	X	-
74	OHX	D1	3485	-	-	-	X
74	OHX	D1	3489	-	-	-	X
74	OHX	D1	3490	-	-	-	X
74	OHX	D1	3496	-	-	-	X
74	OHX	D1	3502	-	-	X	-
74	OHX	D1	3507	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
74	OHX	D1	3508	-	-	-	X
74	OHX	D1	3510	-	-	-	X
74	OHX	D1	3514	-	-	-	X
74	OHX	D1	3516	-	-	-	X
74	OHX	D1	3517	-	-	-	X
74	OHX	D1	3522	-	-	-	X
74	OHX	D1	3524	-	-	-	X
74	OHX	D1	3525	-	-	-	X
74	OHX	D1	3527	-	-	-	X
74	OHX	D1	3532	-	-	-	X
74	OHX	D1	3535	-	-	-	X
74	OHX	D1	3538	-	-	-	X
74	OHX	D1	3543	-	-	X	-
74	OHX	D1	3544	-	-	-	X
74	OHX	D1	3545	-	-	-	X
74	OHX	D1	3546	-	-	-	X
74	OHX	D1	3550	-	-	-	X
74	OHX	D1	3551	-	-	-	X
74	OHX	D1	3552	-	-	-	X
74	OHX	D1	3554	-	-	-	X
74	OHX	D1	3555	-	-	X	-
74	OHX	D1	3558	-	-	-	X
74	OHX	D1	3563	-	-	-	X
74	OHX	D1	3564	-	-	-	X
74	OHX	D1	3567	-	-	X	-
74	OHX	D1	3568	-	-	X	X
74	OHX	D1	3574	-	-	X	-
74	OHX	D1	3579	-	-	-	X
74	OHX	D1	3581	-	-	-	X
74	OHX	D1	3582	-	-	X	-
74	OHX	D1	3583	-	-	X	-
74	OHX	D1	3584	-	-	-	X
74	OHX	D1	3585	-	-	X	-
74	OHX	D1	3586	-	-	-	X
74	OHX	D1	3587	-	-	-	X
74	OHX	D1	3588	-	-	X	-
74	OHX	D1	3589	-	-	X	X
74	OHX	D1	3592	-	-	X	-
74	OHX	D1	3593	-	-	-	X
74	OHX	D1	3594	-	-	-	X
74	OHX	D1	3597	-	-	-	X
74	OHX	D1	3602	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
74	OHX	D1	3603	-	-	-	X
74	OHX	D1	3607	-	-	X	-
74	OHX	D1	3613	-	-	-	X
74	OHX	D1	3615	-	-	-	X
74	OHX	D1	3617	-	-	-	X
74	OHX	D1	3618	-	-	-	X
74	OHX	D1	3620	-	-	-	X
74	OHX	D1	3623	-	-	-	X
74	OHX	D1	3624	-	-	-	X
74	OHX	D1	3625	-	-	X	-
74	OHX	D2	201	-	-	X	-
74	OHX	D2	202	-	-	-	X
74	OHX	D2	207	-	-	X	-
74	OHX	D3	202	-	-	X	-
74	OHX	D3	204	-	-	X	-
74	OHX	D3	205	-	-	X	-
74	OHX	D3	208	-	-	-	X
74	OHX	D3	209	-	-	X	-
74	OHX	D3	210	-	-	-	X
74	OHX	D3	211	-	-	-	X
74	OHX	D3	212	-	-	X	X
74	OHX	DO	301	-	-	X	-

## 2 Entry composition

There are 74 unique types of molecules in this entry. The entry contains 309610 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A1	1789	Total	C	N	O	P	0	0	0
			38107	17037	6732	12549	1789			
1	C1	1789	Total	C	N	O	P	0	0	0
			38107	17037	6732	12549	1789			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	AA	220	Total	C	N	O	0	0	0
			1090	650	220	220			
2	CA	220	Total	C	N	O	0	0	0
			1090	650	220	220			

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	AB	219	Total	C	N	O	0	0	0
			1074	636	219	219			
3	CB	219	Total	C	N	O	0	0	0
			1074	636	219	219			

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	AC	189	Total	C	N	O	0	0	0
			928	550	189	189			
4	CC	189	Total	C	N	O	0	0	0
			928	550	189	189			

- Molecule 5 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	AD	169	Total	C	N	O	0	0	0
			836	498	169	169			
5	CD	169	Total	C	N	O	0	0	0
			836	498	169	169			

- Molecule 6 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	AE	157	Total	C	N	O	0	0	0
			777	463	157	157			
6	CE	157	Total	C	N	O	0	0	0
			777	463	157	157			

- Molecule 7 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	AF	77	Total	C	N	O	0	0	0
			382	228	77	77			
7	CF	77	Total	C	N	O	0	0	0
			382	228	77	77			

- Molecule 8 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	AG	117	Total	C	N	O	0	0	0
			580	346	117	117			
8	CG	117	Total	C	N	O	0	0	0
			580	346	117	117			

- Molecule 9 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AH	128	Total	C	N	O	0	0	0
			627	371	128	128			
9	CH	128	Total	C	N	O	0	0	0
			627	371	128	128			

- Molecule 10 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	AI	121	Total	C	N	O	0	0	0
			596	354	121	121			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CI	121	Total	C	N	O	0	0	0
			596	354	121	121			

- Molecule 11 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	AJ	134	Total	C	N	O	0	0	0
			658	390	134	134			
11	CJ	134	Total	C	N	O	0	0	0
			658	390	134	134			

- Molecule 12 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	AK	67	Total	C	N	O	0	0	0
			332	198	67	67			
12	CK	67	Total	C	N	O	0	0	0
			332	198	67	67			

- Molecule 13 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	AL	120	Total	C	N	O	0	0	0
			591	351	120	120			
13	CL	120	Total	C	N	O	0	0	0
			591	351	120	120			

- Molecule 14 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AM	106	Total	C	N	O	0	0	0
			521	309	106	106			
14	CM	106	Total	C	N	O	0	0	0
			521	309	106	106			

- Molecule 15 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	AN	111	Total	C	N	O	0	0	0
			551	329	111	111			
15	CN	111	Total	C	N	O	0	0	0
			551	329	111	111			

- Molecule 16 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	AO	127	Total	C	N	O	0	0	0
			622	368	127	127			
16	CO	127	Total	C	N	O	0	0	0
			622	368	127	127			

- Molecule 17 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	AP	116	Total	C	N	O	0	0	0
			566	334	116	116			
17	CP	116	Total	C	N	O	0	0	0
			566	334	116	116			

- Molecule 18 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AQ	67	Total	C	N	O	0	0	0
			332	198	67	67			
18	CQ	63	Total	C	N	O	0	0	0
			312	186	63	63			

- Molecule 19 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	AR	47	Total	C	N	O	0	0	0
			230	136	47	47			
19	CR	47	Total	C	N	O	0	0	0
			230	136	47	47			

- Molecule 20 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	AS	39	Total	C	N	O	0	0	0
			190	112	39	39			
20	CS	39	Total	C	N	O	0	0	0
			190	112	39	39			

- Molecule 21 is a protein called Guanine nucleotide-binding protein subunit beta-like protein; RACK-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AT	313	Total 1543	C 917	N 313	O 313	0	0	0
21	CT	313	Total 1543	C 917	N 313	O 313	0	0	0

- Molecule 22 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	Aa	20	Total 100	C 60	N 20	O 20	0	0	0
22	Bo	20	Total 100	C 60	N 20	O 20	0	0	0
22	Ca	20	Total 100	C 60	N 20	O 20	0	0	0

- Molecule 23 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	Ab	105	Total 525	C 315	N 105	O 105	0	0	0
23	Cb	105	Total 525	C 315	N 105	O 105	0	0	0

- Molecule 24 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	Ac	93	Total 465	C 279	N 93	O 93	0	0	0
24	Cc	93	Total 465	C 279	N 93	O 93	0	0	0

- Molecule 25 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	Ad	35	Total 175	C 105	N 35	O 35	0	0	0
25	Cd	35	Total 175	C 105	N 35	O 35	0	0	0

- Molecule 26 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	Ae	21	Total	C	N	O	0	0	0
			105	63	21	21			
26	Bj	21	Total	C	N	O	0	0	0
			105	63	21	21			
26	Dj	21	Total	C	N	O	0	0	0
			105	63	21	21			

- Molecule 27 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	Af	11	Total	C	N	O	0	0	0
			55	33	11	11			

- Molecule 28 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	Ah	41	Total	C	N	O	0	0	0
			205	123	41	41			
28	Ch	41	Total	C	N	O	0	0	0
			205	123	41	41			

- Molecule 29 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B1	3206	Total	C	N	O	P	0	0	0
			68577	30632	12365	22374	3206			
29	D1	3206	Total	C	N	O	P	0	0	0
			68577	30632	12365	22374	3206			

- Molecule 30 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B2	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
30	D2	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 31 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B3	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D3	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 32 is a protein called 60S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
32	BA	213	Total	C	N	O	0	0	0
			1055	629	213	213			
32	DA	213	Total	C	N	O	0	0	0
			1055	629	213	213			

- Molecule 33 is a protein called 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
33	BB	234	Total	C	N	O	0	0	0
			1106	638	234	234			
33	DB	234	Total	C	N	O	0	0	0
			1106	638	234	234			

- Molecule 34 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
34	BC	364	Total	C	N	O	0	0	0
			1791	1063	364	364			
34	DC	364	Total	C	N	O	0	0	0
			1791	1063	364	364			

- Molecule 35 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	BD	268	Total	C	N	O	0	0	0
			1312	776	268	268			
35	DD	268	Total	C	N	O	0	0	0
			1312	776	268	268			

- Molecule 36 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BE	287	Total	C	N	O	0	0	0
			1412	838	287	287			
36	DE	287	Total	C	N	O	0	0	0
			1412	838	287	287			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BE	112	ARG	LYS	CONFLICT	UNP P26321
DE	112	ARG	LYS	CONFLICT	UNP P26321

- Molecule 37 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BF	176	Total	C	N	O	0	0	0
			873	521	176	176			
37	DF	176	Total	C	N	O	0	0	0
			873	521	176	176			

- Molecule 38 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	BG	215	Total	C	N	O	0	0	0
			1061	631	215	215			
38	DG	215	Total	C	N	O	0	0	0
			1061	631	215	215			

- Molecule 39 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	BH	173	Total	C	N	O	0	0	0
			856	510	173	173			
39	DH	173	Total	C	N	O	0	0	0
			856	510	173	173			

- Molecule 40 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	BI	191	Total	C	N	O	0	0	0
			942	560	191	191			
40	DI	191	Total	C	N	O	0	0	0
			942	560	191	191			

- Molecule 41 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	BJ	208	Total	C	N	O	0	0	0
			1027	611	208	208			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	DJ	208	Total	C	N	O	0	0	0
			1027	611	208	208			

- Molecule 42 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	BK	165	Total	C	N	O	0	0	0
			810	480	165	165			
42	DK	165	Total	C	N	O	0	0	0
			810	480	165	165			

- Molecule 43 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BN	120	Total	C	N	O	0	0	0
			593	353	120	120			
43	DN	120	Total	C	N	O	0	0	0
			593	353	120	120			

- Molecule 44 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BO	187	Total	C	N	O	0	0	0
			923	549	187	187			
44	DO	187	Total	C	N	O	0	0	0
			923	549	187	187			

- Molecule 45 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BP	196	Total	C	N	O	0	0	0
			967	575	196	196			
45	DP	196	Total	C	N	O	0	0	0
			967	575	196	196			

- Molecule 46 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BQ	154	Total	C	N	O	0	0	0
			761	453	154	154			
46	DQ	154	Total	C	N	O	0	0	0
			761	453	154	154			

- Molecule 47 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	BR	143	Total	C	N	O	0	0	0
			706	420	143	143			
47	DR	143	Total	C	N	O	0	0	0
			706	420	143	143			

- Molecule 48 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	BS	188	Total	C	N	O	0	0	0
			931	555	188	188			
48	DS	188	Total	C	N	O	0	0	0
			931	555	188	188			

- Molecule 49 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	BT	119	Total	C	N	O	0	0	0
			586	348	119	119			
49	DT	119	Total	C	N	O	0	0	0
			586	348	119	119			

- Molecule 50 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	BU	129	Total	C	N	O	0	0	0
			631	373	129	129			
50	DU	129	Total	C	N	O	0	0	0
			631	373	129	129			

- Molecule 51 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BV	59	Total	C	N	O	0	0	0
			291	173	59	59			
51	DV	59	Total	C	N	O	0	0	0
			291	173	59	59			

- Molecule 52 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	BW	94	Total	C	N	O	0	0	0
			468	280	94	94			
52	DW	94	Total	C	N	O	0	0	0
			468	280	94	94			

- Molecule 53 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	BX	107	Total	C	N	O	0	0	0
			530	316	107	107			
53	DX	107	Total	C	N	O	0	0	0
			530	316	107	107			

- Molecule 54 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	BY	149	Total	C	N	O	0	0	0
			727	429	149	149			
54	DY	149	Total	C	N	O	0	0	0
			727	429	149	149			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BY	38	GLU	GLN	CONFLICT	UNP P02406
DY	38	GLU	GLN	CONFLICT	UNP P02406

- Molecule 55 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	BZ	98	Total	C	N	O	0	0	0
			481	285	98	98			
55	DZ	98	Total	C	N	O	0	0	0
			481	285	98	98			

- Molecule 56 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	Ba	86	Total	C	N	O	0	0	0
			425	253	86	86			
56	Da	86	Total	C	N	O	0	0	0
			425	253	86	86			

- Molecule 57 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
57	Bb	125	Total	C	N	O	0	0	0
			618	368	125	125			
57	Db	125	Total	C	N	O	0	0	0
			618	368	125	125			

- Molecule 58 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	Bc	68	Total	C	N	O	0	0	0
			339	203	68	68			
58	Dc	68	Total	C	N	O	0	0	0
			339	203	68	68			

- Molecule 59 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
59	Bd	72	Total	C	N	O	0	0	0
			352	208	72	72			
59	Dd	72	Total	C	N	O	0	0	0
			352	208	72	72			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
60	Be	48	Total	C	N	O	0	0	0
			240	144	48	48			
60	De	48	Total	C	N	O	0	0	0
			240	144	48	48			

- Molecule 61 is a protein called 60S ribosomal protein L42.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
61	Bf	95	Total	C	N	O	0	0	0
			467	277	95	95			
61	Df	95	Total	C	N	O	0	0	0
			467	277	95	95			

- Molecule 62 is a protein called 60S ribosomal protein L43.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
62	Bg	83	Total	C	N	O	0	0	0
			407	241	83	83			
62	Dg	83	Total	C	N	O	0	0	0
			407	241	83	83			

- Molecule 63 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
63	Bh	44	Total	C	N	O	0	0	0
			220	132	44	44			
63	Dh	44	Total	C	N	O	0	0	0
			220	132	44	44			

- Molecule 64 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
64	Bi	12	Total	C	N	O	0	0	0
			60	36	12	12			
64	Di	12	Total	C	N	O	0	0	0
			60	36	12	12			

- Molecule 65 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
65	Bk	16	Total	C	N	O	0	0	0
			80	48	16	16			
65	Dk	16	Total	C	N	O	0	0	0
			80	48	16	16			

- Molecule 66 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
66	Bl	19	Total	C	N	O	0	0	0
			95	57	19	19			

- Molecule 67 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
67	Bm	9	Total	C	N	O	0	0	0
			45	27	9	9			

- Molecule 68 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
68	Bn	27	Total	C	N	O	0	0	0
			135	81	27	27			

- Molecule 69 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
69	Bp	8	Total	C	N	O	0	0	0
			40	24	8	8			

- Molecule 70 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
70	Bq	17	Total	C	N	O	0	0	0
			85	51	17	17			

- Molecule 71 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
71	Br	23	Total	C	N	O	0	0	0
			115	69	23	23			

- Molecule 72 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
72	DL	138	Total	C	N	O	0	0	0
			679	403	138	138			

- Molecule 73 is a protein called 60S acidic ribosomal protein P0.

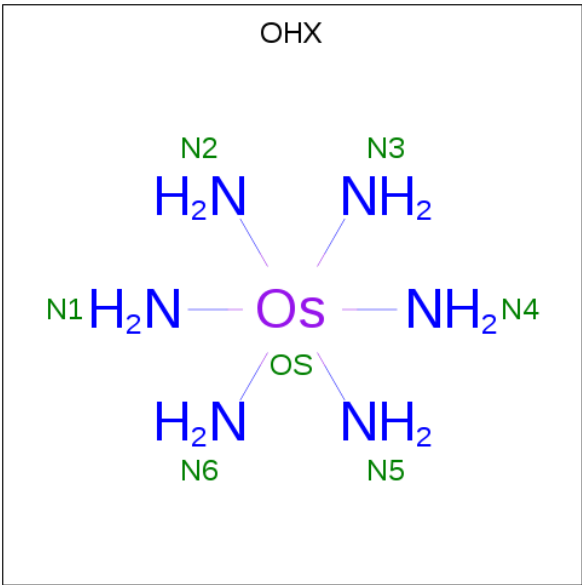
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
73	DM	130	Total	C	N	O	0	0	0
			641	381	130	130			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DM	83	TYR	ASN	CONFLICT	UNP P05317

- Molecule 74 is osmium (III) hexamine (three-letter code: OHX) (formula: H<sub>12</sub>N<sub>6</sub>Os).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	AL	1	Total	N	Os	0	0
			7	6	1		
74	AS	1	Total	N	Os	0	0
			7	6	1		
74	AT	1	Total	N	Os	0	0
			7	6	1		
74	Ac	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B2	1	Total	N	Os	0	0
			7	6	1		
74	B2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B2	1	Total	N	Os	0	0
			7	6	1		
74	B2	1	Total	N	Os	0	0
			7	6	1		
74	B2	1	Total	N	Os	0	0
			7	6	1		
74	B2	1	Total	N	Os	0	0
			7	6	1		
74	B2	1	Total	N	Os	0	0
			7	6	1		
74	B2	1	Total	N	Os	0	0
			7	6	1		
74	B2	1	Total	N	Os	0	0
			7	6	1		
74	B3	1	Total	N	Os	0	0
			7	6	1		
74	B3	1	Total	N	Os	0	0
			7	6	1		
74	B3	1	Total	N	Os	0	0
			7	6	1		
74	B3	1	Total	N	Os	0	0
			7	6	1		
74	B3	1	Total	N	Os	0	0
			7	6	1		
74	B3	1	Total	N	Os	0	0
			7	6	1		
74	B3	1	Total	N	Os	0	0
			7	6	1		
74	B3	1	Total	N	Os	0	0
			7	6	1		
74	B3	1	Total	N	Os	0	0
			7	6	1		
74	BC	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	BO	1	Total	N	Os	0	0
			7	6	1		
74	BT	1	Total	N	Os	0	0
			7	6	1		
74	Bd	1	Total	N	Os	0	0
			7	6	1		
74	Bd	1	Total	N	Os	0	0
			7	6	1		
74	Bg	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	CI	1	Total	N	Os	0	0
			7	6	1		
74	CS	1	Total	N	Os	0	0
			7	6	1		
74	CS	1	Total	N	Os	0	0
			7	6	1		
74	CT	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D2	1	Total	N	Os	0	0
			7	6	1		
74	D2	1	Total	N	Os	0	0
			7	6	1		
74	D2	1	Total	N	Os	0	0
			7	6	1		
74	D2	1	Total	N	Os	0	0
			7	6	1		
74	D2	1	Total	N	Os	0	0
			7	6	1		
74	D2	1	Total	N	Os	0	0
			7	6	1		
74	D2	1	Total	N	Os	0	0
			7	6	1		
74	D3	1	Total	N	Os	0	0
			7	6	1		
74	D3	1	Total	N	Os	0	0
			7	6	1		
74	D3	1	Total	N	Os	0	0
			7	6	1		
74	D3	1	Total	N	Os	0	0
			7	6	1		
74	D3	1	Total	N	Os	0	0
			7	6	1		
74	D3	1	Total	N	Os	0	0
			7	6	1		
74	D3	1	Total	N	Os	0	0
			7	6	1		
74	D3	1	Total	N	Os	0	0
			7	6	1		
74	D3	1	Total	N	Os	0	0
			7	6	1		
74	DC	1	Total	N	Os	0	0
			7	6	1		

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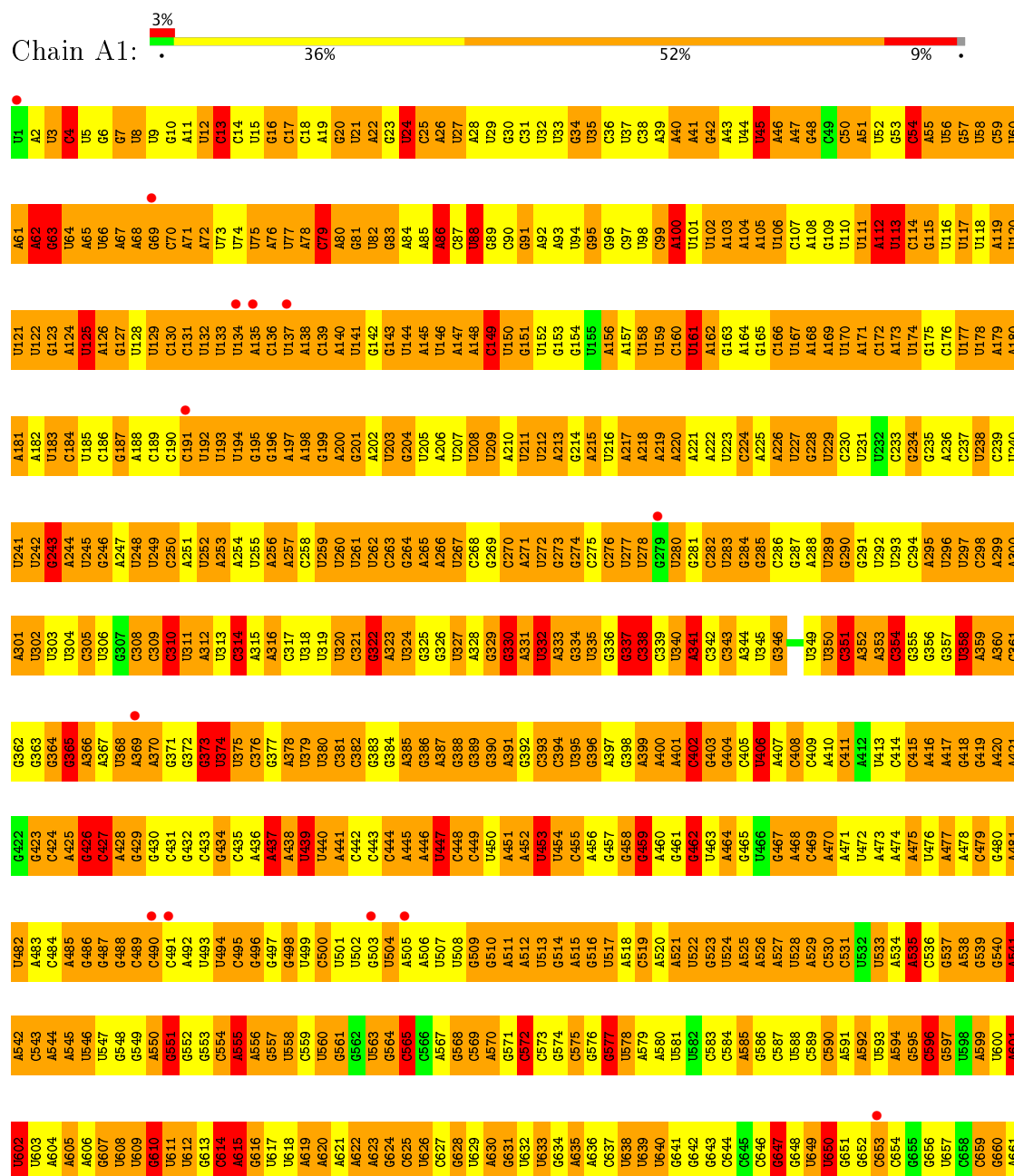
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	DE	1	Total	N	Os	0	0
			7	6	1		
74	DJ	1	Total	N	Os	0	0
			7	6	1		
74	DO	1	Total	N	Os	0	0
			7	6	1		
74	DO	1	Total	N	Os	0	0
			7	6	1		
74	DT	1	Total	N	Os	0	0
			7	6	1		
74	Dd	1	Total	N	Os	0	0
			7	6	1		
74	Dd	1	Total	N	Os	0	0
			7	6	1		
74	Dg	1	Total	N	Os	0	0
			7	6	1		

### 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 the various outlier classes 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



U1564	G1504	A1444	A1384	G1324	G1264	A1204	U1144	A1084	U1024	A963	U903	U843	G783	G723	U662
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C1568	G1508	G1448	G1388	G1328	G1268	A1208	G1148	A1088	C1028	U967	U908	A847	C787	U727	U666
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U1572	G1512	U1452	U1392	C1332	U1272	G1212	A1152	A1092	G1032	A971	U911	U851	C791	U731	U
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C1574	U1514	G1454	C1334	C1274	G1274	G1214	G1154	A1094	C1034	U973	G913	C853	C793	A733	U
G1575	A1515	G1455	U1335	U1335	A1275	C1215	G1155	U1095	G1035	A974	G914	U854	C794	A734	A
A1576	U1516	G1456	A1336	A1336	U1276	C1216	G1156	C1096	A1036	C975	A915	U855	C795	C735	C
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C1581	C1521	A1461	A1401	A1341	G1281	C1221	C1161	G1101	G1041	G980	U920	U860	U800	A740	U
U1582	U1522	G1462	G1402	C1342	U1282	C1222	C1162	G1102	G1042	U981	U921	U861	C801	C741	U
A1583	C1523	C1463	C1403	U1343	U1283	A1223	A1163	U1103	A1043	U982	G922	A862	C802	U742	U
G1584	A1524	G1464	A1404	A1344	C1284	A1224	G1164	U1104	U1044	A983	A923	A863	C803	U743	U
U1585	A1525	G1465	G1405	A1345	U1285	U1225	C1165	U1105	C1045	G984	A924	U864	A804	U744	U
A1586	G1526	G1466	A1406	A1346	U1286	A1226	A1166	U1106	G1046	G985	G925	A865	U805	U745	U
U1587	C1527	U1467	U1407	U1347	A1287	A1227	G1167	G1107	G1047	G986	A926	G866	A806	A746	U
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C1589	C1529	A1469	G1409	C1349	U1289	G1229	G1169	G1109	U1049	A988	U928	C868	U808	U748	C
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G1594	G1534	G1474	U1414	G1354	A1294	A1234	C1174	G1114	U1054	A993	A933	U873	U813	A753	U
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C1598	C1538	G1478	G1418	U1358	U1298	U1238	G1178	G1118	U1058	G997	G937	G877	A817	A757	U
U1599	G1539	A1479	C1359	G1359	G1299	U1239	G1179	G1119	U1059	A998	G938	G878	C818	U758	U
A1600	G1540	G1480	A1360	A1360	A1300	U1240	C1180	U1120	U1060	U999	A939	G879	G819	U759	U
C1601	C1541	C1481	U1361	U1361	U1301	G1241	U1181	C1121	A1061	C1000	A940	C880	U820	A760	U
U1602	G1542	C1482	U1362	U1362	U1302	A1242	U1182	G1122	A1062	A1001	A941	A881	U821	G761	U
C1603	A1543	A1483	U1363	G1363	U1303	G1243	A1183	C1123	U1063	G1002	G942	U882	U822	A762	U
U1604	U1544	G1484	G1364	G1364	G1304	A1244	A1184	A1124	G1064	A1003	C943	C883	G823	G763	U
G1605	A1545	A1485	C1365	C1365	U1305	G1245	U1185	A1125	A1065	U1004	A944	A884	G824	U764	U
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U1607	U1547	A1487	C1367	C1367	U1307	U1247	U1187	G1127	C1067	C1006	U946	U886	U826	U766	U
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U1609	C1549	U1489	U1369	U1369	C1309	U1249	A1189	U1129	A1069	G1008	G948	U888	U828	C768	U
G1610	A1550	C1490	U1370	U1370	U1310	U1250	C1190	G1130	C1070	U1009	C949	U889	A829	A769	U
A1611	U1551	C1431	A1371	A1371	U1311	U1251	U1191	A1131	U1071	C890	C950	C890	U830	A770	U
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C1613	G1553	G1493	C1373	C1373	A1313	U1253	A1193	A1133	G1073	U1012	A952	A892	U832	G772	U
A1614	U1554	C1494	C1374	C1374	U1314	U1254	A1194	C1134	G1074	A1013	G953	U893	U833	C773	U
C1615	A1555	G1495	A1375	U1375	G1255	G1255	C1195	U1135	C1075	G1014	G954	U894	U834	A774	U
G1616	U1556	U1496	G1376	G1376	A1256	A1256	A1196	U1136	A1076	U1015	A955	G895	U835	G775	U
U1617	U1557	U1497	C1377	C1377	U1257	G1257	C1197	A1137	C1077	C1016	C956	U896	U836	G776	U
C1618	G1558	G1498	U1378	G1378	U1258	U1258	G1198	A1138	C1078	U1017	G957	C897	G837	C777	U
U1619	A1559	G1499	C1379	C1379	A1319	U1259	G1199	A1139	U1079	U1018	U958	A898	G838	G778	U
C1620	U1560	C1500	U1380	U1380	U1320	U1260	G1200	G1140	U1080	A1019	U959	G899	U839	U779	U
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G1622	G1562	G1502	A1382	A1382	A1322	U1262	A1142	A1142	C1082	U961	U960	A901	U841	U781	U
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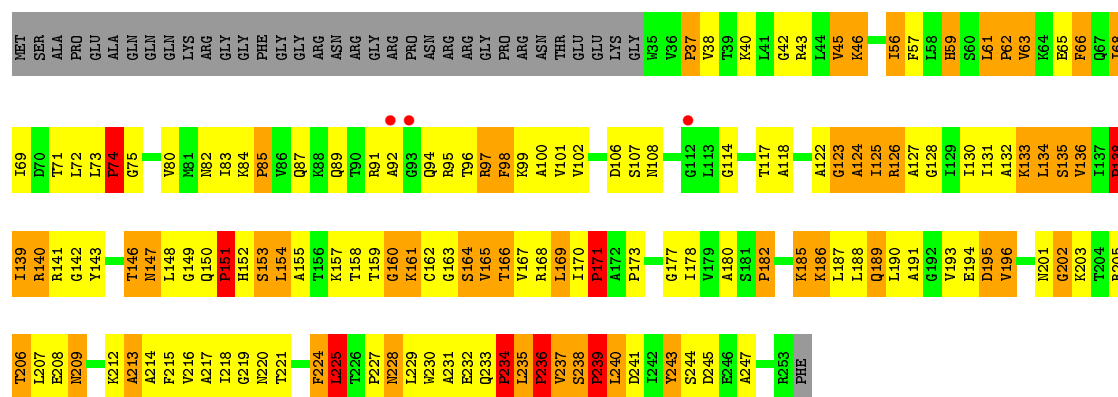
Chain C1:

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A61	A62	A63	A64	A65	A66	A67	A68	A69	A70	A71	A72	A73	A74	A75	A76	A77	A78	A79	A80	A81	A82	A83	A84	A85	A86	A87	A88	A89	A90	A91	A92	A93	A94	A95	A96	A97	A98	A99	A100	A101	A102	A103	A104	A105	A106	A107	A108	A109	A110
U121	U122	U123	U124	U125	U126	U127	U128	U129	U130	U131	U132	U133	U134	U135	U136	U137	U138	U139	U140	U141	U142	U143	U144	U145	U146	U147	U148	U149	U150	U151	U152	U153	U154	U155	U156	U157	U158	U159	U160	U161	U162	U163	U164	U165	U166	U167	U168	U169	U170
A181	A182	U183	U184	U185	U186	U187	A188	A189	A190	A191	A192	U193	U194	U195	A196	A197	A198	A199	A200	A201	U202	U203	U204	U205	A206	U207	U208	U209	A210	U211	U212	A213	U214	U215	U216	A217	A218	A219	A220	A221	A222	U223	U224	U225	A226	A227	U228	A229	U230
U241	U242	U243	U244	U245	U246	A247	U248	U249	U250	U251	U252	U253	U254	U255	U256	A257	U258	U259	U260	U261	U262	U263	U264	A265	A266	U267	U268	U269	U270	A271	U272	U273	U274	U275	U276	U277	U278	U279	U280	U281	U282	U283	U284	U285	U286	U287	U288	U289	
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U481	U482	U483	U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	
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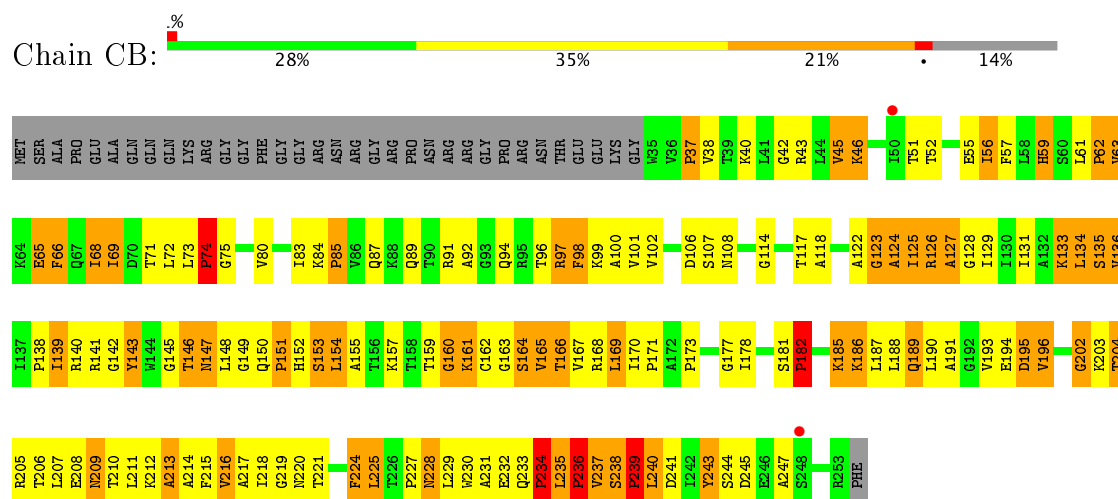
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A1503	G1383	G1323	A1323	G1263	A1203	G1083	A1023	A963	U903	U843	U783	G723	U663
G1504	A1444	A1384	G1324	G1264	A1204	U1084	U1024	U964	G904	A844	C784	G724	U664
A1505	G1445	G1385	A1325	U1265	C1205	G1085	A1025	U965	A905	C845	U785	G725	U665
G1506	A1446	G1386	A1326	U1266	C1206	A1086	A1026	A966	A906	G846	C786	G726	U666
G1507	C1447	G1387	C1327	U1267	C1207	A1087	A1027	A967	A907	A847	G787	U727	U667
U1508	A1448	A1388	G1328	U1268	C1208	A1088	C1028	U968	U908	C848	U788	U728	C
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U1510	U1450	A1390	G1330	U1270	A1210	C1090	A1030	A970	U910	A850	U790	G730	U
U1511	C1451	A1391	A1331	G1271	C1211	A1091	U1031	A971	U911	U851	A791	C731	U
G1512	U1452	U1392	C1332	U1272	G1212	A1092	G1032	G972	U912	C852	U792	G732	U
G1513	G1453	C1393	C1333	G1273	G1213	A1093	C1033	A973	G913	C853	A793	A733	A
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A1515	G1455	U1395	U1335	A1275	C1215	U1095	G1035	C975	A915	A855	U795	A735	U
A1516	C1456	G1396	A1336	U1276	C1216	C1096	A1036	G976	U916	A856	A796	C736	U
C1517	A1457	U1397	A1337	G1277	G1217	U1097	C1037	A977	U917	U857	A797	A737	G
G1518	G1458	U1398	C1338	G1278	G1218	U1098	U1038	A978	U918	C858	C798	G738	A
U1519	C1459	C1399	U1339	C1279	A1219	U1099	A1039	A979	A919	A859	A799	G739	U679
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G1523	C1463	C1403	U1343	U1283	A1223	U1103	A1043	A983	A923	A863	A803	U743	C683
G1524	G1464	A1404	A1344	C1284	A1224	U1104	U1044	G984	A924	U864	A804	U744	A684
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C1527	C1467	U1407	U1347	U1287	A1227	G1107	G1047	G987	C927	G867	A807	C747	G687
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C1541	C1481	A1421	U1361	G1241	G1241	C1121	A1061	A1001	A941	A881	U821	G761	U701
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A1543	A1483	U1423	U1363	G1243	G1243	C1123	U1063	A1003	G943	C883	G823	G763	G703
U1544	G1484	A1424	G1364	A1244	A1244	A1124	G1064	U1004	A944	A884	G824	U764	C704
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A1547	A1487	A1427	G1367	U1247	U1247	G1127	C1067	C1007	U947	A887	C827	U767	A707
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A1550	U1490	U1430	U1370	U1250	U1250	G1130	C1070	C950	C950	C890	U830	A770	U710
U1551	U1491	C1431	A1371	U1251	U1251	A1131	U1071	A951	A951	A891	U831	A771	U711
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G1553	C1493	A1433	C1373	U1253	U1253	A1133	G1073	G953	G953	U893	U833	C773	A713
U1554	C1494	U1434	C1374	U1254	A1254	C1134	G1074	G954	G954	U894	G714	A774	G714
A1555	C1495	A1435	A1375	G1255	G1255	U1135	C1075	A955	A955	G895	U835	G775	U715
A1556	U1496	G1436	C1376	U1256	A1256	U1136	A1076	C956	C956	U896	U836	G776	C716
U1557	U1497	U1437	U1377	U1257	U1257	A1137	C1077	G957	G957	C897	G837	C777	C717
U1558	G1498	G1438	G1378	G1258	U1258	A1138	C1078	U958	U958	A898	G838	G778	C718
A1559	G1499	A1319	C1379	U1259	U1259	A1139	U1079	U959	U959	A899	U779	U779	U719
U1560	C1500	C1440	U1380	U1320	U1260	G1140	U1080	A1020	U960	A900	U840	A780	G720



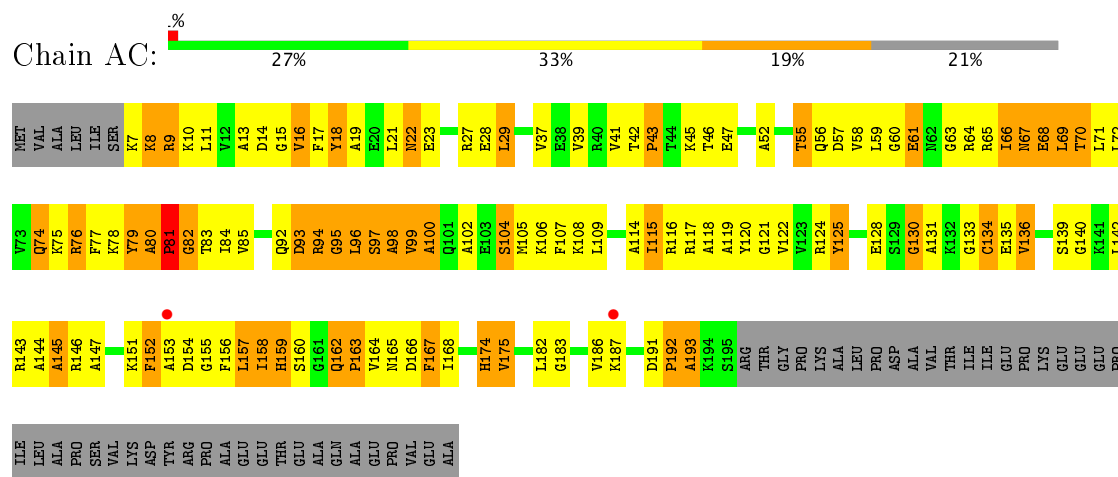




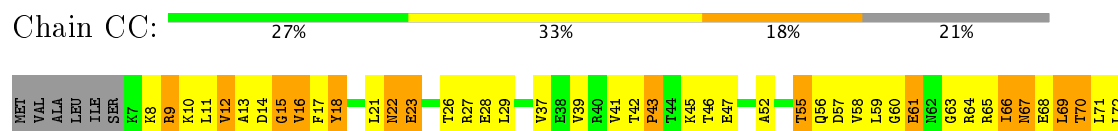
• Molecule 3: 40S ribosomal protein S2



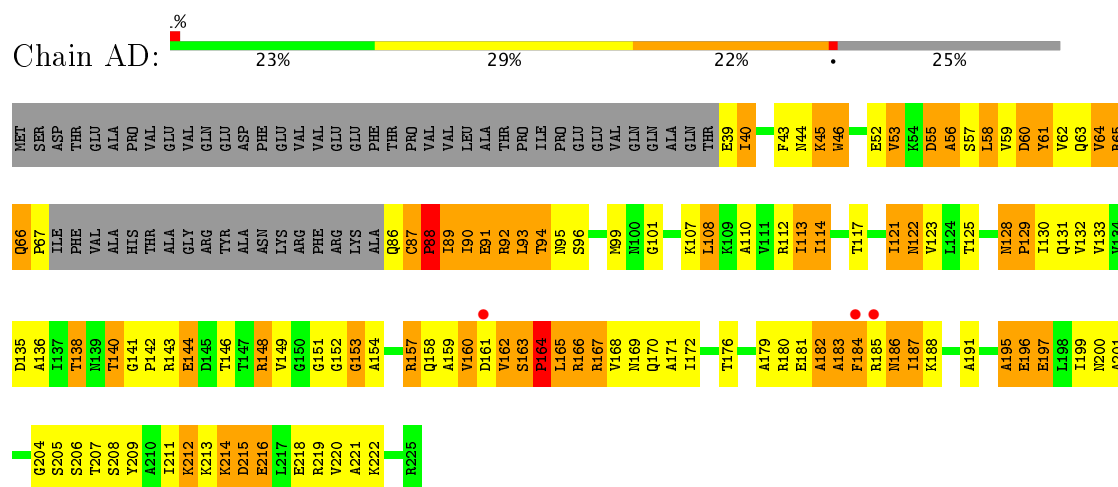
• Molecule 4: 40S ribosomal protein S3



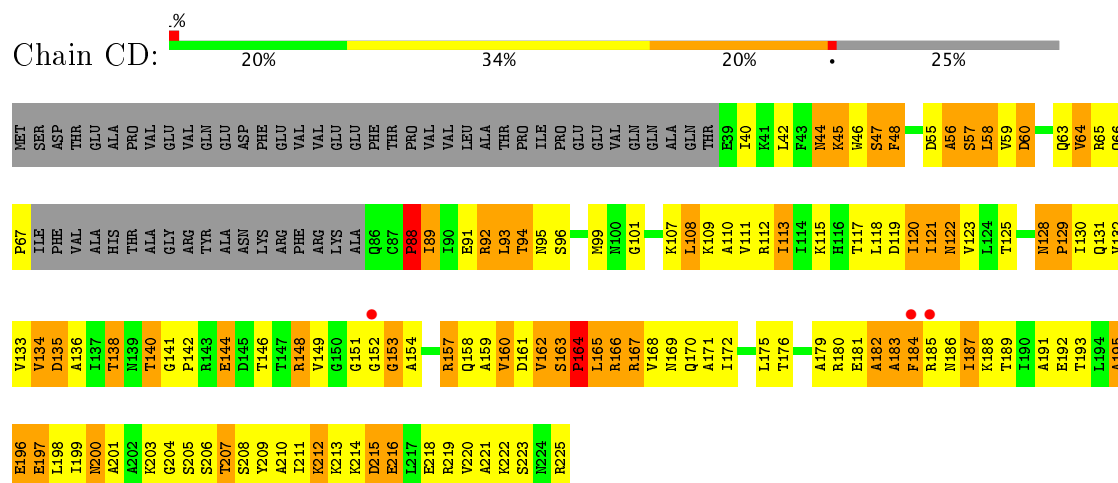
• Molecule 4: 40S ribosomal protein S3



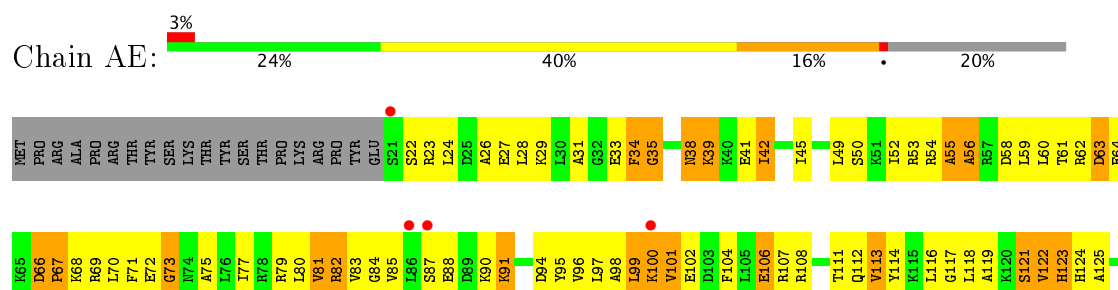
- Molecule 5: 40S ribosomal protein S5



- Molecule 5: 40S ribosomal protein S5

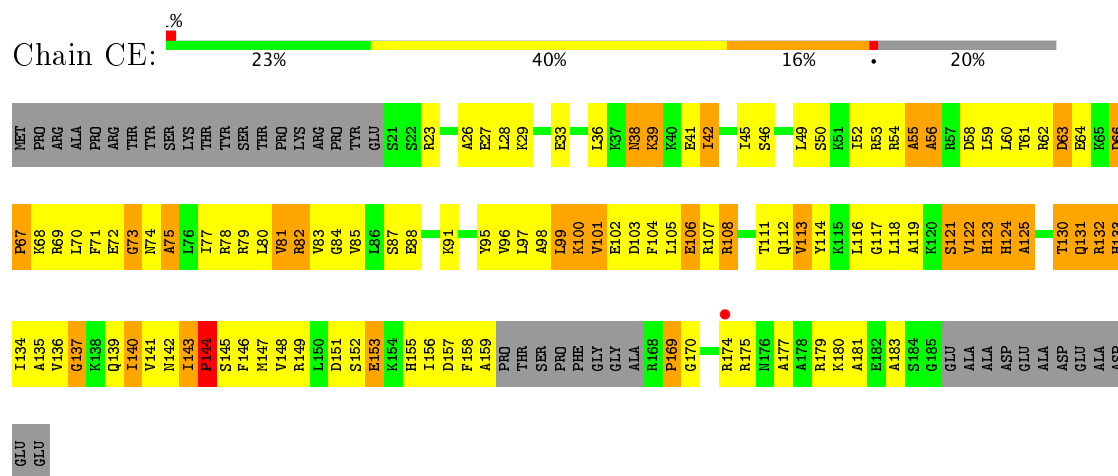


- Molecule 6: 40S ribosomal protein S9-A

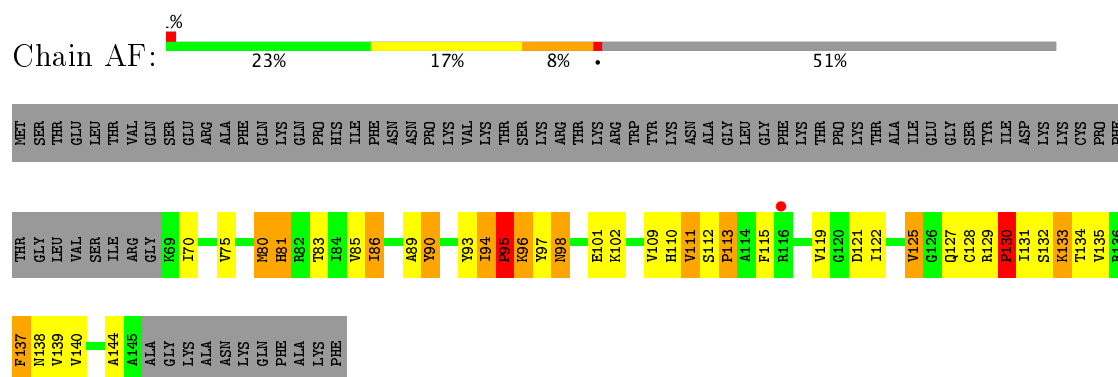




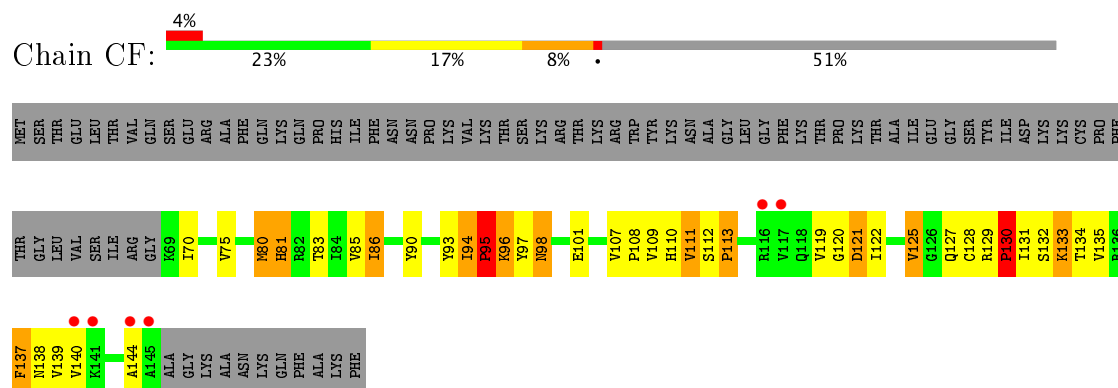
- Molecule 6: 40S ribosomal protein S9-A



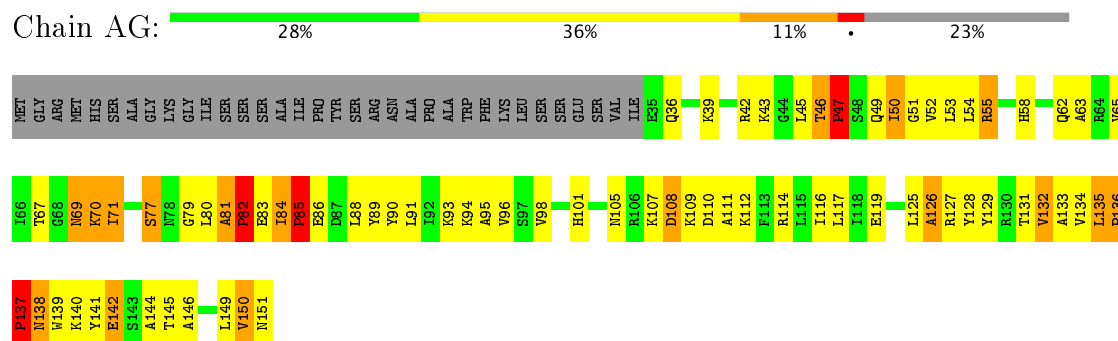
- Molecule 7: 40S ribosomal protein S11



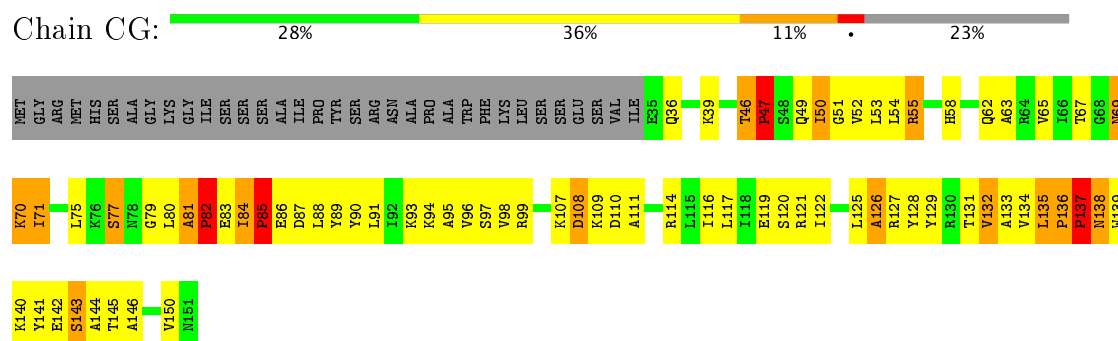
- Molecule 7: 40S ribosomal protein S11



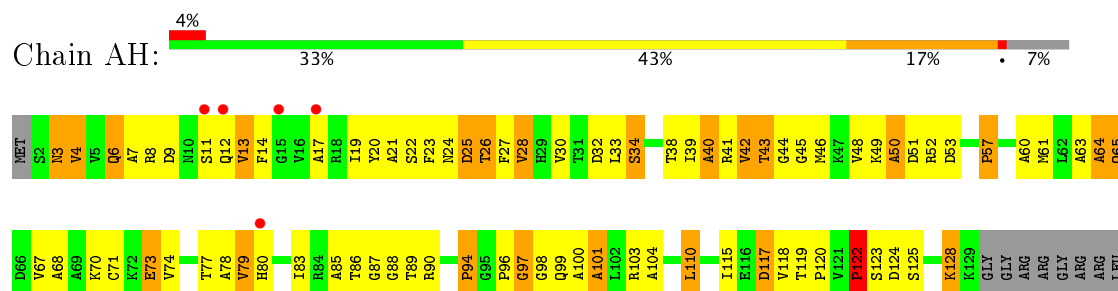
- Molecule 8: 40S ribosomal protein S13



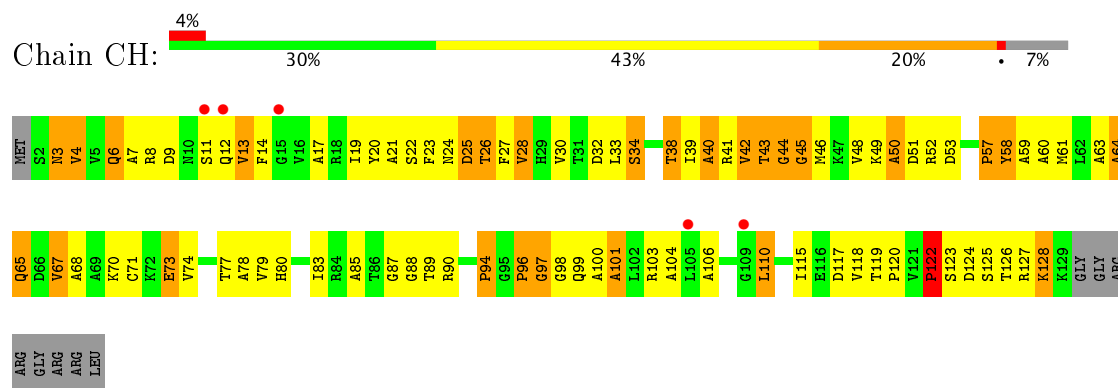
- Molecule 8: 40S ribosomal protein S13



- Molecule 9: 40S ribosomal protein S14-A

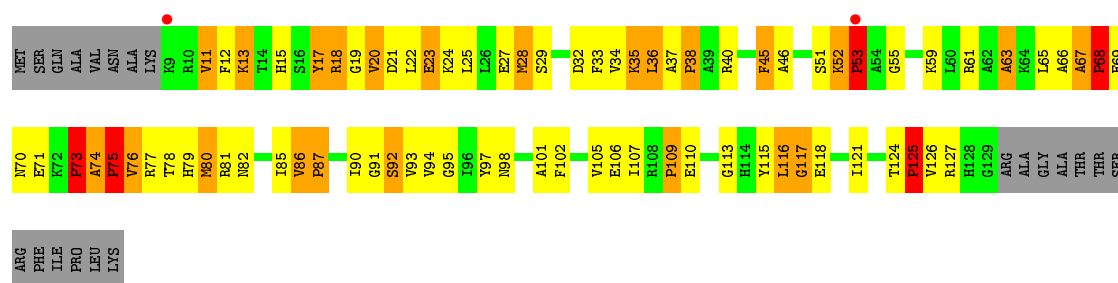


- Molecule 9: 40S ribosomal protein S14-A

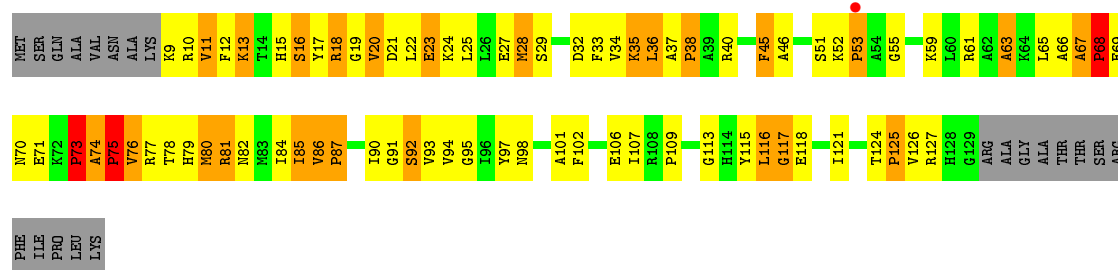


- Molecule 10: 40S ribosomal protein S15

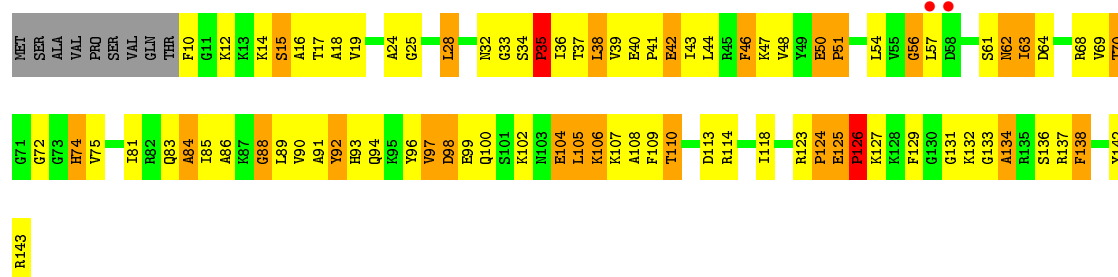




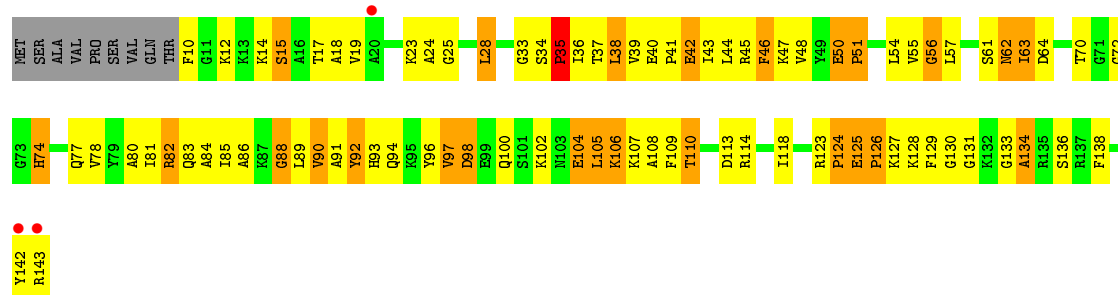
• Molecule 10: 40S ribosomal protein S15



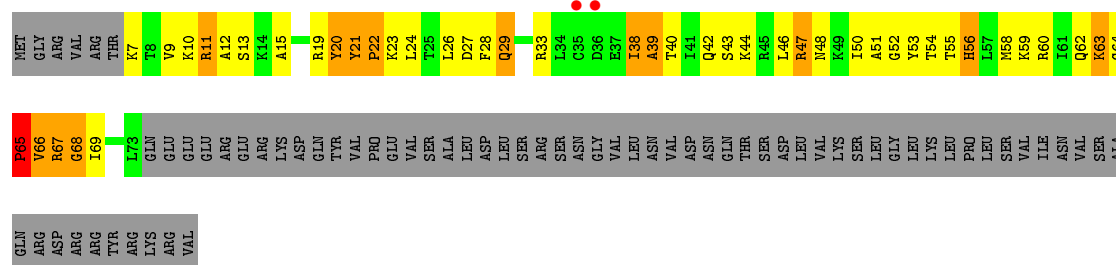
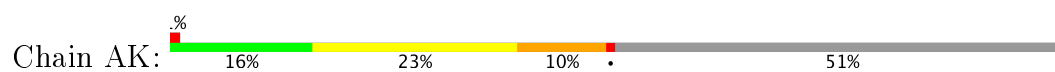
• Molecule 11: 40S ribosomal protein S16



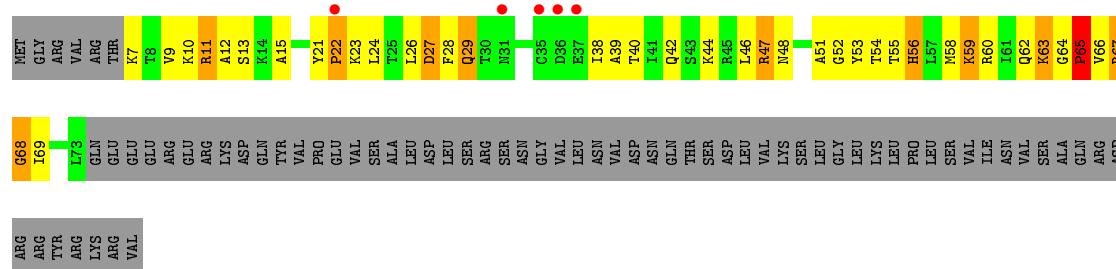
• Molecule 11: 40S ribosomal protein S16



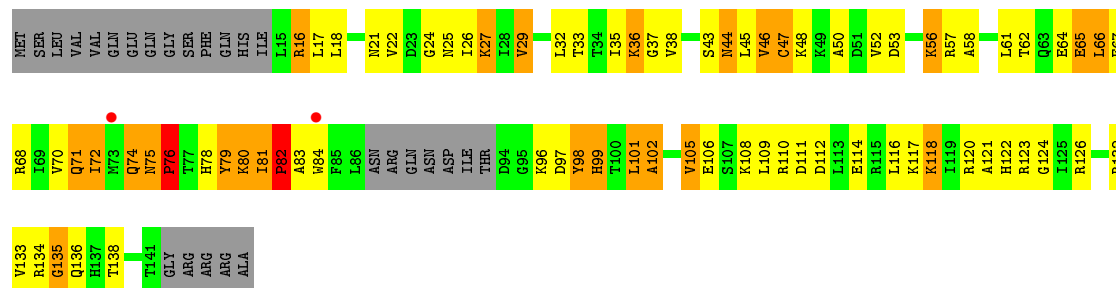
• Molecule 12: 40S ribosomal protein S17-A



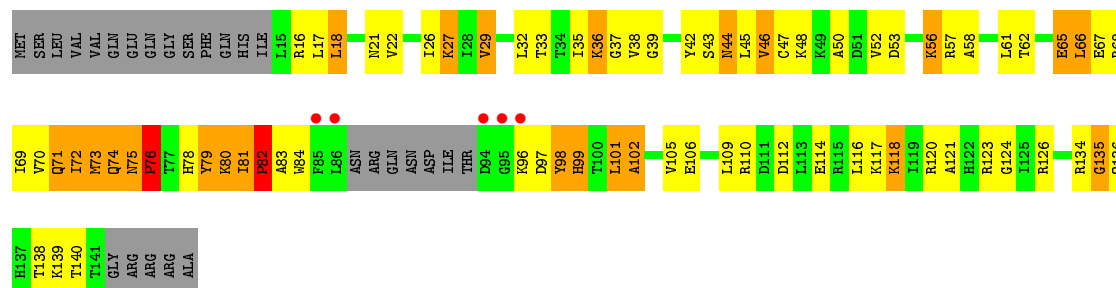
- Molecule 12: 40S ribosomal protein S17-A



- Molecule 13: 40S ribosomal protein S18

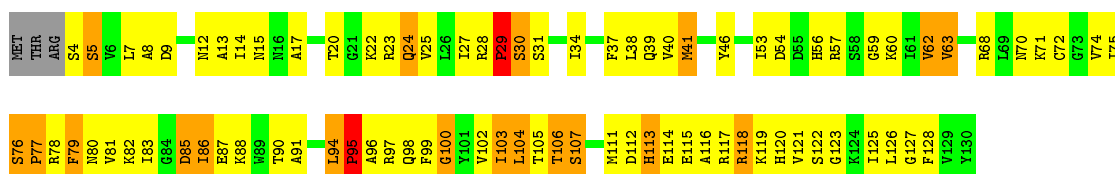


- Molecule 13: 40S ribosomal protein S18



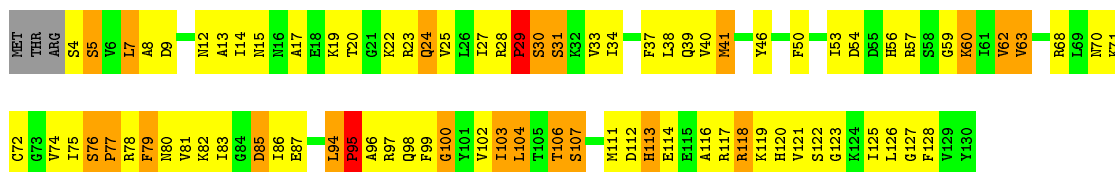
- Molecule 14: 40S ribosomal protein S19-A





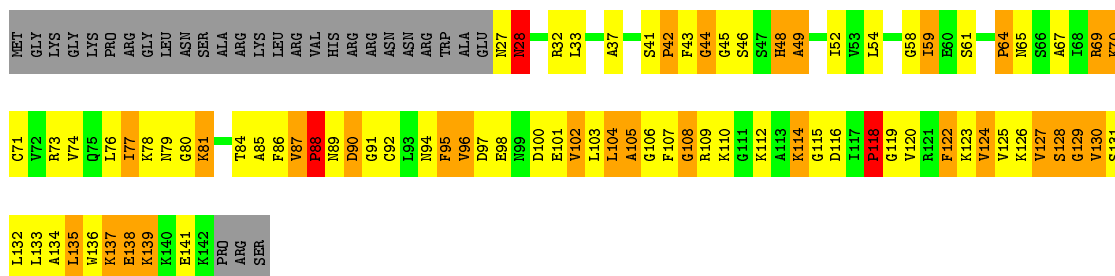
• Molecule 16: 40S ribosomal protein S22-A

Chain CO: 34% 46% 16% . .



