



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 08:52 PM BST

PDB ID : 4V8F
Title : Crystal structure analysis of ribosomal decoding (near-cognate tRNA-ttyr complex with paromomycin).
Authors : Jenner, L.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2011-12-07
Resolution : 3.30 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

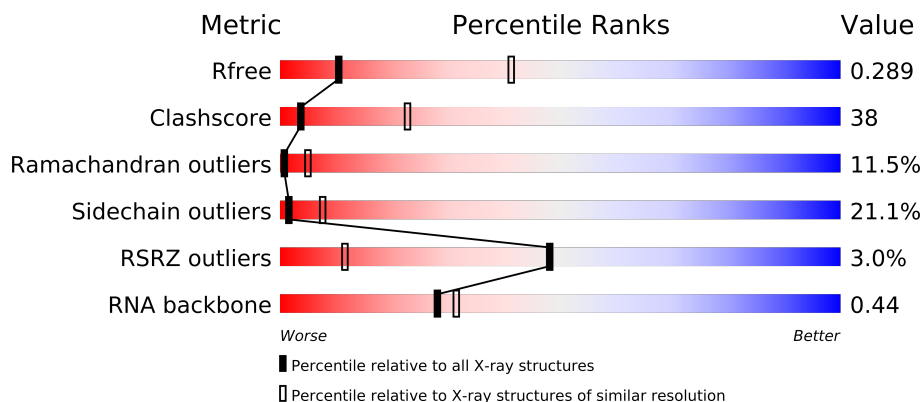
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)
RNA backbone	1838	1042 (3.90-2.70)

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

Mol	Chain	Length	Quality of chain
1	AA	2912	
1	DA	2912	
2	AB	122	
2	DB	122	
3	AD	276	
3	DD	276	
4	AE	206	
4	DE	206	
5	AF	210	
5	DF	210	
6	AG	182	
6	DG	182	

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Mol	Chain	Length	Quality of chain
7	AH	180	
7	DH	180	
8	AK	148	
8	DK	148	
9	AM	140	
9	DM	140	
10	AN	122	
10	DN	122	
11	AO	150	
11	DO	150	
12	AP	141	
12	DP	141	
13	A0	118	
13	D0	118	
14	AQ	112	
14	DQ	112	
15	AR	146	
15	DR	146	
16	A1	118	
16	D1	118	
17	A2	101	
17	D2	101	
18	AS	113	
18	DS	113	
19	AT	96	
19	DT	96	
20	AU	110	
20	DU	110	
21	AV	206	
21	DV	206	
22	A3	85	
22	D3	85	
23	AZ	98	
23	DZ	98	
24	AW	72	
24	DW	72	
25	AX	60	
25	DX	60	
26	A4	71	
26	D4	71	
27	A5	60	
27	D5	60	

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Mol	Chain	Length	Quality of chain
28	A6	54	
28	D6	54	
29	A7	49	
29	D7	49	
30	A8	65	
30	D8	65	
31	BA	1506	
31	CA	1506	
32	BE	256	
32	CE	256	
33	BF	239	
33	CF	239	
34	BG	208	
34	CG	208	
35	BH	162	
35	CH	162	
36	BI	101	
36	CI	101	
37	BJ	156	
37	CJ	156	
38	BK	138	
38	CK	138	
39	BL	128	
39	CL	128	
40	BM	105	
40	CM	105	
41	BN	129	
41	CN	129	
42	BO	132	
42	CO	132	
43	BP	126	
43	CP	126	
44	BQ	61	
44	CQ	61	
45	BR	89	
45	CR	89	
46	BS	88	
46	CS	88	
47	BT	105	
47	CT	105	
48	BU	88	
48	CU	88	

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Mol	Chain	Length	Quality of chain
49	BV	93	
49	CV	93	
50	BW	106	
50	CW	106	
51	BX	27	
51	CX	27	
52	BB	85	
52	BD	85	
52	CB	85	
52	CD	85	
53	BC	77	
53	CC	77	
54	B1	16	
54	C1	16	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 304031 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a RNA chain called RNA (2912-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
1	DA	2907	Total	C	N	O	P	0	0	0
			62607	27866	11712	20123	2906			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	161	U	-	INSERTION	GB AP008226.1
AA	654A	A	G	CONFLICT	GB AP008226.1
AA	654E	C	G	CONFLICT	GB AP008226.1
AA	654P	G	C	CONFLICT	GB AP008226.1
AA	654T	A	C	CONFLICT	GB AP008226.1
AA	1058	U	G	CONFLICT	GB AP008226.1
AA	1080	A	C	CONFLICT	GB AP008226.1
DA	168	U	-	insertion	GB AP008226.1
DA	654A	A	G	CONFLICT	GB AP008226.1
DA	654E	C	G	CONFLICT	GB AP008226.1
DA	654P	G	C	CONFLICT	GB AP008226.1
DA	654T	A	C	CONFLICT	GB AP008226.1
DA	1058	U	G	CONFLICT	GB AP008226.1
DA	1080	A	C	CONFLICT	GB AP008226.1

- Molecule 2 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
2	DB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
3	DD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
4	DE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
5	DF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
6	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
7	DH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	DK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
9	DM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
10	DN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
11	DO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	DP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	A0	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	D0	117	Total	C	N	O	S	0	0	0
			960	599	202	159				

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AQ	111	Total	C	N	O	0	0	0
			882	556	176	150			
14	DQ	111	Total	C	N	O	0	0	0
			882	556	176	150			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
15	DR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	A1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
16	D1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	A2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
17	D2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
18	DS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	AT	92	Total	C	N	O	0	0	0
			725	471	131	123			
19	DT	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
20	DU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AV	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			
21	DV	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	A3	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
22	D3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
23	DZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	DW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AX	59	Total	C	N	O		0	0	0
			469	298	90	81				
25	DX	59	Total	C	N	O		0	0	0
			469	298	90	81				

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A4	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
26	D4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
28	D6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A7	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			
29	D7	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			
30	D8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BA	1502	Total	C	N	O	P	0	0	0
			32284	14370	5982	10431	1501			
31	CA	1502	Total	C	N	O	P	0	0	0
			32287	14370	5982	10433	1502			

- Molecule 32 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
32	CE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- Molecule 33 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BF	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
33	CF	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 34 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
34	CG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 35 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
35	CH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 36 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
36	CI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 37 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
37	CJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 38 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
38	CK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 39 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BL	127	Total	C	N	O		0	0	0
			1010	639	197	174				
39	CL	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- Molecule 40 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	CM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 41 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
41	CN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 42 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
42	CO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 43 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BP	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
43	CP	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 44 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BQ	58	Total	C	N	O	S	0	0	0
			476	303	99	70	4			
44	CQ	58	Total	C	N	O	S	0	0	0
			476	303	99	70	4			

- Molecule 45 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
45	CR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 46 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
46	CS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 47 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
47	CT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 48 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	BU	72	Total	C	N	O	0	0	0
			591	376	117	98			
48	CU	72	Total	C	N	O	0	0	0
			591	376	117	98			

- Molecule 49 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			
49	CV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

- Molecule 50 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
50	CW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 51 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BX	25	Total	C	N	O	0	0	0
			217	134	52	31			
51	CX	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 52 is a RNA chain called TRNA-TYR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
52	BB	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
52	BD	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
52	CB	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
52	CD	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CB	?	-	U	DELETION	GB AP012306.1
CB	?	-	A	DELETION	GB AP012306.1
CB	?	-	A	DELETION	GB AP012306.1
CB	10	C	-	insertion	GB AP012306.1
CB	11	C	-	insertion	GB AP012306.1
CB	12	C	G	CONFLICT	GB AP012306.1
CB	?	-	U	DELETION	GB AP012306.1
CB	?	-	A	DELETION	GB AP012306.1
CB	?	-	A	DELETION	GB AP012306.1
CB	17	G	C	CONFLICT	GB AP012306.1
CB	20	C	U	CONFLICT	GB AP012306.1
CB	22	A	C	CONFLICT	GB AP012306.1
CB	23	A	C	CONFLICT	GB AP012306.1
CB	24	G	U	CONFLICT	GB AP012306.1
CB	25	G	U	CONFLICT	GB AP012306.1
CB	29	C	G	CONFLICT	GB AP012306.1
CB	30	A	U	CONFLICT	GB AP012306.1
CB	32	A	-	insertion	GB AP012306.1
CB	33	C	-	insertion	GB AP012306.1
CB	34	U	-	insertion	GB AP012306.1
CB	38	MIA	-	insertion	GB AP012306.1
CB	39	A	-	insertion	GB AP012306.1
CB	40	U	-	insertion	GB AP012306.1

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Chain	Residue	Modelled	Actual	Comment	Reference
CB	41	C	G	CONFLICT	GB AP012306.1
CB	46	G	-	insertion	GB AP012306.1
CB	47	U	-	insertion	GB AP012306.1
CB	?	-	A	DELETION	GB AP012306.1
CB	?	-	A	DELETION	GB AP012306.1
CB	51	C	G	CONFLICT	GB AP012306.1
CB	53	A	G	CONFLICT	GB AP012306.1
CB	?	-	A	DELETION	GB AP012306.1
CB	59	A	-	insertion	GB AP012306.1
CB	60	A	-	insertion	GB AP012306.1
CB	66	G	A	CONFLICT	GB AP012306.1
CB	68	A	G	CONFLICT	GB AP012306.1
CB	?	-	C	DELETION	GB AP012306.1
CB	72	U	G	CONFLICT	GB AP012306.1
CB	76	C	U	CONFLICT	GB AP012306.1
CB	?	-	G	DELETION	GB AP012306.1
CB	?	-	G	DELETION	GB AP012306.1
CB	78	C	U	CONFLICT	GB AP012306.1
CB	83	C	-	insertion	GB AP012306.1
CB	84	C	-	insertion	GB AP012306.1
CB	85	A	-	insertion	GB AP012306.1
CD	?	-	U	DELETION	GB AP012306.1
CD	?	-	A	DELETION	GB AP012306.1
CD	?	-	A	DELETION	GB AP012306.1
CD	10	C	-	insertion	GB AP012306.1
CD	11	C	-	insertion	GB AP012306.1
CD	12	C	G	CONFLICT	GB AP012306.1
CD	?	-	U	DELETION	GB AP012306.1
CD	?	-	A	DELETION	GB AP012306.1
CD	?	-	A	DELETION	GB AP012306.1
CD	17	G	C	CONFLICT	GB AP012306.1
CD	20	C	U	CONFLICT	GB AP012306.1
CD	22	A	C	CONFLICT	GB AP012306.1
CD	23	A	C	CONFLICT	GB AP012306.1
CD	24	G	U	CONFLICT	GB AP012306.1
CD	25	G	U	CONFLICT	GB AP012306.1
CD	29	C	G	CONFLICT	GB AP012306.1
CD	30	A	U	CONFLICT	GB AP012306.1
CD	32	A	-	insertion	GB AP012306.1
CD	33	C	-	insertion	GB AP012306.1
CD	34	U	-	insertion	GB AP012306.1
CD	38	MIA	-	insertion	GB AP012306.1

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Chain	Residue	Modelled	Actual	Comment	Reference
CD	39	A	-	insertion	GB AP012306.1
CD	40	U	-	insertion	GB AP012306.1
CD	41	C	G	CONFLICT	GB AP012306.1
CD	46	G	-	insertion	GB AP012306.1
CD	47	U	-	insertion	GB AP012306.1
CD	?	-	A	DELETION	GB AP012306.1
CD	?	-	A	DELETION	GB AP012306.1
CD	51	C	G	CONFLICT	GB AP012306.1
CD	53	A	G	CONFLICT	GB AP012306.1
CD	?	-	A	DELETION	GB AP012306.1
CD	59	A	-	insertion	GB AP012306.1
CD	60	A	-	insertion	GB AP012306.1
CD	66	G	A	CONFLICT	GB AP012306.1
CD	68	A	G	CONFLICT	GB AP012306.1
CD	?	-	C	DELETION	GB AP012306.1
CD	72	U	G	CONFLICT	GB AP012306.1
CD	76	C	U	CONFLICT	GB AP012306.1
CD	?	-	G	DELETION	GB AP012306.1
CD	?	-	G	DELETION	GB AP012306.1
CD	78	C	U	CONFLICT	GB AP012306.1
CD	83	C	-	insertion	GB AP012306.1
CD	84	C	-	insertion	GB AP012306.1
CD	85	A	-	insertion	GB AP012306.1

- Molecule 53 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	CC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	18	C	U	CONFLICT	GB AP012306.1

- Molecule 54 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B1	16	Total	C	N	O	P	0	0	0
			347	156	69	106	16			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	C1	16	Total	C	N	O	P	0	0	0
			347	156	69	106	16			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C1	10	G	-	insertion	GB AP012306.1
C1	12	A	-	insertion	GB AP012306.1
C1	13	A	-	insertion	GB AP012306.1
C1	14	A	U	CONFLICT	GB AP012306.1
C1	15	A	U	CONFLICT	GB AP012306.1
C1	20	G	U	CONFLICT	GB AP012306.1
C1	21	C	U	CONFLICT	GB AP012306.1
C1	22	A	U	CONFLICT	GB AP012306.1
C1	23	A	-	insertion	GB AP012306.1
C1	24	A	-	insertion	GB AP012306.1
C1	25	A	-	insertion	GB AP012306.1

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

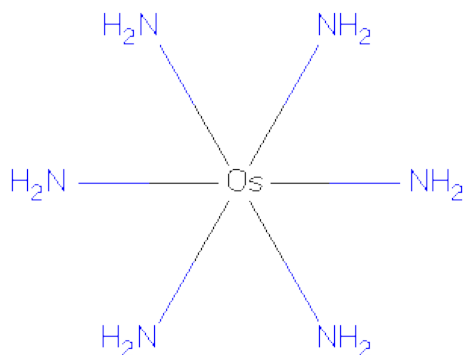
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	BA	114	Total	Mg	0	0
			114	114		
55	CA	121	Total	Mg	0	0
			121	121		
55	AB	6	Total	Mg	0	0
			6	6		
55	B1	1	Total	Mg	0	0
			1	1		
55	C1	2	Total	Mg	0	0
			2	2		
55	BB	13	Total	Mg	0	0
			13	13		
55	AE	3	Total	Mg	0	0
			3	3		
55	BF	1	Total	Mg	0	0
			1	1		
55	AA	332	Total	Mg	0	0
			332	332		
55	A5	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	D7	1	Total 1	Mg 1	0	0
55	BC	4	Total 4	Mg 4	0	0
55	A1	2	Total 2	Mg 2	0	0
55	CN	1	Total 1	Mg 1	0	0
55	D0	1	Total 1	Mg 1	0	0
55	CC	7	Total 7	Mg 7	0	0
55	DA	272	Total 272	Mg 272	0	0
55	A0	1	Total 1	Mg 1	0	0
55	DE	1	Total 1	Mg 1	0	0
55	CB	3	Total 3	Mg 3	0	0
55	BS	1	Total 1	Mg 1	0	0
55	A7	1	Total 1	Mg 1	0	0
55	D5	1	Total 1	Mg 1	0	0
55	BD	1	Total 1	Mg 1	0	0
55	AO	1	Total 1	Mg 1	0	0
55	BW	1	Total 1	Mg 1	0	0
55	A3	1	Total 1	Mg 1	0	0
55	AF	2	Total 2	Mg 2	0	0
55	DB	7	Total 7	Mg 7	0	0

- Molecule 56 is osmium (III) hexammine (three-letter code: OHX) (formula: H₁₂N₆Os).



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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
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56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
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56	AA	1	Total	N	Os	0	0
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56	AA	1	Total	N	Os	0	0
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56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
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56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AB	1	Total	N	Os	0	0
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56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AE	1	Total	N	Os	0	0
			7	6	1		
56	AF	1	Total	N	Os	0	0
			7	6	1		
56	AO	1	Total	N	Os	0	0
			7	6	1		
56	AO	1	Total	N	Os	0	0
			7	6	1		
56	A1	1	Total	N	Os	0	0
			7	6	1		
56	A1	1	Total	N	Os	0	0
			7	6	1		
56	A3	1	Total	N	Os	0	0
			7	6	1		
56	AW	1	Total	N	Os	0	0
			7	6	1		
56	A6	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
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56	BA	1	Total	N	Os	0	0
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56	BA	1	Total	N	Os	0	0
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56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	BA	1	Total	N	Os	0	0
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56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BG	1	Total	N	Os	0	0
			7	6	1		
56	BL	1	Total	N	Os	0	0
			7	6	1		
56	BR	1	Total	N	Os	0	0
			7	6	1		
56	BB	1	Total	N	Os	0	0
			7	6	1		
56	BB	1	Total	N	Os	0	0
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56	BC	1	Total	N	Os	0	0
			7	6	1		
56	BC	1	Total	N	Os	0	0
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56	BC	1	Total	N	Os	0	0
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56	BD	1	Total	N	Os	0	0
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56	BD	1	Total	N	Os	0	0
			7	6	1		
56	BD	1	Total	N	Os	1	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
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56	CA	1	Total	N	Os	0	0
			7	6	1		
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56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CK	1	Total	N	Os	0	0
			7	6	1		
56	CR	1	Total	N	Os	0	0
			7	6	1		
56	CV	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
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56	CB	1	Total	N	Os	0	0
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56	CB	1	Total	N	Os	0	0
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56	CC	1	Total	N	Os	0	0
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56	CC	1	Total	N	Os	0	0
			7	6	1		
56	CC	1	Total	N	Os	0	0
			7	6	1		
56	CD	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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

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

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

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

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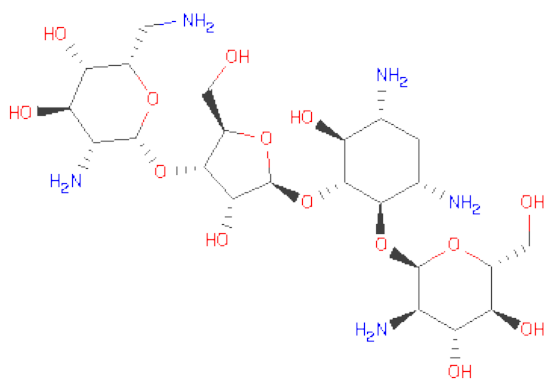
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
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			7	6	1		
56	DB	1	Total	N	Os	0	0
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56	DB	1	Total	N	Os	0	0
			7	6	1		
56	DF	1	Total	N	Os	0	0
			7	6	1		
56	DO	1	Total	N	Os	0	0
			7	6	1		
56	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	D3	1	Total	N	Os	0	0
			7	6	1		
56	D5	1	Total	N	Os	0	0
			7	6	1		
56	D8	1	Total	N	Os	0	0
			7	6	1		

- Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	BA	1	Total	C	N	O	0	0
			42	23	5	14		
57	CA	1	Total	C	N	O	0	0
			42	23	5	14		

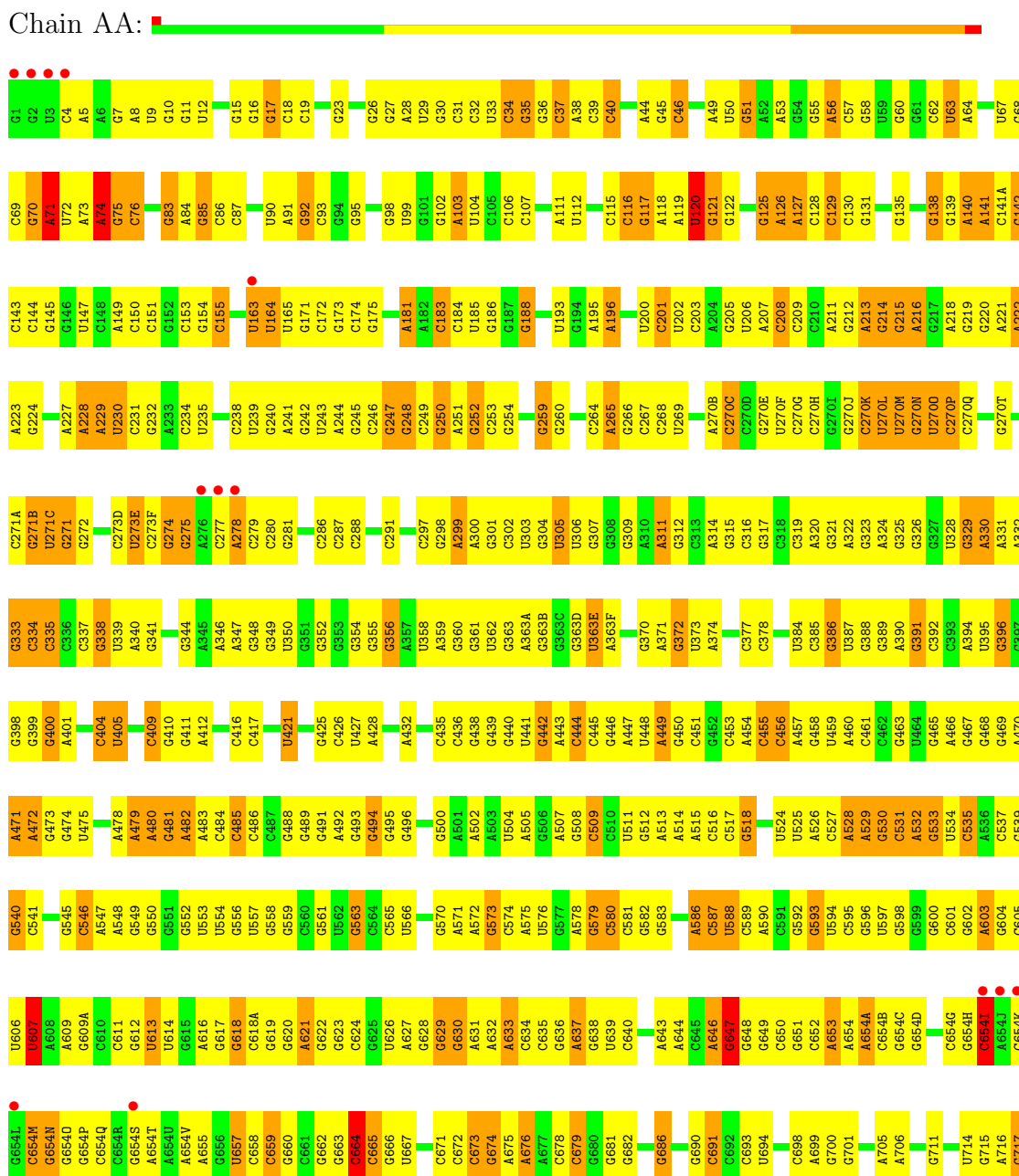
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	BG	1	Total	Zn	0	0
			1	1		
58	BQ	1	Total	Zn	0	0
			1	1		
58	CQ	1	Total	Zn	0	0
			1	1		
58	CG	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