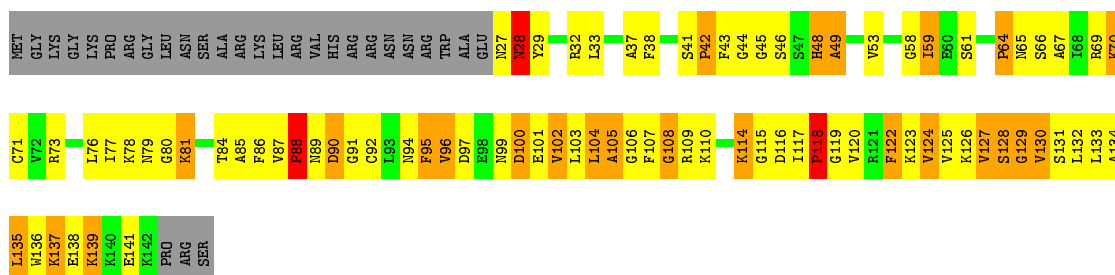
• Molecule 17: 40S ribosomal protein S23

Chain AP: 23% 35% 20% . 20%



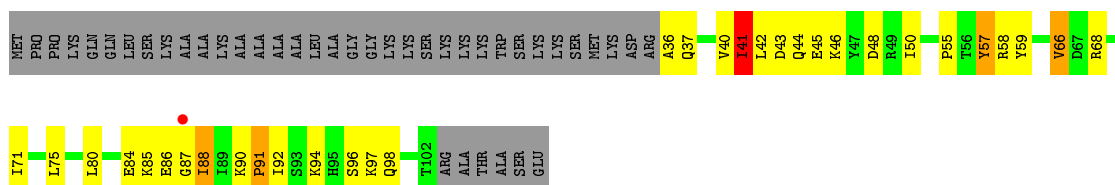
• Molecule 17: 40S ribosomal protein S23

Chain CP: 22% 39% 17% . 20%



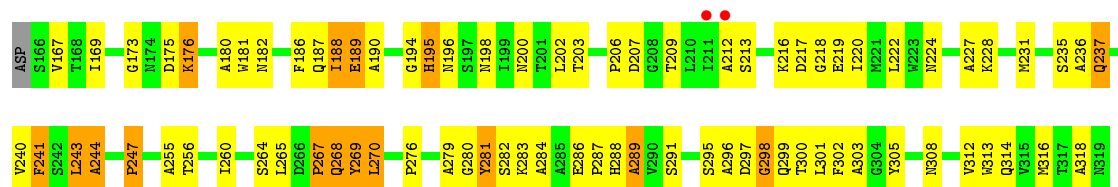
• Molecule 18: 40S ribosomal protein S25-A

Chain AQ: 32% 25% . . 38%

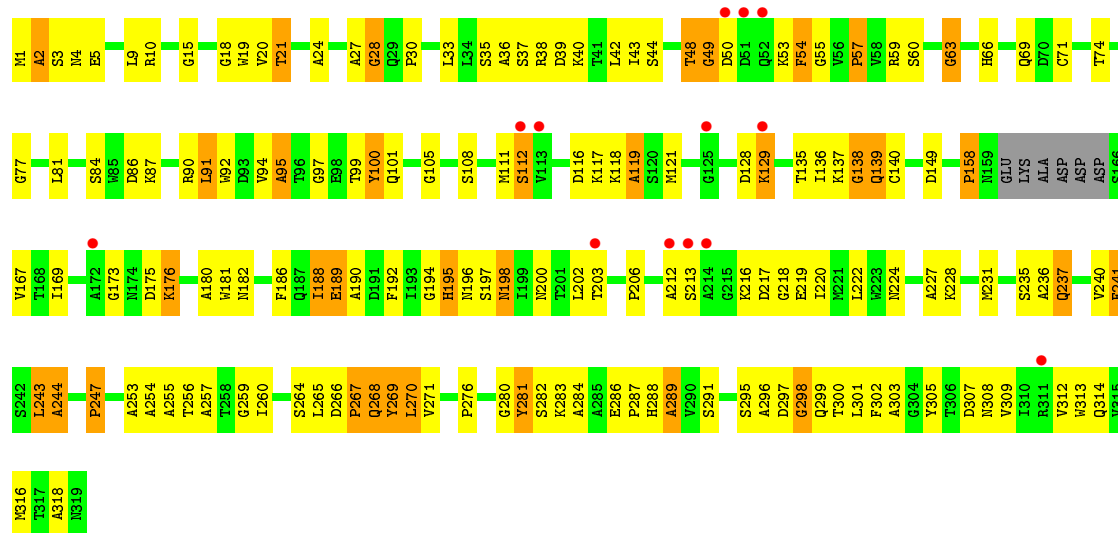




- Chain AT:
- 
- 4% 50% 37% 11%
- 
- Chain AT: 4% 50% 37% 11%



- Molecule 21: Guanine nucleotide-binding protein subunit beta-like protein; RACK-1



- Molecule 22: Unassigned secondary structure



There are no outlier residues recorded for this chain.

- Molecule 22: Unassigned secondary structure



- Molecule 22: Unassigned secondary structure



There are no outlier residues recorded for this chain.

- Molecule 23: Unassigned secondary structure



- Molecule 23: Unassigned secondary structure

Chain Cb:  99%



- Molecule 24: Unassigned secondary structure

Chain Ac:  99%



- Molecule 24: Unassigned secondary structure

Chain Cc:  100%

There are no outlier residues recorded for this chain.

- Molecule 25: Unassigned secondary structure

Chain Ad:  100%

There are no outlier residues recorded for this chain.

- Molecule 25: Unassigned secondary structure

Chain Cd:  100%

There are no outlier residues recorded for this chain.

- Molecule 26: Unassigned secondary structure

Chain Ae:  100%

There are no outlier residues recorded for this chain.

- Molecule 26: Unassigned secondary structure

Chain Bj:  100%

There are no outlier residues recorded for this chain.

- Molecule 26: Unassigned secondary structure

Chain Dj:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: Unassigned secondary structure

Chain Af:  100%

- Molecule 28: Unassigned secondary structure

100%

- Molecule 28: Unassigned secondary structure

100%

- Molecule 29: 25S ribosomal RNA



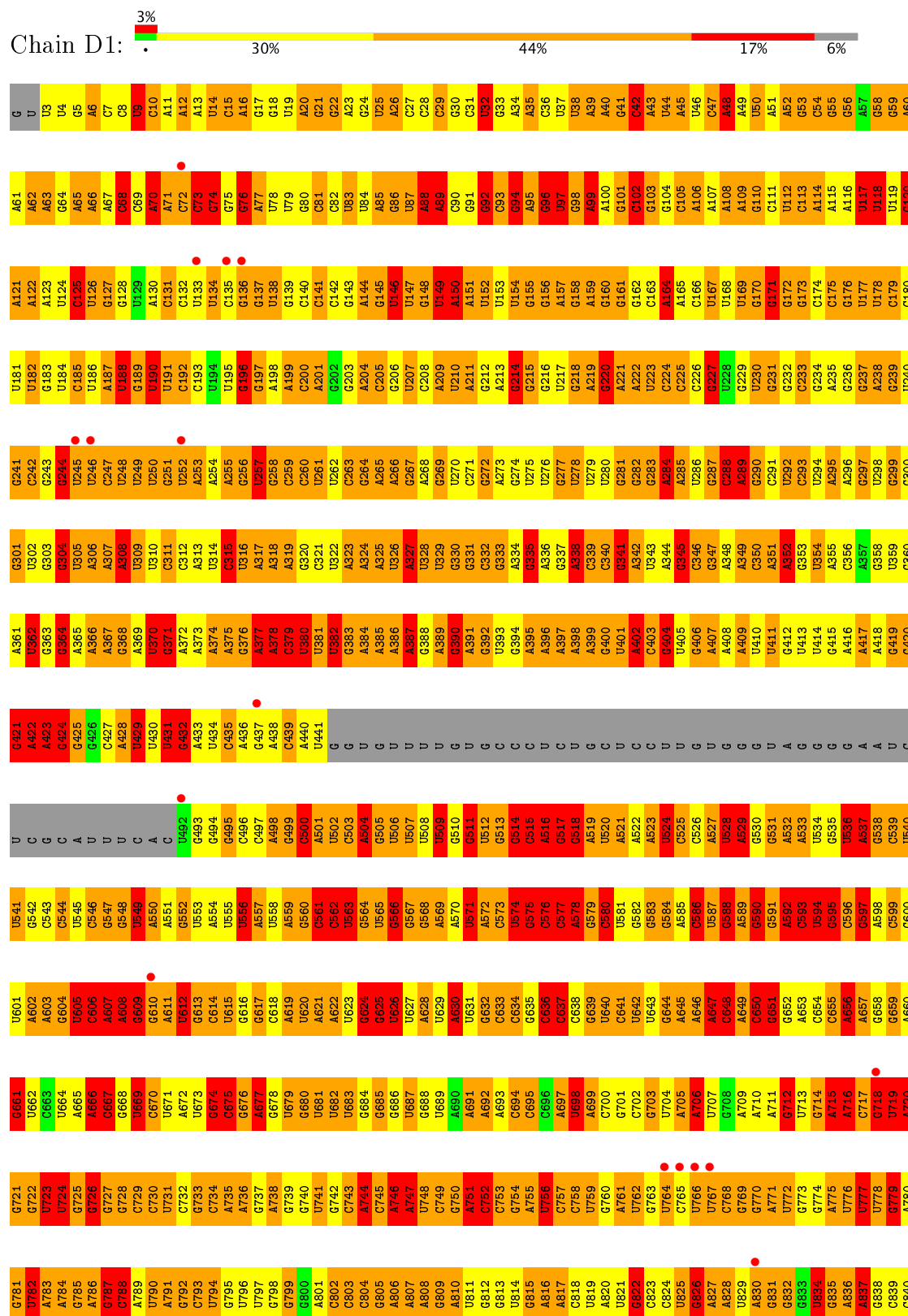
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C1508	G1447	G1387	U1325	U1264	A1204	U1144	A1084	C1023	G953	U903	A783	U723	C663
A1509	G1448	U1388	G1326	U1266	A1205	G1145	A1085	A904	A965	A904	A784	U724	U664
U1511	A1449	G1389	C1327	U1267	G1206	G1146	C1086	A1026	U966	U905	G785	G725	A665
U1512	G1450	A1390	C1328	U1268	U1208	G1147	G1087	A1027	A967	A906	A786	G726	A666
G1513	C1451	C1391	U1329	U1269	G1209	G1148	U1088	A1028	G968	G907	G787	G727	C667
G1514	A1452	G1392	A1330	A1270	U1210	G1149	G1089	U1029	C969	G908	C788	G728	G668
A1515	A1453	A1393	U1331	A1271	U1211	A1150	G1090	A1030	A970	G910	A789	C729	U669
C1516	A1454	A1394	A1332	C1272	A1212	G1151	A1091	C1031	U971	C911	U791	C730	C670
G1517	A1455	G1395	C1333	A1273	G1213	G1152	C1092	A1032	A972	G912	A791	U731	U671
U1518	A1456	C1396	U1334	A1274	U1214	A1153	A1093	G1033	A973	G913	G792	G732	A672
G1519	U1457	C1397	C1335	C1275	U1215	A1154	U1094	U1034	G974	A914	G793	C734	U673
G1520	U1458	U1398	U1336	U1276	U1216	C1155	U1095	U1035	C975	A915	G794	C735	G674
A1521	C1459	A1399	A1337	C1277	A1217	G1156	U1096	G1036	U976	G916	G795	A736	C675
U1522	A1460	G1400	C1338	A1278	U1218	A1157	U1097	U1037	U977	A917	U796	A737	G676
U1523	A1461	A1401	C1339	C1279	C1219	A1158	A1098	C1038	G977	A918	U797	G737	A677
A1524	A1462	C1402	G1340	C1280	U1220	A1159	A1099	U1039	G978	C918	G798	A738	G678
G1525	U1463	C1403	U1341	G1281	U1221	C1160	U1100	U1040	U979	U919	G799	G739	U679
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C1527	A1465	U1405	A1343	C1283	A1223	A1162	A1102	U1042	U981	A921	A801	U741	U681
G1528	G1466	A1406	G1344	C1284	C1224	G1163	A1103	U1043	C982	U922	C802	G742	U682
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A1535	G1473	G1413	U1353	A1291	G1231	G1171	U1111	U1050	U990	U930	G809	C749	U689
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• Molecule 29: 25S ribosomal RNA





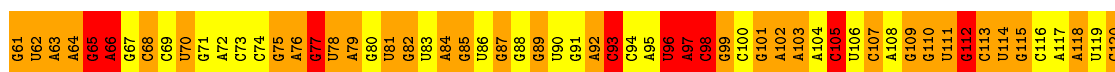
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U1740	G1680	U1620	G1560	G1500	G1440	G1380	C1320	A1260	A1200	G1140	A1080	G1020	U960	G900

G2586	A2583	A2462	U2282	A2222	U2162	U2102	A1922	U1862	U1801	A1741
G2587	A2584	G2403	G2283	A2223	C2163	U2103	C1923	G1863	C1802	U1742
U2588	G2404	G2403	G2284	A2224	A2164	A2104	U1924	A1864	C1803	G1743
G2589	G2405	G2405	C2285	U2225	G2165	G2105	U1925	A1865	A1804	G1744
A2590	G2406	G2406	U2286	U2226	A2166	A2106	C1926	C1866	C1805	C1745
G2591	G2407	G2407	C2287	C2227	A2167	A2107	G1927	A1867	A1806	U1746
G2592	A2408	U2408	C2288	A2228	A2168	C2108	G1928	G1868	G1807	G1747
A2593	G2409	G2409	U2289	A2229	G2169	U2109	G1929	C1869	A1808	G1748
G2594	U2410	C2350	U2290	C2230	U2170	G2110	A1930	C1870	A1809	A1749
A2595	U2411	U2351	U2291	G2231	G2171	U2111	U1931	C1871	A1810	A1750
U2596	U2412	G2352	U2292	A2232	A2172	U2112	A1932	C1872	G1811	G1751
U2597	G2413	G2353	A2293	A2233	U2173	A2113	A1933	U1873	A1812	A1752
G2598	G2414	G2354	U2294	G2234	G2174	C2114	G1934	A1874	A1813	G1753
U2599	G2415	G2355	A2295	C2235	U2175	G2115	G1935	G1875	A1814	G1754
G2600	U2416	A2356	A2296	G2236	G2176	A2116	A1936	U1876	U1815	C1755
A2601	U2417	A2357	U2297	G2237	G2177	G2117	U1937	C1877	A1816	G1756
G2602	G2418	A2358	U2298	G2238	A2178	U2118	G1938	G1878	G1817	A1757
G2603	G2419	C2359	A2299	G2239	C2179	A2119	G1939	A1879	U1818	G1758
U2604	C2420	C2360	G2300	G2240	G2180	A2120	G1940	U1880	U1819	C1759
G2605	G2421	A2361	U2301	U2241	C2181	G2121	C1941	A1881	U1820	A1760
G2606	U2422	G2362	G2302	A2242	C2182	G2122	U1942	G1882	U1821	C1761
G2607	A2423	A2363	A2303	A2243	A2183	G2123	A1883	A1883	C1822	U1762
A2608	A2424	G2364	C2304	A2244	U2184	G2124	U1944	A1884	U1763	C1763
A2609	G2425	C2365	G2305	C2245	G2185	A2125	U1885	U1885	U1764	U1764
G2610	U2426	C2366	C2306	G2246	U2186	A2126	A1946	A1886	U1765	U1765
U2611	U2427	A2367	G2307	G2247	G2187	U2127	G1947	A1887	C1826	U1766
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G2614	A2430	G2370	U2310	G2250	U2190	G2130	U1950	U1890	G1830	G1769
G2615	G2431	G2371	G2311	G2251	U2191	A2131	A1951	A1891	U1831	G1770
G2616	A2432	A2372	A2312	A2252	C2192	G2132	G1952	G1892	C1832	C1771
U2617	U2433	A2373	G2313	G2253	U2193	U2133	U1953	A1893	G1833	U1772
G2618	U2434	G2374	U2314	U2254	G2194	C2134	G	U1894	U1834	C1773
G2619	G2435	G2375	G2315	A2255	G2195	U2135	U	A1895	A1835	C1774
G2620	U2436	G2376	G2316	A2256	C2196	C2136	A	A1896	C1836	G1775
G2621	U2437	G2377	A2317	C2257	C2197	U2137	G	G1897	U1837	G1776
G2622	G2438	C2378	U2318	U2258	A2198	A2138	U	G1898	G1838	U1777
G2623	A2439	U2379	U2319	A2259	C2199	A2139	G	G1899	A1839	G1778
G2624	G2440	U2380	A2320	U2260	U2200	U2140	A	A1900	U1840	C1779
G2625	A2441	G2381	A2321	U2261	G2201	U2141	G	A1901	A1841	G1780
A2626	G2442	G2382	C2322	A2262	C2202	A2142	G	G1902	A1842	C1781
G2627	A2443	C2383	G2323	C2263	U2203	G2143	G	U1903	C1843	U1782
A2628	G2444	A2384	A2324	U2264	C2204	A2144	C	C1904	G1844	U1783
U2629	C2445	G2385	G2325	G2265	U2205	A2145	C	G1905	G1845	G1784
G2630	U2446	A2386	U2326	U2266	G2206	C2146	U	G1906	C1846	U1785
U2631	U2447	A2387	U2327	C2267	A2207	A2147	G	C1907	A1847	G1786
G2632	G2448	U2388	U2328	U2268	A2208	U2148	G	A1908	G1848	A1787
G2633	A2449	C2389	C2329	U2269	U2209	A2149	A	A1909	C1849	G1788
U2634	G2450	A2390	C2330	A2270	G2210	G2150	U	A1910	A1850	G1789
A2635	G2451	G2391	C2331	A2271	U2211	C2151	C	A1911	G1851	G1790
G2636	G2452	C2392	A2332	G2272	C2212	A2152	A	U1912	G1852	C1791
A2637	U2513	G2393	C2333	G2273	A2213	U2153	G	U1913	U1853	C1792
C2638	G2454	G2394	U2334	U2274	A2214	C2094	C	A1914	C1854	C1793
G2639	A2515	G2395	A2335	A2275	A2215	G2155	C	U1915	U1855	G1794
A2640	U2516	G2396	U2336	G2276	G2216	A2096	U	U1916	C1856	U1795
U2641	G2457	A2397	C2337	C2277	U2217	G2157	C	C1917	G1857	G1796
A2642	A2458	A2398	C2338	C2278	G2218	A2158	A	C1918	A1858	A1797
G2643	U2459	G2399	A2339	A2279	A2219	U2159	C	U1919	C1859	A1798
G2644	U2460	G2400	U2340	A2280	A2220	G2160	U	U1920	A1860	A1799
G2645	A2461	A2401	A2341	A2281	G2221	G2161	U	A1921	G1861	A1800

- Molecule 30: 5S ribosomal RNA

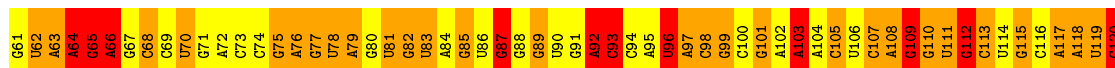
21%

G1	G2	G3	G4	G5	G6	G7	G8	G9	G10	G11	G12	G13	G14	G15	G16	G17	G18	G19	G20	G21	G22	G23	G24	G25	G26	G27	G28	G29	G30	G31	G32	G33	G34	G35	G36	G37	G38	G39	G40	G41	G42	G43	G44	G45	G46	G47	G48	G49	G50	G51	G52	G53	G54	G55	G56	G57	G58	G59	G60
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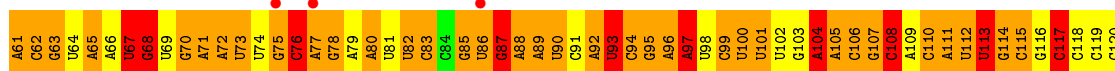
U121

- Molecule 30: 5S ribosomal RNA

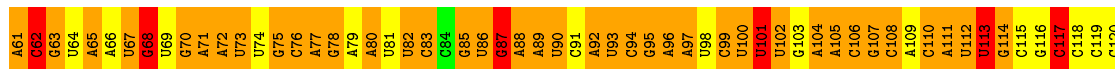


U121

- Molecule 31: 5.8S ribosomal RNA

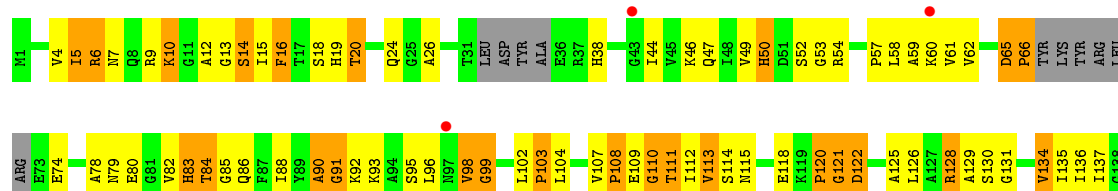


- Molecule 31: 5.8S ribosomal RNA

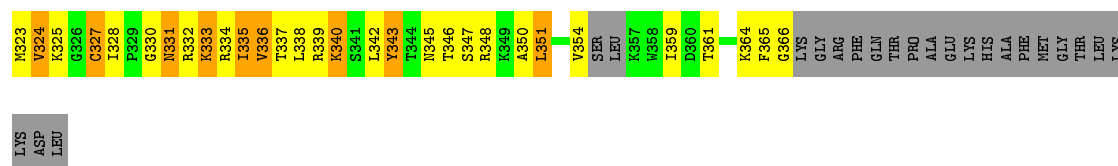


- Molecule 32: 60S ribosomal protein L1

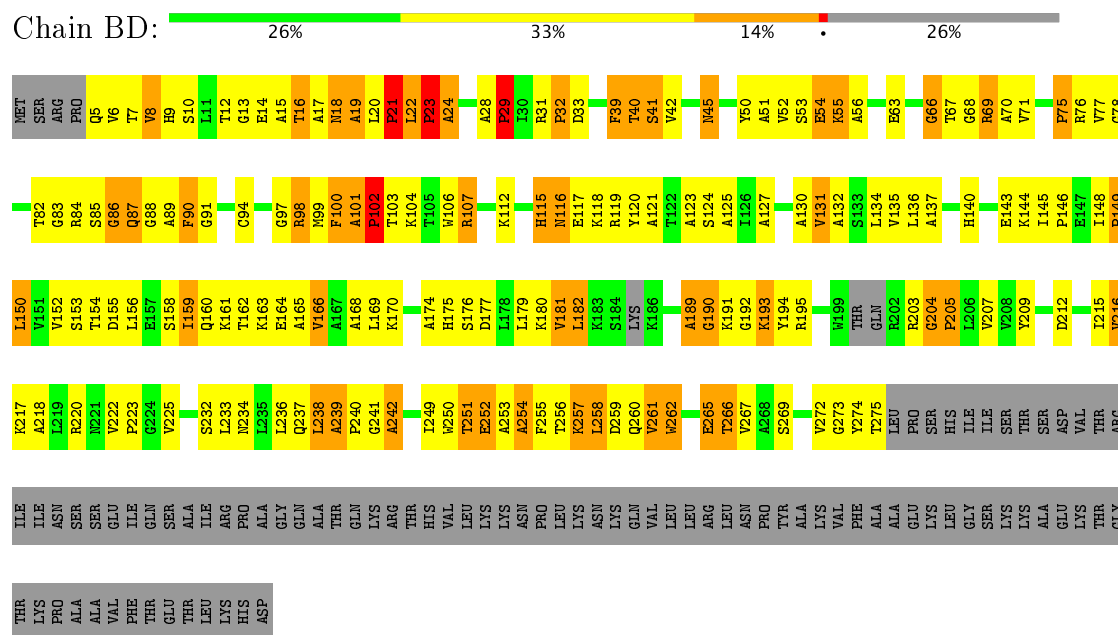




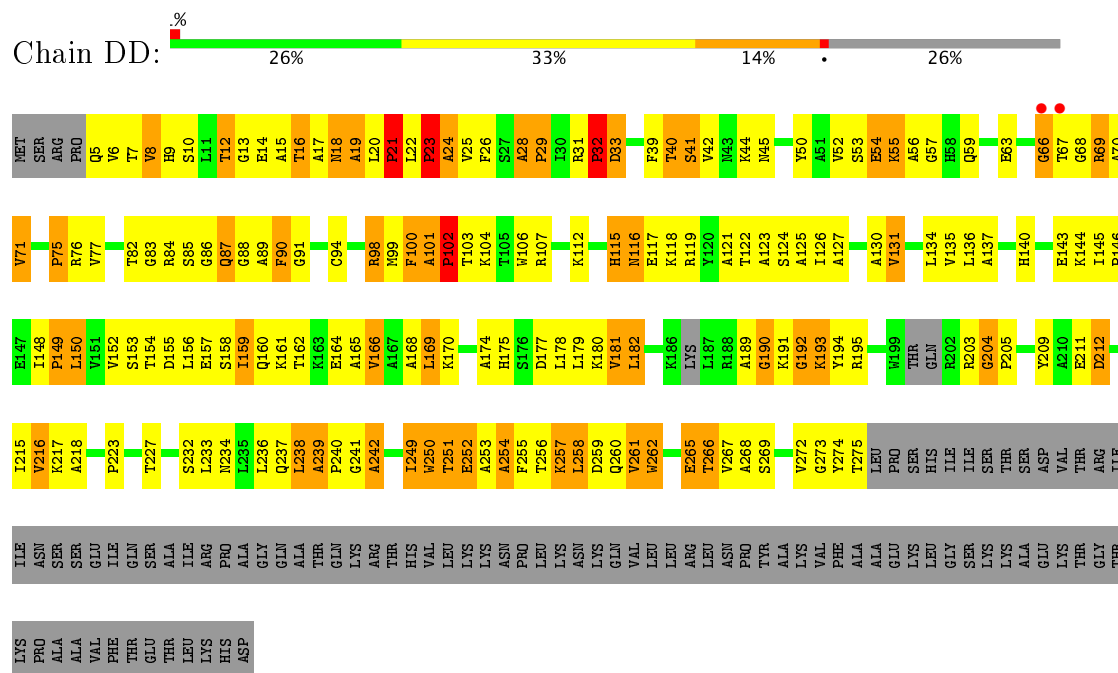




### • Molecule 35: 60S ribosomal protein L4-A



### • Molecule 35: 60S ribosomal protein L4-A

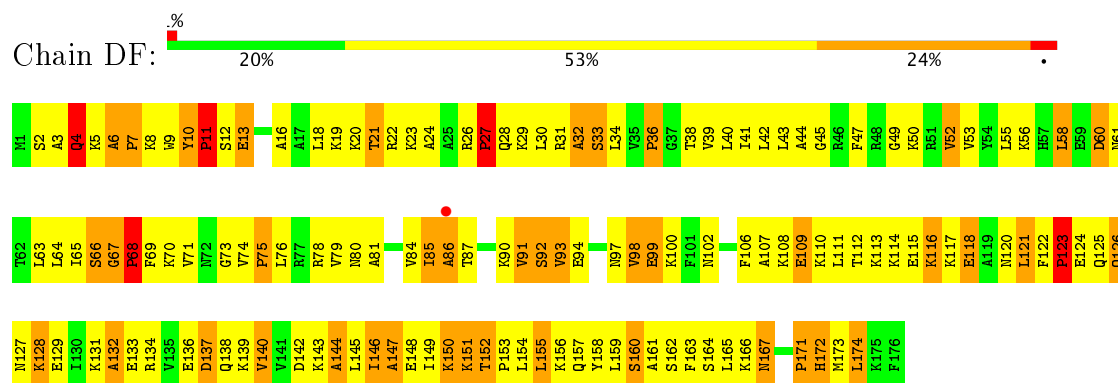


### • Molecule 36: 60S ribosomal protein L5

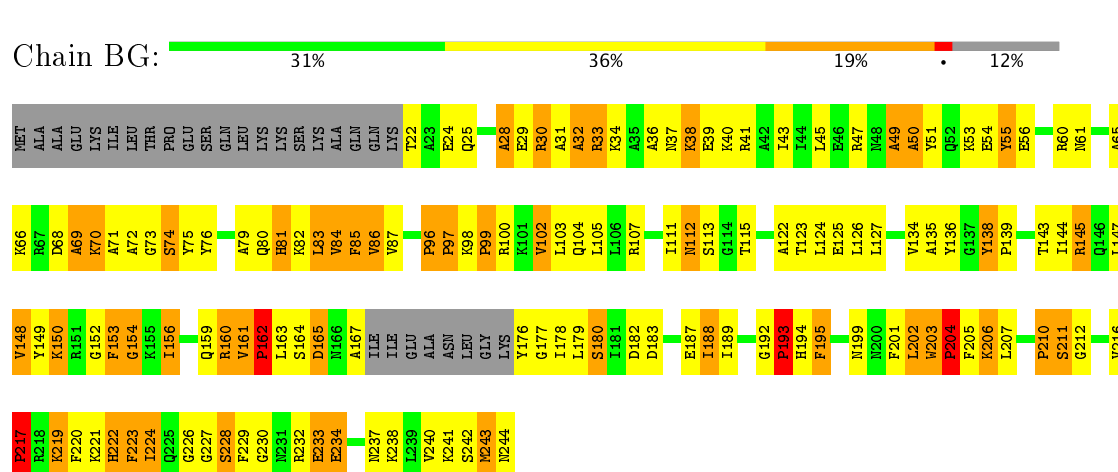




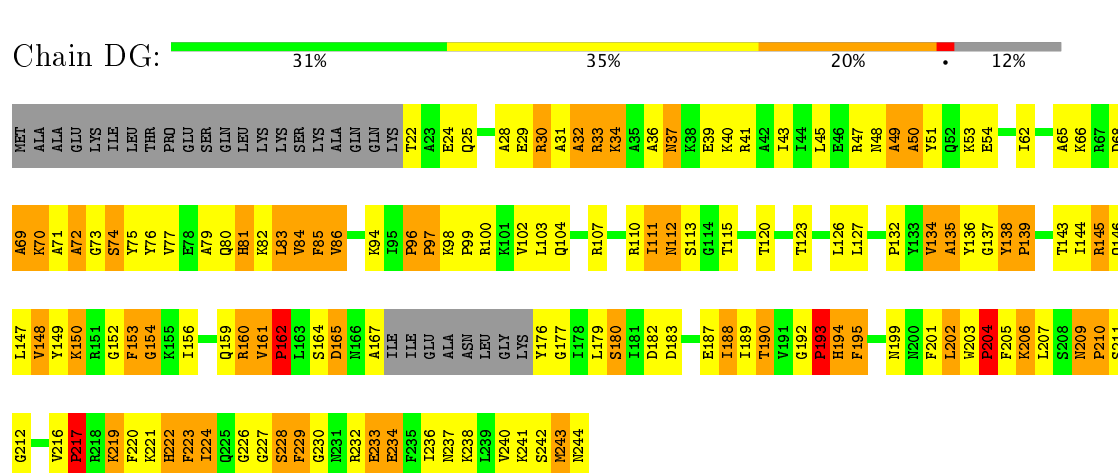
- Molecule 37: 60S ribosomal protein L6-A



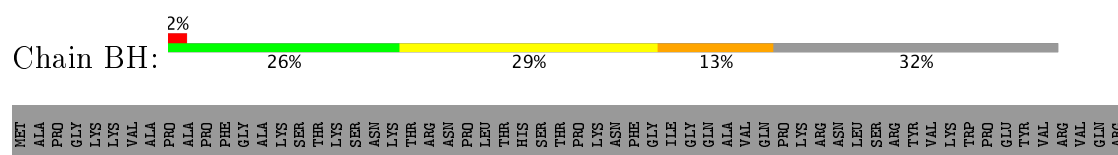
- Molecule 38: 60S ribosomal protein L7-A

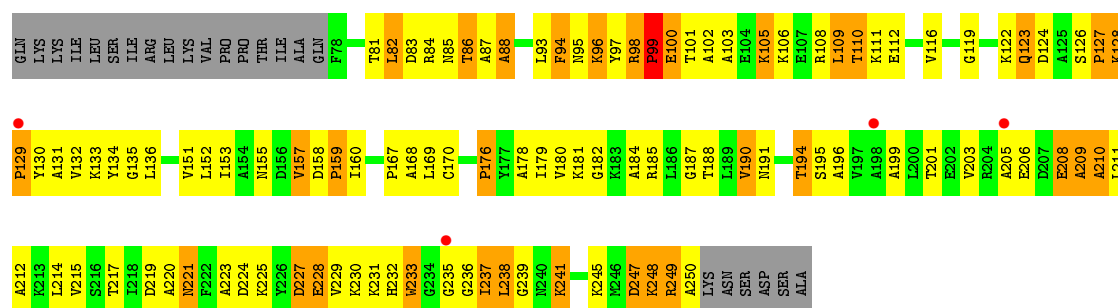


- Molecule 38: 60S ribosomal protein L7-A

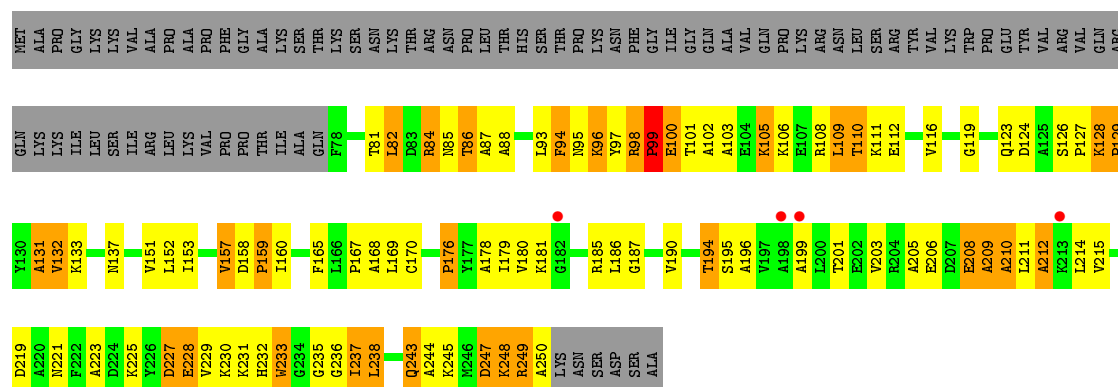
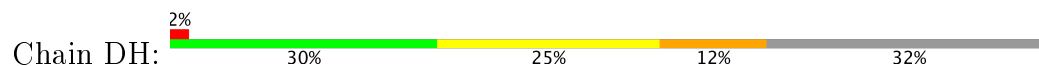


- Molecule 39: 60S ribosomal protein L8-A

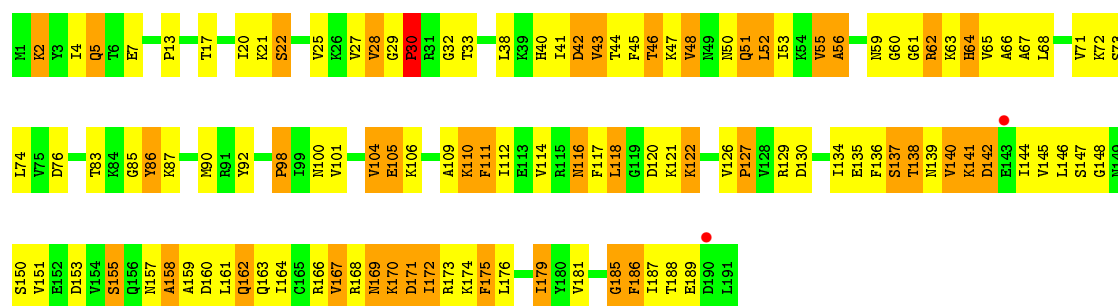




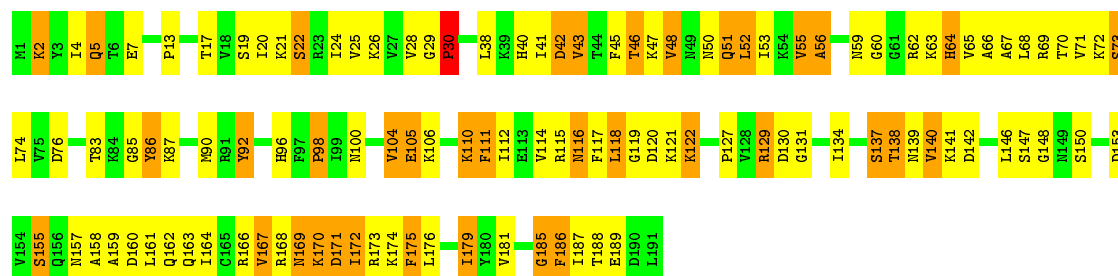
• Molecule 39: 60S ribosomal protein L8-A



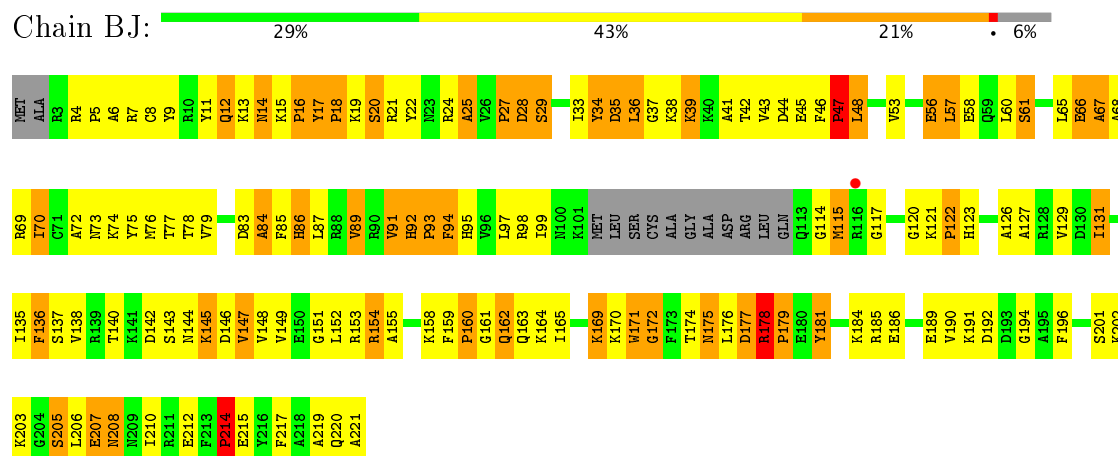
• Molecule 40: 60S ribosomal protein L9-A



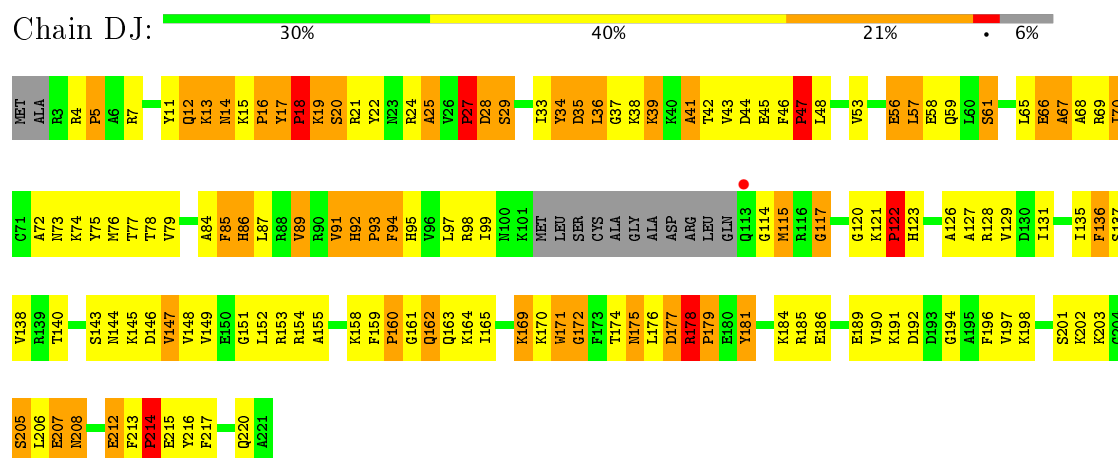
• Molecule 40: 60S ribosomal protein L9-A



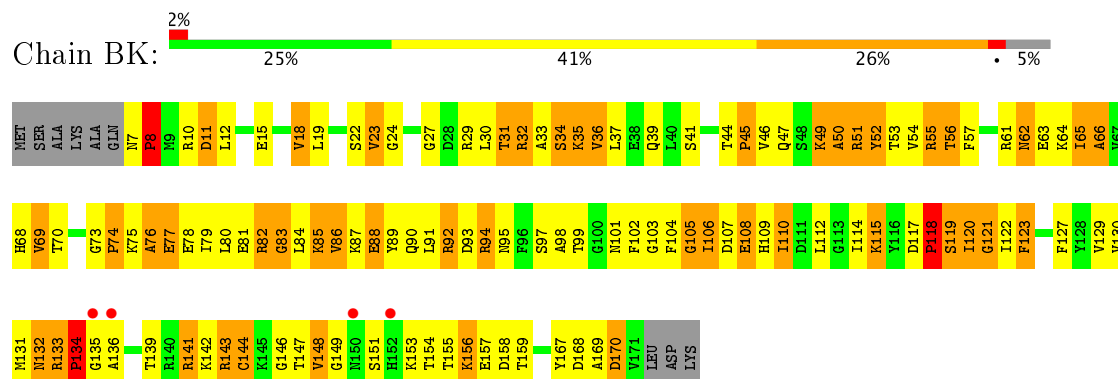
- Molecule 41: 60S ribosomal protein L10



- Molecule 41: 60S ribosomal protein L10

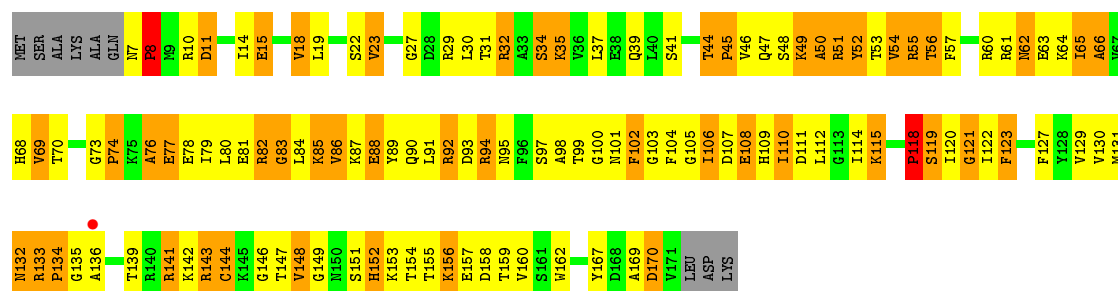


- Molecule 42: 60S ribosomal protein L11-A



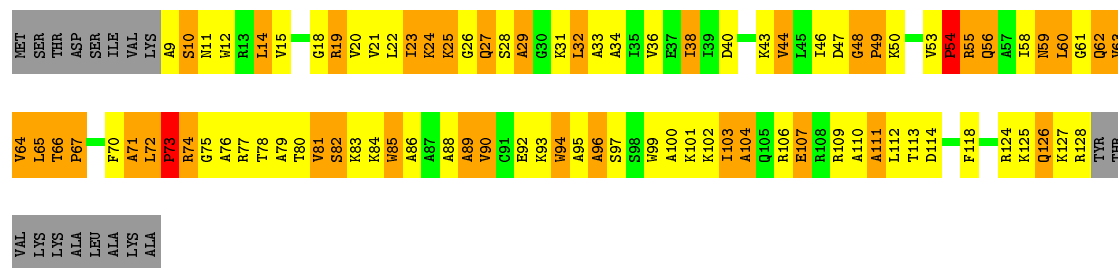
- Molecule 42: 60S ribosomal protein L11-A





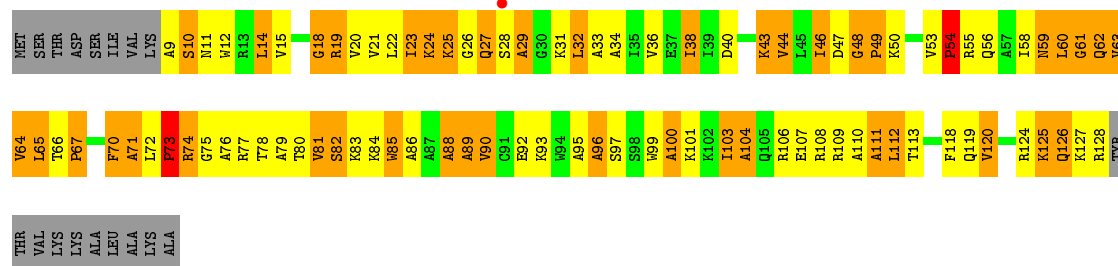
• Molecule 43: 60S ribosomal protein L14-A

Chain BN: 20% 38% 28% 13%



• Molecule 43: 60S ribosomal protein L14-A

Chain DN: 20% 35% 30% 13%



• Molecule 44: 60S ribosomal protein L15-A

Chain BO: 36% 33% 21% 8%

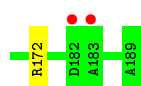


• Molecule 44: 60S ribosomal protein L15-A

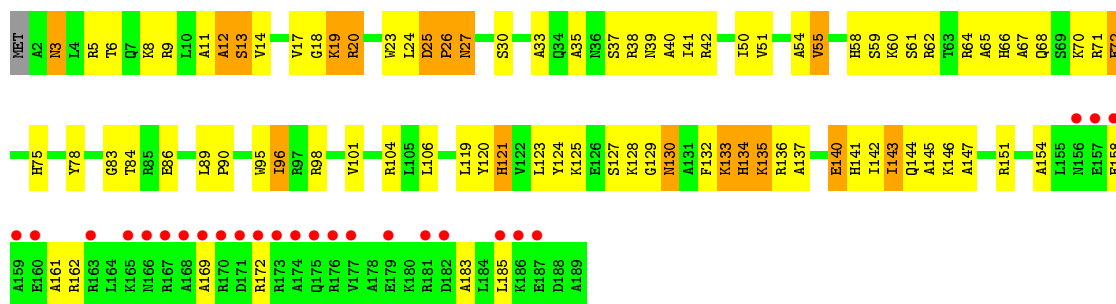
Chain DO: 39% 33% 19% 8%



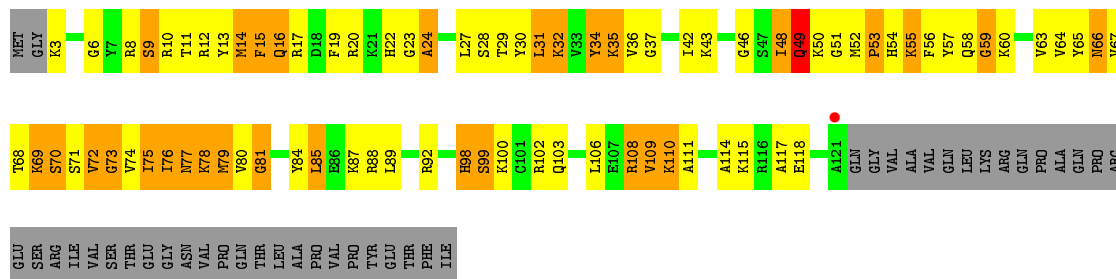
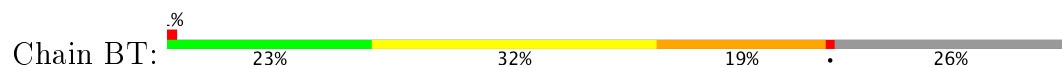




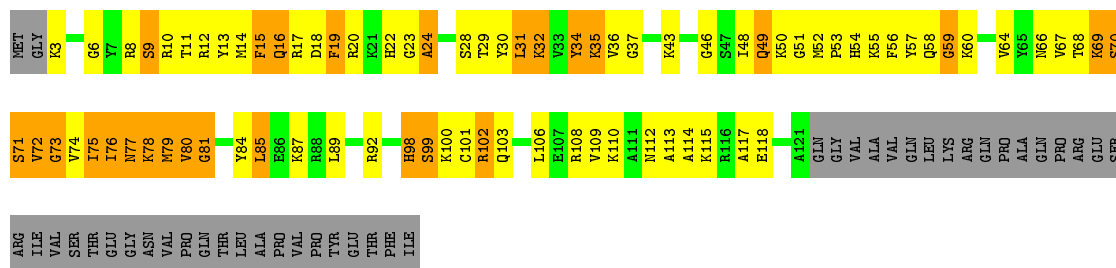
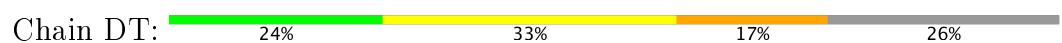
- Molecule 48: 60S ribosomal protein L19



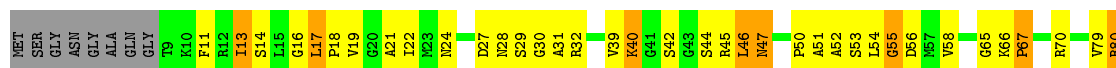
- Molecule 49: 60S ribosomal protein L21-A



- Molecule 49: 60S ribosomal protein L21-A



- Molecule 50: 60S ribosomal protein L23

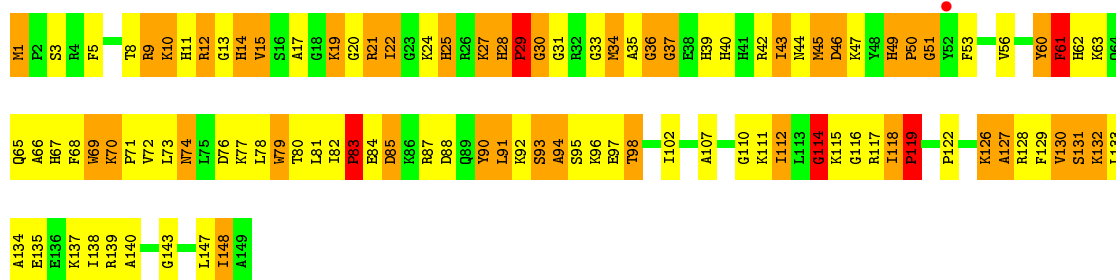




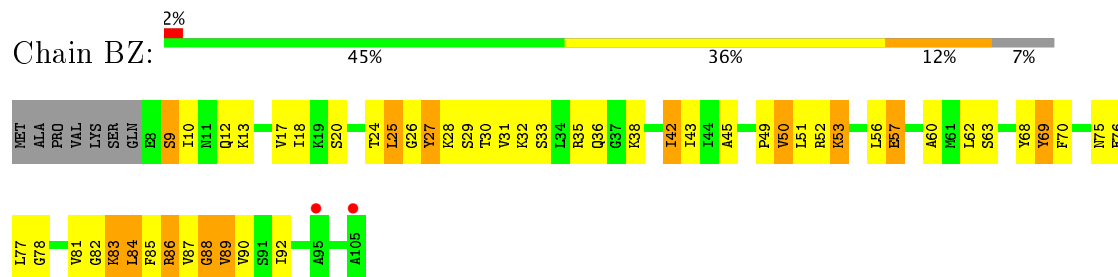


Chain DW: 

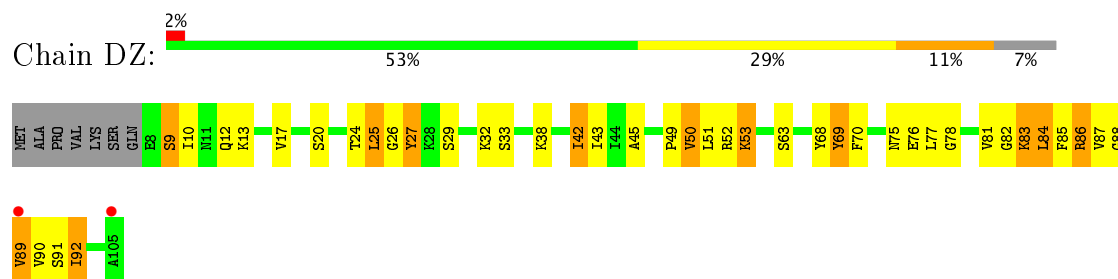




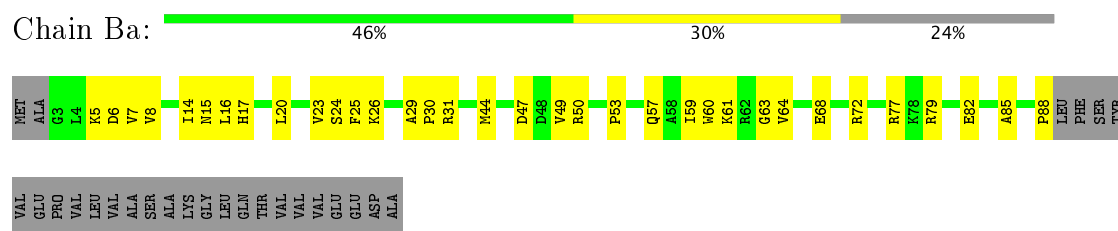
- Molecule 55: 60S ribosomal protein L30



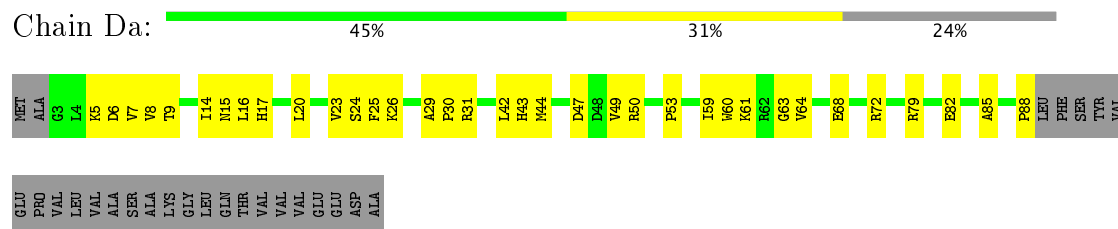
- Molecule 55: 60S ribosomal protein L30



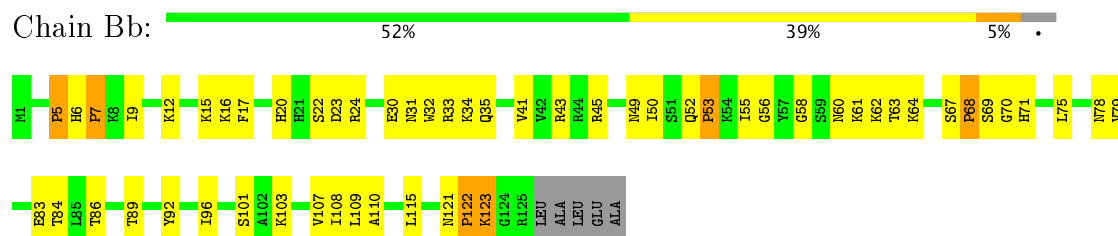
- Molecule 56: 60S ribosomal protein L31-A



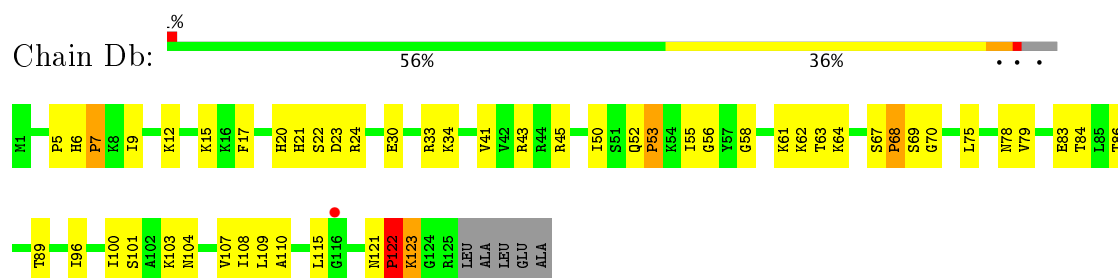
- Molecule 56: 60S ribosomal protein L31-A



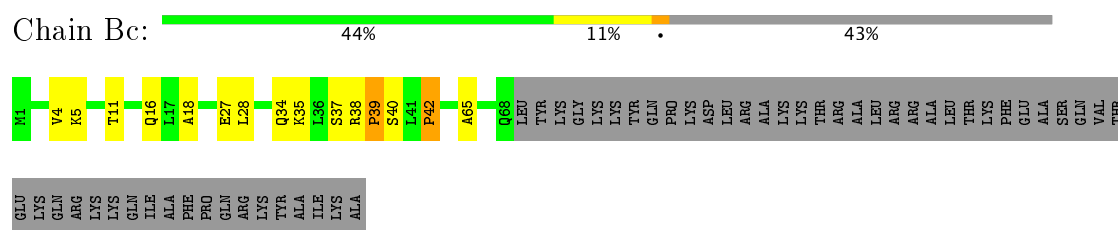
- Molecule 57: 60S ribosomal protein L32



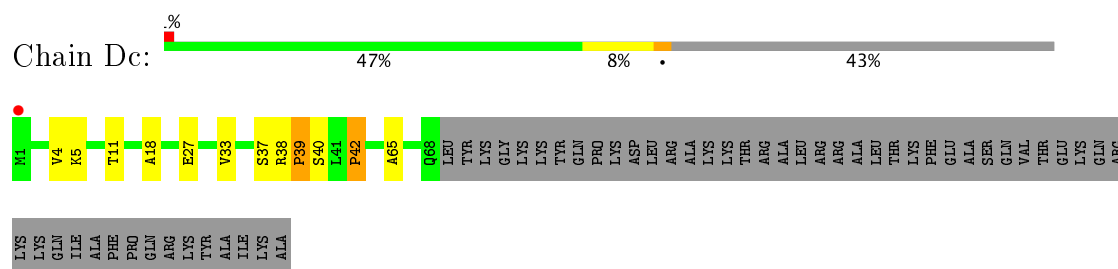
- Molecule 57: 60S ribosomal protein L32



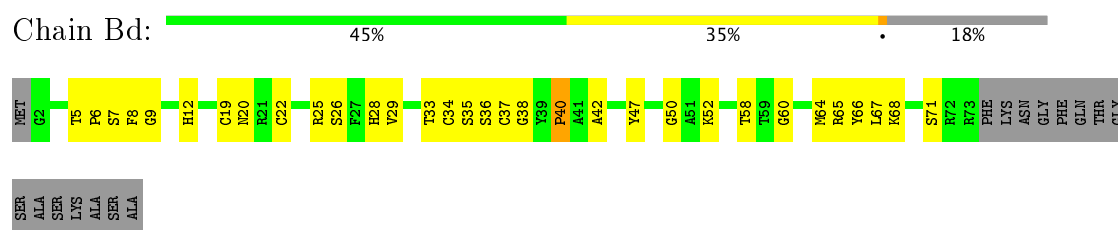
- Molecule 58: 60S ribosomal protein L35



- Molecule 58: 60S ribosomal protein L35

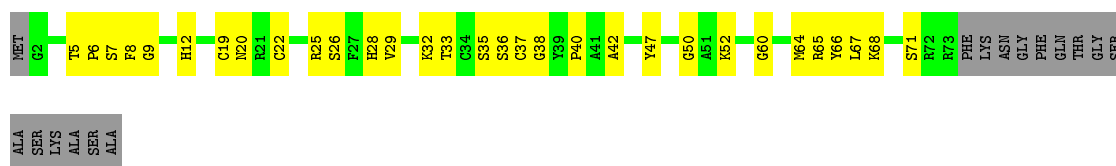


- Molecule 59: 60S ribosomal protein L37-A

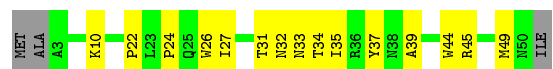


- Molecule 59: 60S ribosomal protein L37-A

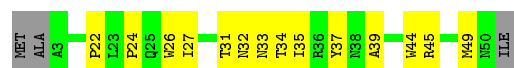




- Molecule 60: 60S ribosomal protein L39



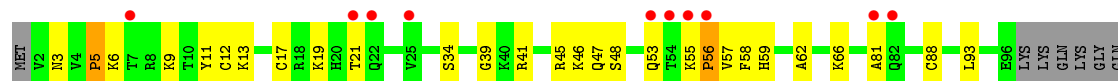
- Molecule 60: 60S ribosomal protein L39



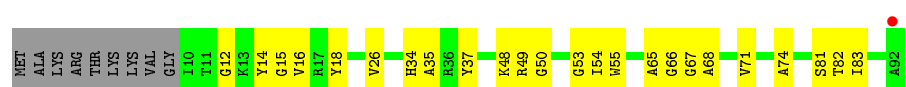
- Molecule 61: 60S ribosomal protein L42



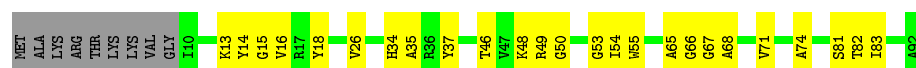
- Molecule 61: 60S ribosomal protein L42



- Molecule 62: 60S ribosomal protein L43



- Molecule 62: 60S ribosomal protein L43



- Molecule 63: Unassigned secondary structure

Chain Bh:  100%

There are no outlier residues recorded for this chain.

- Molecule 63: Unassigned secondary structure

Chain Dh:  100%

There are no outlier residues recorded for this chain.

- Molecule 64: Unassigned secondary structure

Chain Bi:  100%

There are no outlier residues recorded for this chain.

- Molecule 64: Unassigned secondary structure

Chain Di:  100%

There are no outlier residues recorded for this chain.

- Molecule 65: Unassigned secondary structure

Chain Bk:  100%

There are no outlier residues recorded for this chain.

- Molecule 65: Unassigned secondary structure

Chain Dk:  100%

There are no outlier residues recorded for this chain.

- Molecule 66: Unassigned secondary structure

Chain Bl:  100%

There are no outlier residues recorded for this chain.

- Molecule 67: Unassigned secondary structure

Chain Bm:  100%

There are no outlier residues recorded for this chain.