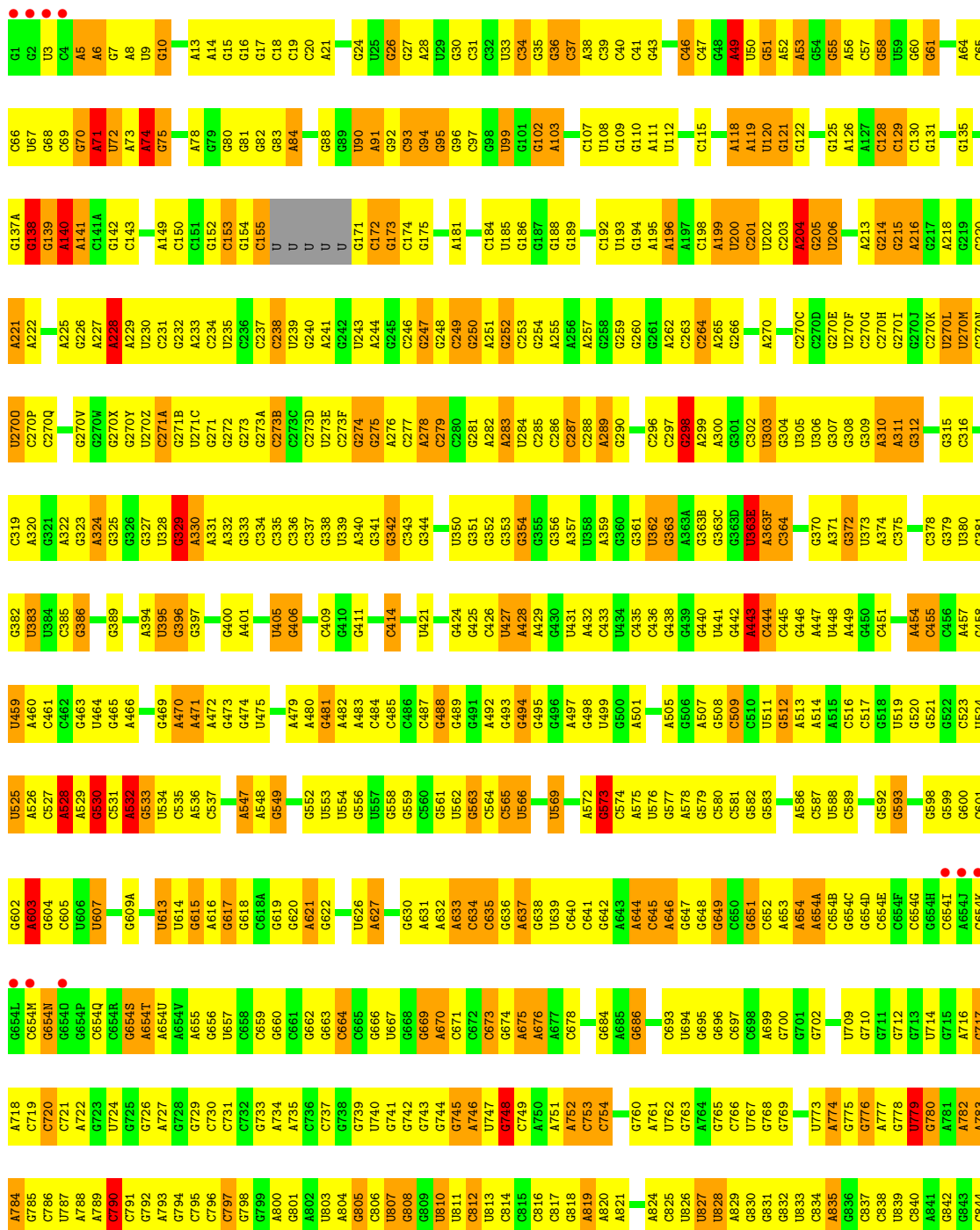
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: RNA (2912-MER)

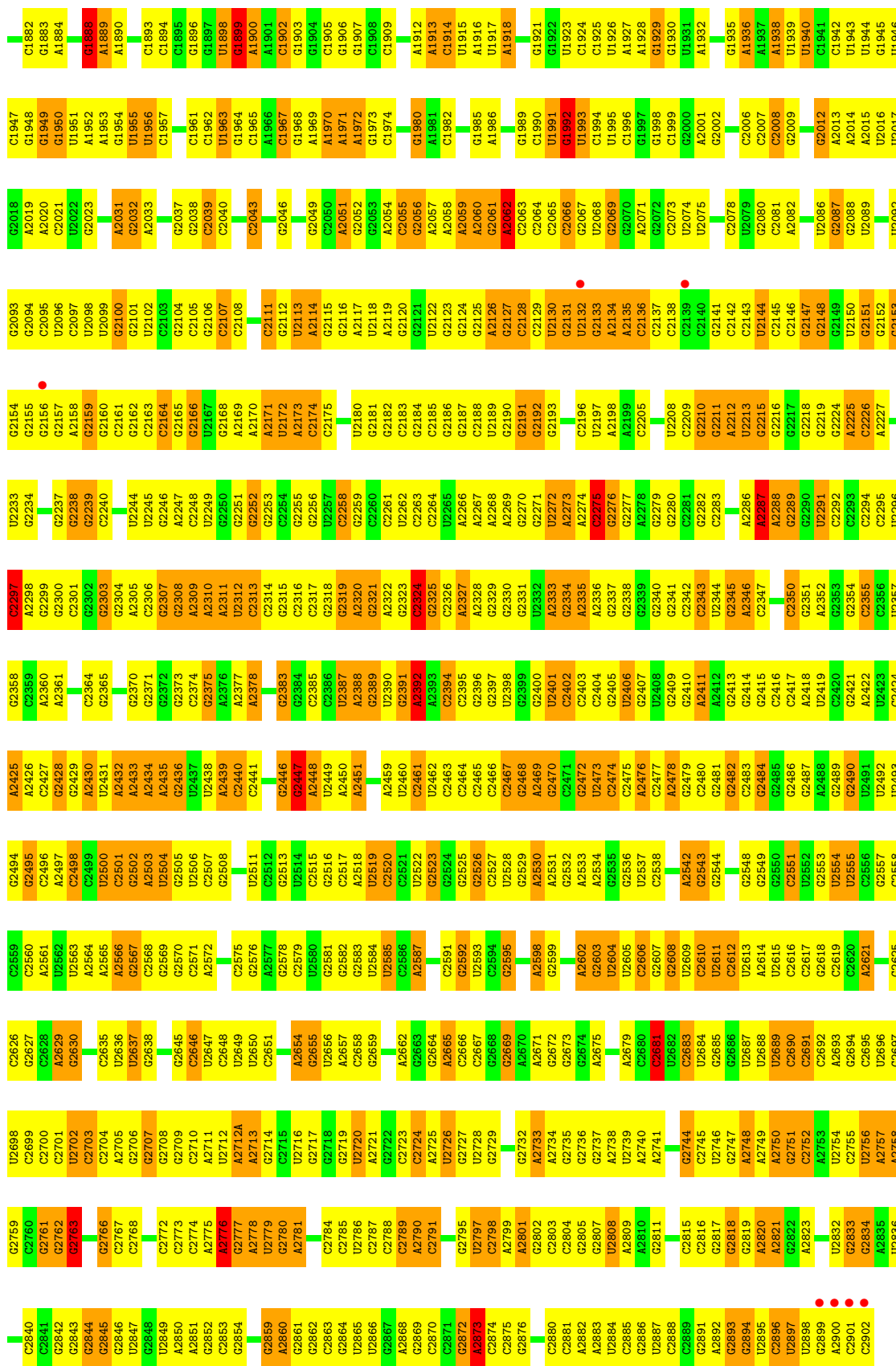




A2734	C2666	A2598	A2531	C2452	G2391	G2325	G2256	A2173	C2111	A2030	A1953	G1888	C1734
U2739	C2667	G2599	G2532	A2453	A2392	G2326	U2257	C2174	G2112	A2031	G1954	A1889	C1735
A2740	G2668	A2600	A2353	G2454	A2393	C2326	G2258		U2113	G2032	A1955	A1810	C1741
A2741	G2669	C2601	G2536	U2457	C2395	A2328	G2259	G2181	A2114	A2033	U1956	G1811	C1742
C2743	A2670	G2603	G2537	C2458	C2396	G2329	U2262	C2183	G2115	U2034	C1957	A1812	G1743
A2744	G2671	U2604	C2538		G2397	G2330	C2263	G2184	G2116	G2035	C1894	G1813	G1746
G2745	G2672	U2605	C2539	C2461	U2398	G2331		C2185	A2117	C2036	G1962	G1814	
G2746	G2673	C2606	C2540	U2462	G2399		A2267	G2186	U2118	G2037	U1963	A1815	A1749
U2747	G2674	G2607	G2541	U2463	G2400	G2334	A2268	C2187	A2119	G2038	G1964	G1816	G1750
G2748	G2675	A2542	A2543	C2467	U2401	A2335	A2269		G2120	C2039	C1965	G1817	C1751
A2749	C2680	G2543	G2544	C2468	C2402	A2336	G2270	G2190	G2121		G1966	A1900	G1752
A2750	C2681	C2610	G2544	A2469	G2403	G2337	G2271	G2191	U2122	C2043	G1967	A1901	G1753
A2751	U2682	G2611	G2545	C2470	C2404	G2338	U2272	G2192	G2123		G1968	C1902	C1754
C2752	C2683	C2612	U2546	G2471	G2405	G2339	A2273	G2193	G2124	G2048	A1969	G1903	A1755
U2753	U2684	U2613	U2547	G2472	U2406	G2340	A2274	G2194	A2126	C2050	A1970	G1904	G1756
G2754	G2685	A2614	G2548	U2473	G2407	G2341	C2275		G2127		A1972	G1905	G1757
C2755	G2686	U2615	G2549	C2474	U2408	C2342	G2276	A2198	G2128	A2054	G1973	G1906	G1758
U2756	U2687	G2616	G2550	C2475	G2409	G2343	G2277	A2199	C2129	G2055	G1973	C1907	A1759
A2757	G2688	C2617	G2553	A2476	G2410	U2344	A2278	C2205	U2130	G2056	G1980	C1908	A1760
A2758	U2689	G2618	U2554	C2477		G2345		C2206	G2131	A2057	A1981	A1829	C1761
	C2690	C2619	C2555	A2478	G2411	A2346	C2281	C2207	U2132	A2058	G1982	G1910	A1762
	G2691	C2620	C2556		G2412	C2347	G2282	U2208	G2133	A2059	G1983	G1911	G1763
			G2557	G2481	G2415		G2283	G2209	A2134	A2060	G1984	A1912	G1764
			C2558	G2482	C2416	C2350	C2284	G2210	A2135	G2061	G1985	A1913	G1765
			C2559		G2417	G2351	C2285	A2212	G2136	A2062		U1915	U1766
	C2626	C2626	C2560	G2486	A2418	A2352	A2286	G2213	C2137	C2063	G1989	U1917	G1769
U2698	G2697	A2561	U2562	G2487	U2419	C2353	A2287	G2215	C2138	C2064	U1991	G1918	G1770
C2699	C2699	G2630	U2563	G2489	G2421	C2356	G2289	G2216	C2140	U2068	G1992	A1919	G1772
C2700	C2701	G2631	A2564	G2490	A2422	U2357	U2291	G2217	G2141	G2069	C1993	C1920	A1773
U2702		A2632	A2565		U2423	C2358	G2294	G2219	C2142	U2070	U1994	G1921	C1774
			A2566	G2494	A2424	C2359	C2294	G2224	C2143	G2078	G1995	G1922	U1775
			C2567		A2425	A2360	C2295	A2225	U2144	G2079	G1996	U1923	G1776
			C2568	C2498	A2426			C2226	C2145	U2079	G1997	C1924	U1777
				C2499	G2427	C2363	A2298		G2146	U2079	A2001	C1925	U1778
				U2500	G2428	C2364	G2299	U2233	G2147	C2081	U2026	G1926	U1779
				C2501	G2429	G2365	G2300	G2234	G2148	A2082	C2006	A1927	U1780
				G2502	A2430	A2366	C2301	G2235	G2149	G2082	G2007	G1928	C1781
				A2503	U2431	C2367	C2302	G2236	U2150	G2083	C2007	G1929	A1848
				U2504	A2432	C2368	G2303	G2237	G2151	U2086	C2008	G1930	G1776
				G2505	A2433		C2303	G2237	G2152	U2086	G2009	U1931	U1777
				U2506	A2434	G2372	A2304	G2238	G2153	G2087		A1859	U1778
				C2507	A2435	G2373	A2305	G2239	G2154		G2012	A1932	U1779
				G2508	G2508	C2374	C2306	G2240	G2155		C2013	G1932	A1786
						G2375	G2307	A2241	G2156	U2092	A2014	C1934	A1787
						C2376	G2308	G2242	G2157	G2093	A2015	G1935	C1788
						A2377	A2309	U2243	A2158	G2094	A2016	A1936	A1789
						A2378	A2310	U2244		C2095	U2016	G1937	C1790
						C2440	C2440			U2096	U2017	A1938	C1870
						A2518	A2311	U2245	G2162	C2097	G2018	A1871	A1791
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						C2521	C2381	G2247	C2164	U2099	C1941	C1879	C1797
						U2522	G2444	G2248	G2165	G2100	C2021	C1880	U1798
						U2523	G2445	U2249	G2166	G2101	U2022	C1881	U1799
						G2524	G2446	G2250	U2167	G2023	G2023	C1882	G1799
						C2525	C2384	G2251	G2168	U2102	G2024	G1883	C1800
						U2528	G2385	G2252	A2169	C2103	G2024	U1946	G1801
						U2529	A2388	G2253	G2170	G2108	C2026	A1884	A1802
						C2530	A2389	C2254	A2171	C2108	G1950	A1885	A1803
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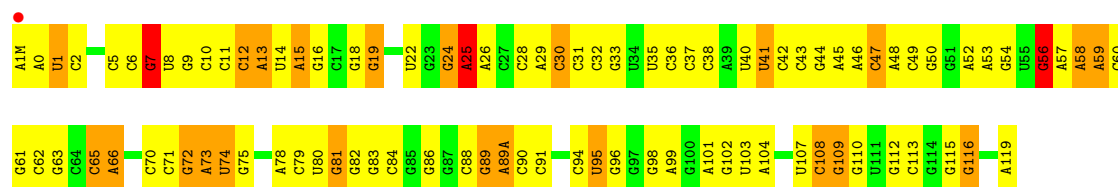


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G1800	G1801	G1727	U1576	C1506	C1575	C1506	G1440	G1369	C1299	G1224	C1161	A1095	G1031	C970	C908	U847
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A1872	C1711		U1638	U1639	C1711	U1638	C1498	A1435	C1362	C1292	A1156	G1089	U1026		G966	C903
G1878	C1712		U1639	C1499	C1712	U1639	C1499	G1435	C1362	U1291	A1156	G1089	A1027		C966	C904
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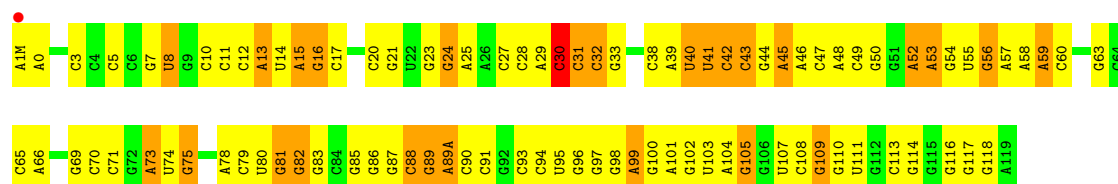
- Molecule 2: 5S RIBOSOMAL RNA

Chain AB:



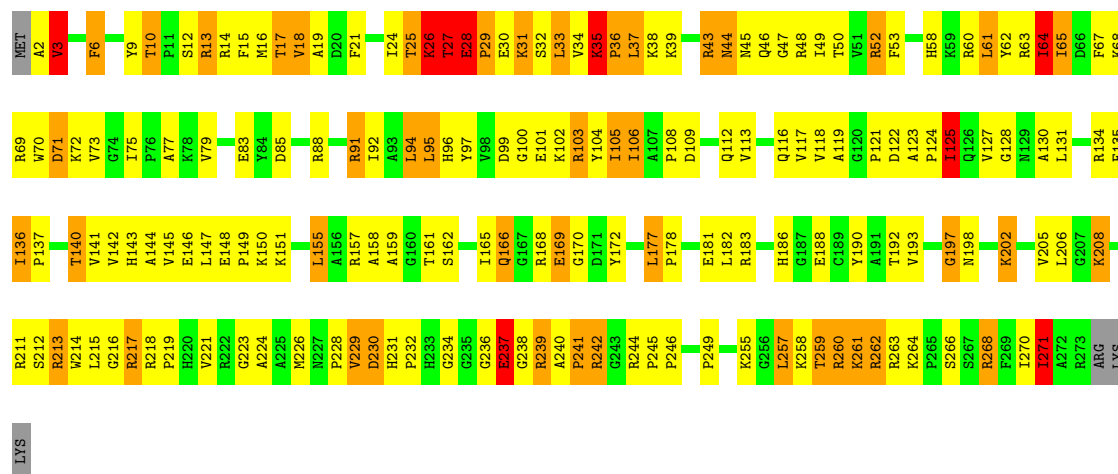
- Molecule 2: 5S RIBOSOMAL RNA

Chain DB:



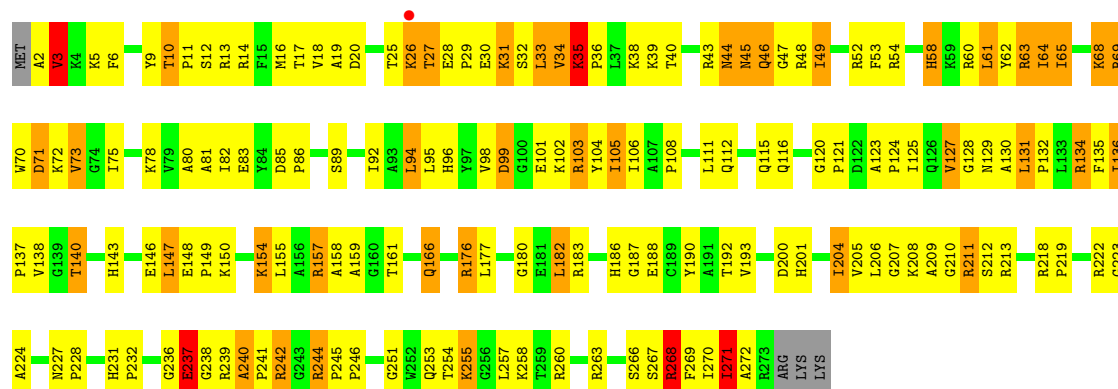
- Molecule 3: 50S ribosomal protein L2

Chain AD:



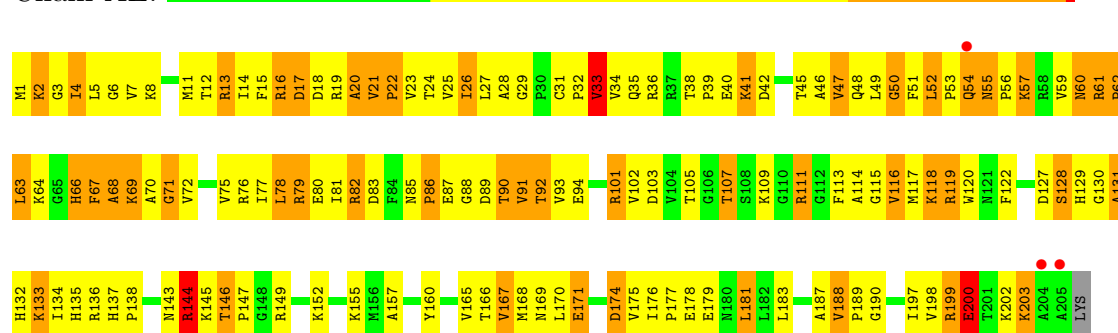
- Molecule 3: 50S ribosomal protein L2

Chain DD:



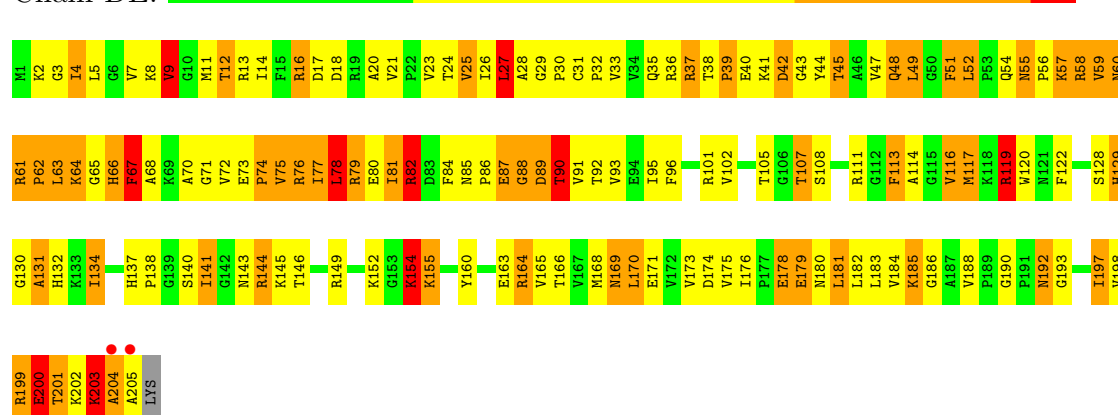
- Molecule 4: 50S ribosomal protein L3

Chain AE:



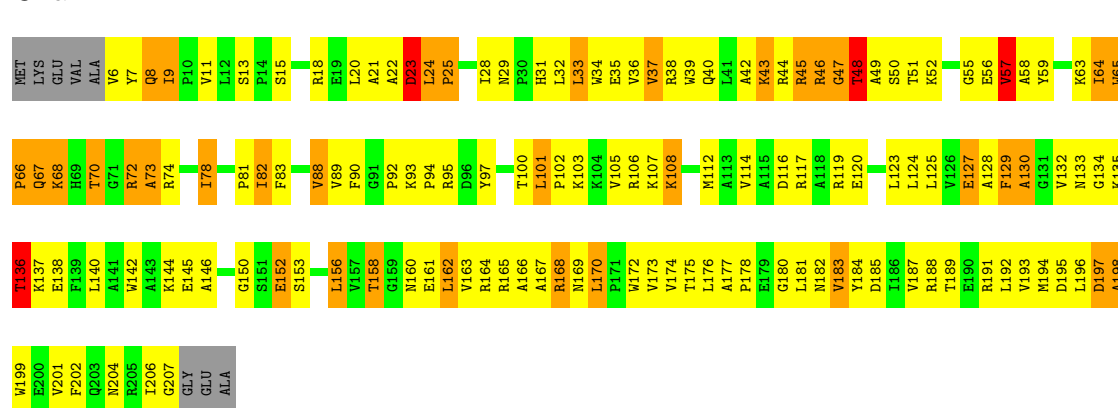
- Molecule 4: 50S ribosomal protein L3

Chain DE:



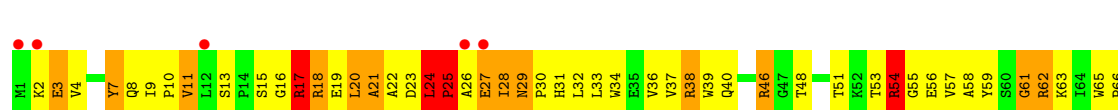
- Molecule 5: 50S ribosomal protein L4

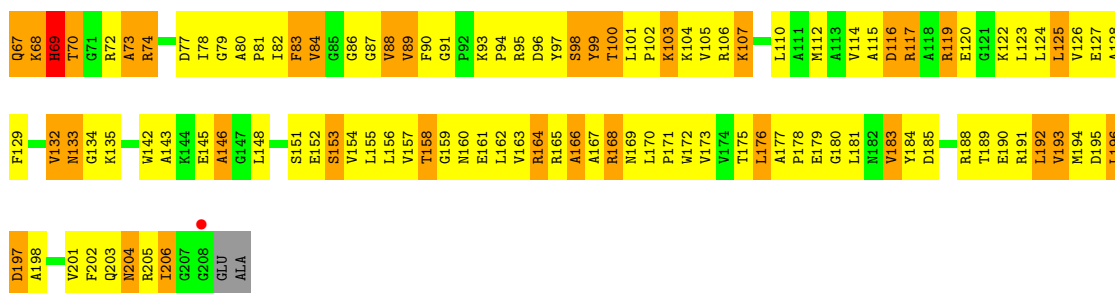
Chain AF:



- Molecule 5: 50S ribosomal protein L4

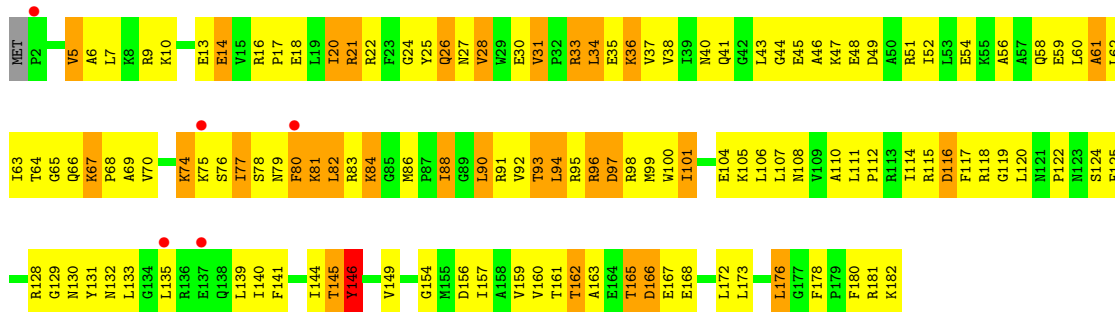
Chain DF:





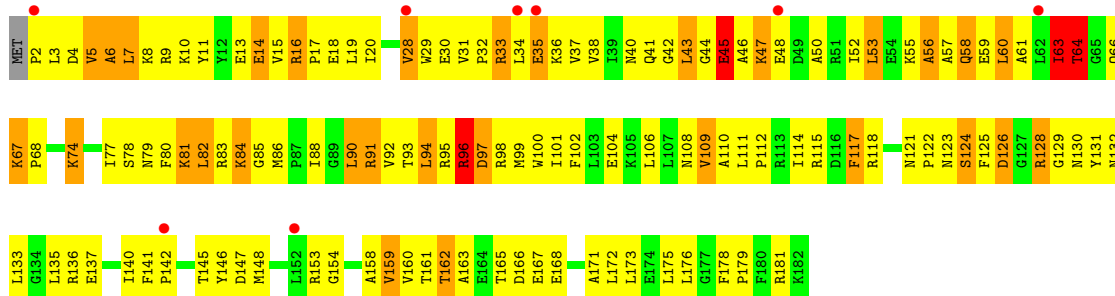
• Molecule 6: 50S ribosomal protein L5

Chain AG:



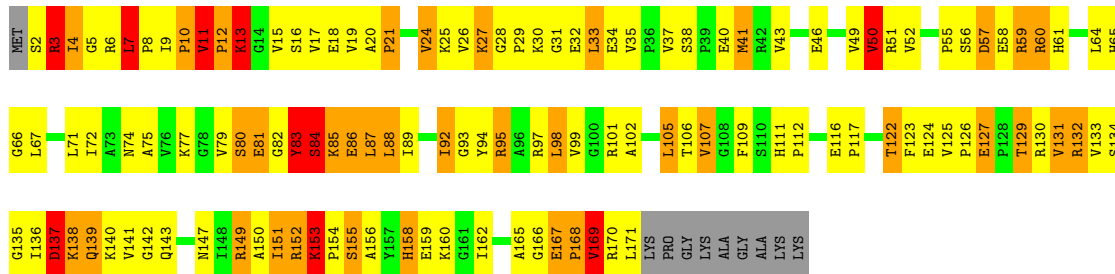
• Molecule 6: 50S ribosomal protein L5

Chain DG:



• Molecule 7: 50S ribosomal protein L6

Chain AH:

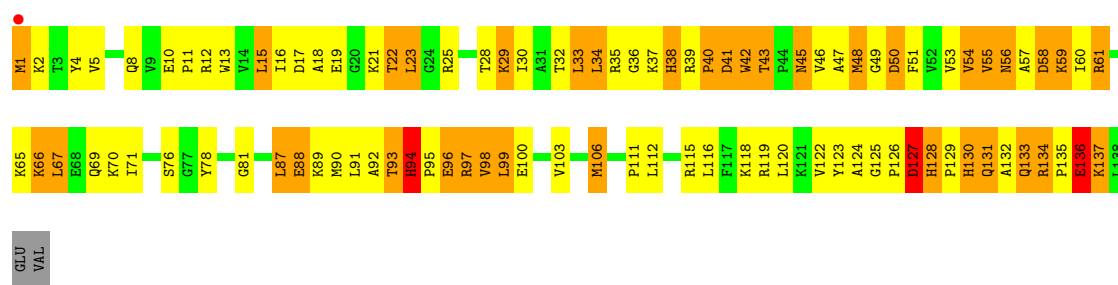


• Molecule 7: 50S ribosomal protein L6

Chain DH:

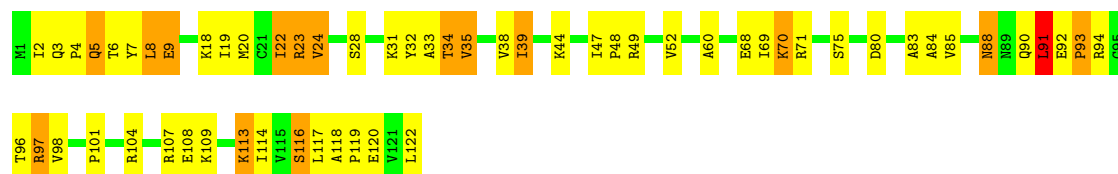






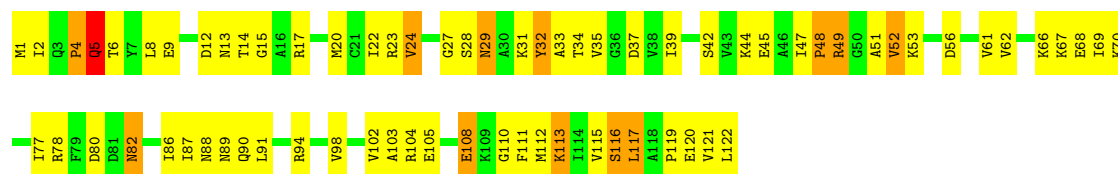
• Molecule 10: 50S ribosomal protein L14

Chain AN: █ █ █ █



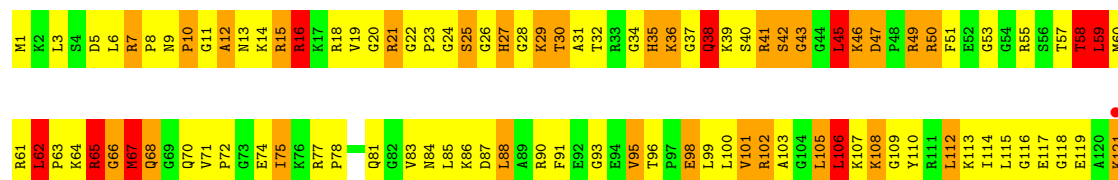
• Molecule 10: 50S ribosomal protein L14

Chain DN: █ █ █ █



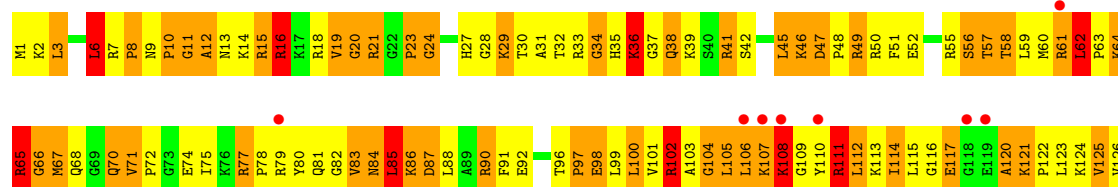
• Molecule 11: 50S ribosomal protein L15

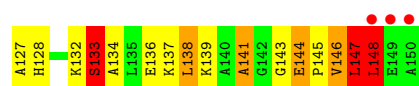
Chain AO: █ █ █ █



• Molecule 11: 50S ribosomal protein L15

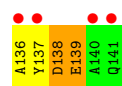
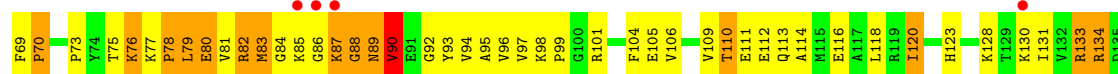
Chain DO: █ █ █ █





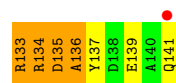
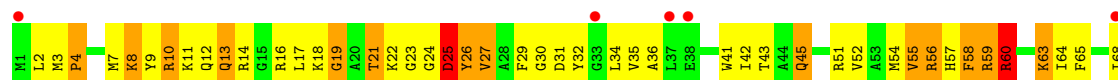
- Molecule 12: 50S ribosomal protein L16

Chain AP:



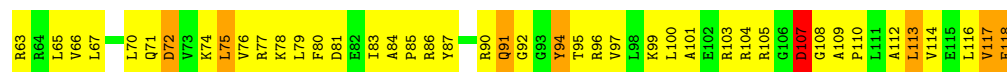
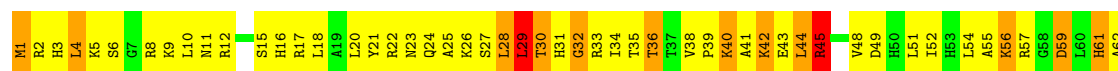
- Molecule 12: 50S ribosomal protein L16

Chain DP:



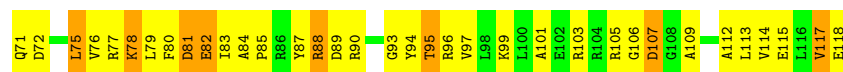
- Molecule 13: 50S ribosomal protein L17

Chain A0:



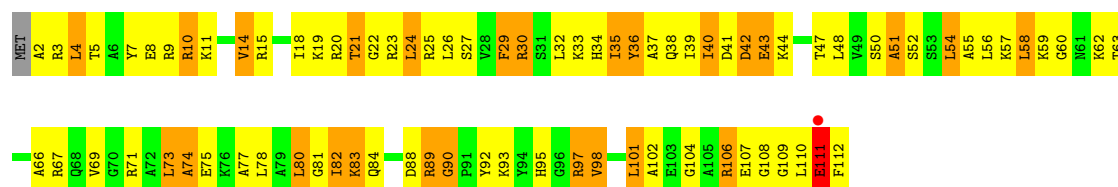
- Molecule 13: 50S ribosomal protein L17

Chain D0:



- Molecule 14: 50S ribosomal protein L18

Chain AQ:



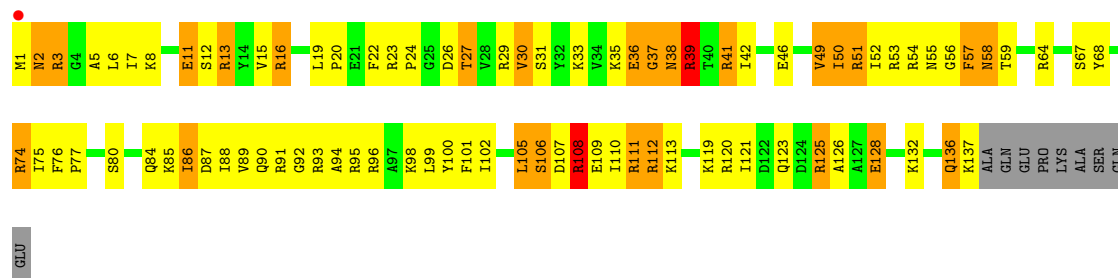
• Molecule 14: 50S ribosomal protein L18

Chain DQ:



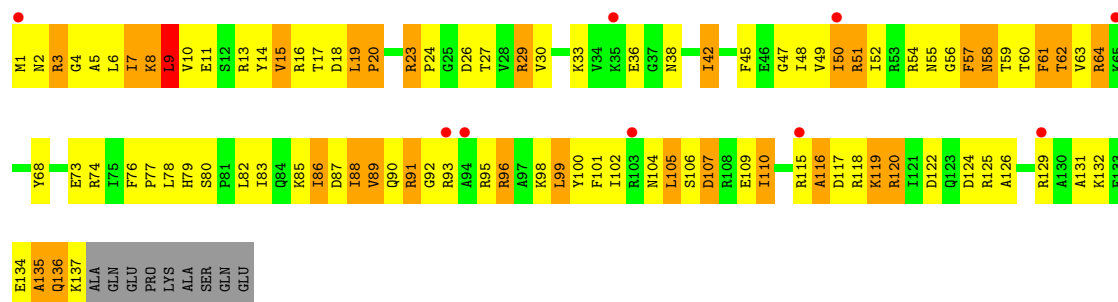
• Molecule 15: 50S ribosomal protein L19

Chain AR:



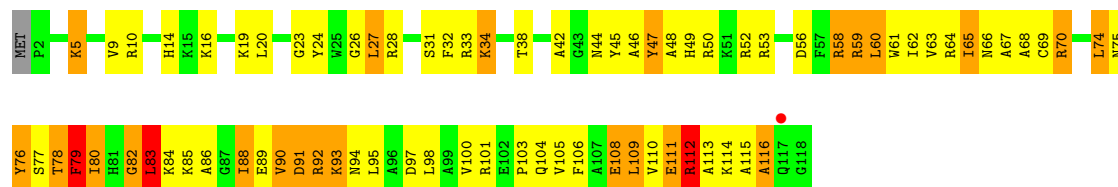
• Molecule 15: 50S ribosomal protein L19

Chain DR:



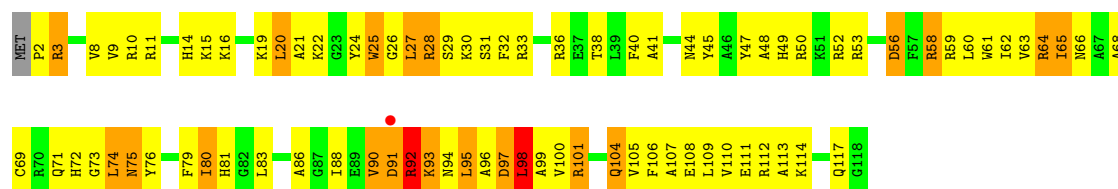
• Molecule 16: 50S ribosomal protein L20

Chain A1:



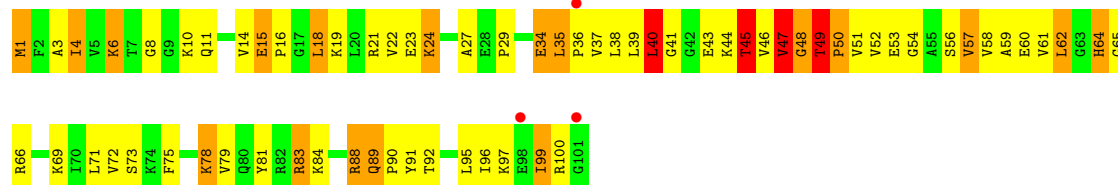
• Molecule 16: 50S ribosomal protein L20

Chain D1: 



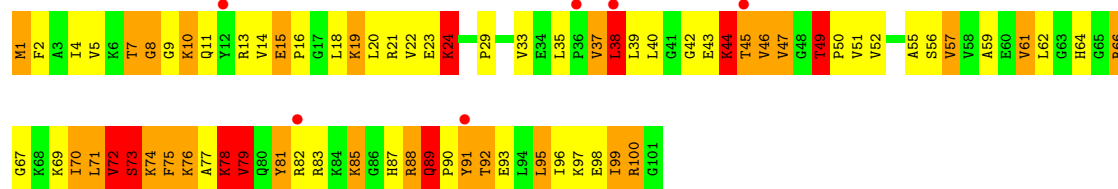
- Molecule 17: 50S ribosomal protein L21

Chain A2: 



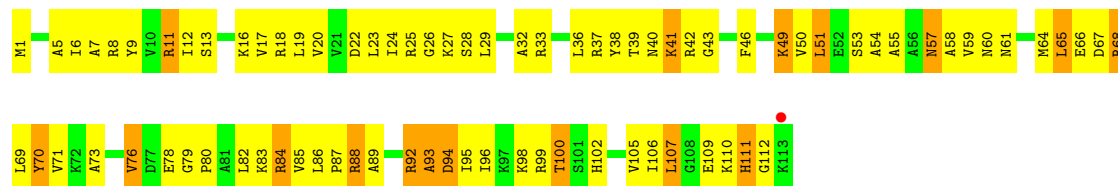
- Molecule 17: 50S ribosomal protein L21

Chain D2: 



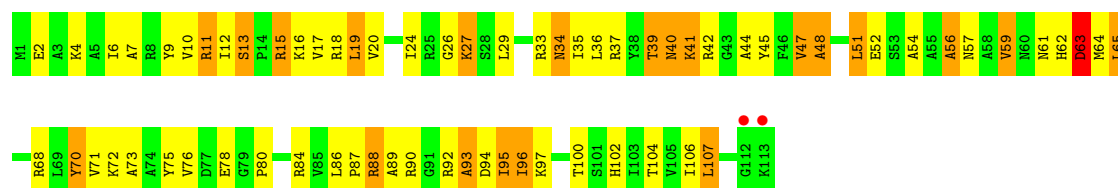
- Molecule 18: 50S ribosomal protein L22

Chain AS: 



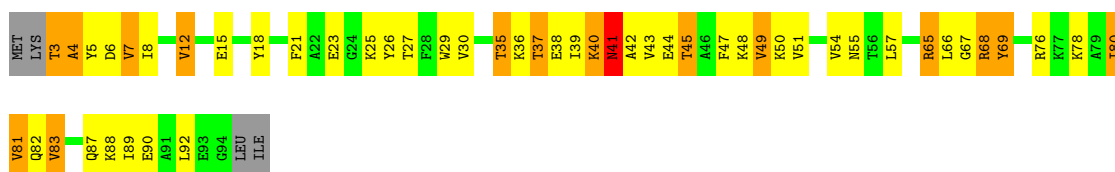
- Molecule 18: 50S ribosomal protein L22

Chain DS: 



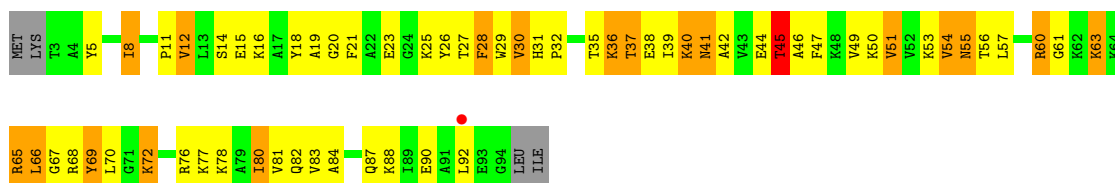
- Molecule 19: 50S ribosomal protein L23

Chain AT: 



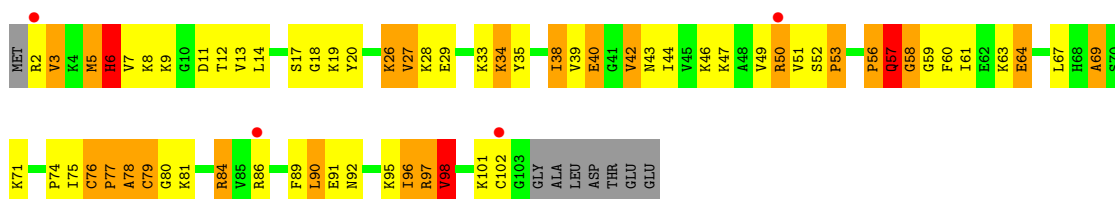
- Molecule 19: 50S ribosomal protein L23

Chain DT:



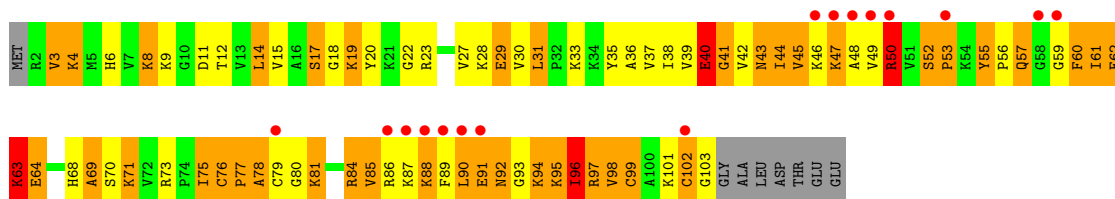
- Molecule 20: 50S ribosomal protein L24

Chain AU:



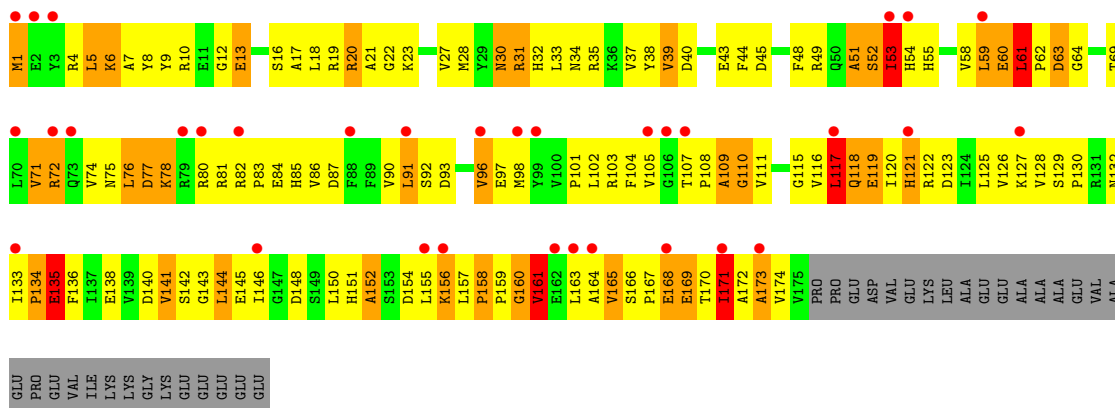
- Molecule 20: 50S ribosomal protein L24

Chain DU:

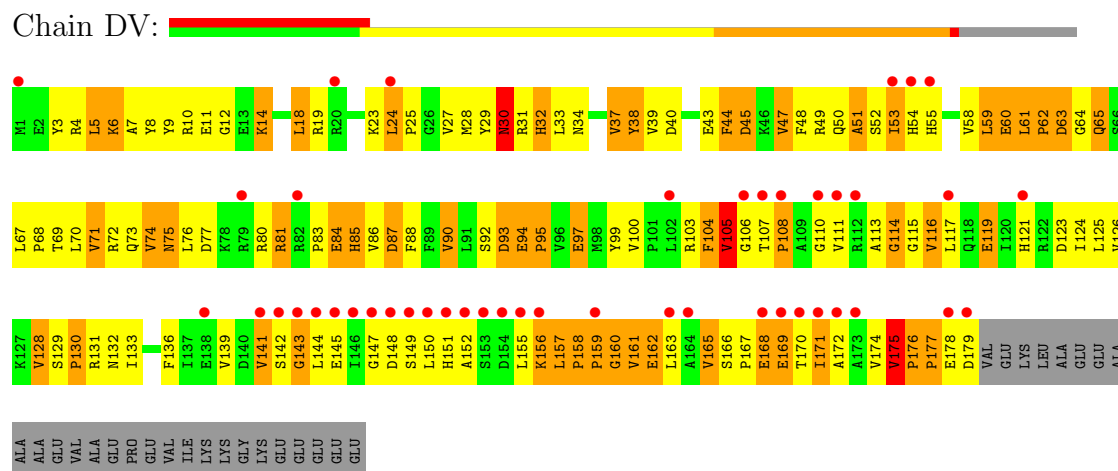


- Molecule 21: 50S ribosomal protein L25

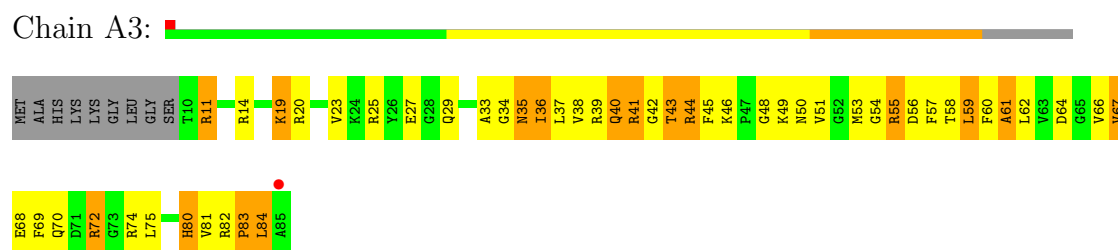
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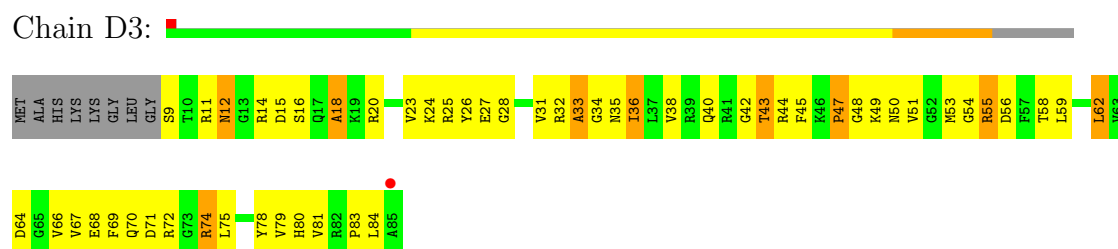
- Molecule 21: 50S ribosomal protein L25



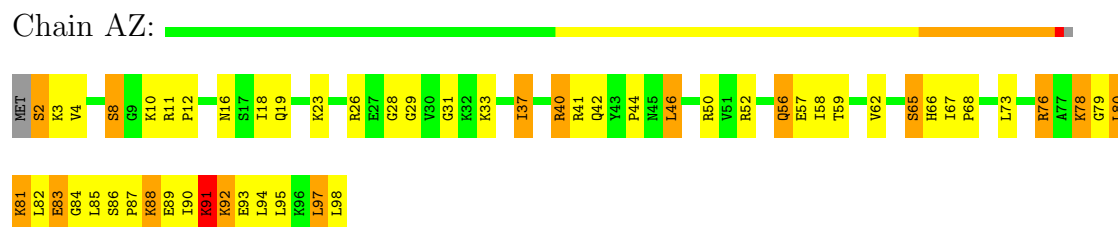
- Molecule 22: 50S ribosomal protein L27



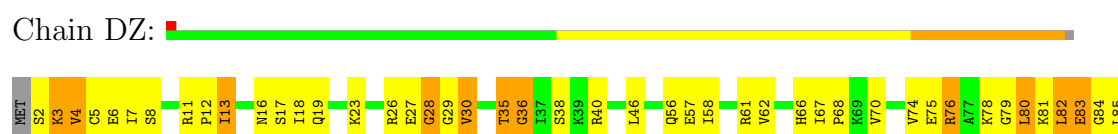
- Molecule 22: 50S ribosomal protein L27

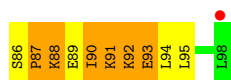


- Molecule 23: 50S ribosomal protein L28



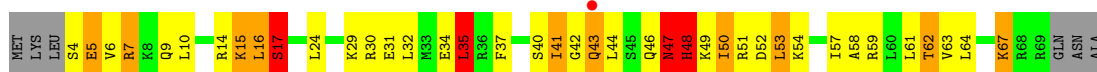
- Molecule 23: 50S ribosomal protein L28





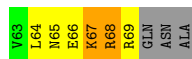
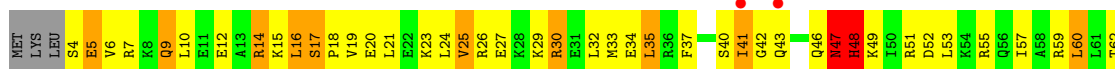
- Molecule 24: 50S ribosomal protein L29

Chain AW:



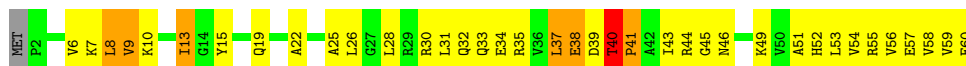
- Molecule 24: 50S ribosomal protein L29

Chain DW:



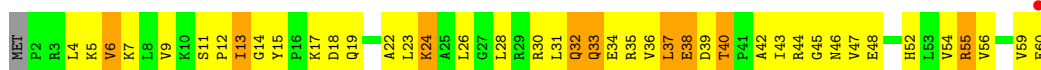
- Molecule 25: 50S ribosomal protein L30

Chain AX:



- Molecule 25: 50S ribosomal protein L30

Chain DX:



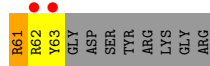
- Molecule 26: 50S ribosomal protein L31

Chain A4:



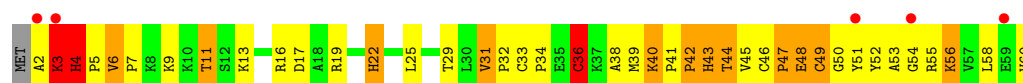
- Molecule 26: 50S ribosomal protein L31

Chain D4:



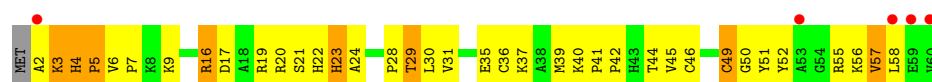
- Molecule 27: 50S ribosomal protein L32

Chain A5: 



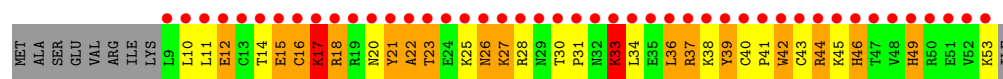
- Molecule 27: 50S ribosomal protein L32

Chain D5: 



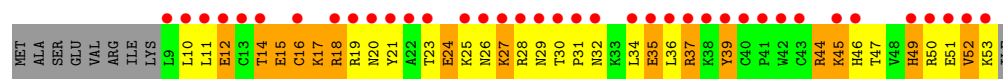
- Molecule 28: 50S ribosomal protein L33

Chain A6: 



- Molecule 28: 50S ribosomal protein L33

Chain D6: 



- Molecule 29: 50S ribosomal protein L34

Chain A7: 



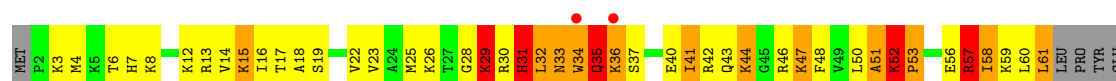
- Molecule 29: 50S ribosomal protein L34

Chain D7: 



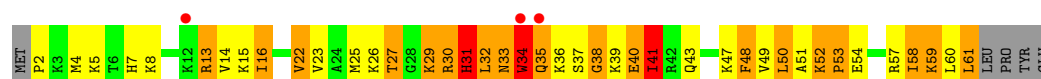
- Molecule 30: 50S ribosomal protein L35

Chain A8: 



- Molecule 30: 50S ribosomal protein L35

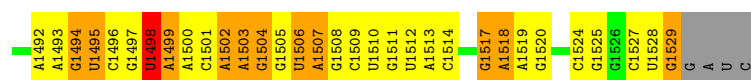
Chain D8: 



Chain BA:

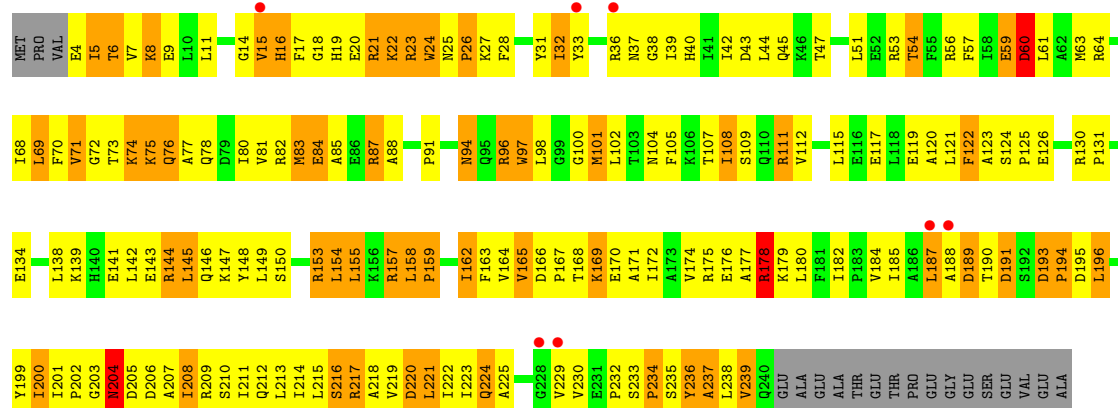


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U1414	U1287	A1225	G1164	C1103	G1042	C984	A923	C957	A782	C708	G639	A572	C504	U427
G1415	A1288	C1226	C1165	G1104	C1043	C985	C924	G958	C783		G640	A573	G505	G428
G1416	A1289	A1227	C1166	A1105	A1044	A986	A859	A859	C784	G711	U641	A574		U429
G1417	U1351	C1228	A1167	G1106	C1045	G987	G926	A860		A712	A642	G575	A509	A430
A1418	G1291	C1229	A1169	C1107	A1046	G988	G927	G861	G791	G713	C643	G576	A510	A431
G1419	U1292	C1230	A1170	G1108	G1047		G927	C962	A792	G714		G577	C511	A432
	G1293	G1231	G1171	C1109	G1048	U991	C930	U863	A793	A715	C647	C578	U512	C433
G1422	G1294	U1232	C1172	A1110	U1049	U992	C931	A864	A794		A648	G579		U434
	G1295	G1233	G1173	G1111	G1050	G993	C932	A865		A716	A649	U580	U516	C435
C1429	G1296	C1234	G1174	C1112	C1051	A994	G933	C966	C797	C719	G650	G581	U517	C436
C1430	U1235	U1235	G1175	C1113	U1052	C995	C934	G867	G798	C720	C651	U582	C518	U437
G1431	A1236	A1236	A1176		G1053	A996	C935	C968	G799	G721	U652	A583	C519	G438
G1432	C1237	C1237	C1177	C1116	C1054	U997	C936	G869	G800	A722	A653	G584	A520	A439
A1433	U1238	A1238	G1178	G1117	A1055		A937	U870	A802	U723	G654	G585	G521	A440
G1434	A1239	A1239	C1179	C1118	U1056	A1000	A938	U871	A802	U724	A655	C586	C522	C442
G1435	U1301	U1239	G1180	C1119	G1057	G1001	G939	A872	G803		C656	G587		C443
A1436	C1362A	G1241	A1181	G1120	G1058	G1002	C940	A873	U804	A728	G657	U591	C526	C444
G1437	C1242	C1242	G1182	U1121	C1059	G1003	G941	G874	C805		G658	G592	G527	C445
	C1243	C1243	A1183	U1122	G1060	A1004	G942	C975	C806	G731	U659	G593	C528	G446
			G1184	U1123	G1061	A1005	U943		A807	C732	G660	G594	U531	C447
			G1185	G1124	U1062	C1006	G944	C978	C812	C735	A663	C599	A533	A450
			A1186	U1125	C1063	C1007	G945	C979	U813	C736	G664	C599	A534	A451
			G1187	G1126	G1064	C1008	A946	C980	C812	C737	A665	C600	U534	A452
			A1188	U1127	U1065	G1009	G947	G981	U813	C738	G666	C601	A535	A453
			G1189	C1128	C1066	G1010	C948	C982	A814	C739	A667		C536	
			G1190	C1129	A1067	G1011	A949	C983	A815		G674	G604	G537	C456
			A1191	U1130	G1068	A1012	U950	U884	C817	G741	U605	U605	G538	C457
			C1192	G1131	C1069	G1013	G951	G885	C817	G742	G606	A539	G540	C458
			G1193	C1132		A1014	U952	G886	A819		U677	G607	G541	G464
			A1194	G1133	U1073	A1015	G953	G987	U820	C745	U678	A608		
			C1195	G1134	U1073	A1016	U954	G988	G821		U678			
			U1196	U1135	G1074	C1017	U955	A889	C824	C748	C679			
			G1197	U1136	C1075	C1018	U956	G990	C824	C749	C680	C612	G542	A465
			C1198	C1137	U1076	C1019	U957	U891	G825	C750	C681	C613	G543	C466
			U1199	G1138	G1077	U1021	A958	C993	C826	U751	A614	C614	G544	C467
			G1200	G1139	U1078	G1021	A959	C994	U827	G752	A694	C615	C545	A468
			A1201	C1140	G1079	G1022	U960	G995	A828	C753	G685	G616	G546	C474
			C1202	G1141	A1080	G1023	U961	C996	U829	C754	U686	G617	A547	G475
			G1203	G1142	G1081	G1024	C962	C997	G830	C755	A687	C618	G550	A477
			A1204	G1143	G1082	U1025	G963	G998	U831	C756	G688	U619	U552	A482
			U1205	G1144	U1083	G1026	A964	C999	C832	C757	C699	C620	A553	C483
			G1206	C1145	G1084	C1027	G965	A900	U833	C758	G690	A621	C554	C484
			U1207	A1146	U1085	C1028	G966	A901	U835	C759	G691	A622	C555	G485
			C1208	C1147	U1086	C1029	C967	A902	C834	A759	G692	A623	C556	G486
			G1209	U1148	G1087	C1028B	A968		U835	C760	U692	G624	G557	U486
			C1210	C1149	G1088	G1029	A969	U905	G836		G693	C625	C558	
			U1211	U1150	G1089	C1030	C970	A906	G837	G765	A694	G626	C559	
			A1151	U1151	U1091	G1031	G971	A907	U841	A766	A695	U626	G559	G491
			C1152	A1152	A1092	A1032	C972	A908	U842	A767	A696	G627	U560	G492
			G1154	C1153	A1093	G1032A	G973	A909	C842	A768	U697	G628	U561	G493
			U1155	G1156	G1094	C1033	A974		U843		G698	G629	U562	C494
			C1217	G1157	U1095	G1034	A975	C912	C848	U772	C699	G630	A563	U495
			A1158	U1158	G1096	A1035	G976	A913	C849	G773	G700	G631	C562	A496
			U1219	C1159	C1097	G1036	A977	A914	U850	G774	C701	A632	C564	A497
			G1220	U1159	C1098	G1037	A978	A915	G851	G775	A702	G633	U565	U497
			G1221	G1160	G1099	C1037	C979	A919	G852	G776	C703	C634	G566	A498
			C1222	G1161	C1100	C1038	C980	A920	G853	A777	U705	G635	G567	C501
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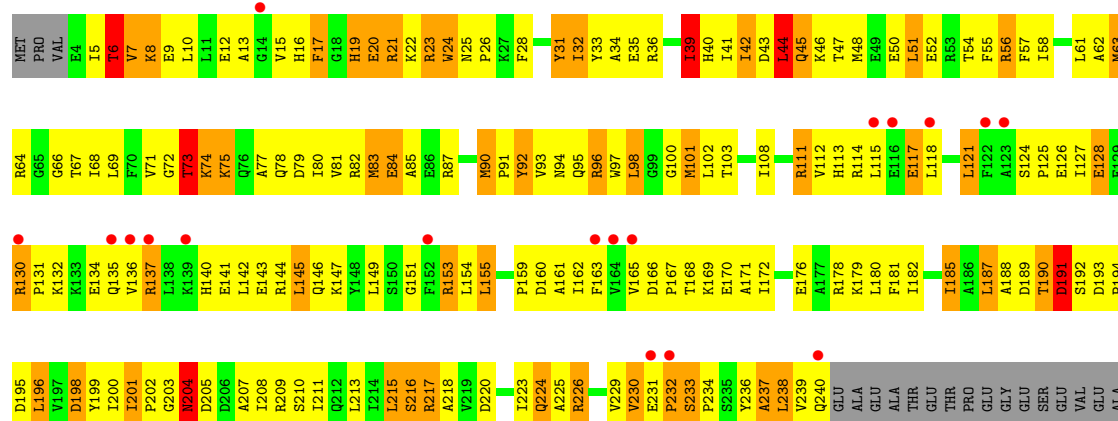
• Molecule 32: 30S RIBOSOMAL PROTEIN S2

Chain BE:



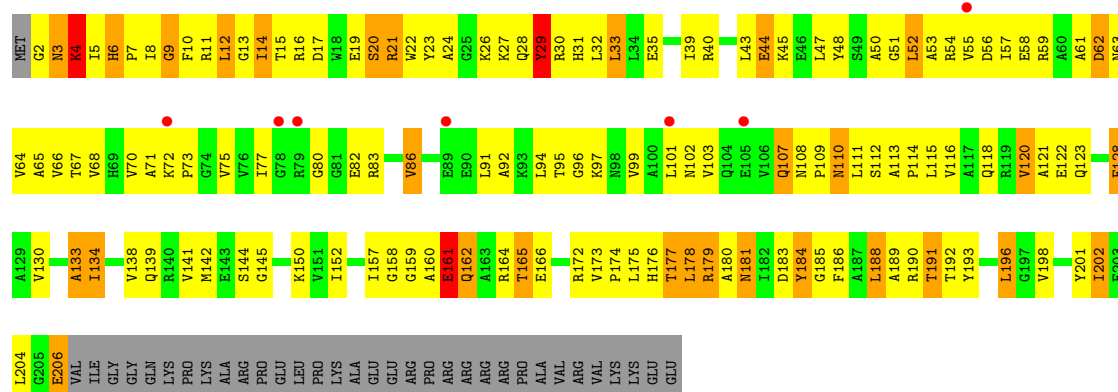
• Molecule 32: 30S RIBOSOMAL PROTEIN S2

Chain CE:



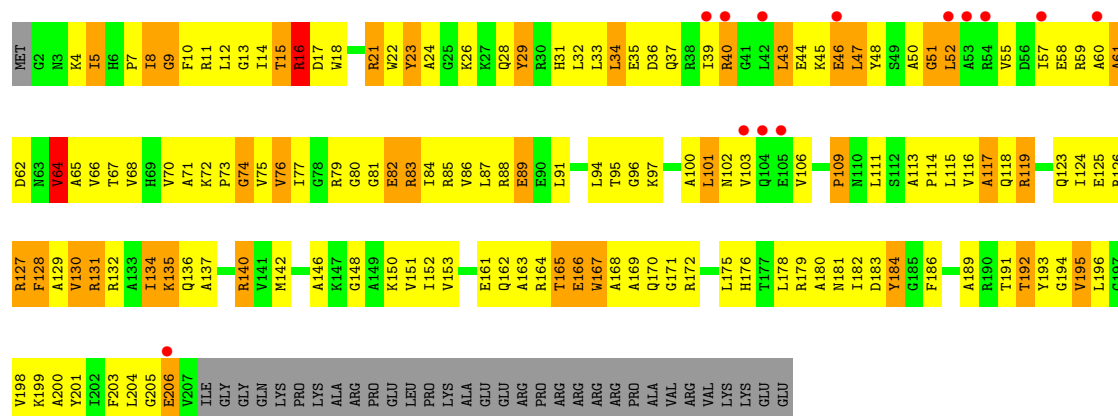
• Molecule 33: 30S RIBOSOMAL PROTEIN S3

Chain BF:



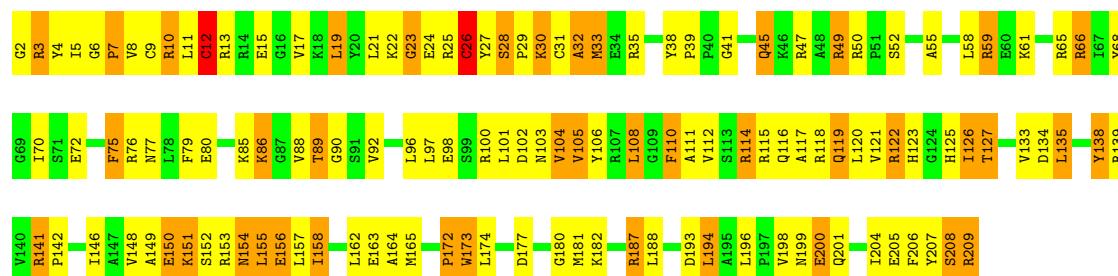
- Molecule 33: 30S RIBOSOMAL PROTEIN S3

Chain CF:



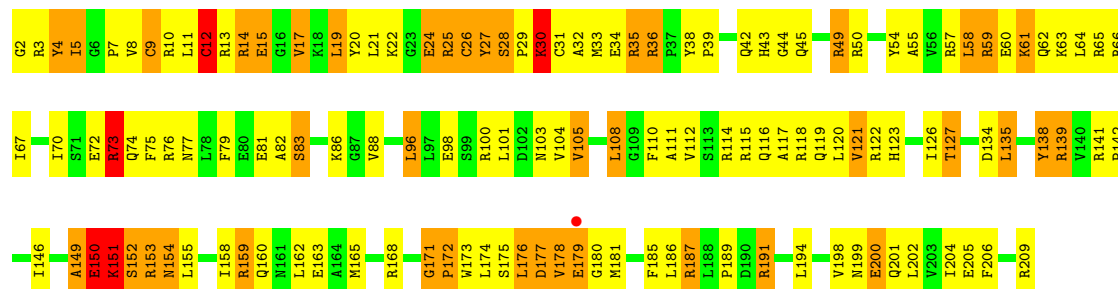
- Molecule 34: 30S RIBOSOMAL PROTEIN S4

Chain BG:



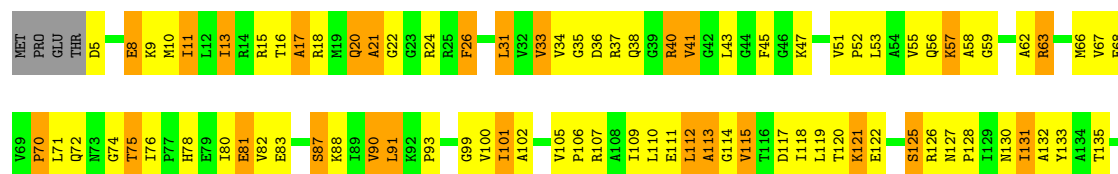
- Molecule 34: 30S RIBOSOMAL PROTEIN S4

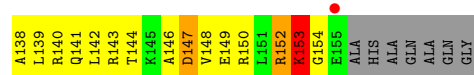
Chain CG:



- Molecule 35: 30S RIBOSOMAL PROTEIN S5

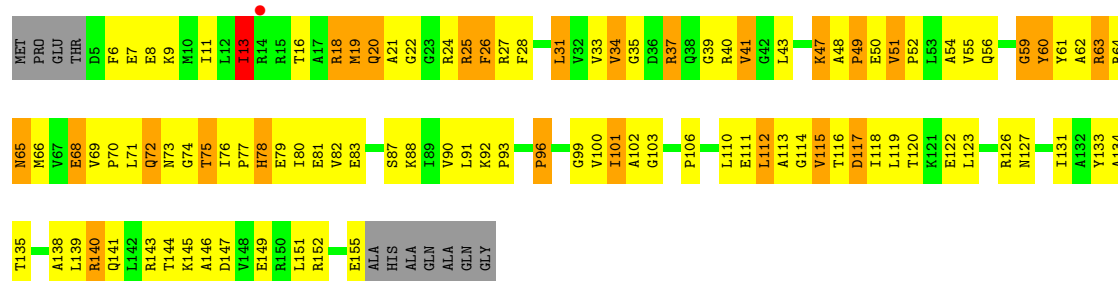
Chain BH:





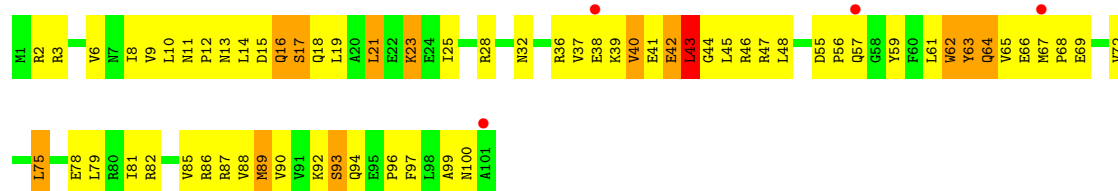
• Molecule 35: 30S RIBOSOMAL PROTEIN S5

Chain CH:



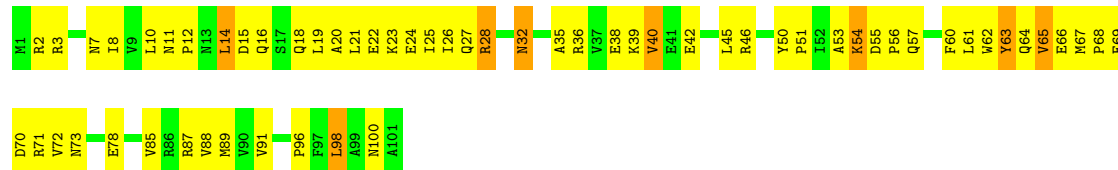
• Molecule 36: 30S RIBOSOMAL PROTEIN S6

Chain BI:



• Molecule 36: 30S RIBOSOMAL PROTEIN S6

Chain CI:



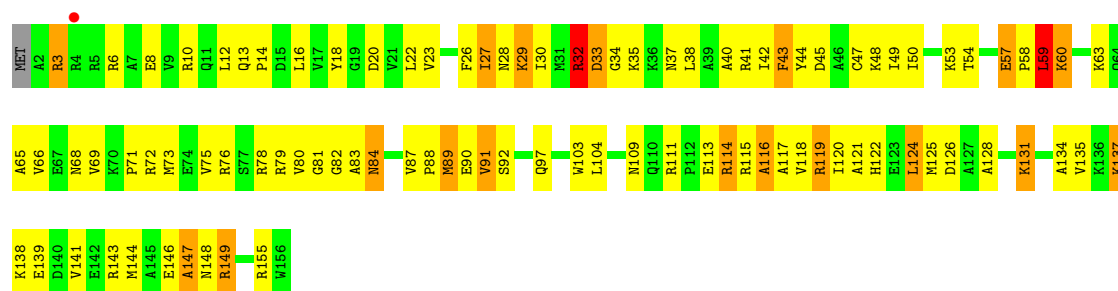
• Molecule 37: 30S RIBOSOMAL PROTEIN S7

Chain BJ:



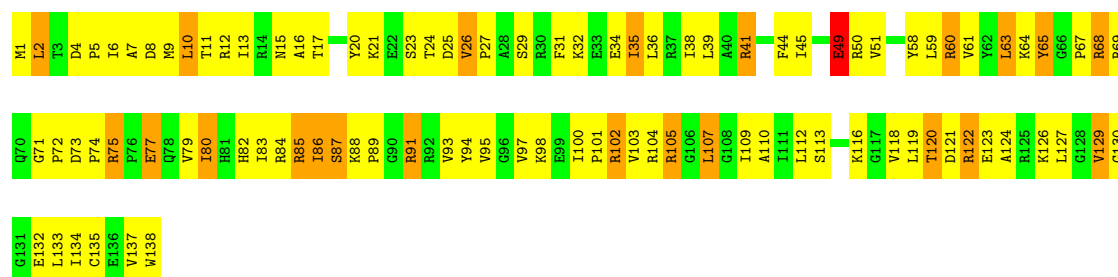
• Molecule 37: 30S RIBOSOMAL PROTEIN S7

Chain CJ:



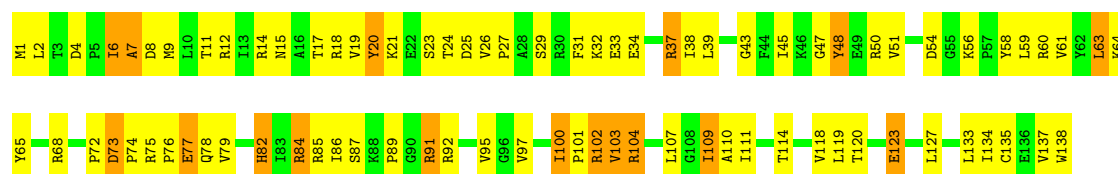
• Molecule 38: 30S RIBOSOMAL PROTEIN S8

Chain BK:



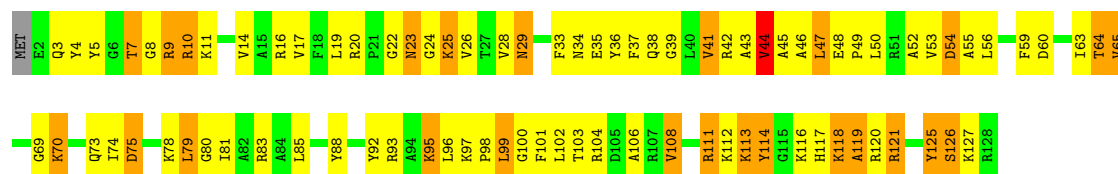
• Molecule 38: 30S RIBOSOMAL PROTEIN S8

Chain CK:



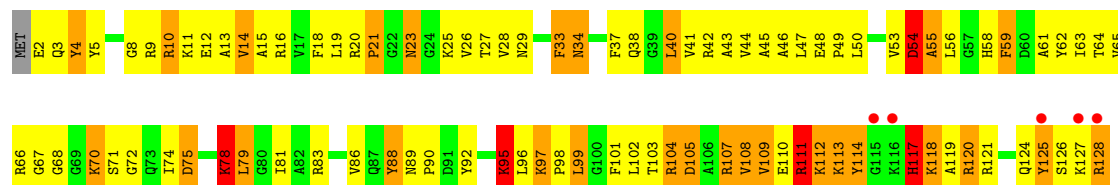
• Molecule 39: 30S RIBOSOMAL PROTEIN S9

Chain BL:



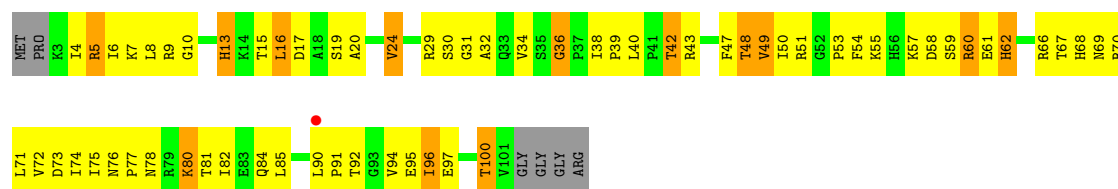
• Molecule 39: 30S RIBOSOMAL PROTEIN S9

Chain CL:



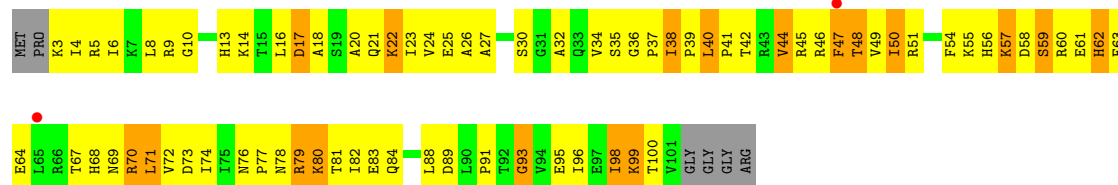
• Molecule 40: 30S RIBOSOMAL PROTEIN S10

Chain BM:



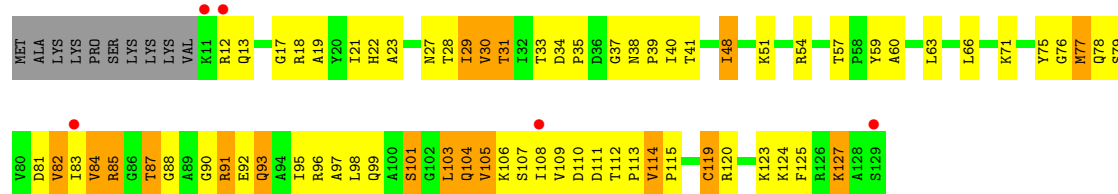
- Molecule 40: 30S RIBOSOMAL PROTEIN S10

Chain CM:



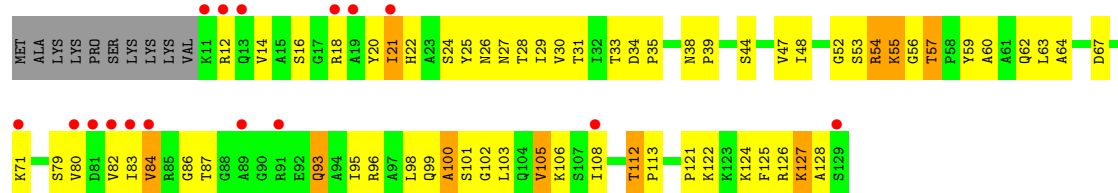
- Molecule 41: 30S RIBOSOMAL PROTEIN S11

Chain BN:



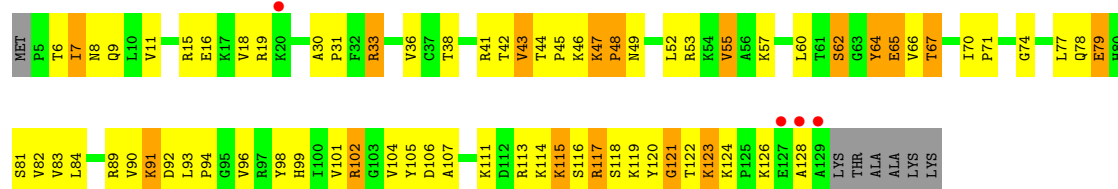
- Molecule 41: 30S RIBOSOMAL PROTEIN S11

Chain CN:



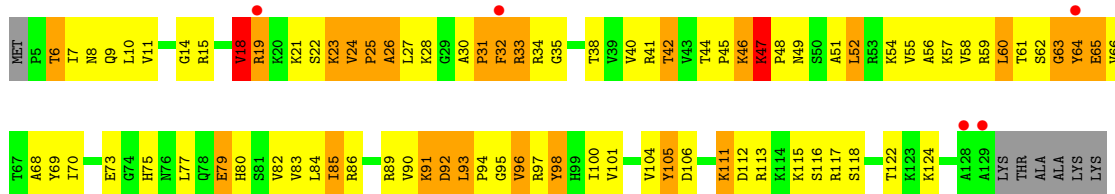
- Molecule 42: 30S RIBOSOMAL PROTEIN S12

Chain BO:



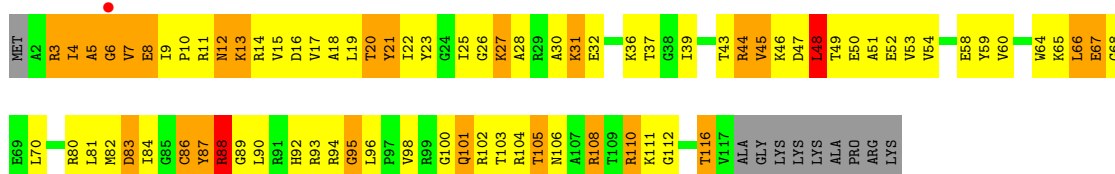
- Molecule 42: 30S RIBOSOMAL PROTEIN S12

Chain CO:



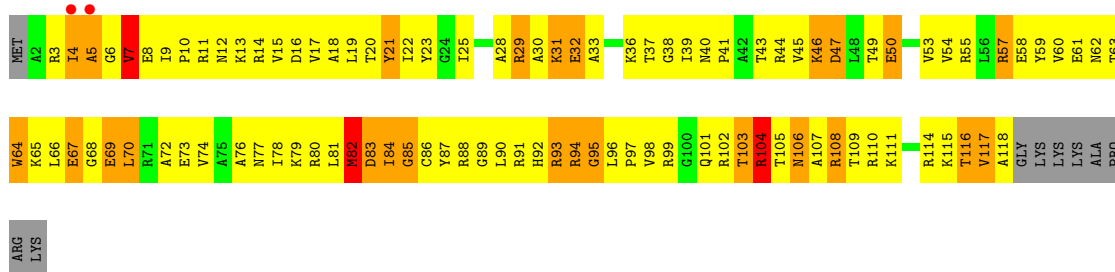
• Molecule 43: 30S RIBOSOMAL PROTEIN S13

Chain BP:



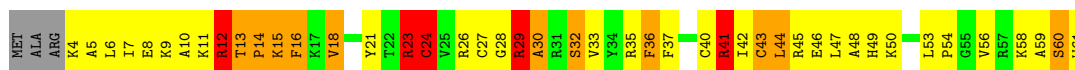
• Molecule 43: 30S RIBOSOMAL PROTEIN S13

Chain CP:



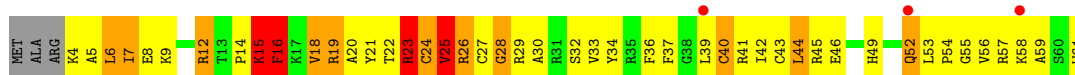
• Molecule 44: 30S RIBOSOMAL PROTEIN S14

Chain BQ:



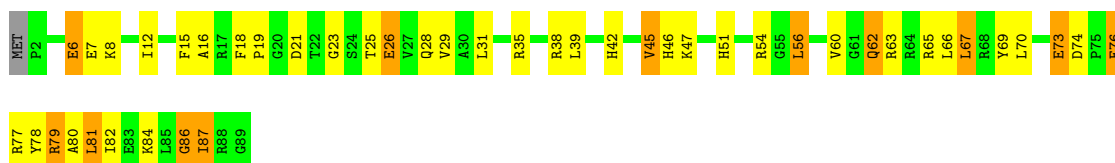
• Molecule 44: 30S RIBOSOMAL PROTEIN S14

Chain CQ:



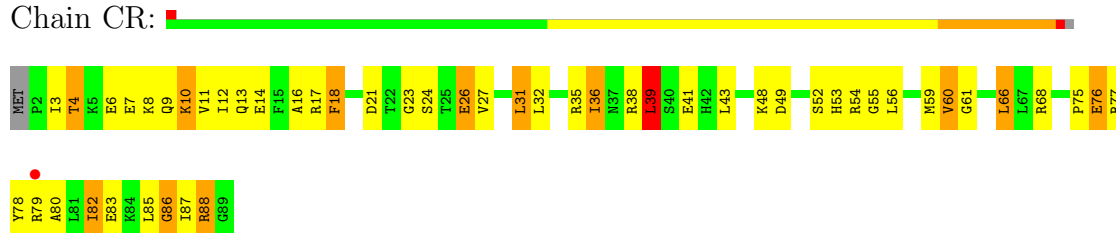
• Molecule 45: 30S RIBOSOMAL PROTEIN S15

Chain BR:



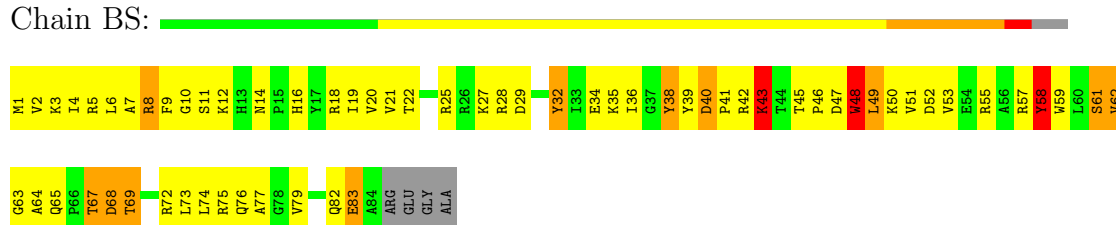
- Molecule 45: 30S RIBOSOMAL PROTEIN S15

Chain CR:



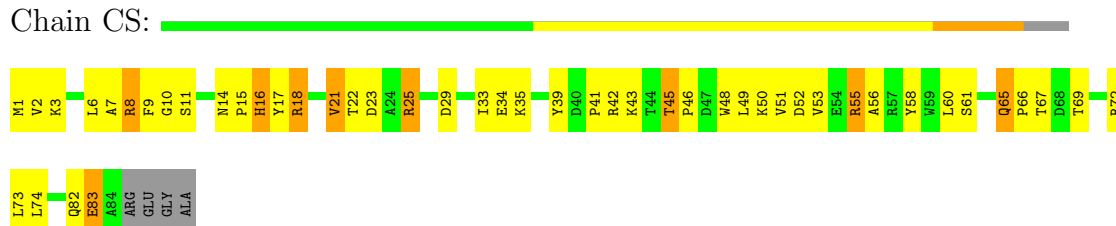
- Molecule 46: 30S RIBOSOMAL PROTEIN S16

Chain BS:



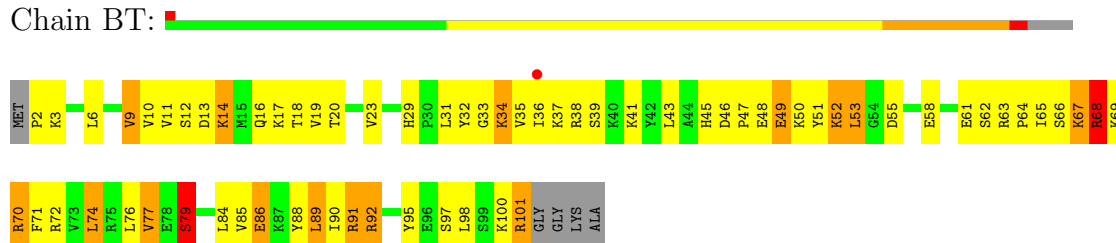
- Molecule 46: 30S RIBOSOMAL PROTEIN S16

Chain CS:



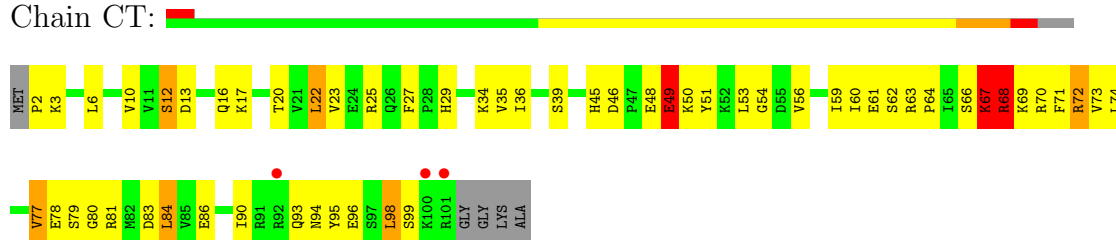
- Molecule 47: 30S RIBOSOMAL PROTEIN S17

Chain BT:



- Molecule 47: 30S RIBOSOMAL PROTEIN S17

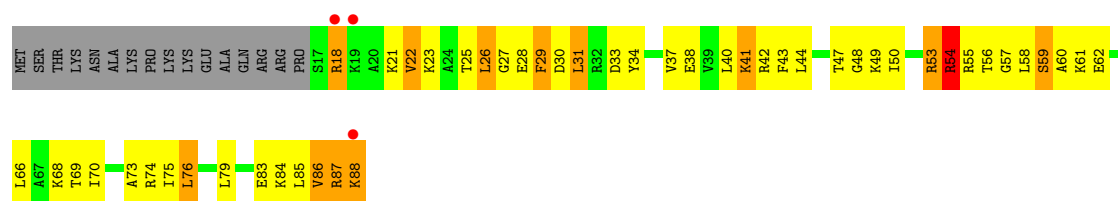
Chain CT:



- Molecule 48: 30S RIBOSOMAL PROTEIN S18

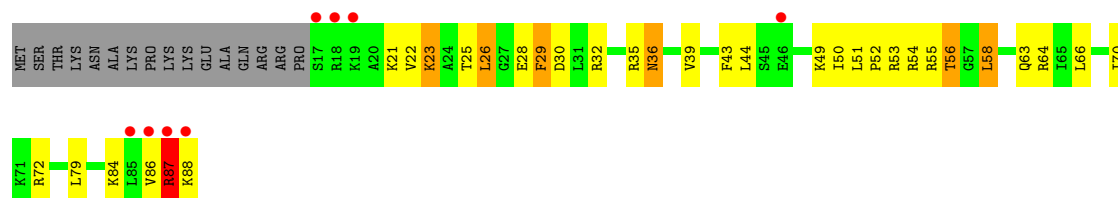
Chain BU:





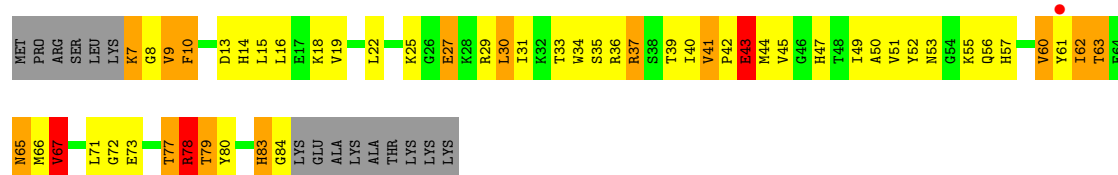
• Molecule 48: 30S RIBOSOMAL PROTEIN S18

Chain CU:



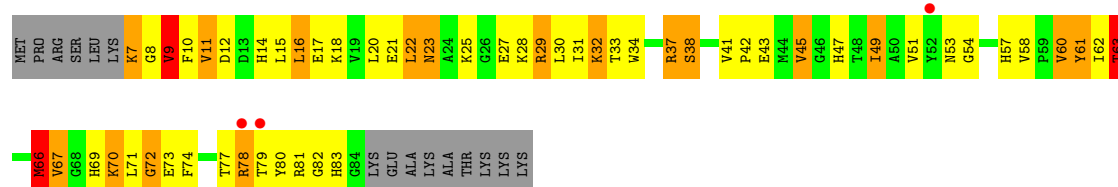
• Molecule 49: 30S RIBOSOMAL PROTEIN S19

Chain BV:



• Molecule 49: 30S RIBOSOMAL PROTEIN S19

Chain CV:



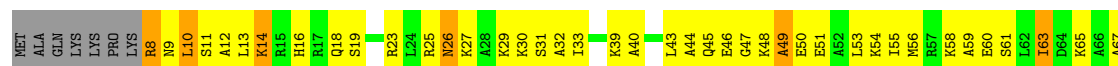
• Molecule 50: 30S RIBOSOMAL PROTEIN S20