- Molecule 68: Unassigned secondary structure

Chain Bn:  100%

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, $\alpha$ , $\beta$ , $\gamma$	437.11Å 288.38Å 306.56Å 90.00° 99.13° 90.00°	Depositor
Resolution (Å)	268.00 – 4.00 268.66 – 4.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (268.00-4.00) 97.9 (268.66-4.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 4.02Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.278 , 0.341 0.277 , 0.341	Depositor DCC
$R_{free}$ test set	12351 reflections (2.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	147.1	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.16 , 259.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	309610	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	A1	0.77	20/42619 (0.0%)	1.32	552/66408 (0.8%)
1	C1	0.83	25/42619 (0.1%)	1.37	627/66408 (0.9%)
2	AA	0.45	0/1089	0.86	16/1517 (1.1%)
2	CA	0.50	0/1089	0.87	15/1517 (1.0%)
3	AB	0.54	0/1073	0.91	13/1488 (0.9%)
3	CB	0.56	0/1073	0.91	10/1488 (0.7%)
4	AC	0.50	0/927	0.68	4/1286 (0.3%)
4	CC	0.47	0/927	0.67	4/1286 (0.3%)
5	AD	0.45	0/834	0.71	5/1159 (0.4%)
5	CD	0.50	0/834	0.79	5/1159 (0.4%)
6	AE	0.49	0/775	0.70	3/1077 (0.3%)
6	CE	0.53	0/775	0.73	3/1077 (0.3%)
7	AF	0.60	0/381	0.88	3/530 (0.6%)
7	CF	0.59	0/381	0.90	4/530 (0.8%)
8	AG	0.51	0/579	0.78	5/806 (0.6%)
8	CG	0.52	0/579	0.79	5/806 (0.6%)
9	AH	0.43	0/626	0.71	4/867 (0.5%)
9	CH	0.44	0/626	0.72	4/867 (0.5%)
10	AI	0.45	0/595	0.90	8/826 (1.0%)
10	CI	0.52	0/595	0.91	7/826 (0.8%)
11	AJ	0.49	0/657	0.78	5/911 (0.5%)
11	CJ	0.55	0/657	0.81	5/911 (0.5%)
12	AK	0.44	0/331	0.74	2/460 (0.4%)
12	CK	0.41	0/331	0.70	2/460 (0.4%)
13	AL	0.47	0/589	0.70	2/816 (0.2%)
13	CL	0.50	0/589	0.72	2/816 (0.2%)
14	AM	0.54	0/518	0.83	3/715 (0.4%)
14	CM	0.68	1/518 (0.2%)	0.89	3/715 (0.4%)
15	AN	0.51	0/550	0.84	5/766 (0.7%)
15	CN	0.52	0/550	0.86	5/766 (0.7%)
16	AO	0.53	0/621	0.83	3/860 (0.3%)
16	CO	0.56	0/621	0.85	3/860 (0.3%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AP	0.61	0/565	0.92	4/781 (0.5%)
17	CP	0.68	0/565	0.97	5/781 (0.6%)
18	AQ	0.41	0/331	0.68	2/460 (0.4%)
18	CQ	0.44	0/311	0.74	2/432 (0.5%)
19	AR	0.40	0/229	0.63	1/316 (0.3%)
19	CR	0.42	0/229	0.68	1/316 (0.3%)
20	AS	0.54	0/189	0.70	0/260
20	CS	0.58	0/189	0.73	0/260
21	AT	0.43	0/1541	0.61	8/2141 (0.4%)
21	CT	0.45	0/1541	0.61	8/2141 (0.4%)
29	B1	1.11	229/76764 (0.3%)	1.79	2866/119684 (2.4%)
29	D1	1.08	218/76764 (0.3%)	1.75	2607/119684 (2.2%)
30	B2	1.06	8/2883 (0.3%)	1.70	90/4491 (2.0%)
30	D2	1.17	10/2883 (0.3%)	1.84	112/4491 (2.5%)
31	B3	0.91	6/3746 (0.2%)	1.41	64/5832 (1.1%)
31	D3	0.79	1/3746 (0.0%)	1.28	40/5832 (0.7%)
32	BA	0.34	0/1054	0.63	9/1468 (0.6%)
32	DA	0.33	0/1054	0.61	9/1468 (0.6%)
33	BB	0.62	0/1103	0.92	11/1501 (0.7%)
33	DB	0.53	0/1103	0.87	11/1501 (0.7%)
34	BC	0.70	0/1790	1.05	9/2487 (0.4%)
34	DC	0.76	0/1790	1.08	12/2487 (0.5%)
35	BD	0.67	0/1311	0.95	9/1817 (0.5%)
35	DD	0.55	0/1311	0.90	12/1817 (0.7%)
36	BE	0.53	0/1411	0.93	9/1960 (0.5%)
36	DE	0.59	0/1411	0.97	9/1960 (0.5%)
37	BF	0.76	0/872	1.20	10/1215 (0.8%)
37	DF	0.85	0/872	1.21	12/1215 (1.0%)
38	BG	0.73	0/1059	1.06	8/1471 (0.5%)
38	DG	0.75	0/1059	1.05	9/1471 (0.6%)
39	BH	0.48	0/855	0.79	6/1190 (0.5%)
39	DH	0.45	0/855	0.76	6/1190 (0.5%)
40	BI	0.64	0/941	0.86	4/1308 (0.3%)
40	DI	0.73	0/941	0.92	5/1308 (0.4%)
41	BJ	0.66	0/1025	0.89	8/1424 (0.6%)
41	DJ	0.71	0/1025	0.91	9/1424 (0.6%)
42	BK	0.56	0/809	0.86	5/1122 (0.4%)
42	DK	0.61	0/809	0.87	4/1122 (0.4%)
43	BN	0.71	0/592	1.05	6/823 (0.7%)
43	DN	0.82	0/592	1.14	6/823 (0.7%)
44	BO	0.59	0/922	0.88	7/1282 (0.5%)
44	DO	0.51	0/922	0.86	7/1282 (0.5%)
45	BP	0.80	0/966	1.12	10/1343 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
45	DP	0.84	1/966 (0.1%)	1.14	12/1343 (0.9%)
46	BQ	0.72	0/760	0.94	5/1057 (0.5%)
46	DQ	0.65	0/760	0.87	4/1057 (0.4%)
47	BR	0.70	0/705	1.00	6/980 (0.6%)
47	DR	0.60	0/705	0.94	7/980 (0.7%)
48	BS	0.52	0/930	0.63	2/1295 (0.2%)
48	DS	0.48	0/930	0.58	2/1295 (0.2%)
49	BT	0.68	0/585	0.85	0/812
49	DT	0.70	0/585	0.87	0/812
50	BU	0.63	0/630	0.86	5/872 (0.6%)
50	DU	0.75	0/630	0.93	5/872 (0.6%)
51	BV	0.54	0/290	0.84	2/402 (0.5%)
51	DV	0.58	0/290	0.85	2/402 (0.5%)
52	BW	0.55	0/467	0.84	2/651 (0.3%)
52	DW	0.49	0/467	0.81	3/651 (0.5%)
53	BX	0.55	0/529	0.78	4/736 (0.5%)
53	DX	0.49	0/529	0.74	3/736 (0.4%)
54	BY	0.70	0/726	1.10	9/1004 (0.9%)
54	DY	0.62	0/726	1.03	8/1004 (0.8%)
55	BZ	0.49	0/480	0.62	1/665 (0.2%)
55	DZ	0.46	0/480	0.62	1/665 (0.2%)
56	Ba	0.62	0/424	0.94	3/589 (0.5%)
56	Da	0.59	0/424	0.92	3/589 (0.5%)
57	Bb	0.72	0/617	1.13	6/858 (0.7%)
57	Db	0.61	0/617	1.07	6/858 (0.7%)
58	Bc	0.53	0/338	0.82	2/471 (0.4%)
58	Dc	0.45	0/338	0.74	2/471 (0.4%)
59	Bd	0.63	0/351	0.97	2/485 (0.4%)
59	Dd	0.54	0/351	0.89	2/485 (0.4%)
60	Be	0.59	0/239	0.85	2/333 (0.6%)
60	De	0.46	0/239	0.79	2/333 (0.6%)
61	Bf	0.47	0/466	0.68	2/646 (0.3%)
61	Df	0.39	0/466	0.66	2/646 (0.3%)
62	Bg	0.53	0/406	0.74	1/562 (0.2%)
62	Dg	0.49	0/406	0.67	0/562
72	DL	0.42	0/678	0.75	7/941 (0.7%)
73	DM	0.48	0/639	0.76	4/886 (0.5%)
All	All	0.92	519/326627 (0.2%)	1.50	7498/496371 (1.5%)

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
3	AB	0	2
3	CB	0	2
17	AP	0	1
17	CP	0	1
18	AQ	0	1
18	CQ	0	1
22	Bo	0	1
23	Ab	0	1
23	Cb	0	1
24	Ac	0	1
29	B1	0	3
29	D1	0	3
34	BC	0	5
34	DC	0	6
35	BD	0	1
35	DD	0	2
36	BE	0	1
36	DE	0	1
37	BF	0	4
37	DF	0	4
38	BG	0	1
38	DG	0	1
42	BK	0	1
42	DK	0	1
44	DO	0	1
45	BP	0	4
45	DP	0	5
49	BT	0	1
49	DT	0	1
51	BV	0	1
51	DV	0	1
54	BY	0	2
54	DY	0	2
56	Ba	0	1
56	Da	0	1
57	Bb	0	1
57	Db	0	1
All	All	0	68

The worst 5 of 519 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D1	3243	A	N9-C4	13.96	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D1	308	A	C6-N1	-13.36	1.26	1.35
29	B1	3184	A	C6-N1	-12.55	1.26	1.35
29	B1	308	A	C6-N1	-11.80	1.27	1.35
29	D1	2845	A	C6-N1	-11.64	1.27	1.35

The worst 5 of 7498 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D1	244	G	N1-C6-O6	43.40	145.94	119.90
29	B1	244	G	N1-C6-O6	41.87	145.02	119.90
29	D1	2845	A	N1-C6-N6	40.75	143.05	118.60
29	D1	2845	A	C6-N1-C2	39.78	142.47	118.60
29	B1	2845	A	N1-C6-N6	39.33	142.20	118.60

There are no chirality outliers.

5 of 68 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AB	224	PHE	Peptide
3	AB	225	LEU	Peptide
17	AP	28	ASN	Peptide
18	AQ	41	ILE	Peptide
23	Ab	14	UNK	Peptide

## 5.2 Too-close contacts [i](#)

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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	38107	0	19170	5867	0
1	C1	38107	0	19169	6035	0
2	AA	1090	0	508	112	0
2	CA	1090	0	508	119	0
3	AB	1074	0	502	131	0
3	CB	1074	0	502	141	0
4	AC	928	0	448	85	0
4	CC	928	0	448	89	0
5	AD	836	0	391	107	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	CD	836	0	391	111	0
6	AE	777	0	362	86	0
6	CE	777	0	362	89	0
7	AF	382	0	164	27	0
7	CF	382	0	164	25	0
8	AG	580	0	266	67	0
8	CG	580	0	266	61	0
9	AH	627	0	312	61	0
9	CH	627	0	312	77	0
10	AI	596	0	272	56	0
10	CI	596	0	272	71	0
11	AJ	658	0	307	80	0
11	CJ	658	0	307	83	0
12	AK	332	0	146	26	0
12	CK	332	0	146	21	0
13	AL	591	0	261	72	0
13	CL	591	0	261	77	0
14	AM	521	0	251	66	0
14	CM	521	0	251	67	0
15	AN	551	0	229	82	0
15	CN	551	0	229	77	0
16	AO	622	0	283	58	0
16	CO	622	0	283	51	0
17	AP	566	0	260	75	0
17	CP	566	0	260	74	0
18	AQ	332	0	149	16	0
18	CQ	312	0	135	17	0
19	AR	230	0	100	10	0
19	CR	230	0	100	11	0
20	AS	190	0	85	47	0
20	CS	190	0	85	45	0
21	AT	1543	0	743	94	0
21	CT	1543	0	743	103	0
22	Aa	100	0	25	0	0
22	Bo	100	0	23	0	0
22	Ca	100	0	23	0	0
23	Ab	525	0	141	0	0
23	Cb	525	0	138	0	0
24	Ac	465	0	122	0	0
24	Cc	465	0	120	0	0
25	Ad	175	0	39	0	0
25	Cd	175	0	41	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	Ae	105	0	25	0	0
26	Bj	105	0	23	0	0
26	Dj	105	0	24	0	0
27	Af	55	0	15	0	0
28	Ah	205	0	51	0	0
28	Ch	205	0	50	0	0
29	B1	68577	0	34452	11488	0
29	D1	68577	0	34452	11458	0
30	B2	2579	0	1304	604	0
30	D2	2579	0	1304	619	0
31	B3	3353	0	1695	663	0
31	D3	3353	0	1695	615	0
32	BA	1055	0	453	34	0
32	DA	1055	0	453	36	0
33	BB	1106	0	512	95	0
33	DB	1106	0	512	108	0
34	BC	1791	0	839	262	0
34	DC	1791	0	839	274	0
35	BD	1312	0	651	166	0
35	DD	1312	0	651	155	0
36	BE	1412	0	670	216	0
36	DE	1412	0	670	207	0
37	BF	873	0	400	151	0
37	DF	873	0	400	144	0
38	BG	1061	0	492	138	0
38	DG	1061	0	492	140	0
39	BH	856	0	432	75	0
39	DH	856	0	432	64	0
40	BI	942	0	414	88	0
40	DI	942	0	414	87	0
41	BJ	1027	0	468	98	0
41	DJ	1027	0	468	99	0
42	BK	810	0	360	126	0
42	DK	810	0	360	122	0
43	BN	593	0	299	99	0
43	DN	593	0	299	112	0
44	BO	923	0	423	128	0
44	DO	923	0	423	114	0
45	BP	967	0	468	145	0
45	DP	967	0	468	154	0
46	BQ	761	0	371	101	0
46	DQ	761	0	371	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	BR	706	0	340	94	0
47	DR	706	0	340	90	0
48	BS	931	0	460	66	0
48	DS	931	0	460	75	0
49	BT	586	0	269	85	0
49	DT	586	0	269	72	0
50	BU	631	0	306	38	0
50	DU	631	0	306	40	0
51	BV	291	0	131	38	0
51	DV	291	0	131	34	0
52	BW	468	0	213	38	0
52	DW	468	0	213	43	0
53	BX	530	0	240	48	0
53	DX	530	0	240	41	0
54	BY	727	0	346	102	0
54	DY	727	0	346	98	0
55	BZ	481	0	224	32	0
55	DZ	481	0	224	31	0
56	Ba	425	0	191	0	0
56	Da	425	0	191	0	0
57	Bb	618	0	284	0	0
57	Db	618	0	284	0	0
58	Bc	339	0	155	0	0
58	Dc	339	0	155	0	0
59	Bd	352	0	161	0	0
59	Dd	352	0	161	0	0
60	Be	240	0	105	0	0
60	De	240	0	105	0	0
61	Bf	467	0	210	0	0
61	Df	467	0	210	0	0
62	Bg	407	0	203	0	0
62	Dg	407	0	203	0	0
63	Bh	220	0	57	0	0
63	Dh	220	0	53	0	0
64	Bi	60	0	16	0	0
64	Di	60	0	14	0	0
65	Bk	80	0	20	0	0
65	Dk	80	0	21	0	0
66	Bl	95	0	21	0	0
67	Bm	45	0	12	0	0
68	Bn	135	0	34	0	0
69	Bp	40	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	Bq	85	0	25	0	0
71	Br	115	0	27	0	0
72	DL	679	0	325	49	0
73	DM	641	0	281	65	0
74	A1	714	0	0	109	0
74	AL	7	0	0	0	0
74	AS	7	0	0	18	0
74	AT	7	0	0	1	0
74	Ac	7	0	0	0	0
74	B1	1547	0	0	220	0
74	B2	70	0	0	12	0
74	B3	84	0	0	14	0
74	BC	7	0	0	1	0
74	BO	7	0	0	0	0
74	BT	7	0	0	2	0
74	Bd	14	0	0	0	0
74	Bg	7	0	0	0	0
74	C1	707	0	0	107	0
74	CI	7	0	0	0	0
74	CS	14	0	0	16	0
74	CT	7	0	0	0	0
74	D1	1575	0	0	223	0
74	D2	63	0	0	18	0
74	D3	84	0	0	28	0
74	DC	7	0	0	0	0
74	DE	7	0	0	0	0
74	DJ	7	0	0	0	0
74	DO	14	0	0	5	0
74	DT	7	0	0	0	0
74	Dd	14	0	0	0	0
74	Dg	7	0	0	0	0
All	All	309610	0	149262	44156	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 99.

The worst 5 of 44156 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B1:592:A:H2'	29:B1:593:C:C4'	1.31	1.55
29:B1:606:C:H3'	29:B1:607:A:C8	1.39	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D1:606:C:H3'	29:D1:607:A:C8	1.43	1.52
1:A1:825:U:C5	1:A1:847:A:N1	1.82	1.45
1:C1:825:U:C5	1:C1:847:A:N1	1.84	1.45

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	218/252 (86%)	75 (34%)	68 (31%)	75 (34%)	0	0
2	CA	218/252 (86%)	78 (36%)	63 (29%)	77 (35%)	0	0
3	AB	217/254 (85%)	85 (39%)	54 (25%)	78 (36%)	0	0
3	CB	217/254 (85%)	81 (37%)	62 (29%)	74 (34%)	0	0
4	AC	187/240 (78%)	72 (38%)	56 (30%)	59 (32%)	0	0
4	CC	187/240 (78%)	69 (37%)	55 (29%)	63 (34%)	0	0
5	AD	165/225 (73%)	55 (33%)	46 (28%)	64 (39%)	0	0
5	CD	165/225 (73%)	58 (35%)	44 (27%)	63 (38%)	0	0
6	AE	153/197 (78%)	48 (31%)	54 (35%)	51 (33%)	0	0
6	CE	153/197 (78%)	48 (31%)	49 (32%)	56 (37%)	0	0
7	AF	75/156 (48%)	32 (43%)	18 (24%)	25 (33%)	0	0
7	CF	75/156 (48%)	31 (41%)	20 (27%)	24 (32%)	0	0
8	AG	115/151 (76%)	46 (40%)	38 (33%)	31 (27%)	0	0
8	CG	115/151 (76%)	49 (43%)	33 (29%)	33 (29%)	0	0
9	AH	126/137 (92%)	52 (41%)	38 (30%)	36 (29%)	0	0
9	CH	126/137 (92%)	51 (40%)	39 (31%)	36 (29%)	0	0
10	AI	119/142 (84%)	38 (32%)	40 (34%)	41 (34%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CI	119/142 (84%)	43 (36%)	35 (29%)	41 (34%)	0	0
11	AJ	132/143 (92%)	57 (43%)	33 (25%)	42 (32%)	0	0
11	CJ	132/143 (92%)	52 (39%)	37 (28%)	43 (33%)	0	0
12	AK	65/136 (48%)	27 (42%)	16 (25%)	22 (34%)	0	0
12	CK	65/136 (48%)	28 (43%)	16 (25%)	21 (32%)	0	0
13	AL	116/146 (80%)	48 (41%)	34 (29%)	34 (29%)	0	0
13	CL	116/146 (80%)	48 (41%)	33 (28%)	35 (30%)	0	0
14	AM	100/144 (69%)	38 (38%)	28 (28%)	34 (34%)	0	0
14	CM	100/144 (69%)	36 (36%)	27 (27%)	37 (37%)	0	0
15	AN	109/121 (90%)	49 (45%)	30 (28%)	30 (28%)	0	0
15	CN	109/121 (90%)	49 (45%)	29 (27%)	31 (28%)	0	0
16	AO	125/130 (96%)	48 (38%)	40 (32%)	37 (30%)	0	0
16	CO	125/130 (96%)	49 (39%)	36 (29%)	40 (32%)	0	0
17	AP	114/145 (79%)	48 (42%)	24 (21%)	42 (37%)	0	0
17	CP	114/145 (79%)	45 (40%)	28 (25%)	41 (36%)	0	0
18	AQ	65/108 (60%)	28 (43%)	21 (32%)	16 (25%)	0	1
18	CQ	61/108 (56%)	28 (46%)	18 (30%)	15 (25%)	0	1
19	AR	45/67 (67%)	17 (38%)	12 (27%)	16 (36%)	0	0
19	CR	45/67 (67%)	17 (38%)	11 (24%)	17 (38%)	0	0
20	AS	37/56 (66%)	8 (22%)	14 (38%)	15 (40%)	0	0
20	CS	37/56 (66%)	8 (22%)	13 (35%)	16 (43%)	0	0
21	AT	309/319 (97%)	180 (58%)	71 (23%)	58 (19%)	0	2
21	CT	309/319 (97%)	184 (60%)	66 (21%)	59 (19%)	0	2
32	BA	211/217 (97%)	76 (36%)	67 (32%)	68 (32%)	0	0
32	DA	211/217 (97%)	76 (36%)	79 (37%)	56 (26%)	0	1
33	BB	228/254 (90%)	80 (35%)	55 (24%)	93 (41%)	0	0
33	DB	228/254 (90%)	83 (36%)	55 (24%)	90 (40%)	0	0
34	BC	362/387 (94%)	112 (31%)	100 (28%)	150 (41%)	0	0
34	DC	362/387 (94%)	109 (30%)	102 (28%)	151 (42%)	0	0
35	BD	266/362 (74%)	111 (42%)	79 (30%)	76 (29%)	0	0
35	DD	266/362 (74%)	109 (41%)	78 (29%)	79 (30%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BE	285/297 (96%)	108 (38%)	82 (29%)	95 (33%)	0	0
36	DE	285/297 (96%)	105 (37%)	79 (28%)	101 (35%)	0	0
37	BF	174/176 (99%)	44 (25%)	62 (36%)	68 (39%)	0	0
37	DF	174/176 (99%)	43 (25%)	61 (35%)	70 (40%)	0	0
38	BG	211/244 (86%)	85 (40%)	62 (29%)	64 (30%)	0	0
38	DG	211/244 (86%)	89 (42%)	60 (28%)	62 (29%)	0	0
39	BH	171/256 (67%)	59 (34%)	58 (34%)	54 (32%)	0	0
39	DH	171/256 (67%)	60 (35%)	62 (36%)	49 (29%)	0	0
40	BI	189/191 (99%)	76 (40%)	60 (32%)	53 (28%)	0	0
40	DI	189/191 (99%)	79 (42%)	57 (30%)	53 (28%)	0	0
41	BJ	204/221 (92%)	80 (39%)	52 (26%)	72 (35%)	0	0
41	DJ	204/221 (92%)	75 (37%)	55 (27%)	74 (36%)	0	0
42	BK	163/174 (94%)	57 (35%)	42 (26%)	64 (39%)	0	0
42	DK	163/174 (94%)	56 (34%)	46 (28%)	61 (37%)	0	0
43	BN	118/138 (86%)	27 (23%)	44 (37%)	47 (40%)	0	0
43	DN	118/138 (86%)	28 (24%)	39 (33%)	51 (43%)	0	0
44	BO	185/204 (91%)	77 (42%)	49 (26%)	59 (32%)	0	0
44	DO	185/204 (91%)	76 (41%)	53 (29%)	56 (30%)	0	0
45	BP	194/199 (98%)	81 (42%)	56 (29%)	57 (29%)	0	0
45	DP	194/199 (98%)	77 (40%)	62 (32%)	55 (28%)	0	0
46	BQ	152/184 (83%)	62 (41%)	44 (29%)	46 (30%)	0	0
46	DQ	152/184 (83%)	62 (41%)	45 (30%)	45 (30%)	0	0
47	BR	141/186 (76%)	63 (45%)	28 (20%)	50 (36%)	0	0
47	DR	141/186 (76%)	59 (42%)	32 (23%)	50 (36%)	0	0
48	BS	186/189 (98%)	104 (56%)	57 (31%)	25 (13%)	0	5
48	DS	186/189 (98%)	101 (54%)	60 (32%)	25 (13%)	0	5
49	BT	117/160 (73%)	53 (45%)	18 (15%)	46 (39%)	0	0
49	DT	117/160 (73%)	50 (43%)	23 (20%)	44 (38%)	0	0
50	BU	127/137 (93%)	64 (50%)	28 (22%)	35 (28%)	0	0
50	DU	127/137 (93%)	70 (55%)	21 (16%)	36 (28%)	0	0
51	BV	57/155 (37%)	14 (25%)	19 (33%)	24 (42%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	DV	57/155 (37%)	15 (26%)	16 (28%)	26 (46%)	0	0
52	BW	92/142 (65%)	30 (33%)	30 (33%)	32 (35%)	0	0
52	DW	92/142 (65%)	32 (35%)	28 (30%)	32 (35%)	0	0
53	BX	105/127 (83%)	53 (50%)	28 (27%)	24 (23%)	0	1
53	DX	105/127 (83%)	55 (52%)	30 (29%)	20 (19%)	0	2
54	BY	147/149 (99%)	37 (25%)	47 (32%)	63 (43%)	0	0
54	DY	147/149 (99%)	36 (24%)	51 (35%)	60 (41%)	0	0
55	BZ	96/105 (91%)	48 (50%)	28 (29%)	20 (21%)	0	2
55	DZ	96/105 (91%)	51 (53%)	28 (29%)	17 (18%)	0	3
56	Ba	84/113 (74%)	27 (32%)	27 (32%)	30 (36%)	0	0
56	Da	84/113 (74%)	25 (30%)	28 (33%)	31 (37%)	0	0
57	Bb	123/130 (95%)	39 (32%)	28 (23%)	56 (46%)	0	0
57	Db	123/130 (95%)	41 (33%)	31 (25%)	51 (42%)	0	0
58	Bc	66/120 (55%)	28 (42%)	23 (35%)	15 (23%)	0	1
58	Dc	66/120 (55%)	28 (42%)	26 (39%)	12 (18%)	0	3
59	Bd	70/88 (80%)	19 (27%)	20 (29%)	31 (44%)	0	0
59	Dd	70/88 (80%)	17 (24%)	24 (34%)	29 (41%)	0	0
60	Be	46/51 (90%)	25 (54%)	8 (17%)	13 (28%)	0	0
60	De	46/51 (90%)	22 (48%)	12 (26%)	12 (26%)	0	1
61	Bf	93/106 (88%)	37 (40%)	28 (30%)	28 (30%)	0	0
61	Df	93/106 (88%)	37 (40%)	28 (30%)	28 (30%)	0	0
62	Bg	81/92 (88%)	31 (38%)	27 (33%)	23 (28%)	0	0
62	Dg	81/92 (88%)	32 (40%)	24 (30%)	25 (31%)	0	0
72	DL	136/165 (82%)	42 (31%)	42 (31%)	52 (38%)	0	0
73	DM	126/312 (40%)	48 (38%)	31 (25%)	47 (37%)	0	0
All	All	14930/18123 (82%)	5798 (39%)	4273 (29%)	4859 (32%)	0	0

5 of 4859 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AA	11	PRO
2	AA	13	ASP
2	AA	14	ALA

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Mol	Chain	Res	Type
2	AA	21	ASN
2	AA	24	LEU

### 5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	1787/1800 (99%)	1003 (56%)	148 (8%)
1	C1	1787/1800 (99%)	990 (55%)	150 (8%)
29	B1	3203/3396 (94%)	1725 (53%)	259 (8%)
29	D1	3203/3396 (94%)	1714 (53%)	257 (8%)
30	B2	120/121 (99%)	70 (58%)	12 (10%)
30	D2	120/121 (99%)	66 (55%)	12 (10%)
31	B3	157/158 (99%)	80 (50%)	9 (5%)
31	D3	157/158 (99%)	79 (50%)	9 (5%)
All	All	10534/10950 (96%)	5727 (54%)	856 (8%)

5 of 5727 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	2	A
1	A1	3	U
1	A1	4	C
1	A1	7	G
1	A1	8	U

5 of 856 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	B1	3179	U
1	C1	400	A
29	D1	3038	U
29	B1	3303	G
1	C1	65	A