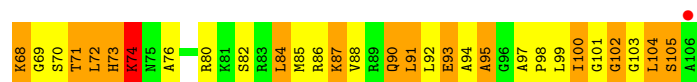
Chain BW:



• Molecule 50: 30S RIBOSOMAL PROTEIN S20

Chain CW:





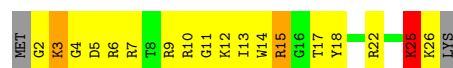
- Molecule 51: 30S RIBOSOMAL PROTEIN THX

Chain BX:



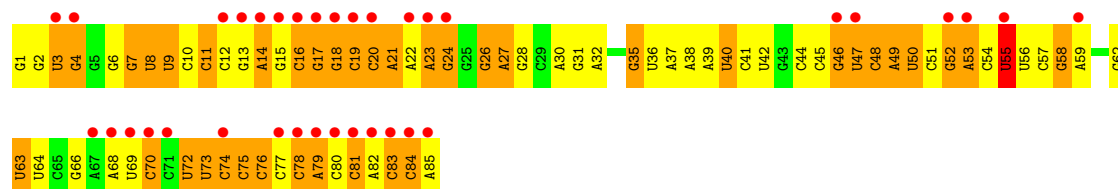
- Molecule 51: 30S RIBOSOMAL PROTEIN THX

Chain CX:



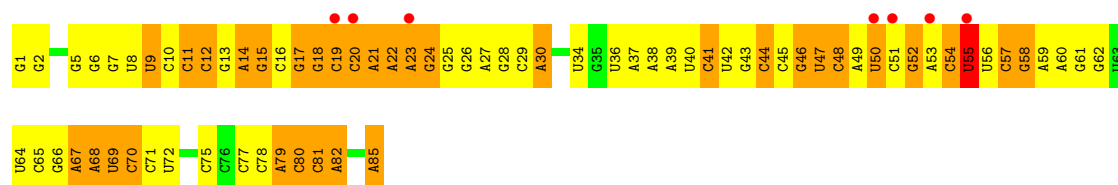
- Molecule 52: TRNA-TYR

Chain BB:



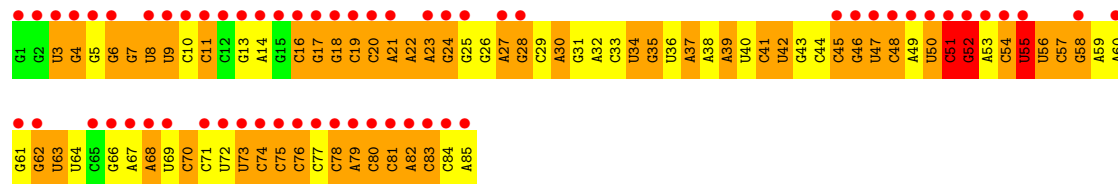
- Molecule 52: TRNA-TYR

Chain BD:



- Molecule 52: TRNA-TYR

Chain CB:



- Molecule 52: TRNA-TYR

Chain CD:





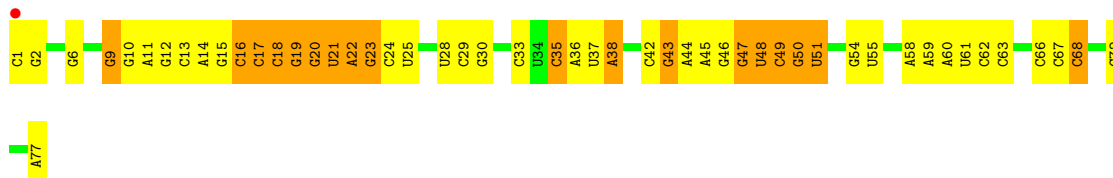
• Molecule 53: TRNA-FMET

Chain BC:



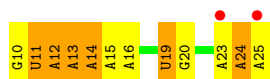
• Molecule 53: TRNA-FMET

Chain CC:



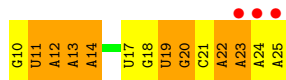
• Molecule 54: MRNA

Chain B1:



• Molecule 54: MRNA

Chain C1:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.00Å 450.33Å 622.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.64 – 3.30 152.64 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (152.64-3.30) 89.2 (152.64-3.00)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.196 , 0.247 0.255 , 0.289	Depositor DCC
R_{free} test set	692 reflections (0.07%)	DCC
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 57.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 1161006 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	304031	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	AA	0.73	18/70233 (0.0%)	1.21	496/109643 (0.5%)
1	DA	0.64	9/70122 (0.0%)	1.10	332/109469 (0.3%)
2	AB	0.60	0/2928	1.24	32/4568 (0.7%)
2	DB	0.50	0/2928	1.03	7/4568 (0.2%)
3	AD	0.56	0/2165	0.81	1/2919 (0.0%)
3	DD	0.52	0/2165	0.75	0/2919
4	AE	0.47	0/1601	0.72	0/2160
4	DE	0.45	0/1601	0.67	0/2160
5	AF	0.51	0/1620	0.71	0/2194
5	DF	0.38	0/1662	0.65	0/2249
6	AG	0.36	0/1499	0.60	0/2016
6	DG	0.28	0/1499	0.52	0/2016
7	AH	0.43	0/1332	0.66	0/1802
7	DH	0.29	0/1332	0.53	0/1802
8	AK	0.36	0/1151	0.63	0/1558
8	DK	0.36	0/1151	0.63	0/1558
9	AM	0.43	0/1131	0.66	0/1525
9	DM	0.34	0/1131	0.58	0/1525
10	AN	0.46	0/943	0.65	0/1269
10	DN	0.42	0/943	0.63	1/1269 (0.1%)
11	AO	0.44	0/1162	0.81	1/1544 (0.1%)
11	DO	0.32	0/1162	0.57	1/1544 (0.1%)
12	AP	0.45	0/1143	0.63	0/1527
12	DP	0.33	0/1143	0.54	0/1527
13	A0	0.42	0/982	0.67	0/1312
13	D0	0.40	0/974	0.66	0/1302
14	AQ	0.45	0/892	0.72	0/1187
14	DQ	0.33	0/892	0.60	0/1187
15	AR	0.46	0/1155	0.66	0/1542
15	DR	0.41	0/1155	0.61	0/1542
16	A1	0.47	0/982	0.72	0/1306
16	D1	0.37	0/982	0.57	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	A2	0.41	0/790	0.71	1/1057 (0.1%)
17	D2	0.32	0/790	0.60	1/1057 (0.1%)
18	AS	0.46	0/911	0.68	0/1220
18	DS	0.44	0/911	0.62	0/1220
19	AT	0.60	1/739 (0.1%)	0.69	0/993
19	DT	0.48	0/739	0.63	0/993
20	AU	0.50	0/798	0.69	0/1064
20	DU	0.42	0/798	0.65	0/1064
21	AV	0.37	0/1427	0.62	1/1935 (0.1%)
21	DV	0.29	0/1460	0.53	0/1982
22	A3	0.49	0/615	0.72	0/819
22	D3	0.41	0/621	0.66	0/827
23	AZ	0.46	0/770	0.70	0/1022
23	DZ	0.44	0/770	0.69	0/1022
24	AW	0.52	0/560	0.75	1/741 (0.1%)
24	DW	0.40	0/560	0.59	0/741
25	AX	0.41	0/474	0.57	0/635
25	DX	0.33	0/474	0.55	0/635
26	A4	0.39	0/545	0.61	1/733 (0.1%)
26	D4	0.34	0/527	0.62	0/709
27	A5	0.44	0/473	0.65	0/639
27	D5	0.41	0/473	0.65	0/639
28	A6	0.48	0/396	0.64	0/529
28	D6	0.45	0/396	0.67	0/529
29	A7	0.57	0/399	0.76	0/526
29	D7	0.50	0/399	0.69	0/526
30	A8	0.55	0/486	0.81	0/638
30	D8	0.42	0/486	0.65	1/638 (0.2%)
31	BA	0.54	0/36139	1.02	97/56406 (0.2%)
31	CA	0.50	0/36142	0.96	59/56410 (0.1%)
32	BE	0.30	0/1959	0.53	0/2642
32	CE	0.28	0/1959	0.52	0/2642
33	BF	0.34	0/1629	0.53	0/2195
33	CF	0.29	0/1636	0.51	0/2205
34	BG	0.44	2/1733 (0.1%)	0.60	1/2318 (0.0%)
34	CG	0.38	0/1733	0.59	1/2318 (0.0%)
35	BH	0.39	0/1171	0.60	0/1576
35	CH	0.36	0/1171	0.58	0/1576
36	BI	0.37	0/856	0.56	0/1154
36	CI	0.36	0/856	0.56	0/1154
37	BJ	0.33	0/1276	0.52	0/1709
37	CJ	0.30	0/1276	0.50	0/1709
38	BK	0.35	0/1136	0.60	0/1527

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	CK	0.30	0/1136	0.54	0/1527
39	BL	0.29	0/1029	0.52	0/1379
39	CL	0.30	0/1029	0.53	0/1379
40	BM	0.32	0/814	0.57	0/1095
40	CM	0.30	0/814	0.55	0/1095
41	BN	0.35	0/900	0.58	0/1213
41	CN	0.35	0/900	0.56	0/1213
42	BO	0.46	0/991	0.71	0/1327
42	CO	0.38	0/991	0.65	0/1327
43	BP	0.35	0/938	0.59	0/1258
43	CP	0.28	0/943	0.52	0/1265
44	BQ	0.44	1/485 (0.2%)	0.67	1/643 (0.2%)
44	CQ	0.31	0/485	0.55	0/643
45	BR	0.38	0/745	0.61	0/992
45	CR	0.36	0/745	0.56	1/992 (0.1%)
46	BS	0.31	0/721	0.56	0/970
46	CS	0.34	0/721	0.58	0/970
47	BT	0.38	0/847	0.57	0/1131
47	CT	0.35	0/847	0.53	0/1131
48	BU	0.36	0/596	0.63	0/790
48	CU	0.36	0/596	0.57	0/790
49	BV	0.32	0/638	0.56	0/860
49	CV	0.31	0/638	0.56	0/860
50	BW	0.30	0/765	0.57	0/1007
50	CW	0.33	0/765	0.58	0/1007
51	BX	0.32	0/221	0.52	0/288
51	CX	0.33	0/221	0.53	0/288
52	BB	0.76	0/1992	0.98	2/3099 (0.1%)
52	BD	0.65	0/1992	0.90	3/3099 (0.1%)
52	CB	0.85	0/1992	0.94	6/3099 (0.2%)
52	CD	0.67	0/1992	0.88	6/3099 (0.2%)
53	BC	0.50	0/1835	0.94	6/2859 (0.2%)
53	CC	0.46	0/1835	0.91	1/2859 (0.0%)
54	B1	0.72	0/390	0.91	1/606 (0.2%)
54	C1	0.71	0/390	0.89	0/606
All	All	0.58	31/324159 (0.0%)	0.99	1062/485455 (0.2%)

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	AD	0	3
3	DD	0	1
4	AE	0	1
5	AF	0	1
5	DF	0	1
7	AH	0	1
8	AK	0	1
8	DK	0	1
11	AO	0	1
11	DO	0	1
24	AW	0	1
30	A8	0	1
30	D8	0	1
42	BO	0	1
All	All	0	16

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	774	A	N9-C4	-9.44	1.32	1.37
1	DA	1342	A	N7-C5	-8.92	1.33	1.39
1	DA	783	A	N9-C4	-8.89	1.32	1.37
1	DA	2873	A	N7-C5	-8.61	1.34	1.39
34	BG	12	CYS	CB-SG	7.57	1.95	1.82

The worst 5 of 1062 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DA	1899	G	N3-C4-N9	-16.88	115.87	126.00
1	AA	1899	G	N3-C4-N9	-14.54	117.28	126.00
1	AA	774	A	C2-N3-C4	-14.31	103.44	110.60
2	AB	81	G	C6-C5-N7	-14.19	121.89	130.40
1	AA	783	A	C5-N7-C8	-13.92	96.94	103.90

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AD	197	GLY	Peptide
3	AD	27	THR	Peptide
3	AD	47	GLY	Peptide
4	AE	20	ALA	Peptide

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Mol	Chain	Res	Type	Group
5	AF	47	GLY	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	62707	0	31614	2894	0
1	DA	62607	0	31564	2901	0
2	AB	2617	0	1328	138	0
2	DB	2617	0	1328	161	0
3	AD	2115	0	2195	271	0
3	DD	2115	0	2195	239	0
4	AE	1568	0	1634	208	0
4	DE	1568	0	1634	214	0
5	AF	1585	0	1632	178	0
5	DF	1627	0	1680	236	0
6	AG	1474	0	1535	158	0
6	DG	1474	0	1535	164	0
7	AH	1307	0	1382	173	0
7	DH	1307	0	1382	136	1
8	AK	1136	0	1223	123	0
8	DK	1136	0	1223	107	0
9	AM	1104	0	1180	134	0
9	DM	1104	0	1180	145	0
10	AN	933	0	996	64	0
10	DN	933	0	996	75	0
11	AO	1145	0	1228	239	0
11	DO	1145	0	1227	311	0
12	AP	1122	0	1179	189	0
12	DP	1122	0	1179	188	0
13	A0	968	0	1033	129	0
13	D0	960	0	1021	94	0
14	AQ	882	0	943	123	0
14	DQ	882	0	943	137	0
15	AR	1141	0	1202	115	0
15	DR	1141	0	1202	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	A1	964	0	1022	120	0
16	D1	964	0	1019	158	0
17	A2	779	0	852	101	0
17	D2	779	0	852	135	0
18	AS	900	0	964	95	0
18	DS	900	0	964	72	0
19	AT	725	0	778	65	0
19	DT	725	0	778	99	0
20	AU	785	0	878	101	0
20	DU	785	0	878	133	0
21	AV	1397	0	1430	168	0
21	DV	1428	0	1454	184	0
22	A3	607	0	628	63	0
22	D3	613	0	633	68	0
23	AZ	763	0	848	71	0
23	DZ	763	0	848	53	0
24	AW	558	0	610	39	0
24	DW	558	0	610	55	0
25	AX	469	0	518	37	0
25	DX	469	0	518	39	0
26	A4	533	0	522	88	0
26	D4	515	0	510	90	0
27	A5	459	0	480	87	0
27	D5	459	0	478	52	0
28	A6	389	0	404	56	0
28	D6	389	0	404	64	0
29	A7	391	0	432	41	0
29	D7	391	0	432	37	0
30	A8	480	0	549	131	0
30	D8	480	0	549	130	0
31	BA	32284	0	16296	1832	1
31	CA	32287	0	16295	1769	0
32	BE	1924	0	1975	195	0
32	CE	1924	0	1975	225	0
33	BF	1605	0	1668	134	0
33	CF	1612	0	1677	179	0
34	BG	1703	0	1763	175	0
34	CG	1703	0	1763	186	0
35	BH	1155	0	1213	115	0
35	CH	1155	0	1213	116	0
36	BI	843	0	857	70	0
36	CI	843	0	857	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	BJ	1257	0	1296	107	0
37	CJ	1257	0	1296	106	0
38	BK	1116	0	1177	113	0
38	CK	1116	0	1177	79	0
39	BL	1010	0	1037	110	0
39	CL	1010	0	1037	156	0
40	BM	801	0	849	94	0
40	CM	801	0	849	130	0
41	BN	885	0	904	65	0
41	CN	885	0	904	71	0
42	BO	975	0	1062	65	0
42	CO	975	0	1062	123	0
43	BP	928	0	987	106	0
43	CP	933	0	992	134	0
44	BQ	476	0	511	58	0
44	CQ	476	0	512	79	0
45	BR	734	0	771	47	0
45	CR	734	0	771	51	0
46	BS	705	0	725	77	0
46	CS	705	0	725	52	0
47	BT	834	0	904	84	0
47	CT	834	0	904	58	0
48	BU	591	0	662	61	0
48	CU	591	0	662	38	0
49	BV	624	0	636	72	0
49	CV	624	0	636	83	0
50	BW	763	0	861	97	0
50	CW	763	0	861	82	0
51	BX	217	0	234	16	0
51	CX	217	0	234	22	0
52	BB	1814	0	931	140	0
52	BD	1814	0	932	148	0
52	CB	1814	0	931	149	0
52	CD	1814	0	932	156	0
53	BC	1643	0	837	55	0
53	CC	1643	0	837	79	0
54	B1	347	0	174	20	0
54	C1	347	0	174	48	0
55	A0	1	0	0	0	0
55	A1	2	0	0	0	0
55	A3	1	0	0	0	0
55	A5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	A7	1	0	0	0	0
55	AA	332	0	0	0	0
55	AB	6	0	0	0	0
55	AE	3	0	0	0	0
55	AF	2	0	0	0	0
55	AO	1	0	0	0	0
55	B1	1	0	0	0	0
55	BA	114	0	0	0	0
55	BB	13	0	0	0	0
55	BC	4	0	0	0	0
55	BD	1	0	0	0	0
55	BF	1	0	0	0	0
55	BS	1	0	0	0	0
55	BW	1	0	0	0	0
55	C1	2	0	0	0	0
55	CA	121	0	0	0	0
55	CB	3	0	0	0	0
55	CC	7	0	0	0	0
55	CN	1	0	0	0	0
55	D0	1	0	0	0	0
55	D5	1	0	0	0	0
55	D7	1	0	0	0	0
55	DA	272	0	0	0	0
55	DB	7	0	0	0	0
55	DE	1	0	0	0	0
56	A1	14	0	0	0	0
56	A3	7	0	0	1	0
56	A6	7	0	0	1	0
56	AA	1659	0	0	140	0
56	AB	91	0	0	6	0
56	AE	7	0	0	0	0
56	AF	7	0	0	3	0
56	AO	14	0	0	2	0
56	AW	7	0	0	0	0
56	BA	693	0	0	66	0
56	BB	14	0	0	0	0
56	BC	21	0	0	2	0
56	BD	21	0	0	1	0
56	BG	7	0	0	2	0
56	BL	7	0	0	0	0
56	BR	7	0	0	0	0
56	CA	651	0	0	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CB	21	0	0	2	0
56	CC	21	0	0	7	0
56	CD	7	0	0	1	0
56	CK	7	0	0	1	0
56	CR	7	0	0	0	0
56	CV	7	0	0	1	0
56	D1	7	0	0	0	0
56	D3	7	0	0	1	0
56	D5	7	0	0	1	0
56	D8	7	0	0	5	0
56	DA	1533	0	0	128	0
56	DB	91	0	0	6	0
56	DF	7	0	0	1	0
56	DO	7	0	0	0	0
57	BA	42	0	45	3	0
57	CA	42	0	45	1	0
58	BG	1	0	0	0	0
58	BQ	1	0	0	0	0
58	CG	1	0	0	0	0
58	CQ	1	0	0	0	0
All	All	304031	0	201063	19321	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 38.

The worst 5 of 19321 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:DO:71:VAL:CG1	11:DO:72:PRO:HD3	1.34	1.57
30:A8:34:TRP:CB	30:A8:35:GLN:HB2	1.34	1.53
20:DU:89:PHE:CE1	20:DU:90:LEU:HG	1.40	1.50
9:DM:17:ASP:HA	9:DM:55:VAL:CG2	1.36	1.49
27:D5:4:HIS:HB3	27:D5:5:PRO:CD	1.40	1.48

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:BA:85:U:O2'	7:DH:100:GLY:O[3_555]	1.86	0.34

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	270/276 (98%)	208 (77%)	45 (17%)	17 (6%)	2	20
3	DD	270/276 (98%)	226 (84%)	31 (12%)	13 (5%)	4	30
4	AE	203/206 (98%)	138 (68%)	33 (16%)	32 (16%)	0	1
4	DE	203/206 (98%)	128 (63%)	34 (17%)	41 (20%)	0	1
5	AF	200/210 (95%)	153 (76%)	28 (14%)	19 (10%)	1	9
5	DF	206/210 (98%)	133 (65%)	46 (22%)	27 (13%)	0	3
6	AG	179/182 (98%)	127 (71%)	36 (20%)	16 (9%)	1	10
6	DG	179/182 (98%)	128 (72%)	30 (17%)	21 (12%)	1	5
7	AH	168/180 (93%)	111 (66%)	25 (15%)	32 (19%)	0	1
7	DH	168/180 (93%)	92 (55%)	52 (31%)	24 (14%)	0	2
8	AK	144/148 (97%)	75 (52%)	44 (31%)	25 (17%)	0	1
8	DK	144/148 (97%)	98 (68%)	27 (19%)	19 (13%)	0	3
9	AM	136/140 (97%)	96 (71%)	21 (15%)	19 (14%)	0	2
9	DM	136/140 (97%)	98 (72%)	21 (15%)	17 (12%)	1	4
10	AN	120/122 (98%)	101 (84%)	15 (12%)	4 (3%)	6	43
10	DN	120/122 (98%)	97 (81%)	15 (12%)	8 (7%)	2	18
11	AO	148/150 (99%)	91 (62%)	29 (20%)	28 (19%)	0	1
11	DO	148/150 (99%)	83 (56%)	21 (14%)	44 (30%)	0	0
12	AP	139/141 (99%)	93 (67%)	27 (19%)	19 (14%)	0	2
12	DP	139/141 (99%)	88 (63%)	29 (21%)	22 (16%)	0	1
13	A0	116/118 (98%)	86 (74%)	21 (18%)	9 (8%)	1	14
13	D0	115/118 (98%)	83 (72%)	18 (16%)	14 (12%)	1	4
14	AQ	109/112 (97%)	74 (68%)	26 (24%)	9 (8%)	1	12
14	DQ	109/112 (97%)	60 (55%)	32 (29%)	17 (16%)	0	1
15	AR	135/146 (92%)	101 (75%)	19 (14%)	15 (11%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	DR	135/146 (92%)	101 (75%)	23 (17%)	11 (8%)	1	13
16	A1	115/118 (98%)	82 (71%)	19 (16%)	14 (12%)	1	4
16	D1	115/118 (98%)	73 (64%)	29 (25%)	13 (11%)	1	5
17	A2	99/101 (98%)	81 (82%)	10 (10%)	8 (8%)	1	13
17	D2	99/101 (98%)	64 (65%)	19 (19%)	16 (16%)	0	1
18	AS	111/113 (98%)	94 (85%)	13 (12%)	4 (4%)	5	40
18	DS	111/113 (98%)	89 (80%)	13 (12%)	9 (8%)	1	13
19	AT	90/96 (94%)	78 (87%)	8 (9%)	4 (4%)	4	32
19	DT	90/96 (94%)	67 (74%)	15 (17%)	8 (9%)	1	10
20	AU	100/110 (91%)	65 (65%)	18 (18%)	17 (17%)	0	1
20	DU	100/110 (91%)	56 (56%)	18 (18%)	26 (26%)	0	0
21	AV	173/206 (84%)	105 (61%)	42 (24%)	26 (15%)	0	2
21	DV	177/206 (86%)	100 (56%)	35 (20%)	42 (24%)	0	0
22	A3	74/85 (87%)	58 (78%)	11 (15%)	5 (7%)	2	18
22	D3	75/85 (88%)	54 (72%)	15 (20%)	6 (8%)	1	13
23	AZ	95/98 (97%)	75 (79%)	14 (15%)	6 (6%)	2	20
23	DZ	95/98 (97%)	72 (76%)	12 (13%)	11 (12%)	1	5
24	AW	64/72 (89%)	55 (86%)	3 (5%)	6 (9%)	1	9
24	DW	64/72 (89%)	46 (72%)	11 (17%)	7 (11%)	1	6
25	AX	57/60 (95%)	47 (82%)	8 (14%)	2 (4%)	6	41
25	DX	57/60 (95%)	44 (77%)	9 (16%)	4 (7%)	2	17
26	A4	64/71 (90%)	33 (52%)	14 (22%)	17 (27%)	0	0
26	D4	61/71 (86%)	23 (38%)	12 (20%)	26 (43%)	0	0
27	A5	57/60 (95%)	39 (68%)	10 (18%)	8 (14%)	0	2
27	D5	57/60 (95%)	44 (77%)	7 (12%)	6 (10%)	1	6
28	A6	43/54 (80%)	21 (49%)	13 (30%)	9 (21%)	0	1
28	D6	43/54 (80%)	23 (54%)	9 (21%)	11 (26%)	0	0
29	A7	43/49 (88%)	41 (95%)	0	2 (5%)	4	30
29	D7	43/49 (88%)	38 (88%)	3 (7%)	2 (5%)	4	30
30	A8	58/65 (89%)	39 (67%)	11 (19%)	8 (14%)	0	2
30	D8	58/65 (89%)	40 (69%)	8 (14%)	10 (17%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BE	235/256 (92%)	155 (66%)	44 (19%)	36 (15%)	0	1
32	CE	235/256 (92%)	152 (65%)	49 (21%)	34 (14%)	0	2
33	BF	203/239 (85%)	137 (68%)	47 (23%)	19 (9%)	1	9
33	CF	204/239 (85%)	124 (61%)	55 (27%)	25 (12%)	1	4
34	BG	206/208 (99%)	152 (74%)	34 (16%)	20 (10%)	1	8
34	CG	206/208 (99%)	152 (74%)	31 (15%)	23 (11%)	1	5
35	BH	149/162 (92%)	115 (77%)	26 (17%)	8 (5%)	3	26
35	CH	149/162 (92%)	115 (77%)	25 (17%)	9 (6%)	2	22
36	BI	99/101 (98%)	71 (72%)	23 (23%)	5 (5%)	3	28
36	CI	99/101 (98%)	85 (86%)	12 (12%)	2 (2%)	11	58
37	BJ	153/156 (98%)	111 (72%)	32 (21%)	10 (6%)	2	19
37	CJ	153/156 (98%)	118 (77%)	22 (14%)	13 (8%)	1	11
38	BK	136/138 (99%)	105 (77%)	24 (18%)	7 (5%)	3	28
38	CK	136/138 (99%)	100 (74%)	24 (18%)	12 (9%)	1	11
39	BL	125/128 (98%)	89 (71%)	25 (20%)	11 (9%)	1	11
39	CL	125/128 (98%)	80 (64%)	29 (23%)	16 (13%)	0	3
40	BM	97/105 (92%)	76 (78%)	20 (21%)	1 (1%)	22	74
40	CM	97/105 (92%)	73 (75%)	19 (20%)	5 (5%)	3	27
41	BN	117/129 (91%)	85 (73%)	24 (20%)	8 (7%)	2	18
41	CN	117/129 (91%)	93 (80%)	19 (16%)	5 (4%)	4	34
42	BO	123/132 (93%)	93 (76%)	18 (15%)	12 (10%)	1	8
42	CO	123/132 (93%)	79 (64%)	27 (22%)	17 (14%)	0	2
43	BP	114/126 (90%)	69 (60%)	27 (24%)	18 (16%)	0	1
43	CP	115/126 (91%)	71 (62%)	24 (21%)	20 (17%)	0	1
44	BQ	56/61 (92%)	38 (68%)	5 (9%)	13 (23%)	0	0
44	CQ	56/61 (92%)	32 (57%)	13 (23%)	11 (20%)	0	1
45	BR	86/89 (97%)	62 (72%)	19 (22%)	5 (6%)	3	23
45	CR	86/89 (97%)	72 (84%)	11 (13%)	3 (4%)	6	41
46	BS	82/88 (93%)	57 (70%)	15 (18%)	10 (12%)	1	4
46	CS	82/88 (93%)	55 (67%)	21 (26%)	6 (7%)	2	16
47	BT	98/105 (93%)	74 (76%)	17 (17%)	7 (7%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	CT	98/105 (93%)	83 (85%)	9 (9%)	6 (6%)	2	22
48	BU	70/88 (80%)	53 (76%)	11 (16%)	6 (9%)	1	11
48	CU	70/88 (80%)	58 (83%)	10 (14%)	2 (3%)	7	47
49	BV	76/93 (82%)	56 (74%)	13 (17%)	7 (9%)	1	9
49	CV	76/93 (82%)	49 (64%)	18 (24%)	9 (12%)	1	4
50	BW	97/106 (92%)	65 (67%)	21 (22%)	11 (11%)	1	5
50	CW	97/106 (92%)	70 (72%)	13 (13%)	14 (14%)	0	2
51	BX	23/27 (85%)	15 (65%)	5 (22%)	3 (13%)	0	3
51	CX	23/27 (85%)	15 (65%)	6 (26%)	2 (9%)	1	11
All	All	11319/12052 (94%)	7969 (70%)	2044 (18%)	1306 (12%)	1	5

5 of 1306 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AD	3	VAL
3	AD	28	GLU
3	AD	29	PRO
3	AD	33	LEU
3	AD	37	LEU

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AD	214/218 (98%)	154 (72%)	60 (28%)	0	2
3	DD	214/218 (98%)	164 (77%)	50 (23%)	1	4
4	AE	165/166 (99%)	131 (79%)	34 (21%)	2	8
4	DE	165/166 (99%)	120 (73%)	45 (27%)	0	2
5	AF	161/166 (97%)	126 (78%)	35 (22%)	1	7
5	DF	165/166 (99%)	130 (79%)	35 (21%)	1	7
6	AG	155/156 (99%)	124 (80%)	31 (20%)	2	9
6	DG	155/156 (99%)	128 (83%)	27 (17%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AH	142/148 (96%)	112 (79%)	30 (21%)	1	7
7	DH	142/148 (96%)	116 (82%)	26 (18%)	2	12
8	AK	122/124 (98%)	97 (80%)	25 (20%)	2	8
8	DK	122/124 (98%)	100 (82%)	22 (18%)	2	13
9	AM	117/119 (98%)	87 (74%)	30 (26%)	1	3
9	DM	117/119 (98%)	82 (70%)	35 (30%)	0	1
10	AN	100/100 (100%)	81 (81%)	19 (19%)	2	11
10	DN	100/100 (100%)	84 (84%)	16 (16%)	3	18
11	AO	116/116 (100%)	81 (70%)	35 (30%)	0	1
11	DO	116/116 (100%)	77 (66%)	39 (34%)	0	1
12	AP	111/111 (100%)	88 (79%)	23 (21%)	2	8
12	DP	111/111 (100%)	79 (71%)	32 (29%)	0	2
13	A0	101/101 (100%)	77 (76%)	24 (24%)	1	4
13	D0	100/101 (99%)	80 (80%)	20 (20%)	2	9
14	AQ	87/88 (99%)	63 (72%)	24 (28%)	0	2
14	DQ	87/88 (99%)	66 (76%)	21 (24%)	1	4
15	AR	120/127 (94%)	97 (81%)	23 (19%)	2	10
15	DR	120/127 (94%)	90 (75%)	30 (25%)	1	3
16	A1	93/94 (99%)	71 (76%)	22 (24%)	1	4
16	D1	93/94 (99%)	77 (83%)	16 (17%)	3	15
17	A2	82/82 (100%)	58 (71%)	24 (29%)	0	2
17	D2	82/82 (100%)	53 (65%)	29 (35%)	0	1
18	AS	92/92 (100%)	69 (75%)	23 (25%)	1	3
18	DS	92/92 (100%)	72 (78%)	20 (22%)	1	7
19	AT	74/78 (95%)	58 (78%)	16 (22%)	1	7
19	DT	74/78 (95%)	56 (76%)	18 (24%)	1	3
20	AU	85/91 (93%)	65 (76%)	20 (24%)	1	4
20	DU	85/91 (93%)	57 (67%)	28 (33%)	0	1
21	AV	154/179 (86%)	126 (82%)	28 (18%)	2	12
21	DV	158/179 (88%)	133 (84%)	25 (16%)	4	18
22	A3	61/67 (91%)	48 (79%)	13 (21%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	D3	62/67 (92%)	55 (89%)	7 (11%)	9	36
23	AZ	82/83 (99%)	64 (78%)	18 (22%)	1	6
23	DZ	82/83 (99%)	64 (78%)	18 (22%)	1	6
24	AW	62/67 (92%)	44 (71%)	18 (29%)	0	2
24	DW	62/67 (92%)	48 (77%)	14 (23%)	1	5
25	AX	51/52 (98%)	42 (82%)	9 (18%)	3	13
25	DX	51/52 (98%)	41 (80%)	10 (20%)	2	9
26	A4	59/63 (94%)	49 (83%)	10 (17%)	3	15
26	D4	57/63 (90%)	45 (79%)	12 (21%)	1	7
27	A5	51/52 (98%)	39 (76%)	12 (24%)	1	4
27	D5	51/52 (98%)	43 (84%)	8 (16%)	4	19
28	A6	44/52 (85%)	32 (73%)	12 (27%)	0	2
28	D6	44/52 (85%)	38 (86%)	6 (14%)	5	26
29	A7	38/42 (90%)	32 (84%)	6 (16%)	4	18
29	D7	38/42 (90%)	29 (76%)	9 (24%)	1	4
30	A8	50/55 (91%)	36 (72%)	14 (28%)	0	2
30	D8	50/55 (91%)	35 (70%)	15 (30%)	0	1
32	BE	205/220 (93%)	167 (82%)	38 (18%)	2	11
32	CE	205/220 (93%)	168 (82%)	37 (18%)	2	13
33	BF	159/188 (85%)	127 (80%)	32 (20%)	2	8
33	CF	160/188 (85%)	132 (82%)	28 (18%)	3	14
34	BG	180/180 (100%)	149 (83%)	31 (17%)	3	15
34	CG	180/180 (100%)	143 (79%)	37 (21%)	2	8
35	BH	116/123 (94%)	89 (77%)	27 (23%)	1	5
35	CH	116/123 (94%)	89 (77%)	27 (23%)	1	5
36	BI	90/90 (100%)	80 (89%)	10 (11%)	9	37
36	CI	90/90 (100%)	78 (87%)	12 (13%)	6	27
37	BJ	126/127 (99%)	96 (76%)	30 (24%)	1	4
37	CJ	126/127 (99%)	103 (82%)	23 (18%)	2	12
38	BK	119/119 (100%)	95 (80%)	24 (20%)	2	8
38	CK	119/119 (100%)	101 (85%)	18 (15%)	4	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	BL	98/99 (99%)	77 (79%)	21 (21%)	1	7
39	CL	98/99 (99%)	73 (74%)	25 (26%)	1	3
40	BM	89/92 (97%)	73 (82%)	16 (18%)	2	13
40	CM	89/92 (97%)	72 (81%)	17 (19%)	2	10
41	BN	90/99 (91%)	76 (84%)	14 (16%)	4	19
41	CN	90/99 (91%)	79 (88%)	11 (12%)	7	32
42	BO	104/109 (95%)	84 (81%)	20 (19%)	2	10
42	CO	104/109 (95%)	80 (77%)	24 (23%)	1	5
43	BP	94/101 (93%)	77 (82%)	17 (18%)	2	12
43	CP	94/101 (93%)	76 (81%)	18 (19%)	2	10
44	BQ	48/50 (96%)	35 (73%)	13 (27%)	1	2
44	CQ	48/50 (96%)	38 (79%)	10 (21%)	2	8
45	BR	79/80 (99%)	69 (87%)	10 (13%)	6	30
45	CR	79/80 (99%)	65 (82%)	14 (18%)	3	13
46	BS	72/74 (97%)	58 (81%)	14 (19%)	2	10
46	CS	72/74 (97%)	60 (83%)	12 (17%)	3	16
47	BT	95/97 (98%)	78 (82%)	17 (18%)	2	13
47	CT	95/97 (98%)	82 (86%)	13 (14%)	5	26
48	BU	63/77 (82%)	53 (84%)	10 (16%)	4	18
48	CU	63/77 (82%)	53 (84%)	10 (16%)	4	18
49	BV	67/80 (84%)	50 (75%)	17 (25%)	1	3
49	CV	67/80 (84%)	47 (70%)	20 (30%)	0	1
50	BW	76/82 (93%)	64 (84%)	12 (16%)	4	18
50	CW	76/82 (93%)	63 (83%)	13 (17%)	3	15
51	BX	20/22 (91%)	20 (100%)	0	100	100
51	CX	20/22 (91%)	18 (90%)	2 (10%)	11	43
All	All	9565/9996 (96%)	7550 (79%)	2015 (21%)	1	7

5 of 2015 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	BP	86	CYS
35	CH	65	ASN

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Mol	Chain	Res	Type
19	DT	80	ILE
45	BR	67	LEU
32	CE	73	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 288 such sidechains are listed below:

Mol	Chain	Res	Type
47	BT	16	GLN
38	CK	82	HIS
21	DV	132	ASN
50	BW	26	ASN
34	CG	43	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2911/2912 (99%)	694 (23%)	62 (2%)
1	DA	2905/2912 (99%)	731 (25%)	60 (2%)
2	AB	121/122 (99%)	23 (19%)	0
2	DB	121/122 (99%)	28 (23%)	1 (0%)
31	BA	1501/1506 (99%)	351 (23%)	39 (2%)
31	CA	1501/1506 (99%)	351 (23%)	49 (3%)
52	BB	83/85 (97%)	45 (54%)	5 (6%)
52	BD	83/85 (97%)	38 (45%)	5 (6%)
52	CB	83/85 (97%)	49 (59%)	8 (9%)
52	CD	83/85 (97%)	35 (42%)	6 (7%)
53	BC	76/77 (98%)	17 (22%)	3 (3%)
53	CC	76/77 (98%)	20 (26%)	3 (3%)
54	B1	15/16 (93%)	7 (46%)	2 (13%)
54	C1	15/16 (93%)	8 (53%)	3 (20%)
All	All	9574/9606 (99%)	2397 (25%)	246 (2%)

5 of 2397 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	U
1	AA	17	G
1	AA	23	G
1	AA	34	C
1	AA	35	G

5 of 246 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	BD	21	A
31	CA	686	U
1	DA	2225	A
54	B1	11	U
31	CA	243	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
52	MIA	BB	38	52	29,31,32	1.69	3 (10%)	41,44,47	2.14	12 (29%)
52	MIA	BD	38	52	29,31,32	1.69	3 (10%)	41,44,47	2.61	10 (24%)
52	MIA	CB	38	52	29,31,32	1.85	5 (17%)	41,44,47	2.48	9 (21%)
52	MIA	CD	38	52	29,31,32	1.65	3 (10%)	41,44,47	2.50	10 (24%)

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
52	MIA	BB	38	52	-	0/16/33/34	0/3/3/3
52	MIA	BD	38	52	-	0/16/33/34	0/3/3/3
52	MIA	CB	38	52	-	0/16/33/34	0/3/3/3
52	MIA	CD	38	52	-	0/16/33/34	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	CB	38	MIA	C6-N6	7.19	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	BB	38	MIA	C6-N6	6.51	1.46	1.34
52	BD	38	MIA	C6-N6	6.46	1.46	1.34
52	CD	38	MIA	C6-N6	6.39	1.46	1.34
52	CB	38	MIA	P-OP1	5.19	1.52	1.46