## 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 ⓘ

715 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
74	OHX	A1	1901	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1902	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1903	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1904	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1905	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1906	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1907	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1908	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1909	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1910	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1911	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1912	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1913	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1914	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1915	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1916	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1917	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1918	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1919	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1920	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1921	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1922	-	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
74	OHX	A1	1923	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1924	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1925	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1926	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1927	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1928	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1929	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1930	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1931	1	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1932	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1933	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1934	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1935	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1936	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1937	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1938	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1939	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1940	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1941	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1942	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1943	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1944	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1945	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1946	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1947	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1948	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1949	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1950	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1951	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1952	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1953	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1954	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1955	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1956	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1957	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1958	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1959	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1960	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1961	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1962	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1963	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1964	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1965	-	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
74	OHX	A1	1966	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1967	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1968	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1969	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1970	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1971	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1972	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1973	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1974	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1975	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1976	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1977	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1978	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1979	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1980	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1981	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1982	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1983	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1984	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1985	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1986	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1987	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1988	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1989	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1990	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1991	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1992	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1993	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1994	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1995	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1996	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1997	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1998	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	1999	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	2000	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	2001	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	A1	2002	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	AL	201	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	AS	101	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	AT	401	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	Ac	100	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3401	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3402	-	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
74	OHX	B1	3403	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3404	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3405	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3406	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3407	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3408	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3409	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3410	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3411	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3412	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3413	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3414	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3415	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3416	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3417	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3418	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3419	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3420	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3421	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3422	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3423	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3424	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3426	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3427	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3428	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3429	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3430	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3431	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3432	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3433	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3434	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3435	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3437	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3438	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3439	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3440	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3441	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3442	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3443	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3444	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3445	-	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
74	OHX	B1	3446	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3447	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3448	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3449	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3450	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3451	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3452	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3453	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3454	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3455	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3456	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3457	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3458	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3459	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3460	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3461	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3462	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3463	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3464	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3465	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3466	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3467	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3468	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3469	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3470	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3471	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3472	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3473	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3474	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3475	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3476	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3477	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3478	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3479	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3480	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3481	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3482	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3483	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3485	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3486	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3487	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3488	-	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
74	OHX	B1	3489	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3491	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3492	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3493	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3494	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3495	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3496	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3497	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3498	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3499	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3500	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3501	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3502	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3503	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3504	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3505	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3506	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3507	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3508	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3509	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3510	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3511	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3512	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3513	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3514	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3515	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3516	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3517	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3518	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3519	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3520	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3521	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3522	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3523	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3524	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3525	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3526	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3527	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3528	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3529	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3530	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3531	-	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
74	OHX	B1	3532	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3533	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3534	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3535	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3536	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3537	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3538	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3539	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3540	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3541	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3542	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3543	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3544	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3545	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3546	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3547	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3548	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3549	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3550	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3551	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3552	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3553	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3554	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3555	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3556	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3557	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3558	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3559	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3560	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3561	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3562	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3563	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3564	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3565	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3566	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3567	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3568	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3569	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3570	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3571	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3572	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3573	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3574	-	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
74	OHX	B1	3575	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3576	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3577	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3578	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3579	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3580	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3581	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3582	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3583	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3584	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3585	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3586	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3587	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3588	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3589	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3590	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3591	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3592	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3593	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3594	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3595	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3596	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3597	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3598	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3599	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3600	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3601	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3602	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3603	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3604	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3605	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3606	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3607	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3608	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3609	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3610	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3611	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3612	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3613	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3614	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3615	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3616	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3617	-	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
74	OHX	B1	3618	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3619	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3620	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B1	3621	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B2	202	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B2	203	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B2	204	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B2	205	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B2	206	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B2	207	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B2	208	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B2	209	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B2	210	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B3	204	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B3	205	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B3	206	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B3	207	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B3	208	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B3	209	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B3	210	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B3	211	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	B3	212	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	BC	401	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	BO	301	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	BT	201	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	Bd	101	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	Bd	102	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	Bg	101	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1901	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1902	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1903	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1904	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1905	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1906	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1907	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1908	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1909	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1910	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1911	-	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
74	OHX	C1	1912	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1913	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1914	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1915	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1916	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1917	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1918	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1919	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1920	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1921	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1922	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1923	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1924	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1925	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1926	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1927	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1928	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1929	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1930	1	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1931	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1932	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1933	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1934	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1935	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1936	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1937	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1938	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1939	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1940	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1941	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1942	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1943	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1944	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1945	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1946	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1947	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1948	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1949	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1950	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1951	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1952	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1953	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1954	-	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
74	OHX	C1	1955	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1956	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1957	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1958	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1959	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1960	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1961	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1962	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1963	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1964	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1965	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1966	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1967	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1968	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1969	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1970	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1971	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1972	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1973	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1974	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1975	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1976	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1977	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1978	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1979	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1980	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1981	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1982	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1983	1	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1984	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1985	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1986	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1987	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1988	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1989	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1990	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1991	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1992	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1993	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1994	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1995	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1996	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1997	-	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
74	OHX	C1	1998	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	1999	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	2000	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	C1	2001	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	CI	201	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	CS	101	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	CS	102	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	CT	401	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3401	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3402	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3403	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3404	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3405	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3406	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3407	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3408	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3409	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3410	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3411	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3412	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3413	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3414	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3415	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3416	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3417	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3418	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3419	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3420	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3421	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3422	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3423	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3424	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3426	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3427	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3428	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3429	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3430	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3431	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3432	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3433	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3434	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3435	-	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
74	OHX	D1	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3437	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3438	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3439	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3440	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3441	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3442	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3443	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3444	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3445	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3446	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3447	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3448	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3449	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3450	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3451	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3452	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3453	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3454	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3455	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3456	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3457	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3458	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3459	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3460	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3461	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3462	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3463	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3464	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3465	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3466	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3467	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3468	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3469	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3470	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3471	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3472	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3473	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3474	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3475	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3476	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3477	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3478	-	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
74	OHX	D1	3479	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3480	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3481	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3482	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3483	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3485	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3486	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3487	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3488	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3489	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3491	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3492	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3493	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3494	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3495	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3496	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3497	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3498	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3499	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3500	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3501	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3502	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3503	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3504	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3505	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3506	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3507	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3508	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3509	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3510	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3511	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3512	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3513	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3514	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3515	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3516	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3517	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3518	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3519	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3520	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3521	-	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
74	OHX	D1	3522	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3523	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3524	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3525	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3526	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3527	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3528	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3529	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3530	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3531	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3532	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3533	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3534	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3535	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3536	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3537	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3538	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3539	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3540	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3541	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3542	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3543	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3544	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3545	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3546	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3547	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3548	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3549	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3550	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3551	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3552	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3553	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3554	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3555	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3556	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3557	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3558	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3559	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3560	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3561	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3562	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3563	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3564	-	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
74	OHX	D1	3565	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3566	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3567	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3568	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3569	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3570	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3571	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3572	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3573	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3574	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3575	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3576	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3577	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3578	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3579	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3580	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3581	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3582	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3583	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3584	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3585	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3586	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3587	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3588	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3589	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3590	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3591	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3592	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3593	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3594	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3595	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3596	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3597	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3598	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3599	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3600	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3601	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3602	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3603	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3604	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3605	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3606	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3607	-	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
74	OHX	D1	3608	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3609	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3610	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3611	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3612	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3613	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3614	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3615	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3616	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3617	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3618	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3619	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3620	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3621	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3622	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3623	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3624	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D1	3625	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D2	202	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D2	203	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D2	204	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D2	205	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D2	206	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D2	207	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D2	208	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D2	209	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D3	204	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D3	205	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D3	206	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D3	207	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D3	208	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D3	209	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D3	210	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D3	211	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	D3	212	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	DC	401	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	DE	301	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	DJ	301	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	DO	301	-	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
74	OHX	DO	302	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	DT	201	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	Dd	101	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	Dd	102	-	0,6,6	0.00	-	0,15,15	0.00	-
74	OHX	Dg	101	-	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
74	OHX	A1	1901	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1902	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1903	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1904	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1905	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1906	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1907	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1908	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1909	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1910	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1911	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1912	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1913	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1914	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1915	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1916	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1917	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1918	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1919	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1920	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1921	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1922	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1923	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1924	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1925	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1926	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1927	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1928	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1929	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1930	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1931	1	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	OHX	A1	1932	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1933	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1934	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1935	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1936	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1937	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1938	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1939	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1940	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1941	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1942	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1943	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1944	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1945	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1946	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1947	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1948	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1949	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1950	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1951	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1952	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1953	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1954	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1955	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1956	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1957	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1958	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1959	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1960	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1961	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1962	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1963	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1964	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1965	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1966	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1967	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1968	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1969	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1970	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1971	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1972	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1973	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	OHX	A1	1974	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1975	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1976	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1977	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1978	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1979	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1980	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1981	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1982	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1983	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1984	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1985	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1986	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1987	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1988	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1989	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1990	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1991	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1992	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1993	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1994	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1995	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1996	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1997	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1998	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	1999	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	2000	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	2001	-	-	0/0/0/0	0/0/0/0
74	OHX	A1	2002	-	-	0/0/0/0	0/0/0/0
74	OHX	AL	201	-	-	0/0/0/0	0/0/0/0
74	OHX	AS	101	-	-	0/0/0/0	0/0/0/0
74	OHX	AT	401	-	-	0/0/0/0	0/0/0/0
74	OHX	Ac	100	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3401	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3402	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3403	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3404	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3405	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3406	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3407	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3408	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3409	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	OHX	B1	3410	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3411	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3412	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3413	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3414	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3415	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3416	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3417	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3418	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3419	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3420	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3421	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3422	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3423	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3424	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3425	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3426	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3427	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3428	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3429	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3430	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3431	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3432	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3433	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3434	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3435	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3436	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3437	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3438	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3439	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3440	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3441	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3442	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3443	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3444	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3445	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3446	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3447	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3448	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3449	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3450	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3451	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	OHX	B1	3452	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3453	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3454	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3455	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3456	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3457	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3458	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3459	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3460	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3461	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3462	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3463	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3464	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3465	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3466	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3467	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3468	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3469	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3470	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3471	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3472	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3473	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3474	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3475	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3476	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3477	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3478	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3479	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3480	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3481	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3482	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3483	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3484	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3485	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3486	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3487	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3488	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3489	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3490	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3491	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3492	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3493	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	OHX	B1	3494	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3495	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3496	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3497	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3498	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3499	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3500	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3501	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3502	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3503	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3504	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3505	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3506	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3507	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3508	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3509	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3510	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3511	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3512	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3513	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3514	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3515	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3516	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3517	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3518	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3519	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3520	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3521	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3522	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3523	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3524	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3525	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3526	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3527	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3528	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3529	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3530	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3531	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3532	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3533	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3534	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3535	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	OHX	B1	3536	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3537	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3538	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3539	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3540	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3541	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3542	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3543	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3544	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3545	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3546	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3547	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3548	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3549	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3550	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3551	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3552	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3553	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3554	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3555	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3556	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3557	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3558	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3559	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3560	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3561	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3562	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3563	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3564	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3565	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3566	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3567	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3568	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3569	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3570	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3571	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3572	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3573	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3574	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3575	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3576	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3577	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	OHX	B1	3578	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3579	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3580	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3581	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3582	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3583	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3584	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3585	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3586	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3587	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3588	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3589	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3590	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3591	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3592	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3593	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3594	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3595	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3596	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3597	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3598	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3599	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3600	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3601	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3602	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3603	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3604	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3605	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3606	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3607	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3608	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3609	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3610	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3611	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3612	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3613	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3614	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3615	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3616	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3617	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3618	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3619	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	OHX	B1	3620	-	-	0/0/0/0	0/0/0/0
74	OHX	B1	3621	-	-	0/0/0/0	0/0/0/0
74	OHX	B2	201	-	-	0/0/0/0	0/0/0/0
74	OHX	B2	202	-	-	0/0/0/0	0/0/0/0
74	OHX	B2	203	-	-	0/0/0/0	0/0/0/0
74	OHX	B2	204	-	-	0/0/0/0	0/0/0/0
74	OHX	B2	205	-	-	0/0/0/0	0/0/0/0
74	OHX	B2	206	-	-	0/0/0/0	0/0/0/0
74	OHX	B2	207	-	-	0/0/0/0	0/0/0/0
74	OHX	B2	208	-	-	0/0/0/0	0/0/0/0
74	OHX	B2	209	-	-	0/0/0/0	0/0/0/0
74	OHX	B2	210	-	-	0/0/0/0	0/0/0/0
74	OHX	B3	201	-	-	0/0/0/0	0/0/0/0
74	OHX	B3	202	-	-	0/0/0/0	0/0/0/0
74	OHX	B3	203	-	-	0/0/0/0	0/0/0/0
74	OHX	B3	204	-	-	0/0/0/0	0/0/0/0
74	OHX	B3	205	-	-	0/0/0/0	0/0/0/0
74	OHX	B3	206	-	-	0/0/0/0	0/0/0/0
74	OHX	B3	207	-	-	0/0/0/0	0/0/0/0
74	OHX	B3	208	-	-	0/0/0/0	0/0/0/0
74	OHX	B3	209	-	-	0/0/0/0	0/0/0/0
74	OHX	B3	210	-	-	0/0/0/0	0/0/0/0
74	OHX	B3	211	-	-	0/0/0/0	0/0/0/0
74	OHX	B3	212	-	-	0/0/0/0	0/0/0/0
74	OHX	BC	401	-	-	0/0/0/0	0/0/0/0
74	OHX	BO	301	-	-	0/0/0/0	0/0/0/0
74	OHX	BT	201	-	-	0/0/0/0	0/0/0/0
74	OHX	Bd	101	-	-	0/0/0/0	0/0/0/0
74	OHX	Bd	102	-	-	0/0/0/0	0/0/0/0
74	OHX	Bg	101	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1901	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1902	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1903	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1904	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1905	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1906	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1907	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1908	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1909	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1910	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1911	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1912	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	OHX	C1	1913	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1914	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1915	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1916	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1917	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1918	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1919	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1920	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1921	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1922	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1923	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1924	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1925	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1926	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1927	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1928	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1929	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1930	1	-	0/0/0/0	0/0/0/0
74	OHX	C1	1931	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1932	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1933	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1934	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1935	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1936	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1937	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1938	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1939	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1940	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1941	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1942	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1943	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1944	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1945	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1946	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1947	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1948	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1949	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1950	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1951	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1952	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1953	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1954	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	OHX	C1	1955	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1956	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1957	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1958	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1959	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1960	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1961	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1962	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1963	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1964	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1965	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1966	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1967	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1968	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1969	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1970	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1971	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1972	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1973	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1974	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1975	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1976	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1977	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1978	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1979	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1980	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1981	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1982	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1983	1	-	0/0/0/0	0/0/0/0
74	OHX	C1	1984	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1985	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1986	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1987	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1988	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1989	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1990	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1991	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1992	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1993	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1994	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1995	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1996	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	OHX	C1	1997	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1998	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	1999	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	2000	-	-	0/0/0/0	0/0/0/0
74	OHX	C1	2001	-	-	0/0/0/0	0/0/0/0
74	OHX	CI	201	-	-	0/0/0/0	0/0/0/0
74	OHX	CS	101	-	-	0/0/0/0	0/0/0/0
74	OHX	CS	102	-	-	0/0/0/0	0/0/0/0
74	OHX	CT	401	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3401	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3402	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3403	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3404	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3405	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3406	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3407	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3408	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3409	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3410	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3411	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3412	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3413	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3414	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3415	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3416	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3417	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3418	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3419	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3420	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3421	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3422	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3423	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3424	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3425	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3426	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3427	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3428	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3429	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3430	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3431	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3432	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3433	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	OHX	D1	3434	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3435	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3436	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3437	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3438	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3439	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3440	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3441	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3442	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3443	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3444	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3445	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3446	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3447	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3448	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3449	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3450	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3451	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3452	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3453	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3454	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3455	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3456	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3457	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3458	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3459	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3460	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3461	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3462	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3463	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3464	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3465	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3466	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3467	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3468	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3469	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3470	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3471	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3472	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3473	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3474	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3475	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	OHX	D1	3476	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3477	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3478	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3479	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3480	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3481	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3482	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3483	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3484	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3485	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3486	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3487	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3488	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3489	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3490	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3491	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3492	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3493	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3494	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3495	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3496	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3497	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3498	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3499	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3500	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3501	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3502	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3503	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3504	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3505	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3506	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3507	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3508	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3509	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3510	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3511	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3512	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3513	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3514	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3515	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3516	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3517	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	OHX	D1	3518	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3519	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3520	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3521	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3522	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3523	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3524	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3525	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3526	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3527	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3528	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3529	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3530	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3531	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3532	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3533	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3534	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3535	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3536	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3537	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3538	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3539	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3540	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3541	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3542	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3543	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3544	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3545	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3546	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3547	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3548	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3549	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3550	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3551	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3552	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3553	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3554	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3555	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3556	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3557	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3558	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3559	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	OHX	D1	3560	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3561	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3562	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3563	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3564	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3565	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3566	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3567	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3568	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3569	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3570	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3571	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3572	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3573	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3574	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3575	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3576	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3577	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3578	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3579	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3580	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3581	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3582	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3583	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3584	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3585	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3586	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3587	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3588	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3589	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3590	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3591	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3592	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3593	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3594	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3595	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3596	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3597	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3598	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3599	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3600	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3601	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	OHX	D1	3602	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3603	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3604	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3605	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3606	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3607	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3608	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3609	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3610	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3611	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3612	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3613	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3614	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3615	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3616	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3617	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3618	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3619	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3620	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3621	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3622	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3623	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3624	-	-	0/0/0/0	0/0/0/0
74	OHX	D1	3625	-	-	0/0/0/0	0/0/0/0
74	OHX	D2	201	-	-	0/0/0/0	0/0/0/0
74	OHX	D2	202	-	-	0/0/0/0	0/0/0/0
74	OHX	D2	203	-	-	0/0/0/0	0/0/0/0
74	OHX	D2	204	-	-	0/0/0/0	0/0/0/0
74	OHX	D2	205	-	-	0/0/0/0	0/0/0/0
74	OHX	D2	206	-	-	0/0/0/0	0/0/0/0
74	OHX	D2	207	-	-	0/0/0/0	0/0/0/0
74	OHX	D2	208	-	-	0/0/0/0	0/0/0/0
74	OHX	D2	209	-	-	0/0/0/0	0/0/0/0
74	OHX	D3	201	-	-	0/0/0/0	0/0/0/0
74	OHX	D3	202	-	-	0/0/0/0	0/0/0/0
74	OHX	D3	203	-	-	0/0/0/0	0/0/0/0
74	OHX	D3	204	-	-	0/0/0/0	0/0/0/0
74	OHX	D3	205	-	-	0/0/0/0	0/0/0/0
74	OHX	D3	206	-	-	0/0/0/0	0/0/0/0
74	OHX	D3	207	-	-	0/0/0/0	0/0/0/0
74	OHX	D3	208	-	-	0/0/0/0	0/0/0/0
74	OHX	D3	209	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	OHX	D3	210	-	-	0/0/0/0	0/0/0/0
74	OHX	D3	211	-	-	0/0/0/0	0/0/0/0
74	OHX	D3	212	-	-	0/0/0/0	0/0/0/0
74	OHX	DC	401	-	-	0/0/0/0	0/0/0/0
74	OHX	DE	301	-	-	0/0/0/0	0/0/0/0
74	OHX	DJ	301	-	-	0/0/0/0	0/0/0/0
74	OHX	DO	301	-	-	0/0/0/0	0/0/0/0
74	OHX	DO	302	-	-	0/0/0/0	0/0/0/0
74	OHX	DT	201	-	-	0/0/0/0	0/0/0/0
74	OHX	Dd	101	-	-	0/0/0/0	0/0/0/0
74	OHX	Dd	102	-	-	0/0/0/0	0/0/0/0
74	OHX	Dg	101	-	-	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.

250 monomers are involved in 774 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	A1	1901	OHX	6	0
74	A1	1902	OHX	1	0
74	A1	1903	OHX	1	0
74	A1	1905	OHX	1	0
74	A1	1908	OHX	1	0
74	A1	1909	OHX	3	0
74	A1	1910	OHX	5	0
74	A1	1913	OHX	6	0
74	A1	1915	OHX	5	0
74	A1	1916	OHX	5	0
74	A1	1917	OHX	4	0
74	A1	1923	OHX	2	0
74	A1	1929	OHX	7	0
74	A1	1931	OHX	7	0
74	A1	1932	OHX	2	0
74	A1	1935	OHX	8	0
74	A1	1936	OHX	3	0
74	A1	1937	OHX	2	0
74	A1	1939	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	A1	1941	OHX	1	0
74	A1	1943	OHX	5	0
74	A1	1949	OHX	4	0
74	A1	1950	OHX	2	0
74	A1	1951	OHX	4	0
74	A1	1952	OHX	2	0
74	A1	1958	OHX	3	0
74	A1	1959	OHX	9	0
74	A1	1969	OHX	2	0
74	A1	1970	OHX	1	0
74	A1	1972	OHX	1	0
74	A1	1975	OHX	4	0
74	A1	1976	OHX	5	0
74	A1	1978	OHX	1	0
74	A1	1979	OHX	6	0
74	A1	1986	OHX	6	0
74	A1	1989	OHX	2	0
74	A1	1990	OHX	3	0
74	A1	1991	OHX	4	0
74	AS	101	OHX	18	0
74	AT	401	OHX	1	0
74	B1	3404	OHX	2	0
74	B1	3405	OHX	2	0
74	B1	3406	OHX	2	0
74	B1	3413	OHX	1	0
74	B1	3415	OHX	2	0
74	B1	3417	OHX	3	0
74	B1	3420	OHX	2	0
74	B1	3428	OHX	8	0
74	B1	3429	OHX	2	0
74	B1	3433	OHX	1	0
74	B1	3434	OHX	2	0
74	B1	3438	OHX	12	0
74	B1	3440	OHX	1	0
74	B1	3442	OHX	1	0
74	B1	3447	OHX	1	0
74	B1	3449	OHX	7	0
74	B1	3450	OHX	17	0
74	B1	3451	OHX	1	0
74	B1	3456	OHX	2	0
74	B1	3459	OHX	6	0
74	B1	3460	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	B1	3464	OHX	1	0
74	B1	3469	OHX	2	0
74	B1	3471	OHX	1	0
74	B1	3478	OHX	1	0
74	B1	3479	OHX	10	0
74	B1	3481	OHX	1	0
74	B1	3483	OHX	3	0
74	B1	3485	OHX	1	0
74	B1	3489	OHX	3	0
74	B1	3490	OHX	1	0
74	B1	3492	OHX	10	0
74	B1	3496	OHX	5	0
74	B1	3503	OHX	1	0
74	B1	3505	OHX	4	0
74	B1	3506	OHX	1	0
74	B1	3513	OHX	3	0
74	B1	3519	OHX	5	0
74	B1	3523	OHX	1	0
74	B1	3524	OHX	4	0
74	B1	3527	OHX	1	0
74	B1	3529	OHX	4	0
74	B1	3536	OHX	8	0
74	B1	3537	OHX	8	0
74	B1	3539	OHX	2	0
74	B1	3540	OHX	1	0
74	B1	3544	OHX	5	0
74	B1	3552	OHX	2	0
74	B1	3553	OHX	1	0
74	B1	3558	OHX	6	0
74	B1	3559	OHX	1	0
74	B1	3561	OHX	1	0
74	B1	3563	OHX	5	0
74	B1	3567	OHX	7	0
74	B1	3568	OHX	2	0
74	B1	3574	OHX	1	0
74	B1	3576	OHX	2	0
74	B1	3578	OHX	1	0
74	B1	3581	OHX	7	0
74	B1	3583	OHX	3	0
74	B1	3585	OHX	2	0
74	B1	3587	OHX	8	0
74	B1	3592	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	B1	3593	OHX	1	0
74	B1	3595	OHX	1	0
74	B1	3599	OHX	4	0
74	B1	3605	OHX	5	0
74	B1	3607	OHX	2	0
74	B1	3609	OHX	1	0
74	B1	3614	OHX	3	0
74	B1	3615	OHX	2	0
74	B1	3616	OHX	4	0
74	B1	3617	OHX	4	0
74	B1	3619	OHX	6	0
74	B1	3620	OHX	4	0
74	B2	201	OHX	7	0
74	B2	204	OHX	2	0
74	B2	209	OHX	3	0
74	B3	202	OHX	1	0
74	B3	205	OHX	2	0
74	B3	206	OHX	8	0
74	B3	211	OHX	1	0
74	B3	212	OHX	2	0
74	BC	401	OHX	1	0
74	BT	201	OHX	2	0
74	C1	1901	OHX	3	0
74	C1	1902	OHX	1	0
74	C1	1903	OHX	2	0
74	C1	1905	OHX	1	0
74	C1	1907	OHX	1	0
74	C1	1908	OHX	2	0
74	C1	1910	OHX	1	0
74	C1	1912	OHX	7	0
74	C1	1914	OHX	1	0
74	C1	1915	OHX	1	0
74	C1	1916	OHX	4	0
74	C1	1917	OHX	6	0
74	C1	1918	OHX	2	0
74	C1	1924	OHX	8	0
74	C1	1927	OHX	3	0
74	C1	1928	OHX	5	0
74	C1	1929	OHX	1	0
74	C1	1930	OHX	10	0
74	C1	1933	OHX	7	0
74	C1	1939	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	C1	1944	OHX	1	0
74	C1	1951	OHX	2	0
74	C1	1952	OHX	1	0
74	C1	1953	OHX	3	0
74	C1	1955	OHX	5	0
74	C1	1961	OHX	2	0
74	C1	1964	OHX	6	0
74	C1	1970	OHX	6	0
74	C1	1973	OHX	1	0
74	C1	1983	OHX	4	0
74	C1	1984	OHX	1	0
74	C1	1985	OHX	1	0
74	C1	1991	OHX	1	0
74	C1	1993	OHX	3	0
74	C1	1994	OHX	1	0
74	C1	1995	OHX	3	0
74	C1	1997	OHX	1	0
74	C1	1999	OHX	3	0
74	C1	2001	OHX	8	0
74	CS	101	OHX	16	0
74	D1	3402	OHX	3	0
74	D1	3406	OHX	1	0
74	D1	3407	OHX	1	0
74	D1	3408	OHX	8	0
74	D1	3413	OHX	3	0
74	D1	3415	OHX	13	0
74	D1	3416	OHX	1	0
74	D1	3419	OHX	1	0
74	D1	3428	OHX	2	0
74	D1	3430	OHX	4	0
74	D1	3431	OHX	7	0
74	D1	3434	OHX	1	0
74	D1	3442	OHX	5	0
74	D1	3446	OHX	7	0
74	D1	3447	OHX	3	0
74	D1	3448	OHX	2	0
74	D1	3452	OHX	12	0
74	D1	3454	OHX	1	0
74	D1	3455	OHX	1	0
74	D1	3456	OHX	1	0
74	D1	3462	OHX	1	0
74	D1	3463	OHX	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	D1	3464	OHX	2	0
74	D1	3465	OHX	3	0
74	D1	3470	OHX	2	0
74	D1	3471	OHX	6	0
74	D1	3473	OHX	5	0
74	D1	3477	OHX	8	0
74	D1	3480	OHX	4	0
74	D1	3489	OHX	2	0
74	D1	3492	OHX	3	0
74	D1	3495	OHX	2	0
74	D1	3502	OHX	5	0
74	D1	3510	OHX	3	0
74	D1	3514	OHX	3	0
74	D1	3523	OHX	3	0
74	D1	3524	OHX	2	0
74	D1	3526	OHX	1	0
74	D1	3527	OHX	3	0
74	D1	3530	OHX	2	0
74	D1	3537	OHX	3	0
74	D1	3539	OHX	1	0
74	D1	3543	OHX	6	0
74	D1	3547	OHX	1	0
74	D1	3551	OHX	1	0
74	D1	3555	OHX	4	0
74	D1	3556	OHX	3	0
74	D1	3557	OHX	3	0
74	D1	3559	OHX	3	0
74	D1	3567	OHX	5	0
74	D1	3568	OHX	4	0
74	D1	3570	OHX	1	0
74	D1	3574	OHX	13	0
74	D1	3576	OHX	2	0
74	D1	3577	OHX	1	0
74	D1	3578	OHX	1	0
74	D1	3582	OHX	10	0
74	D1	3583	OHX	6	0
74	D1	3585	OHX	4	0
74	D1	3588	OHX	13	0
74	D1	3589	OHX	5	0
74	D1	3591	OHX	3	0
74	D1	3592	OHX	5	0
74	D1	3597	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	D1	3598	OHX	1	0
74	D1	3599	OHX	3	0
74	D1	3607	OHX	6	0
74	D1	3608	OHX	1	0
74	D1	3615	OHX	3	0
74	D1	3616	OHX	3	0
74	D1	3619	OHX	1	0
74	D1	3625	OHX	7	0
74	D2	201	OHX	8	0
74	D2	202	OHX	2	0
74	D2	204	OHX	1	0
74	D2	205	OHX	1	0
74	D2	207	OHX	6	0
74	D2	209	OHX	2	0
74	D3	201	OHX	3	0
74	D3	202	OHX	7	0
74	D3	204	OHX	7	0
74	D3	205	OHX	4	0
74	D3	209	OHX	7	0
74	D3	212	OHX	12	0
74	DO	301	OHX	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	Cb	4
23	Ab	4
63	Dh	1
68	Bn	1
28	Ch	1
24	Cc	1
24	Ac	1
28	Ah	1
63	Bh	1

The worst 5 of 15 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Bh	23:UNK	C	34:UNK	N	29.25
1	Dh	23:UNK	C	34:UNK	N	28.80
1	Ch	25:UNK	C	50:UNK	N	22.77
1	Ab	19:UNK	C	21:UNK	N	20.41
1	Bn	19:UNK	C	27:UNK	N	20.28

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A1	1789/1800 (99%)	0.03	49 (2%) 55 44	45, 138, 429, 753	0
1	C1	1789/1800 (99%)	0.13	60 (3%) 46 36	42, 120, 419, 674	0
2	AA	220/252 (87%)	-0.53	5 (2%) 61 52	64, 150, 323, 474	0
2	CA	220/252 (87%)	-0.54	2 (0%) 84 77	66, 119, 336, 538	0
3	AB	219/254 (86%)	-0.39	3 (1%) 75 66	42, 117, 298, 500	0
3	CB	219/254 (86%)	-0.55	2 (0%) 84 77	50, 108, 288, 386	0
4	AC	189/240 (78%)	-0.35	2 (1%) 80 72	52, 120, 278, 403	0
4	CC	189/240 (78%)	-0.54	0 100 100	41, 120, 262, 460	0
5	AD	169/225 (75%)	-0.58	3 (1%) 69 60	58, 150, 355, 516	0
5	CD	169/225 (75%)	-0.63	3 (1%) 69 60	33, 108, 269, 383	0
6	AE	157/197 (79%)	-0.47	6 (3%) 41 32	44, 140, 362, 438	0
6	CE	157/197 (79%)	-0.47	1 (0%) 89 84	31, 99, 330, 482	0
7	AF	77/156 (49%)	-0.56	1 (1%) 77 68	45, 95, 205, 412	0
7	CF	77/156 (49%)	0.08	6 (7%) 14 11	56, 91, 267, 342	0
8	AG	117/151 (77%)	-0.78	0 100 100	35, 108, 284, 362	0
8	CG	117/151 (77%)	-0.76	0 100 100	47, 97, 263, 458	0
9	AH	128/137 (93%)	-0.22	5 (3%) 40 31	53, 186, 349, 436	0
9	CH	128/137 (93%)	-0.22	5 (3%) 40 31	39, 132, 354, 482	0
10	AI	121/142 (85%)	-0.51	2 (1%) 70 61	55, 140, 329, 419	0
10	CI	121/142 (85%)	-0.45	1 (0%) 86 79	46, 116, 273, 447	0
11	AJ	134/143 (93%)	-0.56	2 (1%) 74 64	74, 144, 302, 340	0
11	CJ	134/143 (93%)	-0.47	3 (2%) 62 53	44, 99, 288, 381	0
12	AK	67/136 (49%)	-0.43	2 (2%) 51 40	52, 142, 319, 407	0
12	CK	67/136 (49%)	0.17	5 (7%) 15 12	64, 199, 350, 401	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AL	120/146 (82%)	-0.46	2 (1%) 70 61	55, 146, 298, 514	0
13	CL	120/146 (82%)	-0.41	5 (4%) 37 29	52, 96, 293, 519	0
14	AM	106/144 (73%)	-0.54	2 (1%) 67 58	71, 138, 348, 425	0
14	CM	106/144 (73%)	-0.58	2 (1%) 67 58	42, 81, 260, 338	0
15	AN	111/121 (91%)	-0.34	3 (2%) 55 44	68, 129, 336, 412	0
15	CN	111/121 (91%)	-0.35	1 (0%) 84 77	32, 111, 286, 424	0
16	AO	127/130 (97%)	-0.39	0 100 100	53, 95, 256, 411	0
16	CO	127/130 (97%)	-0.76	0 100 100	54, 91, 229, 441	0
17	AP	116/145 (80%)	-0.63	0 100 100	29, 95, 247, 384	0
17	CP	116/145 (80%)	-0.64	0 100 100	29, 71, 190, 418	0
18	AQ	67/108 (62%)	-0.43	1 (1%) 74 64	94, 210, 332, 355	0
18	CQ	63/108 (58%)	-0.34	2 (3%) 48 38	68, 150, 282, 307	0
19	AR	47/67 (70%)	0.11	4 (8%) 11 10	107, 245, 393, 457	0
19	CR	47/67 (70%)	0.36	5 (10%) 7 6	51, 221, 381, 425	0
20	AS	39/56 (69%)	-0.49	0 100 100	58, 108, 181, 260	0
20	CS	39/56 (69%)	-0.49	0 100 100	37, 95, 140, 292	0
21	AT	313/319 (98%)	-0.23	12 (3%) 41 32	106, 195, 286, 348	0
21	CT	313/319 (98%)	-0.20	13 (4%) 37 29	67, 158, 257, 328	0
22	Aa	0/20	-	-	-	-
22	Bo	0/20	-	-	-	-
22	Ca	0/20	-	-	-	-
23	Ab	0/105	-	-	-	-
23	Cb	0/105	-	-	-	-
24	Ac	0/93	-	-	-	-
24	Cc	0/93	-	-	-	-
25	Ad	0/35	-	-	-	-
25	Cd	0/35	-	-	-	-
26	Ae	0/21	-	-	-	-
26	Bj	0/21	-	-	-	-
26	Dj	0/21	-	-	-	-
27	Af	0/11	-	-	-	-
28	Ah	0/41	-	-	-	-
28	Ch	0/41	-	-	-	-
29	B1	3206/3396 (94%)	0.03	81 (2%) 58 47	33, 86, 395, 634	0
29	D1	3206/3396 (94%)	0.08	87 (2%) 55 44	30, 94, 427, 674	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
30	B2	121/121 (100%)	-0.10	0 100 100	46, 118, 189, 323	0
30	D2	121/121 (100%)	-0.07	1 (0%) 86 79	36, 95, 180, 349	0
31	B3	158/158 (100%)	-0.01	6 (3%) 41 32	46, 108, 258, 619	0
31	D3	158/158 (100%)	-0.03	2 (1%) 77 68	59, 136, 358, 586	0
32	BA	213/217 (98%)	0.50	33 (15%) 2 3	137, 327, 441, 483	0
32	DA	213/217 (98%)	0.73	42 (19%) 1 2	159, 354, 442, 484	0
33	BB	234/254 (92%)	-0.47	3 (1%) 77 68	25, 83, 246, 419	0
33	DB	234/254 (92%)	-0.24	5 (2%) 64 54	54, 108, 254, 417	0
34	BC	364/387 (94%)	-0.61	1 (0%) 93 91	20, 66, 216, 560	0
34	DC	364/387 (94%)	-0.70	0 100 100	29, 58, 208, 543	0
35	BD	268/362 (74%)	-0.71	0 100 100	34, 70, 207, 500	0
35	DD	268/362 (74%)	-0.53	2 (0%) 87 82	50, 102, 274, 463	0
36	BE	287/297 (96%)	-0.47	2 (0%) 87 82	58, 119, 355, 497	0
36	DE	287/297 (96%)	-0.61	6 (2%) 64 54	38, 91, 302, 478	0
37	BF	176/176 (100%)	-0.62	2 (1%) 80 72	25, 81, 305, 519	0
37	DF	176/176 (100%)	-0.50	1 (0%) 89 84	31, 69, 342, 518	0
38	BG	215/244 (88%)	-0.86	0 100 100	21, 59, 226, 486	0
38	DG	215/244 (88%)	-0.90	0 100 100	25, 49, 167, 330	0
39	BH	173/256 (67%)	-0.45	4 (2%) 61 52	45, 110, 297, 429	0
39	DH	173/256 (67%)	-0.39	4 (2%) 61 52	70, 146, 316, 422	0
40	BI	191/191 (100%)	-0.52	2 (1%) 82 74	27, 83, 237, 347	0
40	DI	191/191 (100%)	-0.90	0 100 100	22, 49, 164, 286	0
41	BJ	208/221 (94%)	-0.64	1 (0%) 90 86	39, 93, 251, 452	0
41	DJ	208/221 (94%)	-0.73	1 (0%) 90 86	25, 64, 257, 456	0
42	BK	165/174 (94%)	-0.49	4 (2%) 59 49	56, 125, 348, 497	0
42	DK	165/174 (94%)	-0.61	1 (0%) 89 84	45, 97, 330, 532	0
43	BN	120/138 (86%)	-0.59	0 100 100	34, 77, 260, 387	0
43	DN	120/138 (86%)	-0.69	1 (0%) 86 79	33, 60, 262, 325	0
44	BO	187/204 (91%)	-0.56	1 (0%) 90 86	38, 86, 178, 383	0
44	DO	187/204 (91%)	-0.37	4 (2%) 64 54	57, 119, 255, 327	0
45	BP	196/199 (98%)	-0.84	0 100 100	23, 48, 152, 409	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
45	DP	196/199 (98%)	-0.75	1 (0%) 90 86	23, 45, 111, 424	0
46	BQ	154/184 (83%)	-0.73	0 100 100	30, 55, 144, 337	0
46	DQ	154/184 (83%)	-0.79	0 100 100	37, 77, 243, 373	0
47	BR	143/186 (76%)	-0.72	1 (0%) 87 82	38, 70, 200, 421	0
47	DR	143/186 (76%)	-0.30	4 (2%) 53 43	60, 87, 244, 378	0
48	BS	188/189 (99%)	-0.50	3 (1%) 72 63	52, 101, 419, 569	0
48	DS	188/189 (99%)	0.16	25 (13%) 4 4	59, 109, 589, 657	0
49	BT	119/160 (74%)	-0.58	1 (0%) 86 79	42, 73, 221, 310	0
49	DT	119/160 (74%)	-0.62	0 100 100	36, 72, 184, 282	0
50	BU	129/137 (94%)	-0.55	0 100 100	27, 70, 208, 391	0
50	DU	129/137 (94%)	-0.62	0 100 100	20, 48, 151, 235	0
51	BV	59/155 (38%)	-0.69	0 100 100	29, 84, 259, 363	0
51	DV	59/155 (38%)	-0.48	1 (1%) 70 61	53, 73, 197, 320	0
52	BW	94/142 (66%)	-0.44	0 100 100	53, 91, 211, 312	0
52	DW	94/142 (66%)	-0.45	1 (1%) 80 72	64, 124, 247, 337	0
53	BX	107/127 (84%)	-0.70	0 100 100	58, 91, 182, 233	0
53	DX	107/127 (84%)	-0.48	2 (1%) 67 58	56, 106, 248, 361	0
54	BY	149/149 (100%)	-0.47	3 (2%) 65 56	30, 76, 331, 456	0
54	DY	149/149 (100%)	-0.52	1 (0%) 87 82	49, 95, 277, 409	0
55	BZ	98/105 (93%)	-0.34	2 (2%) 65 56	52, 128, 269, 360	0
55	DZ	98/105 (93%)	-0.30	2 (2%) 65 56	56, 134, 272, 365	0
56	Ba	86/113 (76%)	-0.68	0 100 100	38, 83, 232, 396	0
56	Da	86/113 (76%)	-0.64	0 100 100	51, 82, 274, 430	0
57	Bb	125/130 (96%)	-0.78	0 100 100	26, 54, 138, 435	0
57	Db	125/130 (96%)	-0.48	1 (0%) 86 79	39, 77, 168, 380	0
58	Bc	68/120 (56%)	-0.66	0 100 100	46, 89, 202, 381	0
58	Dc	68/120 (56%)	-0.74	1 (1%) 74 64	50, 123, 270, 348	0
59	Bd	72/88 (81%)	-0.53	0 100 100	36, 79, 322, 434	0
59	Dd	72/88 (81%)	-0.62	0 100 100	30, 103, 268, 336	0
60	Be	48/51 (94%)	-0.66	0 100 100	30, 72, 159, 290	0
60	De	48/51 (94%)	-0.58	0 100 100	40, 118, 222, 333	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
61	Bf	95/106 (89%)	-0.19	3 (3%) 48 38	57, 145, 363, 475	0
61	Df	95/106 (89%)	0.21	10 (10%) 7 6	62, 195, 389, 486	0
62	Bg	83/92 (90%)	-0.69	1 (1%) 79 71	35, 98, 311, 431	0
62	Dg	83/92 (90%)	-0.64	0 100 100	42, 103, 241, 369	0
63	Bh	0/44	-	-	-	-
63	Dh	0/44	-	-	-	-
64	Bi	0/12	-	-	-	-
64	Di	0/12	-	-	-	-
65	Bk	0/16	-	-	-	-
65	Dk	0/16	-	-	-	-
66	Bl	0/19	-	-	-	-
67	Bm	0/9	-	-	-	-
68	Bn	0/27	-	-	-	-
69	Bp	0/8	-	-	-	-
70	Bq	0/17	-	-	-	-
71	Br	0/23	-	-	-	-
72	DL	138/165 (83%)	-0.58	2 (1%) 75 66	84, 172, 387, 465	0
73	DM	130/312 (41%)	-0.53	2 (1%) 74 64	47, 121, 305, 409	0
All	All	25728/30002 (85%)	-0.26	584 (2%) 61 52	20, 105, 353, 753	0

The worst 5 of 584 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	B1	136	G	14.8
1	C1	681	U	14.5
29	D1	2495	C	14.2
1	A1	1701	A	13.5
29	D1	2494	A	13.5

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
74	OHX	B1	3498	7/7	0.92	0.32	35.93	83,83,83,83	7
74	OHX	B1	3577	7/7	0.82	0.47	24.29	148,148,148,148	7
74	OHX	C1	1998	7/7	0.81	0.62	17.50	129,129,129,129	7
74	OHX	A1	2002	7/7	0.86	0.43	17.08	185,185,185,185	7
74	OHX	D1	3507	7/7	0.86	0.28	17.05	133,133,133,133	7
74	OHX	D1	3586	7/7	0.79	0.62	16.79	115,115,115,115	7
74	OHX	B1	3504	7/7	0.92	0.35	16.23	140,140,140,140	7
74	OHX	B3	210	7/7	0.93	0.40	15.05	64,64,64,64	7
74	OHX	D1	3563	7/7	0.87	0.34	14.75	99,99,99,99	7
74	OHX	B1	3542	7/7	0.96	0.38	14.65	64,64,64,64	7
74	OHX	B2	203	7/7	0.93	0.36	14.62	174,174,174,174	7
74	OHX	A1	1930	7/7	0.74	0.43	14.27	228,228,228,228	7
74	OHX	D1	3550	7/7	0.89	0.45	13.80	100,100,100,100	7
74	OHX	D1	3552	7/7	0.90	0.39	13.70	115,115,115,115	7
74	OHX	B1	3575	7/7	0.91	0.35	13.26	123,123,123,123	7
74	OHX	D3	208	7/7	0.79	0.28	12.81	135,135,135,135	7
74	OHX	B1	3594	7/7	0.92	0.33	12.61	100,100,100,100	7
74	OHX	D1	3545	7/7	0.93	0.42	12.60	77,77,77,77	7
74	OHX	B1	3571	7/7	0.74	0.48	11.84	176,176,176,176	7
74	OHX	B1	3589	7/7	0.91	0.50	11.44	85,85,85,85	7
74	OHX	D1	3618	7/7	0.80	0.34	10.22	62,62,62,62	7
74	OHX	A1	1993	7/7	0.86	0.33	10.16	108,108,108,108	7
74	OHX	B1	3562	7/7	0.85	0.59	10.02	130,130,130,130	7
74	OHX	B1	3551	7/7	0.96	0.43	10.00	84,84,84,84	7
74	OHX	A1	1988	7/7	0.93	0.36	9.98	25,25,25,25	7
74	OHX	B1	3608	7/7	0.93	0.58	9.98	75,75,75,75	7
74	OHX	B1	3528	7/7	0.95	0.36	9.63	158,158,158,158	7
74	OHX	D1	3593	7/7	0.70	0.52	9.52	99,99,99,99	7
74	OHX	B1	3582	7/7	0.94	0.27	9.20	83,83,83,83	7
74	OHX	D1	3546	7/7	0.90	0.32	9.19	105,105,105,105	7
74	OHX	D1	3525	7/7	0.72	0.27	9.11	106,106,106,106	7
74	OHX	B1	3549	7/7	0.93	0.29	9.09	86,86,86,86	7
74	OHX	B1	3501	7/7	0.96	0.31	9.02	99,99,99,99	7
74	OHX	A1	1925	7/7	0.88	0.37	8.93	165,165,165,165	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
74	OHX	D1	3544	7/7	0.96	0.43	8.90	127,127,127,127	7
74	OHX	D1	3535	7/7	0.80	0.32	8.83	142,142,142,142	7
74	OHX	B1	3615	7/7	0.91	0.34	8.82	49,49,49,49	7
74	OHX	A1	1952	7/7	0.92	0.32	8.79	110,110,110,110	7
74	OHX	D1	3437	7/7	0.99	0.24	8.41	103,103,103,103	7
74	OHX	D1	3568	7/7	0.92	0.35	8.26	92,92,92,92	7
74	OHX	D1	3603	7/7	0.95	0.43	8.06	114,114,114,114	7
74	OHX	D1	3475	7/7	0.91	0.34	8.03	142,142,142,142	7
74	OHX	B1	3604	7/7	0.92	0.30	7.98	53,53,53,53	7
74	OHX	D1	3564	7/7	0.80	0.38	7.85	85,85,85,85	7
74	OHX	D1	3579	7/7	0.93	0.30	7.51	44,44,44,44	7
74	OHX	B1	3599	7/7	0.83	0.28	7.41	87,87,87,87	7
74	OHX	B1	3469	7/7	0.93	0.33	7.40	169,169,169,169	7
74	OHX	D1	3597	7/7	0.89	0.64	7.27	222,222,222,222	7
74	OHX	B1	3611	7/7	0.92	0.33	7.27	68,68,68,68	7
74	OHX	D1	3517	7/7	0.95	0.29	7.25	126,126,126,126	7
74	OHX	B1	3572	7/7	0.90	0.35	7.17	56,56,56,56	7
74	OHX	A1	1959	7/7	0.94	0.27	6.91	110,110,110,110	7
74	OHX	B1	3544	7/7	0.88	0.30	6.85	130,130,130,130	7
74	OHX	B1	3580	7/7	0.85	0.37	6.50	84,84,84,84	7
74	OHX	D1	3558	7/7	0.88	0.29	6.45	127,127,127,127	7
74	OHX	B1	3506	7/7	0.92	0.29	6.36	53,53,53,53	7
74	OHX	D1	3617	7/7	0.91	0.26	6.28	50,50,50,50	7
74	OHX	D1	3581	7/7	0.94	0.26	6.28	60,60,60,60	7
74	OHX	C1	1995	7/7	0.92	0.32	6.20	51,51,51,51	7
74	OHX	A1	1966	7/7	0.89	0.42	6.09	120,120,120,120	7
74	OHX	B3	209	7/7	0.92	0.30	6.08	99,99,99,99	7
74	OHX	D1	3532	7/7	0.92	0.26	5.84	102,102,102,102	7
74	OHX	D1	3489	7/7	0.94	0.32	5.84	75,75,75,75	7
74	OHX	C1	1919	7/7	0.94	0.26	5.80	159,159,159,159	7
74	OHX	C1	1979	7/7	0.77	0.33	5.75	190,190,190,190	7
74	OHX	C1	1992	7/7	0.93	0.41	5.73	76,76,76,76	7
74	OHX	B1	3539	7/7	0.87	0.33	5.60	137,137,137,137	7
74	OHX	D1	3587	7/7	0.83	0.58	5.51	111,111,111,111	7
74	OHX	A1	1999	7/7	0.79	0.38	5.50	99,99,99,99	7
74	OHX	A1	1991	7/7	0.93	0.31	5.35	98,98,98,98	7
74	OHX	D1	3602	7/7	0.91	0.30	5.35	109,109,109,109	7
74	OHX	B1	3484	7/7	0.95	0.25	5.20	143,143,143,143	7
74	OHX	D1	3479	7/7	0.97	0.24	5.15	99,99,99,99	7
74	OHX	B1	3486	7/7	0.96	0.22	5.09	104,104,104,104	7
74	OHX	B1	3595	7/7	0.89	0.32	5.04	73,73,73,73	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
74	OHX	A1	1977	7/7	0.92	0.30	5.03	119,119,119,119	7
74	OHX	B1	3556	7/7	0.91	0.25	4.97	104,104,104,104	7
74	OHX	A1	1978	7/7	0.87	0.35	4.96	139,139,139,139	7
74	OHX	C1	1975	7/7	0.94	0.24	4.96	119,119,119,119	7
74	OHX	B1	3616	7/7	0.95	0.27	4.95	103,103,103,103	7
74	OHX	A1	1907	7/7	0.98	0.21	4.92	111,111,111,111	7
74	OHX	D1	3485	7/7	0.89	0.28	4.77	90,90,90,90	7
74	OHX	D1	3510	7/7	0.95	0.23	4.77	108,108,108,108	7
74	OHX	C1	1963	7/7	0.94	0.27	4.73	94,94,94,94	7
74	OHX	D1	3623	7/7	0.96	0.33	4.71	23,23,23,23	7
74	OHX	D1	3594	7/7	0.91	0.30	4.69	30,30,30,30	7
74	OHX	A1	1970	7/7	0.90	0.23	4.68	66,66,66,66	7
74	OHX	C1	1947	7/7	0.92	0.28	4.66	70,70,70,70	7
74	OHX	B1	3479	7/7	0.97	0.35	4.66	145,145,145,145	7
74	OHX	B1	3401	7/7	0.99	0.21	4.66	90,90,90,90	0
74	OHX	B1	3423	7/7	0.99	0.21	4.63	91,91,91,91	7
74	OHX	D1	3624	7/7	0.88	0.42	4.61	95,95,95,95	7
74	OHX	B1	3495	7/7	0.96	0.31	4.47	108,108,108,108	7
74	OHX	C1	1974	7/7	0.83	0.33	4.46	118,118,118,118	7
74	OHX	D1	3405	7/7	0.98	0.20	4.43	110,110,110,110	0
74	OHX	B1	3581	7/7	0.88	0.34	4.40	106,106,106,106	7
74	OHX	A1	1940	7/7	0.93	0.34	4.34	166,166,166,166	7
74	OHX	B1	3579	7/7	0.89	0.30	4.13	47,47,47,47	7
74	OHX	D1	3439	7/7	0.97	0.23	4.08	107,107,107,107	7
74	OHX	D1	3413	7/7	0.97	0.23	4.07	114,114,114,114	7
74	OHX	D1	3527	7/7	0.89	0.19	4.06	146,146,146,146	7
74	OHX	D1	3524	7/7	0.89	0.27	4.01	162,162,162,162	7
74	OHX	D1	3514	7/7	0.94	0.30	3.97	173,173,173,173	7
74	OHX	D3	211	7/7	0.70	0.41	3.93	137,137,137,137	7
74	OHX	A1	1969	7/7	0.91	0.26	3.92	87,87,87,87	7
74	OHX	D3	212	7/7	0.97	0.27	3.87	71,71,71,71	7
74	OHX	A1	1923	7/7	0.96	0.17	3.79	98,98,98,98	7
74	OHX	B1	3583	7/7	0.87	0.28	3.77	126,126,126,126	7
74	OHX	D1	3401	7/7	0.98	0.24	3.76	96,96,96,96	0
74	OHX	D1	3584	7/7	0.96	0.27	3.75	47,47,47,47	7
74	OHX	B1	3468	7/7	0.97	0.28	3.75	89,89,89,89	7
74	OHX	D1	3410	7/7	0.99	0.21	3.60	96,96,96,96	0
74	OHX	A1	1951	7/7	0.89	0.29	3.59	259,259,259,259	7
74	OHX	B1	3456	7/7	0.96	0.25	3.54	106,106,106,106	7
74	OHX	B1	3524	7/7	0.94	0.24	3.51	97,97,97,97	7
74	OHX	D1	3613	7/7	0.93	0.33	3.49	57,57,57,57	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
74	OHX	C1	1940	7/7	0.96	0.25	3.47	139,139,139,139	7
74	OHX	C1	1967	7/7	0.89	0.25	3.36	100,100,100,100	7
74	OHX	B1	3520	7/7	0.92	0.33	3.36	109,109,109,109	7
74	OHX	D1	3538	7/7	0.93	0.25	3.35	87,87,87,87	7
74	OHX	B1	3530	7/7	0.90	0.30	3.33	138,138,138,138	7
74	OHX	B1	3435	7/7	0.98	0.28	3.32	130,130,130,130	7
74	OHX	B1	3521	7/7	0.94	0.25	3.32	107,107,107,107	7
74	OHX	D1	3615	7/7	0.95	0.27	3.31	73,73,73,73	7
74	OHX	C1	1973	7/7	0.90	0.21	3.23	95,95,95,95	7
74	OHX	D2	202	7/7	0.93	0.25	3.15	106,106,106,106	7
74	OHX	D1	3490	7/7	0.86	0.35	3.14	167,167,167,167	7
74	OHX	A1	1967	7/7	0.97	0.29	3.12	96,96,96,96	7
74	OHX	B1	3525	7/7	0.93	0.25	2.99	54,54,54,54	7
74	OHX	C1	1972	7/7	0.67	0.30	2.98	216,216,216,216	7
74	OHX	B1	3560	7/7	0.85	0.33	2.97	105,105,105,105	7
74	OHX	A1	1904	7/7	0.98	0.17	2.94	137,137,137,137	7
74	OHX	B1	3403	7/7	0.98	0.25	2.94	126,126,126,126	0
74	OHX	C1	1929	7/7	0.98	0.19	2.93	90,90,90,90	7
74	OHX	B1	3566	7/7	0.92	0.26	2.88	107,107,107,107	7
74	OHX	D3	210	7/7	0.89	0.22	2.87	74,74,74,74	7
74	OHX	D1	3459	7/7	0.95	0.21	2.86	96,96,96,96	7
74	OHX	A1	1932	7/7	0.93	0.20	2.86	142,142,142,142	7
74	OHX	D1	3554	7/7	0.93	0.26	2.85	122,122,122,122	7
74	OHX	C1	1997	7/7	0.92	0.23	2.81	36,36,36,36	7
74	OHX	A1	1905	7/7	0.97	0.17	2.80	118,118,118,118	0
74	OHX	AT	401	7/7	0.94	0.36	2.78	207,207,207,207	7
74	OHX	D1	3620	7/7	0.91	0.26	2.76	78,78,78,78	7
74	OHX	B1	3512	7/7	0.96	0.22	2.74	113,113,113,113	7
74	OHX	C1	1903	7/7	0.98	0.17	2.74	115,115,115,115	0
74	OHX	C1	1958	7/7	0.82	0.23	2.73	153,153,153,153	7
74	OHX	B1	3568	7/7	0.84	0.22	2.66	94,94,94,94	7
74	OHX	A1	1934	7/7	0.95	0.25	2.64	122,122,122,122	7
74	OHX	B1	3441	7/7	0.98	0.20	2.62	129,129,129,129	7
74	OHX	A1	1972	7/7	0.96	0.17	2.59	87,87,87,87	7
74	OHX	B1	3461	7/7	0.96	0.19	2.57	101,101,101,101	7
74	OHX	B1	3563	7/7	0.92	0.19	2.54	152,152,152,152	7
74	OHX	C1	1993	7/7	0.85	0.28	2.44	93,93,93,93	7
74	OHX	D1	3589	7/7	0.81	0.32	2.44	56,56,56,56	7
74	OHX	D1	3435	7/7	0.97	0.17	2.39	92,92,92,92	7
74	OHX	B1	3536	7/7	0.96	0.28	2.38	324,324,324,324	7
74	OHX	D1	3409	7/7	0.98	0.17	2.36	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
74	OHX	D1	3522	7/7	0.78	0.27	2.33	133,133,133,133	7
74	OHX	D1	3476	7/7	0.91	0.28	2.28	100,100,100,100	7
74	OHX	B1	3476	7/7	0.94	0.20	2.26	102,102,102,102	7
74	OHX	A1	1965	7/7	0.90	0.25	2.25	114,114,114,114	7
74	OHX	D1	3402	7/7	0.98	0.23	2.25	100,100,100,100	0
74	OHX	C1	1986	7/7	0.94	0.20	2.23	169,169,169,169	7
74	OHX	B1	3402	7/7	0.98	0.18	2.22	99,99,99,99	0
74	OHX	B1	3537	7/7	0.96	0.20	2.20	56,56,56,56	7
74	OHX	B1	3453	7/7	0.97	0.24	2.18	127,127,127,127	7
74	OHX	D1	3516	7/7	0.92	0.33	2.15	138,138,138,138	7
74	OHX	D1	3508	7/7	0.90	0.22	2.08	88,88,88,88	7
74	OHX	D1	3551	7/7	0.76	0.30	2.07	120,120,120,120	7
74	OHX	C1	2000	7/7	0.91	0.37	2.06	82,82,82,82	7
74	OHX	A1	1938	7/7	0.92	0.20	2.06	155,155,155,155	7
74	OHX	D1	3496	7/7	0.95	0.27	2.04	155,155,155,155	7
74	OHX	B1	3534	7/7	0.88	0.27	2.03	128,128,128,128	7
74	OHX	A1	1914	7/7	0.96	0.21	2.02	145,145,145,145	7
74	OHX	A1	1958	7/7	0.86	0.19	2.00	116,116,116,116	7
74	OHX	D1	3436	7/7	0.99	0.19	2.00	125,125,125,125	7
74	OHX	B1	3526	7/7	0.88	0.25	1.99	174,174,174,174	7
74	OHX	D1	3585	7/7	0.87	0.24	1.98	102,102,102,102	7
74	OHX	D1	3433	7/7	0.93	0.23	1.96	128,128,128,128	7
74	OHX	C1	1920	7/7	0.98	0.19	1.92	103,103,103,103	7
74	OHX	D1	3483	7/7	0.93	0.22	1.92	98,98,98,98	7
74	OHX	D1	3612	7/7	0.96	0.23	1.90	36,36,36,36	7
74	OHX	B1	3618	7/7	0.96	0.24	1.89	109,109,109,109	7
74	OHX	C1	1999	7/7	0.91	0.26	1.88	41,41,41,41	7
74	OHX	B1	3443	7/7	0.97	0.21	1.85	134,134,134,134	7
74	OHX	D1	3417	7/7	0.98	0.23	1.79	91,91,91,91	7
74	OHX	D1	3560	7/7	0.96	0.23	1.78	82,82,82,82	7
74	OHX	B1	3448	7/7	0.95	0.19	1.77	124,124,124,124	7
74	OHX	B1	3591	7/7	0.90	0.29	1.76	55,55,55,55	7
74	OHX	B1	3590	7/7	0.96	0.21	1.76	69,69,69,69	7
74	OHX	C1	1985	7/7	0.88	0.30	1.76	153,153,153,153	7
74	OHX	B1	3607	7/7	0.91	0.31	1.73	44,44,44,44	7
74	OHX	A1	1926	7/7	0.95	0.23	1.72	87,87,87,87	7
74	OHX	D1	3608	7/7	0.97	0.22	1.72	14,14,14,14	7
74	OHX	D1	3596	7/7	0.86	0.21	1.72	114,114,114,114	7
74	OHX	D1	3494	7/7	0.95	0.25	1.71	105,105,105,105	7
74	OHX	A1	1919	7/7	0.95	0.24	1.69	141,141,141,141	7
74	OHX	B1	3547	7/7	0.94	0.28	1.69	117,117,117,117	7
74	OHX	D1	3418	7/7	0.98	0.22	1.56	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
74	OHX	D1	3450	7/7	0.98	0.21	1.54	112,112,112,112	7
74	OHX	D1	3460	7/7	0.89	0.21	1.53	138,138,138,138	7
74	OHX	B1	3509	7/7	0.94	0.23	1.53	124,124,124,124	7
74	OHX	B1	3610	7/7	0.90	0.27	1.53	68,68,68,68	7
74	OHX	D1	3621	7/7	0.92	0.24	1.52	67,67,67,67	7
74	OHX	B1	3405	7/7	0.99	0.18	1.51	101,101,101,101	0
74	OHX	B1	3559	7/7	0.92	0.23	1.50	68,68,68,68	7
74	OHX	D1	3466	7/7	0.90	0.21	1.47	103,103,103,103	7
74	OHX	B1	3490	7/7	0.90	0.24	1.44	109,109,109,109	7
74	OHX	B1	3472	7/7	0.96	0.25	1.42	132,132,132,132	7
74	OHX	C1	1923	7/7	0.96	0.23	1.40	123,123,123,123	7
74	OHX	A1	1979	7/7	0.96	0.18	1.40	81,81,81,81	7
74	OHX	B1	3527	7/7	0.94	0.21	1.39	84,84,84,84	7
74	OHX	D1	3598	7/7	0.92	0.28	1.39	65,65,65,65	7
74	OHX	D1	3480	7/7	0.93	0.19	1.38	127,127,127,127	7
74	OHX	A1	1953	7/7	0.83	0.39	1.34	122,122,122,122	7
74	OHX	C1	1906	7/7	0.99	0.17	1.32	101,101,101,101	7
74	OHX	A1	1986	7/7	0.96	0.18	1.30	98,98,98,98	7
74	OHX	B1	3419	7/7	0.98	0.17	1.29	109,109,109,109	7
74	OHX	D1	3569	7/7	0.88	0.28	1.28	88,88,88,88	7
74	OHX	D1	3539	7/7	0.92	0.24	1.27	69,69,69,69	7
74	OHX	C1	1910	7/7	0.95	0.20	1.27	138,138,138,138	7
74	OHX	C1	1949	7/7	0.94	0.18	1.25	97,97,97,97	7
74	OHX	D2	207	7/7	0.93	0.21	1.21	111,111,111,111	7
74	OHX	D1	3488	7/7	0.85	0.20	1.17	141,141,141,141	7
74	OHX	D3	207	7/7	0.94	0.22	1.16	123,123,123,123	7
74	OHX	B1	3586	7/7	0.91	0.34	1.15	116,116,116,116	7
74	OHX	B1	3433	7/7	0.97	0.18	1.13	98,98,98,98	7
74	OHX	B1	3619	7/7	0.94	0.22	1.11	85,85,85,85	7
74	OHX	D3	204	7/7	0.97	0.19	1.08	120,120,120,120	7
74	OHX	A1	1935	7/7	0.91	0.24	1.08	156,156,156,156	7
74	OHX	B1	3513	7/7	0.95	0.23	1.05	171,171,171,171	7
74	OHX	B1	3427	7/7	0.98	0.21	1.04	95,95,95,95	7
74	OHX	D1	3588	7/7	0.92	0.24	1.03	336,336,336,336	7
74	OHX	B1	3432	7/7	0.98	0.18	1.03	79,79,79,79	7
74	OHX	B1	3493	7/7	0.87	0.21	0.98	135,135,135,135	7
74	OHX	B3	203	7/7	0.95	0.20	0.92	140,140,140,140	7
74	OHX	DO	301	7/7	0.86	0.24	0.91	285,285,285,285	7
74	OHX	A1	1984	7/7	0.91	0.21	0.90	65,65,65,65	7
74	OHX	B1	3438	7/7	0.94	0.17	0.89	168,168,168,168	7
74	OHX	DC	401	7/7	0.96	0.23	0.88	93,93,93,93	7
74	OHX	B1	3612	7/7	0.92	0.28	0.84	45,45,45,45	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
74	OHX	B1	3477	7/7	0.98	0.19	0.82	101,101,101,101	7
74	OHX	C1	1926	7/7	0.95	0.21	0.81	96,96,96,96	7
74	OHX	C1	1902	7/7	0.99	0.22	0.81	108,108,108,108	0
74	OHX	B1	3585	7/7	0.94	0.29	0.81	197,197,197,197	7
74	OHX	B1	3518	7/7	0.90	0.21	0.79	105,105,105,105	7
74	OHX	A1	1996	7/7	0.91	0.24	0.78	100,100,100,100	7
74	OHX	D1	3509	7/7	0.85	0.33	0.76	120,120,120,120	7
74	OHX	C1	1928	7/7	0.97	0.17	0.74	165,165,165,165	7
74	OHX	D1	3447	7/7	0.97	0.19	0.72	142,142,142,142	7
74	OHX	D1	3486	7/7	0.96	0.24	0.70	143,143,143,143	7
74	OHX	D1	3445	7/7	0.98	0.20	0.67	101,101,101,101	7
74	OHX	B1	3406	7/7	0.98	0.22	0.66	106,106,106,106	0
74	OHX	A1	1911	7/7	0.97	0.20	0.65	112,112,112,112	7
74	OHX	A1	1909	7/7	0.97	0.16	0.64	115,115,115,115	7
74	OHX	B1	3409	7/7	0.98	0.18	0.64	122,122,122,122	0
74	OHX	C1	1913	7/7	0.96	0.21	0.63	149,149,149,149	7
74	OHX	A1	2001	7/7	0.95	0.24	0.63	26,26,26,26	7
74	OHX	B1	3452	7/7	0.98	0.19	0.60	134,134,134,134	7
74	OHX	A1	1917	7/7	0.96	0.14	0.56	130,130,130,130	7
74	OHX	C1	1954	7/7	0.87	0.25	0.52	116,116,116,116	7
74	OHX	D1	3440	7/7	0.98	0.18	0.52	137,137,137,137	7
74	OHX	B1	3470	7/7	0.94	0.19	0.48	122,122,122,122	7
74	OHX	D1	3556	7/7	0.79	0.23	0.47	146,146,146,146	7
74	OHX	C1	1977	7/7	0.92	0.25	0.47	102,102,102,102	7
74	OHX	C1	1904	7/7	0.98	0.16	0.47	113,113,113,113	0
74	OHX	B2	206	7/7	0.86	0.21	0.46	128,128,128,128	7
74	OHX	A1	1943	7/7	0.90	0.19	0.45	176,176,176,176	7
74	OHX	D2	205	7/7	0.94	0.22	0.42	84,84,84,84	7
74	OHX	D1	3520	7/7	0.96	0.18	0.42	109,109,109,109	7
74	OHX	D1	3458	7/7	0.96	0.17	0.40	103,103,103,103	7
74	OHX	A1	1973	7/7	0.94	0.28	0.40	101,101,101,101	7
74	OHX	D1	3469	7/7	0.92	0.23	0.40	152,152,152,152	7
74	OHX	D1	3456	7/7	0.98	0.20	0.39	131,131,131,131	7
74	OHX	B1	3482	7/7	0.97	0.18	0.39	111,111,111,111	7
74	OHX	A1	1949	7/7	0.94	0.20	0.38	101,101,101,101	7
74	OHX	C1	1916	7/7	0.96	0.23	0.38	169,169,169,169	7
74	OHX	A1	1918	7/7	0.97	0.18	0.36	94,94,94,94	7
74	OHX	B1	3440	7/7	0.98	0.19	0.35	105,105,105,105	7
74	OHX	B1	3410	7/7	0.97	0.18	0.34	111,111,111,111	0
74	OHX	C1	1932	7/7	0.95	0.18	0.32	115,115,115,115	7
74	OHX	C1	1933	7/7	0.94	0.21	0.32	111,111,111,111	7
74	OHX	D2	206	7/7	0.97	0.16	0.30	85,85,85,85	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
74	OHX	D1	3583	7/7	0.85	0.28	0.29	88,88,88,88	7
74	OHX	A1	1957	7/7	0.96	0.18	0.27	129,129,129,129	7
74	OHX	D1	3499	7/7	0.90	0.24	0.26	114,114,114,114	7
74	OHX	A1	1944	7/7	0.94	0.21	0.25	108,108,108,108	7
74	OHX	B1	3455	7/7	0.96	0.20	0.25	134,134,134,134	7
74	OHX	B1	3507	7/7	0.92	0.25	0.24	104,104,104,104	7
74	OHX	A1	1980	7/7	0.94	0.19	0.23	136,136,136,136	7
74	OHX	D1	3411	7/7	0.98	0.15	0.22	117,117,117,117	0
74	OHX	A1	1936	7/7	0.95	0.20	0.19	129,129,129,129	7
74	OHX	D1	3506	7/7	0.89	0.32	0.18	131,131,131,131	7
74	OHX	D1	3503	7/7	0.89	0.25	0.18	120,120,120,120	7
74	OHX	B2	205	7/7	0.90	0.18	0.16	159,159,159,159	7
74	OHX	Bg	101	7/7	0.98	0.17	0.14	79,79,79,79	7
74	OHX	B1	3503	7/7	0.94	0.17	0.14	86,86,86,86	7
74	OHX	DT	201	7/7	0.99	0.18	0.13	100,100,100,100	0
74	OHX	C1	1942	7/7	0.93	0.20	0.13	112,112,112,112	7
74	OHX	D1	3412	7/7	0.99	0.18	0.12	126,126,126,126	0
74	OHX	B1	3420	7/7	0.99	0.19	0.12	93,93,93,93	7
74	OHX	D1	3419	7/7	0.98	0.17	0.11	92,92,92,92	0
74	OHX	D1	3543	7/7	0.97	0.19	0.11	45,45,45,45	7
74	OHX	D1	3404	7/7	0.99	0.21	0.10	99,99,99,99	0
74	OHX	A1	1950	7/7	0.93	0.17	0.10	127,127,127,127	7
74	OHX	D3	203	7/7	0.97	0.17	0.10	86,86,86,86	7
74	OHX	D1	3484	7/7	0.89	0.22	0.08	116,116,116,116	7
74	OHX	C1	1994	7/7	0.92	0.29	0.08	47,47,47,47	7
74	OHX	D1	3537	7/7	0.95	0.23	0.08	74,74,74,74	7
74	OHX	B3	211	7/7	0.98	0.16	0.07	67,67,67,67	7
74	OHX	C1	1918	7/7	0.99	0.14	0.06	123,123,123,123	7
74	OHX	B1	3437	7/7	0.95	0.24	0.05	156,156,156,156	7
74	OHX	D1	3562	7/7	0.93	0.18	0.05	121,121,121,121	7
74	OHX	A1	1912	7/7	0.97	0.16	0.05	125,125,125,125	7
74	OHX	C1	1922	7/7	0.97	0.18	0.04	142,142,142,142	7
74	OHX	B1	3436	7/7	0.97	0.17	0.04	104,104,104,104	7
74	OHX	D1	3530	7/7	0.95	0.18	0.03	51,51,51,51	7
74	OHX	D1	3426	7/7	0.99	0.17	0.03	112,112,112,112	7
74	OHX	C1	1964	7/7	0.99	0.14	0.03	88,88,88,88	7
74	OHX	B1	3499	7/7	0.97	0.16	0.01	123,123,123,123	7
74	OHX	D1	3574	7/7	0.96	0.19	-0.00	114,114,114,114	7
74	OHX	CT	401	7/7	0.92	0.23	-0.01	117,117,117,117	7
74	OHX	A1	1994	7/7	0.92	0.24	-0.02	123,123,123,123	7
74	OHX	C1	1952	7/7	0.84	0.21	-0.03	239,239,239,239	7
74	OHX	D1	3432	7/7	0.98	0.18	-0.04	100,100,100,100	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
74	OHX	C1	1901	7/7	0.99	0.16	-0.05	100,100,100,100	0
74	OHX	D1	3518	7/7	0.96	0.21	-0.05	108,108,108,108	7
74	OHX	B1	3418	7/7	0.98	0.16	-0.06	106,106,106,106	0
74	OHX	B1	3480	7/7	0.97	0.18	-0.06	85,85,85,85	7
74	OHX	B1	3442	7/7	0.99	0.17	-0.07	89,89,89,89	7
74	OHX	B1	3426	7/7	0.97	0.17	-0.07	111,111,111,111	7
74	OHX	C1	1983	7/7	0.95	0.18	-0.09	59,59,59,59	7
74	OHX	C1	1955	7/7	0.95	0.20	-0.10	106,106,106,106	7
74	OHX	B1	3416	7/7	0.99	0.18	-0.10	113,113,113,113	0
74	OHX	B1	3421	7/7	0.99	0.17	-0.12	141,141,141,141	0
74	OHX	D1	3442	7/7	0.98	0.16	-0.13	126,126,126,126	7
74	OHX	D1	3444	7/7	0.99	0.18	-0.15	72,72,72,72	7
74	OHX	D1	3492	7/7	0.98	0.16	-0.19	112,112,112,112	7
74	OHX	D1	3561	7/7	0.95	0.20	-0.20	65,65,65,65	7
74	OHX	A1	1937	7/7	0.95	0.15	-0.22	158,158,158,158	7
74	OHX	B1	3447	7/7	0.99	0.16	-0.22	126,126,126,126	7
74	OHX	C1	1931	7/7	0.95	0.19	-0.22	130,130,130,130	7
74	OHX	D1	3540	7/7	0.96	0.20	-0.24	85,85,85,85	7
74	OHX	B1	3496	7/7	0.97	0.14	-0.27	122,122,122,122	7
74	OHX	A1	1924	7/7	0.93	0.21	-0.28	150,150,150,150	7
74	OHX	B1	3473	7/7	0.96	0.17	-0.31	91,91,91,91	7
74	OHX	B1	3540	7/7	0.99	0.18	-0.32	58,58,58,58	7
74	OHX	B1	3553	7/7	0.95	0.18	-0.33	66,66,66,66	7
74	OHX	A1	1910	7/7	0.96	0.15	-0.34	146,146,146,146	7
74	OHX	D1	3604	7/7	0.94	0.14	-0.35	44,44,44,44	7
74	OHX	D1	3425	7/7	0.97	0.16	-0.35	126,126,126,126	7
74	OHX	C1	1948	7/7	0.94	0.20	-0.39	117,117,117,117	7
74	OHX	C1	1941	7/7	0.96	0.18	-0.39	109,109,109,109	7
74	OHX	B3	208	7/7	0.94	0.19	-0.39	79,79,79,79	7
74	OHX	B3	204	7/7	0.99	0.15	-0.39	84,84,84,84	7
74	OHX	DE	301	7/7	0.79	0.24	-0.40	302,302,302,302	7
74	OHX	C1	1912	7/7	0.97	0.14	-0.41	117,117,117,117	7
74	OHX	D1	3446	7/7	0.98	0.15	-0.42	83,83,83,83	7
74	OHX	D1	3526	7/7	0.92	0.18	-0.42	158,158,158,158	7
74	OHX	B1	3487	7/7	0.90	0.23	-0.42	116,116,116,116	7
74	OHX	CS	101	7/7	0.97	0.18	-0.43	46,46,46,46	7
74	OHX	D1	3448	7/7	0.97	0.21	-0.45	107,107,107,107	7
74	OHX	Bd	101	7/7	0.99	0.19	-0.46	32,32,32,32	7
74	OHX	D1	3502	7/7	0.97	0.14	-0.47	79,79,79,79	7
74	OHX	B1	3500	7/7	0.96	0.15	-0.47	116,116,116,116	7
74	OHX	D1	3455	7/7	0.99	0.13	-0.48	110,110,110,110	7
74	OHX	B1	3451	7/7	0.97	0.17	-0.48	86,86,86,86	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
74	OHX	A1	1902	7/7	0.99	0.14	-0.49	112,112,112,112	0
74	OHX	A1	1901	7/7	0.99	0.15	-0.50	100,100,100,100	0
74	OHX	B1	3505	7/7	0.93	0.17	-0.51	134,134,134,134	7
74	OHX	D1	3407	7/7	0.99	0.13	-0.53	113,113,113,113	0
74	OHX	D1	3478	7/7	0.96	0.17	-0.55	117,117,117,117	7
74	OHX	C1	1917	7/7	0.99	0.15	-0.60	130,130,130,130	7
74	OHX	B1	3459	7/7	0.95	0.16	-0.61	160,160,160,160	7
74	OHX	A1	1975	7/7	0.97	0.17	-0.63	67,67,67,67	7
74	OHX	B1	3587	7/7	0.95	0.14	-0.63	154,154,154,154	7
74	OHX	B1	3478	7/7	0.97	0.13	-0.64	110,110,110,110	7
74	OHX	C1	1930	7/7	0.95	0.17	-0.65	112,112,112,112	7
74	OHX	D1	3495	7/7	0.89	0.17	-0.65	160,160,160,160	7
74	OHX	D1	3434	7/7	0.99	0.13	-0.65	77,77,77,77	7
74	OHX	B1	3529	7/7	0.87	0.14	-0.66	171,171,171,171	7
74	OHX	C1	1907	7/7	0.99	0.14	-0.66	123,123,123,123	7
74	OHX	C1	1935	7/7	0.94	0.17	-0.68	93,93,93,93	7
74	OHX	BT	201	7/7	0.99	0.15	-0.68	91,91,91,91	7
74	OHX	A1	1945	7/7	0.96	0.18	-0.72	108,108,108,108	7
74	OHX	B1	3460	7/7	0.98	0.16	-0.74	137,137,137,137	7
74	OHX	Dd	101	7/7	0.99	0.15	-0.74	32,32,32,32	7
74	OHX	A1	1931	7/7	0.98	0.14	-0.76	96,96,96,96	7
74	OHX	D1	3571	7/7	0.97	0.17	-0.77	77,77,77,77	7
74	OHX	D1	3465	7/7	0.97	0.16	-0.78	101,101,101,101	7
74	OHX	D1	3443	7/7	0.97	0.16	-0.81	96,96,96,96	7
74	OHX	C1	1908	7/7	0.98	0.15	-0.82	104,104,104,104	7
74	OHX	D1	3473	7/7	0.91	0.16	-0.82	123,123,123,123	7
74	OHX	B1	3492	7/7	0.97	0.14	-0.83	70,70,70,70	7
74	OHX	AS	101	7/7	0.99	0.14	-0.84	29,29,29,29	7
74	OHX	B1	3411	7/7	0.98	0.15	-0.85	105,105,105,105	0
74	OHX	B1	3412	7/7	0.99	0.14	-0.86	121,121,121,121	0
74	OHX	B1	3445	7/7	0.99	0.12	-0.87	113,113,113,113	7
74	OHX	D1	3427	7/7	0.98	0.15	-0.89	90,90,90,90	7
74	OHX	B1	3494	7/7	0.96	0.18	-0.89	118,118,118,118	7
74	OHX	A1	1906	7/7	0.97	0.14	-0.91	97,97,97,97	7
74	OHX	A1	1913	7/7	0.98	0.11	-0.93	135,135,135,135	7
74	OHX	C1	1905	7/7	0.97	0.13	-0.96	114,114,114,114	7
74	OHX	C1	1937	7/7	0.96	0.17	-0.97	124,124,124,124	7
74	OHX	AL	201	7/7	0.95	0.19	-1.00	122,122,122,122	7
74	OHX	B1	3404	7/7	0.98	0.15	-1.01	114,114,114,114	0
74	OHX	Dg	101	7/7	0.96	0.16	-1.01	69,69,69,69	7
74	OHX	B1	3413	7/7	0.99	0.12	-1.03	106,106,106,106	7
74	OHX	D1	3428	7/7	0.99	0.15	-1.04	80,80,80,80	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
74	OHX	B1	3407	7/7	0.98	0.14	-1.05	105,105,105,105	0
74	OHX	D1	3504	7/7	0.95	0.16	-1.05	101,101,101,101	7
74	OHX	A1	1903	7/7	0.99	0.11	-1.13	122,122,122,122	7
74	OHX	BC	401	7/7	0.94	0.21	-1.15	66,66,66,66	7
74	OHX	D2	201	7/7	0.99	0.13	-1.18	94,94,94,94	7
74	OHX	D3	201	7/7	0.99	0.14	-1.19	93,93,93,93	0
74	OHX	B1	3567	7/7	0.94	0.10	-1.20	126,126,126,126	7
74	OHX	B1	3450	7/7	0.99	0.12	-1.24	91,91,91,91	7
74	OHX	B1	3424	7/7	0.99	0.14	-1.24	105,105,105,105	7
74	OHX	D1	3582	7/7	0.98	0.13	-1.28	71,71,71,71	7
74	OHX	B1	3415	7/7	0.99	0.14	-1.28	93,93,93,93	7
74	OHX	C1	1953	7/7	0.98	0.12	-1.29	56,56,56,56	7
74	OHX	D1	3424	7/7	0.98	0.13	-1.31	125,125,125,125	7
74	OHX	D1	3420	7/7	0.99	0.11	-1.42	112,112,112,112	0
74	OHX	C1	1914	7/7	0.98	0.12	-1.44	128,128,128,128	7
74	OHX	C1	1944	7/7	0.95	0.12	-1.45	134,134,134,134	7
74	OHX	B1	3417	7/7	0.98	0.12	-1.46	102,102,102,102	0
74	OHX	B2	201	7/7	0.98	0.10	-1.49	141,141,141,141	7
74	OHX	D1	3438	7/7	0.99	0.12	-1.52	98,98,98,98	7
74	OHX	B1	3471	7/7	0.98	0.11	-1.57	130,130,130,130	7
74	OHX	D3	202	7/7	0.99	0.13	-1.59	116,116,116,116	0
74	OHX	D1	3408	7/7	0.98	0.12	-1.67	143,143,143,143	0
74	OHX	D1	3414	7/7	0.99	0.11	-1.72	114,114,114,114	0
74	OHX	D1	3477	7/7	0.91	0.15	-1.72	142,142,142,142	7
74	OHX	D1	3406	7/7	0.97	0.13	-1.86	107,107,107,107	0
74	OHX	D1	3452	7/7	0.98	0.09	-1.87	94,94,94,94	7
74	OHX	D1	3421	7/7	0.98	0.15	-1.90	98,98,98,98	7
74	OHX	C1	1970	7/7	0.73	0.29	-2.20	176,176,176,176	7
74	OHX	A1	1961	7/7	0.97	0.10	-2.44	105,105,105,105	7
74	OHX	D1	3423	7/7	0.99	0.12	-2.65	88,88,88,88	7
74	OHX	B1	3430	7/7	0.97	0.14	-2.75	99,99,99,99	7
74	OHX	B1	3422	7/7	0.99	0.12	-3.57	93,93,93,93	7
74	OHX	B2	207	7/7	0.90	0.49	-	104,104,104,104	7
74	OHX	D1	3519	7/7	0.92	0.37	-	111,111,111,111	7
74	OHX	B1	3569	7/7	0.95	0.18	-	95,95,95,95	7
74	OHX	B3	205	7/7	0.96	0.14	-	123,123,123,123	7
74	OHX	B1	3558	7/7	0.94	0.21	-	130,130,130,130	7
74	OHX	D1	3497	7/7	0.96	0.36	-	99,99,99,99	7
74	OHX	B1	3408	7/7	0.99	0.20	-	98,98,98,98	0
74	OHX	Ac	100	7/7	0.98	0.29	-	131,131,131,131	7
74	OHX	D1	3616	7/7	0.87	0.46	-	150,150,150,150	7
74	OHX	D1	3487	7/7	0.97	0.24	-	103,103,103,103	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
74	OHX	B1	3605	7/7	0.96	0.26	-	52,52,52,52	7
74	OHX	D2	203	7/7	0.94	0.25	-	94,94,94,94	7
74	OHX	A1	1982	7/7	0.93	0.18	-	148,148,148,148	7
74	OHX	A1	1998	7/7	0.83	0.32	-	125,125,125,125	7
74	OHX	B1	3428	7/7	0.98	0.15	-	109,109,109,109	7
74	OHX	B1	3603	7/7	0.87	0.29	-	63,63,63,63	7
74	OHX	B1	3429	7/7	0.97	0.17	-	93,93,93,93	7
74	OHX	A1	1948	7/7	0.94	0.26	-	106,106,106,106	7
74	OHX	A1	1956	7/7	0.97	0.12	-	159,159,159,159	7
74	OHX	B1	3511	7/7	0.86	0.39	-	160,160,160,160	7
74	OHX	D1	3457	7/7	0.91	0.32	-	130,130,130,130	7
74	OHX	D1	3403	7/7	0.99	0.21	-	96,96,96,96	0
74	OHX	BO	301	7/7	0.87	0.38	-	110,110,110,110	7
74	OHX	C1	1988	7/7	0.80	0.27	-	146,146,146,146	7
74	OHX	D1	3416	7/7	0.97	0.15	-	108,108,108,108	7
74	OHX	A1	1915	7/7	0.95	0.18	-	129,129,129,129	7
74	OHX	B1	3546	7/7	0.91	0.41	-	148,148,148,148	7
74	OHX	C1	1982	7/7	0.93	0.27	-	106,106,106,106	7
74	OHX	D1	3453	7/7	0.97	0.24	-	124,124,124,124	7
74	OHX	B2	210	7/7	0.84	0.43	-	131,131,131,131	7
74	OHX	B1	3449	7/7	0.97	0.18	-	105,105,105,105	7
74	OHX	C1	1969	7/7	0.88	0.30	-	133,133,133,133	7
74	OHX	D1	3501	7/7	0.94	0.17	-	102,102,102,102	7
74	OHX	D1	3422	7/7	0.98	0.17	-	114,114,114,114	7
74	OHX	A1	1985	7/7	0.89	0.33	-	86,86,86,86	7
74	OHX	D1	3614	7/7	0.95	0.48	-	83,83,83,83	7
74	OHX	A1	1922	7/7	0.94	0.23	-	133,133,133,133	7
74	OHX	DO	302	7/7	0.94	0.24	-	77,77,77,77	7
74	OHX	B1	3464	7/7	0.99	0.17	-	89,89,89,89	7
74	OHX	B1	3497	7/7	0.94	0.24	-	103,103,103,103	7
74	OHX	DJ	301	7/7	0.88	0.29	-	138,138,138,138	7
74	OHX	C1	1927	7/7	0.96	0.14	-	149,149,149,149	7
74	OHX	D1	3534	7/7	0.93	0.41	-	142,142,142,142	7
74	OHX	D1	3595	7/7	0.90	0.35	-	90,90,90,90	7
74	OHX	A1	1955	7/7	0.89	0.34	-	110,110,110,110	7
74	OHX	D1	3474	7/7	0.97	0.29	-	118,118,118,118	7
74	OHX	A1	1989	7/7	0.91	0.25	-	70,70,70,70	7
74	OHX	B1	3588	7/7	0.92	0.31	-	78,78,78,78	7
74	OHX	A1	1983	7/7	0.75	0.58	-	122,122,122,122	7
74	OHX	B1	3439	7/7	0.96	0.24	-	90,90,90,90	7
74	OHX	B1	3515	7/7	0.90	0.39	-	119,119,119,119	7
74	OHX	D1	3464	7/7	0.96	0.18	-	92,92,92,92	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
74	OHX	D1	3515	7/7	0.87	0.24	-	173,173,173,173	7
74	OHX	B1	3463	7/7	0.96	0.16	-	137,137,137,137	7
74	OHX	A1	1976	7/7	0.97	0.18	-	51,51,51,51	7
74	OHX	B1	3554	7/7	0.83	0.69	-	156,156,156,156	7
74	OHX	C1	1965	7/7	0.90	0.42	-	101,101,101,101	7
74	OHX	B3	206	7/7	0.80	0.37	-	201,201,201,201	7
74	OHX	D1	3548	7/7	0.89	0.25	-	77,77,77,77	7
74	OHX	B1	3531	7/7	0.95	0.30	-	65,65,65,65	7
74	OHX	D1	3573	7/7	0.77	0.42	-	135,135,135,135	7
74	OHX	C1	1950	7/7	0.72	0.28	-	215,215,215,215	7
74	OHX	D1	3429	7/7	0.98	0.21	-	82,82,82,82	7
74	OHX	D3	206	7/7	0.74	0.36	-	77,77,77,77	7
74	OHX	D1	3590	7/7	0.85	0.39	-	55,55,55,55	7
74	OHX	C1	1959	7/7	0.87	0.29	-	166,166,166,166	7
74	OHX	D1	3449	7/7	0.99	0.27	-	124,124,124,124	7
74	OHX	B3	212	7/7	0.93	0.21	-	98,98,98,98	7
74	OHX	B1	3444	7/7	0.97	0.15	-	111,111,111,111	7
74	OHX	D1	3523	7/7	0.95	0.19	-	106,106,106,106	7
74	OHX	D1	3610	7/7	0.92	0.46	-	94,94,94,94	7
74	OHX	B1	3517	7/7	0.93	0.30	-	111,111,111,111	7
74	OHX	A1	1962	7/7	0.84	0.49	-	193,193,193,193	7
74	OHX	B1	3535	7/7	0.81	0.28	-	170,170,170,170	7
74	OHX	D1	3609	7/7	0.83	0.45	-	73,73,73,73	7
74	OHX	A1	1947	7/7	0.90	0.30	-	143,143,143,143	7
74	OHX	B1	3502	7/7	0.91	0.28	-	166,166,166,166	7
74	OHX	A1	1927	7/7	0.94	0.22	-	139,139,139,139	7
74	OHX	D1	3513	7/7	0.92	0.26	-	160,160,160,160	7
74	OHX	B1	3578	7/7	0.94	0.24	-	112,112,112,112	7
74	OHX	B1	3621	7/7	0.85	0.36	-	83,83,83,83	7
74	OHX	D1	3547	7/7	0.93	0.18	-	64,64,64,64	7
74	OHX	B1	3467	7/7	0.97	0.15	-	119,119,119,119	7
74	OHX	B1	3519	7/7	0.97	0.28	-	115,115,115,115	7
74	OHX	A1	1946	7/7	0.89	0.19	-	153,153,153,153	7
74	OHX	D1	3605	7/7	0.78	0.46	-	93,93,93,93	7
74	OHX	B1	3475	7/7	0.97	0.20	-	84,84,84,84	7
74	OHX	B2	209	7/7	0.67	0.33	-	148,148,148,148	7
74	OHX	CS	102	7/7	0.82	0.35	-	184,184,184,184	7
74	OHX	D1	3553	7/7	0.87	0.25	-	145,145,145,145	7
74	OHX	C1	1909	7/7	0.98	0.14	-	130,130,130,130	7
74	OHX	C1	1960	7/7	0.96	0.13	-	111,111,111,111	7
74	OHX	B1	3555	7/7	0.84	0.30	-	103,103,103,103	7
74	OHX	C1	1956	7/7	0.91	0.30	-	170,170,170,170	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
74	OHX	D3	205	7/7	0.74	0.25	-	199,199,199,199	7
74	OHX	B1	3617	7/7	0.92	0.38	-	90,90,90,90	7
74	OHX	B1	3485	7/7	0.97	0.23	-	110,110,110,110	7
74	OHX	D1	3471	7/7	0.92	0.28	-	260,260,260,260	7
74	OHX	B1	3606	7/7	0.93	0.37	-	74,74,74,74	7
74	OHX	B1	3545	7/7	0.89	0.34	-	82,82,82,82	7
74	OHX	D1	3591	7/7	0.94	0.22	-	43,43,43,43	7
74	OHX	D1	3482	7/7	0.93	0.21	-	107,107,107,107	7
74	OHX	B1	3481	7/7	0.95	0.23	-	133,133,133,133	7
74	OHX	A1	1964	7/7	0.88	0.74	-	85,85,85,85	7
74	OHX	B1	3508	7/7	0.97	0.24	-	113,113,113,113	7
74	OHX	D1	3536	7/7	0.91	0.24	-	140,140,140,140	7
74	OHX	D1	3467	7/7	0.93	0.27	-	129,129,129,129	7
74	OHX	A1	1995	7/7	0.92	0.35	-	80,80,80,80	7
74	OHX	B1	3609	7/7	0.93	0.35	-	80,80,80,80	7
74	OHX	B1	3532	7/7	0.93	0.43	-	172,172,172,172	7
74	OHX	D1	3576	7/7	0.95	0.20	-	76,76,76,76	7
74	OHX	B2	202	7/7	0.95	0.18	-	106,106,106,106	7
74	OHX	B1	3457	7/7	0.95	0.23	-	147,147,147,147	7
74	OHX	C1	1991	7/7	0.89	0.28	-	77,77,77,77	7
74	OHX	B1	3600	7/7	0.85	0.34	-	135,135,135,135	7
74	OHX	B1	3491	7/7	0.94	0.31	-	99,99,99,99	7
74	OHX	C1	1936	7/7	0.96	0.33	-	126,126,126,126	7
74	OHX	D1	3572	7/7	0.88	0.34	-	91,91,91,91	7
74	OHX	B1	3550	7/7	0.93	0.19	-	137,137,137,137	7
74	OHX	A1	1941	7/7	0.94	0.19	-	124,124,124,124	7
74	OHX	B1	3489	7/7	0.97	0.11	-	129,129,129,129	7
74	OHX	B1	3543	7/7	0.94	0.15	-	102,102,102,102	7
74	OHX	C1	1961	7/7	0.96	0.18	-	101,101,101,101	7
74	OHX	A1	1920	7/7	0.96	0.15	-	126,126,126,126	7
74	OHX	A1	1929	7/7	0.96	0.14	-	114,114,114,114	7
74	OHX	C1	1989	7/7	0.92	0.53	-	114,114,114,114	7
74	OHX	D1	3555	7/7	0.88	0.31	-	150,150,150,150	7
74	OHX	D1	3472	7/7	0.95	0.21	-	185,185,185,185	7
74	OHX	C1	1943	7/7	0.96	0.15	-	141,141,141,141	7
74	OHX	D1	3451	7/7	0.97	0.22	-	112,112,112,112	7
74	OHX	D1	3599	7/7	0.85	0.36	-	93,93,93,93	7
74	OHX	B1	3576	7/7	0.93	0.21	-	86,86,86,86	7
74	OHX	C1	1981	7/7	0.92	0.38	-	87,87,87,87	7
74	OHX	C1	1945	7/7	0.88	0.23	-	122,122,122,122	7
74	OHX	B1	3458	7/7	0.98	0.29	-	114,114,114,114	7
74	OHX	C1	1966	7/7	0.87	0.42	-	127,127,127,127	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
74	OHX	D1	3533	7/7	0.95	0.27	-	92,92,92,92	7
74	OHX	A1	2000	7/7	0.84	0.44	-	75,75,75,75	7
74	OHX	C1	1915	7/7	0.97	0.21	-	120,120,120,120	7
74	OHX	D1	3557	7/7	0.89	0.25	-	148,148,148,148	7
74	OHX	B1	3620	7/7	0.91	0.30	-	58,58,58,58	7
74	OHX	A1	1968	7/7	0.91	0.29	-	180,180,180,180	7
74	OHX	A1	1990	7/7	0.86	0.28	-	117,117,117,117	7
74	OHX	D1	3461	7/7	0.96	0.18	-	128,128,128,128	7
74	OHX	C1	1911	7/7	0.99	0.13	-	96,96,96,96	7
74	OHX	D1	3470	7/7	0.97	0.14	-	84,84,84,84	7
74	OHX	B1	3601	7/7	0.85	0.35	-	158,158,158,158	7
74	OHX	A1	1974	7/7	0.81	0.40	-	136,136,136,136	7
74	OHX	D1	3430	7/7	0.98	0.14	-	101,101,101,101	7
74	OHX	B1	3516	7/7	0.96	0.21	-	136,136,136,136	7
74	OHX	B1	3613	7/7	0.91	0.46	-	93,93,93,93	7
74	OHX	C1	1971	7/7	0.92	0.29	-	131,131,131,131	7
74	OHX	A1	1916	7/7	0.97	0.14	-	91,91,91,91	7
74	OHX	Dd	102	7/7	0.91	0.23	-	118,118,118,118	7
74	OHX	B1	3523	7/7	0.89	0.30	-	150,150,150,150	7
74	OHX	C1	1957	7/7	0.77	0.37	-	226,226,226,226	7
74	OHX	B1	3434	7/7	0.99	0.16	-	102,102,102,102	7
74	OHX	C1	1990	7/7	0.85	0.27	-	105,105,105,105	7
74	OHX	B1	3574	7/7	0.94	0.44	-	136,136,136,136	7
74	OHX	A1	1981	7/7	0.92	0.26	-	128,128,128,128	7
74	OHX	D1	3611	7/7	0.88	0.36	-	82,82,82,82	7
74	OHX	A1	1921	7/7	0.93	0.27	-	148,148,148,148	7
74	OHX	D1	3481	7/7	0.88	0.29	-	137,137,137,137	7
74	OHX	A1	1971	7/7	0.92	0.21	-	94,94,94,94	7
74	OHX	B1	3573	7/7	0.93	0.23	-	111,111,111,111	7
74	OHX	D1	3570	7/7	0.96	0.29	-	49,49,49,49	7
74	OHX	B1	3596	7/7	0.95	0.34	-	56,56,56,56	7
74	OHX	C1	1996	7/7	0.92	0.43	-	86,86,86,86	7
74	OHX	B1	3431	7/7	0.96	0.19	-	125,125,125,125	7
74	OHX	A1	1960	7/7	0.95	0.38	-	70,70,70,70	7
74	OHX	D2	208	7/7	0.87	0.39	-	105,105,105,105	7
74	OHX	B1	3454	7/7	0.97	0.33	-	123,123,123,123	7
74	OHX	D1	3511	7/7	0.95	0.28	-	85,85,85,85	7
74	OHX	C1	1968	7/7	0.85	0.30	-	103,103,103,103	7
74	OHX	D1	3542	7/7	0.70	0.38	-	198,198,198,198	7
74	OHX	B1	3510	7/7	0.91	0.33	-	153,153,153,153	7
74	OHX	B1	3597	7/7	0.89	0.34	-	137,137,137,137	7
74	OHX	D2	209	7/7	0.87	0.31	-	74,74,74,74	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
74	OHX	D1	3415	7/7	0.99	0.12	-	139,139,139,139	0
74	OHX	C1	2001	7/7	0.96	0.25	-	130,130,130,130	7
74	OHX	D1	3500	7/7	0.93	0.29	-	139,139,139,139	7
74	OHX	B1	3414	7/7	0.98	0.14	-	106,106,106,106	0
74	OHX	B1	3564	7/7	0.96	0.24	-	126,126,126,126	7
74	OHX	C1	1976	7/7	0.80	0.37	-	118,118,118,118	7
74	OHX	B1	3446	7/7	0.95	0.23	-	113,113,113,113	7
74	OHX	D1	3600	7/7	0.86	0.29	-	96,96,96,96	7
74	OHX	A1	1933	7/7	0.91	0.20	-	152,152,152,152	7
74	OHX	A1	1954	7/7	0.90	0.19	-	153,153,153,153	7
74	OHX	Bd	102	7/7	0.95	0.19	-	73,73,73,73	7
74	OHX	A1	1963	7/7	0.90	0.34	-	137,137,137,137	7
74	OHX	A1	1928	7/7	0.96	0.15	-	99,99,99,99	7
74	OHX	B1	3548	7/7	0.79	0.60	-	153,153,153,153	7
74	OHX	B1	3565	7/7	0.90	0.26	-	120,120,120,120	7
74	OHX	C1	1987	7/7	0.88	0.35	-	108,108,108,108	7
74	OHX	B1	3592	7/7	0.90	0.39	-	106,106,106,106	7
74	OHX	B1	3557	7/7	0.90	0.48	-	46,46,46,46	7
74	OHX	B3	201	7/7	0.99	0.19	-	117,117,117,117	0
74	OHX	C1	1938	7/7	0.85	0.29	-	191,191,191,191	7
74	OHX	D1	3441	7/7	0.98	0.20	-	124,124,124,124	7
74	OHX	B1	3465	7/7	0.95	0.17	-	142,142,142,142	7
74	OHX	B1	3466	7/7	0.98	0.17	-	120,120,120,120	7
74	OHX	D1	3549	7/7	0.95	0.27	-	127,127,127,127	7
74	OHX	D1	3567	7/7	0.94	0.14	-	106,106,106,106	7
74	OHX	D3	209	7/7	0.92	0.20	-	127,127,127,127	7
74	OHX	B1	3538	7/7	0.90	0.28	-	93,93,93,93	7
74	OHX	D1	3498	7/7	0.93	0.28	-	103,103,103,103	7
74	OHX	D1	3521	7/7	0.87	0.23	-	163,163,163,163	7
74	OHX	D1	3578	7/7	0.82	0.70	-	222,222,222,222	7
74	OHX	C1	1924	7/7	0.97	0.14	-	82,82,82,82	7
74	OHX	C1	1946	7/7	0.95	0.21	-	63,63,63,63	7
74	OHX	B1	3561	7/7	0.86	0.50	-	280,280,280,280	7
74	OHX	C1	1951	7/7	0.95	0.15	-	152,152,152,152	7
74	OHX	D1	3575	7/7	0.93	0.29	-	84,84,84,84	7
74	OHX	B1	3570	7/7	0.96	0.28	-	91,91,91,91	7
74	OHX	D1	3541	7/7	0.83	0.31	-	141,141,141,141	7
74	OHX	D1	3431	7/7	0.98	0.12	-	109,109,109,109	7
74	OHX	B3	207	7/7	0.96	0.18	-	68,68,68,68	7
74	OHX	A1	1987	7/7	0.94	0.23	-	72,72,72,72	7
74	OHX	B1	3474	7/7	0.88	0.26	-	179,179,179,179	7
74	OHX	D1	3528	7/7	0.94	0.35	-	96,96,96,96	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
74	OHX	D1	3566	7/7	0.79	0.36	-	88,88,88,88	7
74	OHX	D1	3580	7/7	0.84	0.29	-	114,114,114,114	7
74	OHX	C1	1921	7/7	0.97	0.09	-	145,145,145,145	7
74	OHX	B1	3598	7/7	0.94	0.22	-	100,100,100,100	7
74	OHX	C1	1925	7/7	0.98	0.12	-	116,116,116,116	7
74	OHX	D1	3463	7/7	0.96	0.18	-	140,140,140,140	7
74	OHX	B1	3533	7/7	0.88	0.34	-	149,149,149,149	7
74	OHX	B1	3541	7/7	0.89	0.28	-	117,117,117,117	7
74	OHX	C1	1939	7/7	0.91	0.28	-	103,103,103,103	7
74	OHX	D1	3531	7/7	0.90	0.32	-	136,136,136,136	7
74	OHX	D1	3619	7/7	0.95	0.20	-	86,86,86,86	7
74	OHX	D1	3505	7/7	0.92	0.36	-	160,160,160,160	7
74	OHX	B1	3602	7/7	0.73	0.44	-	75,75,75,75	7
74	OHX	A1	1992	7/7	0.96	0.43	-	45,45,45,45	7
74	OHX	D1	3622	7/7	0.89	0.30	-	142,142,142,142	7
74	OHX	A1	1942	7/7	0.91	0.30	-	97,97,97,97	7
74	OHX	C1	1934	7/7	0.93	0.20	-	141,141,141,141	7
74	OHX	D1	3454	7/7	0.95	0.19	-	117,117,117,117	7
74	OHX	D1	3512	7/7	0.95	0.19	-	108,108,108,108	7
74	OHX	D1	3462	7/7	0.96	0.16	-	114,114,114,114	7
74	OHX	C1	1978	7/7	0.76	0.29	-	145,145,145,145	7
74	OHX	B3	202	7/7	0.98	0.15	-	116,116,116,116	0
74	OHX	C1	1962	7/7	0.82	0.30	-	180,180,180,180	7
74	OHX	D1	3565	7/7	0.97	0.23	-	60,60,60,60	7
74	OHX	C1	1984	7/7	0.94	0.27	-	78,78,78,78	7
74	OHX	A1	1939	7/7	0.90	0.19	-	100,100,100,100	7
74	OHX	D1	3592	7/7	0.96	0.22	-	118,118,118,118	7
74	OHX	B2	204	7/7	0.88	0.23	-	132,132,132,132	7
74	OHX	B1	3614	7/7	0.86	0.34	-	163,163,163,163	7
74	OHX	B1	3462	7/7	0.96	0.21	-	90,90,90,90	7
74	OHX	D1	3529	7/7	0.87	0.28	-	130,130,130,130	7
74	OHX	D1	3601	7/7	0.91	0.57	-	99,99,99,99	7
74	OHX	B1	3584	7/7	0.90	0.48	-	99,99,99,99	7
74	OHX	D1	3559	7/7	0.90	0.21	-	116,116,116,116	7
74	OHX	B1	3483	7/7	0.97	0.28	-	71,71,71,71	7
74	OHX	B1	3522	7/7	0.95	0.16	-	129,129,129,129	7
74	OHX	B2	208	7/7	0.82	0.48	-	152,152,152,152	7
74	OHX	D1	3625	7/7	0.90	0.24	-	100,100,100,100	7
74	OHX	B1	3593	7/7	0.91	0.24	-	46,46,46,46	7
74	OHX	B1	3425	7/7	0.96	0.17	-	108,108,108,108	7
74	OHX	CI	201	7/7	0.95	0.31	-	143,143,143,143	7
74	OHX	B1	3552	7/7	0.77	0.32	-	138,138,138,138	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
74	OHX	D1	3493	7/7	0.94	0.17	-	126,126,126,126	7
74	OHX	D1	3577	7/7	0.90	0.25	-	198,198,198,198	7
74	OHX	A1	1908	7/7	0.96	0.23	-	96,96,96,96	7
74	OHX	B1	3514	7/7	0.85	0.30	-	123,123,123,123	7
74	OHX	D1	3607	7/7	0.95	0.29	-	78,78,78,78	7
74	OHX	D1	3468	7/7	0.95	0.26	-	130,130,130,130	7
74	OHX	C1	1980	7/7	0.89	0.34	-	162,162,162,162	7
74	OHX	D1	3606	7/7	0.90	0.24	-	63,63,63,63	7
74	OHX	D1	3491	7/7	0.96	0.24	-	37,37,37,37	7
74	OHX	A1	1997	7/7	0.90	0.39	-	100,100,100,100	7
74	OHX	D2	204	7/7	0.90	0.20	-	116,116,116,116	7
74	OHX	B1	3488	7/7	0.95	0.18	-	104,104,104,104	7

## 6.5 Other polymers [i](#)

There are no such residues in this entry.