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	BD	38	MIA	C11-S10-C2	12.29	111.16	102.23
52	CD	38	MIA	C11-S10-C2	11.06	110.27	102.23
52	CB	38	MIA	C11-S10-C2	10.34	109.75	102.23
52	CB	38	MIA	C5-C4-N3	-6.82	118.22	126.07
52	BD	38	MIA	C5-C4-N3	-6.39	118.71	126.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1619 ligands modelled in this entry, 907 are monoatomic - leaving 712 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	OHX	A1	203	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	A1	204	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	A3	102	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	A6	101	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3326	-	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	$\# Z > 2$
56	OHX	AA	3327	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3328	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3329	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3330	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3331	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3332	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3333	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3335	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3336	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3338	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3340	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3341	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3342	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3344	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3345	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3346	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3347	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3348	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3349	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3350	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3351	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3352	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3353	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3354	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3355	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3358	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3359	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3360	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3361	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3362	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3363	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3364	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3365	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3366	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3367	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3368	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3369	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3370	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3371	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3373	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3374	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3375	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3376	-	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	$\# Z > 2$
56	OHX	AA	3377	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3378	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3379	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3380	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3381	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3382	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3383	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3384	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3385	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3386	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3387	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3388	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3389	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3390	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3391	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3392	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3393	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3394	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3395	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3396	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3397	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3398	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3399	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3400	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3401	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3402	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3403	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3404	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3405	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3406	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3407	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3408	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3409	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3410	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3411	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3412	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3413	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3414	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3415	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3416	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3417	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3418	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3419	-	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	$\# Z > 2$
56	OHX	AA	3420	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3421	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3422	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3423	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3424	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3426	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3427	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3428	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3429	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3430	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3431	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3432	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3433	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3434	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3435	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3437	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3438	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3439	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3440	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3441	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3442	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3443	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3444	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3445	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3446	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3447	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3448	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3449	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3450	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3451	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3452	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3453	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3454	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3455	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3456	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3457	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3458	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3459	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3460	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3461	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3462	-	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	$\# Z > 2$
56	OHX	AA	3463	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3464	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3465	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3466	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3467	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3468	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3469	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3470	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3471	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3472	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3473	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3474	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3475	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3476	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3477	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3478	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3479	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3480	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3481	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3482	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3483	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3485	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3486	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3487	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3488	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3489	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3491	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3492	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3493	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3494	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3495	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3496	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3497	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3498	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3499	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3500	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3501	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3502	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3503	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3504	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3505	-	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	$\# Z > 2$
56	OHX	AA	3506	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3507	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3508	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3509	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3510	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3511	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3512	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3513	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3514	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3515	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3516	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3517	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3518	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3519	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3520	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3521	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3522	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3523	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3524	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3525	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3526	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3527	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3528	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3529	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3530	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3531	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3532	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3533	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3534	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3535	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3536	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3537	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3538	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3539	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3540	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3541	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3542	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3543	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3544	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3545	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3546	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3547	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3548	-	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
56	OHX	AA	3549	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3550	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3551	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3552	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3553	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3554	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3555	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3556	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3557	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3558	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3559	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3560	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3561	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3562	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3563	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3564	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3565	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3566	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3567	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3568	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3569	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	207	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	208	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	209	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	210	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	211	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	212	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	213	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	214	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	215	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	216	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	217	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	218	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AB	219	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AE	304	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AF	303	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AO	202	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AO	203	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AW	101	-	0,6,6	0.00	-	0,15,15	0.00	-
57	PAR	BA	1715	-	45,45,45	0.68	1 (2%)	67,67,67	1.72	13 (19%)
56	OHX	BA	1716	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1717	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1718	-	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	$\# Z > 2$
56	OHX	BA	1719	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1720	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1721	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1722	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1723	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1724	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1725	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1726	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1727	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1728	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1729	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1730	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1731	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1732	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1733	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1734	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1735	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1736	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1737	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1738	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1739	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1740	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1741	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1742	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1743	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1744	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1745	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1746	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1747	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1748	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1749	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1750	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1751	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1752	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1753	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1754	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1755	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1756	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1757	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1758	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1759	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1760	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1761	-	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	$\# Z > 2$
56	OHX	BA	1762	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1763	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1764	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1765	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1766	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1767	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1768	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1769	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1770	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1771	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1772	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1773	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1774	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1775	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1776	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1777	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1778	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1779	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1780	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1781	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1782	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1783	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1784	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1785	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1786	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1787	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1788	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1789	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1790	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1791	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1792	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1793	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1794	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1795	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1796	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1797	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1798	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1799	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1800	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1801	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1802	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1803	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1804	-	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
56	OHX	BA	1805	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1806	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1807	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1808	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1809	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1810	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1811	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1812	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1813	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1814	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BB	114	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BB	115	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BC	105	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BC	106	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BC	107	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BD	102	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BD	103	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BD	104	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BG	302	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BL	201	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BR	101	-	0,6,6	0.00	-	0,15,15	0.00	-
57	PAR	CA	1722	-	45,45,45	0.68	0	67,67,67	1.82	15 (22%)
56	OHX	CA	1723	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1724	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1725	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1726	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1727	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1728	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1729	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1730	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1731	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1732	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1733	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1734	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1735	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1736	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1737	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1738	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1739	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1740	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1741	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1742	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1743	-	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
56	OHX	CA	1744	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1745	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1746	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1747	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1748	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1749	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1750	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1751	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1752	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1753	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1754	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1755	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1756	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1757	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1758	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1759	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1760	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1761	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1762	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1763	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1764	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1765	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1766	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1767	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1768	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1769	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1770	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1771	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1772	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1773	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1774	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1775	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1776	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1777	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1778	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1779	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1780	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1781	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1782	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1783	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1784	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1785	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1786	-	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	$\# Z > 2$
56	OHX	CA	1787	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1788	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1789	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1790	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1791	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1792	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1793	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1794	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1795	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1796	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1797	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1798	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1799	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1800	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1801	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1802	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1803	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1804	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1805	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1806	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1807	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1808	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1809	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1810	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1811	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1812	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1813	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1814	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	1815	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	104	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	105	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	106	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CC	108	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CC	109	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CC	110	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CD	101	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CK	201	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CR	101	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CV	101	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	D1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	D3	101	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	D5	102	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	D8	101	-	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	$\# Z > 2$
56	OHX	DA	3061	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3062	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3064	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3065	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3068	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3071	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3073	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3075	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3081	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3082	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3083	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3084	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3087	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3091	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3094	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3099	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3103	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3105	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3109	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3111	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3118	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3124	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3127	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3132	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3134	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3136	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3157	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3159	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3160	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3162	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3163	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3165	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3166	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3168	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3169	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3170	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3171	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3172	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3173	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3174	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3176	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3212	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3214	-	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	$\# Z > 2$
56	OHX	DA	3215	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3217	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3218	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3220	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3221	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3223	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3224	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3226	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3243	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3245	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3246	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3248	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3249	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3251	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3253	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3254	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3255	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3257	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3258	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3335	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3336	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3337	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3338	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3339	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3340	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3341	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3342	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3343	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3344	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3345	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3346	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3347	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3348	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3349	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3350	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3351	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3352	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3353	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3354	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3355	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3356	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3357	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3358	-	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	$\# Z > 2$
56	OHX	DA	3359	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3360	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3361	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3362	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3363	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3364	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3365	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3366	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3367	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3368	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3369	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3370	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3371	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3372	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3373	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3374	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3375	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3376	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3377	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3378	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3379	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3380	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3381	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3382	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3383	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3384	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3385	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3386	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3387	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3388	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3389	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3390	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3391	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3392	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3393	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3394	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3395	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3396	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3397	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3398	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3399	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3400	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3401	-	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	$\# Z > 2$
56	OHX	DA	3402	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3403	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3404	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3405	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3406	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3407	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3408	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3409	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3410	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3411	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3412	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3413	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3414	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3415	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3416	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3417	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3418	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3419	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3420	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3421	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3422	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3423	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3424	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3426	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3427	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3428	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3429	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3430	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3431	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3432	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3433	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3434	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3435	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3437	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3438	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3439	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3440	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3441	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3442	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3443	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3444	-	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	$\# Z > 2$
56	OHX	DA	3445	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3446	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3447	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3448	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3449	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3450	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3451	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3452	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3453	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3454	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3455	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3456	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3457	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3458	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3459	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3460	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3461	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3462	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3463	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3464	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3465	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3466	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3467	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3468	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3469	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3470	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3471	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3472	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3473	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3474	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3475	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3476	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3477	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3478	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3479	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3480	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3481	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3482	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3483	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3485	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3486	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3487	-	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
56	OHX	DA	3488	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3489	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	3491	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DB	208	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DB	209	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DB	210	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DB	211	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DB	212	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DB	213	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DB	214	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DB	215	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DB	216	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DB	217	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DB	218	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DB	219	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DB	220	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DF	301	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DO	201	-	0,6,6	0.00	-	0,15,15	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	A1	203	-	-	0/0/0/0	0/0/0/0
56	OHX	A1	204	-	-	0/0/0/0	0/0/0/0
56	OHX	A3	102	-	-	0/0/0/0	0/0/0/0
56	OHX	A6	101	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3326	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3327	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3328	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3329	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3330	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3331	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3332	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3333	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3335	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3336	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3338	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3340	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3341	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	AA	3342	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3344	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3345	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3346	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3347	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3348	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3349	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3350	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3351	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3352	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3353	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3354	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3355	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3358	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3359	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3360	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3361	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3362	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3363	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3364	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3365	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3366	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3367	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3368	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3369	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3370	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3371	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3373	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3374	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3375	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3376	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3377	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3378	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3379	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3380	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3381	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3382	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3383	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3384	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3385	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3386	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3387	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	AA	3388	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3389	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3390	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3391	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3392	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3393	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3394	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3395	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3396	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3397	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3398	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3399	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3400	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3401	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3402	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3403	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3404	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3405	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3406	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3407	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3408	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3409	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3410	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3411	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3412	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3413	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3414	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3415	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3416	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3417	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3418	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3419	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3420	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3421	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3422	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3423	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3424	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3425	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3426	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3427	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3428	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3429	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	AA	3430	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3431	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3432	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3433	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3434	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3435	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3436	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3437	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3438	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3439	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3440	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3441	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3442	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3443	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3444	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3445	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3446	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3447	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3448	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3449	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3450	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3451	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3452	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3453	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3454	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3455	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3456	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3457	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3458	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3459	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3460	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3461	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3462	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3463	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3464	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3465	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3466	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3467	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3468	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3469	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3470	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3471	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	AA	3472	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3473	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3474	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3475	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3476	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3477	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3478	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3479	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3480	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3481	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3482	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3483	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3484	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3485	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3486	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3487	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3488	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3489	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3490	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3491	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3492	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3493	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3494	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3495	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3496	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3497	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3498	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3499	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3500	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3501	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3502	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3503	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3504	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3505	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3506	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3507	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3508	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3509	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3510	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3511	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3512	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3513	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	AA	3514	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3515	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3516	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3517	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3518	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3519	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3520	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3521	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3522	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3523	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3524	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3525	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3526	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3527	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3528	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3529	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3530	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3531	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3532	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3533	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3534	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3535	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3536	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3537	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3538	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3539	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3540	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3541	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3542	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3543	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3544	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3545	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3546	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3547	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3548	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3549	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3550	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3551	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3552	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3553	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3554	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3555	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	AA	3556	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3557	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3558	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3559	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3560	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3561	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3562	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3563	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3564	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3565	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3566	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3567	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3568	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3569	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	207	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	208	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	209	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	210	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	211	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	212	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	213	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	214	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	215	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	216	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	217	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	218	-	-	0/0/0/0	0/0/0/0
56	OHX	AB	219	-	-	0/0/0/0	0/0/0/0
56	OHX	AE	304	-	-	0/0/0/0	0/0/0/0
56	OHX	AF	303	-	-	0/0/0/0	0/0/0/0
56	OHX	AO	202	-	-	0/0/0/0	0/0/0/0
56	OHX	AO	203	-	-	0/0/0/0	0/0/0/0
56	OHX	AW	101	-	-	0/0/0/0	0/0/0/0
57	PAR	BA	1715	-	-	0/18/94/94	0/4/4/4
56	OHX	BA	1716	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1717	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1718	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1719	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1720	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1721	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1722	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1723	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1724	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	BA	1725	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1726	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1727	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1728	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1729	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1730	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1731	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1732	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1733	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1734	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1735	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1736	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1737	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1738	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1739	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1740	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1741	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1742	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1743	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1744	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1745	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1746	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1747	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1748	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1749	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1750	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1751	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1752	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1753	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1754	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1755	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1756	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1757	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1758	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1759	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1760	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1761	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1762	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1763	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1764	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1765	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1766	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	BA	1767	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1768	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1769	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1770	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1771	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1772	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1773	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1774	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1775	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1776	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1777	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1778	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1779	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1780	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1781	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1782	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1783	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1784	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1785	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1786	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1787	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1788	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1789	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1790	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1791	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1792	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1793	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1794	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1795	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1796	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1797	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1798	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1799	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1800	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1801	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1802	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1803	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1804	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1805	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1806	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1807	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1808	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	BA	1809	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1810	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1811	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1812	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1813	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1814	-	-	0/0/0/0	0/0/0/0
56	OHX	BB	114	-	-	0/0/0/0	0/0/0/0
56	OHX	BB	115	-	-	0/0/0/0	0/0/0/0
56	OHX	BC	105	-	-	0/0/0/0	0/0/0/0
56	OHX	BC	106	-	-	0/0/0/0	0/0/0/0
56	OHX	BC	107	-	-	0/0/0/0	0/0/0/0
56	OHX	BD	102	-	-	0/0/0/0	0/0/0/0
56	OHX	BD	103	-	-	0/0/0/0	0/0/0/0
56	OHX	BD	104	-	-	0/0/0/0	0/0/0/0
56	OHX	BG	302	-	-	0/0/0/0	0/0/0/0
56	OHX	BL	201	-	-	0/0/0/0	0/0/0/0
56	OHX	BR	101	-	-	0/0/0/0	0/0/0/0
57	PAR	CA	1722	-	-	0/18/94/94	0/4/4/4
56	OHX	CA	1723	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1724	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1725	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1726	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1727	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1728	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1729	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1730	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1731	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1732	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1733	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1734	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1735	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1736	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1737	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1738	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1739	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1740	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1741	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1742	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1743	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1744	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1745	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1746	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	CA	1747	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1748	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1749	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1750	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1751	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1752	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1753	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1754	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1755	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1756	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1757	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1758	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1759	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1760	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1761	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1762	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1763	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1764	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1765	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1766	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1767	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1768	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1769	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1770	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1771	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1772	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1773	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1774	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1775	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1776	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1777	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1778	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1779	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1780	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1781	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1782	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1783	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1784	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1785	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1786	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1787	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1788	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	CA	1789	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1790	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1791	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1792	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1793	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1794	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1795	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1796	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1797	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1798	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1799	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1800	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1801	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1802	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1803	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1804	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1805	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1806	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1807	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1808	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1809	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1810	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1811	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1812	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1813	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1814	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	1815	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	104	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	105	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	106	-	-	0/0/0/0	0/0/0/0
56	OHX	CC	108	-	-	0/0/0/0	0/0/0/0
56	OHX	CC	109	-	-	0/0/0/0	0/0/0/0
56	OHX	CC	110	-	-	0/0/0/0	0/0/0/0
56	OHX	CD	101	-	-	0/0/0/0	0/0/0/0
56	OHX	CK	201	-	-	0/0/0/0	0/0/0/0
56	OHX	CR	101	-	-	0/0/0/0	0/0/0/0
56	OHX	CV	101	-	-	0/0/0/0	0/0/0/0
56	OHX	D1	201	-	-	0/0/0/0	0/0/0/0
56	OHX	D3	101	-	-	0/0/0/0	0/0/0/0
56	OHX	D5	102	-	-	0/0/0/0	0/0/0/0
56	OHX	D8	101	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3061	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	DA	3062	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3064	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3065	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3068	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3071	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3073	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3075	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3081	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3082	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3083	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3084	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3087	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3091	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3094	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3099	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3103	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3105	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3109	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3111	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3118	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3124	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3127	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3132	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3134	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3136	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3157	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3159	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3160	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3162	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3163	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3165	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3166	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3168	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3169	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3170	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3171	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3172	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3173	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3174	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3176	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3212	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3214	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	DA	3215	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3217	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3218	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3220	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3221	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3223	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3224	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3226	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3243	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3245	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3246	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3248	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3249	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3251	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3253	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3254	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3255	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3257	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3258	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3335	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3336	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3337	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3338	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3339	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3340	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3341	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3342	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3343	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3344	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3345	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3346	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3347	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3348	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3349	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3350	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3351	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3352	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3353	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3354	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3355	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3356	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3357	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	DA	3358	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3359	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3360	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3361	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3362	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3363	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3364	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3365	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3366	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3367	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3368	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3369	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3370	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3371	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3372	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3373	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3374	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3375	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3376	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3377	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3378	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3379	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3380	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3381	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3382	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3383	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3384	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3385	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3386	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3387	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3388	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3389	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3390	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3391	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3392	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3393	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3394	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3395	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3396	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3397	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3398	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3399	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	DA	3400	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3401	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3402	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3403	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3404	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3405	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3406	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3407	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3408	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3409	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3410	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3411	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3412	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3413	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3414	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3415	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3416	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3417	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3418	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3419	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3420	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3421	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3422	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3423	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3424	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3425	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3426	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3427	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3428	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3429	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3430	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3431	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3432	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3433	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3434	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3435	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3436	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3437	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3438	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3439	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3440	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3441	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	DA	3442	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3443	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3444	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3445	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3446	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3447	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3448	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3449	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3450	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3451	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3452	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3453	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3454	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3455	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3456	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3457	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3458	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3459	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3460	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3461	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3462	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3463	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3464	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3465	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3466	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3467	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3468	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3469	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3470	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3471	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3472	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3473	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3474	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3475	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3476	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3477	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3478	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3479	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3480	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3481	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3482	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3483	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	DA	3484	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3485	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3486	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3487	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3488	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3489	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3490	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	3491	-	-	0/0/0/0	0/0/0/0
56	OHX	DB	208	-	-	0/0/0/0	0/0/0/0
56	OHX	DB	209	-	-	0/0/0/0	0/0/0/0
56	OHX	DB	210	-	-	0/0/0/0	0/0/0/0
56	OHX	DB	211	-	-	0/0/0/0	0/0/0/0
56	OHX	DB	212	-	-	0/0/0/0	0/0/0/0
56	OHX	DB	213	-	-	0/0/0/0	0/0/0/0
56	OHX	DB	214	-	-	0/0/0/0	0/0/0/0
56	OHX	DB	215	-	-	0/0/0/0	0/0/0/0
56	OHX	DB	216	-	-	0/0/0/0	0/0/0/0
56	OHX	DB	217	-	-	0/0/0/0	0/0/0/0
56	OHX	DB	218	-	-	0/0/0/0	0/0/0/0
56	OHX	DB	219	-	-	0/0/0/0	0/0/0/0
56	OHX	DB	220	-	-	0/0/0/0	0/0/0/0
56	OHX	DF	301	-	-	0/0/0/0	0/0/0/0
56	OHX	DO	201	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	BA	1715	PAR	C21-N21	-2.16	1.43	1.47

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	CA	1722	PAR	C11-O51-C51	5.09	123.58	113.73
57	CA	1722	PAR	C62-C12-N12	-4.40	102.59	110.90
57	CA	1722	PAR	C13-O52-C52	-4.34	106.98	118.00
57	BA	1715	PAR	C11-O51-C51	4.32	122.08	113.73
57	CA	1722	PAR	C41-C31-C21	-4.14	104.22	111.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	2912/2912 (100%)	-0.48	25 (0%) 81 37	44, 79, 216, 250	0
1	DA	2907/2912 (99%)	-0.42	26 (0%) 81 37	56, 94, 236, 252	0
2	AB	122/122 (100%)	-0.65	1 (0%) 83 39	77, 99, 118, 184	0
2	DB	122/122 (100%)	-0.56	1 (0%) 83 39	98, 129, 153, 204	0
3	AD	272/276 (98%)	-0.00	0 100 100	42, 67, 88, 106	0
3	DD	272/276 (98%)	0.13	1 (0%) 90 57	52, 78, 98, 130	0
4	AE	205/206 (99%)	0.05	3 (1%) 70 24	54, 90, 135, 147	0
4	DE	205/206 (99%)	0.10	2 (0%) 79 33	61, 102, 153, 167	0
5	AF	202/210 (96%)	-0.14	0 100 100	49, 84, 121, 136	0
5	DF	208/210 (99%)	0.22	6 (2%) 49 12	63, 108, 164, 189	0
6	AG	181/182 (99%)	0.24	5 (2%) 50 12	90, 112, 143, 155	0
6	DG	181/182 (99%)	0.48	8 (4%) 33 7	122, 146, 169, 175	0
7	AH	170/180 (94%)	0.04	0 100 100	89, 116, 133, 162	0
7	DH	170/180 (94%)	0.50	6 (3%) 42 10	162, 204, 226, 236	0
8	AK	146/148 (98%)	0.07	0 100 100	79, 134, 153, 155	0
8	DK	146/148 (98%)	0.11	3 (2%) 60 17	88, 135, 157, 163	0
9	AM	138/140 (98%)	0.16	1 (0%) 84 42	68, 92, 129, 141	0
9	DM	138/140 (98%)	-0.03	1 (0%) 84 42	83, 117, 146, 159	0
10	AN	122/122 (100%)	0.22	0 100 100	61, 79, 96, 107	0
10	DN	122/122 (100%)	0.34	0 100 100	75, 97, 114, 124	0
11	AO	150/150 (100%)	0.04	1 (0%) 84 42	46, 93, 120, 166	0
11	DO	150/150 (100%)	0.64	11 (7%) 15 4	45, 106, 147, 183	0
12	AP	141/141 (100%)	0.27	9 (6%) 19 5	58, 86, 108, 136	0
12	DP	141/141 (100%)	0.59	9 (6%) 19 5	58, 111, 143, 164	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	A0	118/118 (100%)	-0.03	0 100 100	57, 86, 110, 118	0
13	D0	117/118 (99%)	-0.18	0 100 100	68, 89, 109, 124	0
14	AQ	111/112 (99%)	-0.15	1 (0%) 81 37	67, 97, 120, 133	0
14	DQ	111/112 (99%)	-0.17	0 100 100	85, 126, 150, 162	0
15	AR	137/146 (93%)	0.15	1 (0%) 84 42	75, 96, 149, 175	0
15	DR	137/146 (93%)	0.57	9 (6%) 18 4	81, 106, 168, 189	0
16	A1	117/118 (99%)	-0.12	1 (0%) 81 37	58, 81, 110, 142	0
16	D1	117/118 (99%)	0.14	1 (0%) 81 37	71, 109, 145, 167	0
17	A2	101/101 (100%)	0.16	3 (2%) 48 11	51, 104, 126, 143	0
17	D2	101/101 (100%)	0.49	6 (5%) 22 5	65, 134, 147, 155	0
18	AS	113/113 (100%)	0.10	1 (0%) 81 37	61, 77, 108, 161	0
18	DS	113/113 (100%)	0.16	2 (1%) 65 20	66, 82, 116, 162	0
19	AT	92/96 (95%)	-0.12	0 100 100	59, 73, 99, 111	0
19	DT	92/96 (95%)	0.12	1 (1%) 77 30	74, 92, 117, 133	0
20	AU	102/110 (92%)	0.43	4 (3%) 37 8	79, 105, 156, 168	0
20	DU	102/110 (92%)	0.55	16 (15%) 3 1	97, 122, 169, 185	0
21	AV	175/206 (84%)	1.20	33 (18%) 2 1	90, 131, 195, 198	0
21	DV	179/206 (86%)	1.40	45 (25%) 1 1	127, 165, 214, 226	0
22	A3	76/85 (89%)	0.09	1 (1%) 74 27	65, 78, 95, 130	0
22	D3	77/85 (90%)	0.28	1 (1%) 74 27	78, 97, 119, 152	0
23	AZ	97/98 (98%)	-0.08	0 100 100	59, 79, 131, 161	0
23	DZ	97/98 (98%)	0.05	1 (1%) 79 33	69, 89, 136, 157	0
24	AW	66/72 (91%)	-0.07	1 (1%) 70 24	63, 87, 103, 128	0
24	DW	66/72 (91%)	0.14	2 (3%) 48 11	88, 112, 132, 142	0
25	AX	59/60 (98%)	-0.27	0 100 100	66, 86, 119, 134	0
25	DX	59/60 (98%)	0.19	1 (1%) 67 21	87, 113, 146, 167	0
26	A4	66/71 (92%)	1.11	12 (18%) 2 1	130, 162, 180, 188	0
26	D4	63/71 (88%)	1.93	28 (44%) 1 0	149, 192, 200, 204	0
27	A5	59/60 (98%)	0.27	5 (8%) 11 3	54, 95, 172, 174	0
27	D5	59/60 (98%)	0.29	5 (8%) 11 3	61, 96, 179, 195	0
28	A6	45/54 (83%)	5.10	45 (100%) 0 0	129, 159, 174, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	D6	45/54 (83%)	4.26	38 (84%) 0 0	146, 174, 190, 192	0
29	A7	45/49 (91%)	0.06	0 100 100	46, 55, 72, 78	0
29	D7	45/49 (91%)	0.11	0 100 100	56, 66, 79, 96	0
30	A8	60/65 (92%)	0.30	2 (3%) 44 10	56, 74, 97, 120	0
30	D8	60/65 (92%)	0.82	3 (5%) 28 6	75, 91, 113, 138	0
31	BA	1502/1506 (99%)	-0.63	3 (0%) 93 70	58, 111, 193, 251	0
31	CA	1502/1506 (99%)	-0.64	2 (0%) 93 77	69, 122, 195, 251	0
32	BE	237/256 (92%)	0.25	7 (2%) 48 11	117, 150, 188, 200	0
32	CE	237/256 (92%)	0.57	18 (7%) 14 4	128, 166, 201, 216	0
33	BF	205/239 (85%)	0.31	7 (3%) 43 10	95, 124, 157, 167	0
33	CF	206/239 (86%)	0.58	13 (6%) 19 5	130, 151, 179, 185	0
34	BG	208/208 (100%)	-0.19	0 100 100	95, 119, 141, 152	0
34	CG	208/208 (100%)	-0.01	1 (0%) 88 51	94, 114, 136, 151	0
35	BH	151/162 (93%)	-0.07	1 (0%) 84 42	81, 109, 130, 166	0
35	CH	151/162 (93%)	0.11	1 (0%) 84 42	106, 124, 148, 171	0
36	BI	101/101 (100%)	0.51	4 (3%) 36 8	86, 111, 127, 152	0
36	CI	101/101 (100%)	-0.08	0 100 100	83, 108, 131, 149	0
37	BJ	155/156 (99%)	0.30	9 (5%) 22 5	109, 127, 154, 167	0
37	CJ	155/156 (99%)	0.05	1 (0%) 86 46	120, 136, 159, 167	0
38	BK	138/138 (100%)	-0.25	0 100 100	90, 115, 128, 133	0
38	CK	138/138 (100%)	-0.00	0 100 100	105, 129, 141, 151	0
39	BL	127/128 (99%)	-0.17	0 100 100	98, 148, 166, 173	0
39	CL	127/128 (99%)	-0.13	5 (3%) 37 8	118, 160, 175, 179	0
40	BM	99/105 (94%)	0.34	1 (1%) 79 33	93, 149, 177, 178	0
40	CM	99/105 (94%)	0.11	2 (2%) 62 19	128, 165, 180, 184	0
41	BN	119/129 (92%)	0.53	5 (4%) 35 8	81, 109, 138, 167	0
41	CN	119/129 (92%)	0.94	16 (13%) 4 2	89, 116, 144, 172	0
42	BO	125/132 (94%)	0.24	4 (3%) 45 11	73, 86, 118, 162	0
42	CO	125/132 (94%)	0.41	5 (4%) 36 8	91, 113, 138, 172	0
43	BP	116/126 (92%)	-0.07	1 (0%) 81 37	97, 135, 151, 157	0
43	CP	117/126 (92%)	0.02	2 (1%) 67 21	108, 162, 175, 177	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	58/61 (95%)	-0.14	0 100 100	96, 113, 128, 134	0
44	CQ	58/61 (95%)	0.64	3 (5%) 26 6	132, 145, 162, 167	0
45	BR	88/89 (98%)	0.09	0 100 100	81, 103, 125, 130	0
45	CR	88/89 (98%)	0.20	1 (1%) 77 30	88, 116, 138, 145	0
46	BS	84/88 (95%)	0.28	0 100 100	105, 122, 147, 180	0
46	CS	84/88 (95%)	0.10	0 100 100	96, 108, 131, 164	0
47	BT	100/105 (95%)	0.09	1 (1%) 79 33	95, 114, 128, 135	0
47	CT	100/105 (95%)	0.22	3 (3%) 48 11	96, 117, 138, 149	0
48	BU	72/88 (81%)	0.45	3 (4%) 35 8	94, 111, 147, 169	0
48	CU	72/88 (81%)	0.47	8 (11%) 6 2	98, 120, 160, 178	0
49	BV	78/93 (83%)	-0.03	1 (1%) 74 27	113, 135, 155, 159	0
49	CV	78/93 (83%)	0.25	3 (3%) 38 9	146, 170, 187, 192	0
50	BW	99/106 (93%)	-0.26	0 100 100	113, 129, 159, 167	0
50	CW	99/106 (93%)	0.03	1 (1%) 79 33	100, 122, 157, 170	0
51	BX	25/27 (92%)	-0.29	0 100 100	110, 123, 139, 157	0
51	CX	25/27 (92%)	-0.02	0 100 100	126, 148, 165, 175	0
52	BB	84/85 (98%)	2.06	35 (41%) 1 0	98, 138, 163, 176	0
52	BD	84/85 (98%)	0.28	7 (8%) 11 3	78, 144, 223, 233	0
52	CB	84/85 (98%)	3.57	60 (71%) 0 0	113, 143, 166, 176	0
52	CD	84/85 (98%)	-0.30	0 100 100	86, 144, 222, 230	0
53	BC	77/77 (100%)	-0.30	1 (1%) 74 27	82, 117, 146, 159	0
53	CC	77/77 (100%)	-0.30	1 (1%) 74 27	92, 127, 156, 164	0
54	B1	16/16 (100%)	0.79	2 (12%) 5 2	81, 117, 161, 169	0
54	C1	16/16 (100%)	1.08	3 (18%) 2 1	90, 122, 168, 176	0
All	All	21100/21658 (97%)	-0.06	629 (2%) 48 11	42, 108, 188, 252	0

The worst 5 of 629 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA	2901	C	11.6
1	DA	2901	C	11.0
52	CB	52	G	10.6
52	CB	80	C	10.5
28	A6	18	ARG	10.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
52	MIA	BD	38	29/30	0.27	-	126,140,181,195	0
52	MIA	CB	38	29/30	0.37	-	99,111,127,136	0
52	MIA	BB	38	29/30	0.22	-	92,99,110,128	0
52	MIA	CD	38	29/30	0.21	-	127,140,183,200	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	OHX	AO	203	7/7	0.16	-	83,92,110,152	1
56	OHX	CA	1785	7/7	0.22	-	125,126,143,155	1
55	MG	AA	3290	1/1	0.31	-	66,66,66,66	0
55	MG	DA	3283	1/1	0.29	-	86,86,86,86	0
56	OHX	AA	3433	7/7	0.14	-	77,91,106,131	2
56	OHX	DA	3372	7/7	0.18	-	90,96,108,138	1
55	MG	AO	201	1/1	0.12	-	66,66,66,66	0
56	OHX	DA	3480	7/7	0.09	-	125,130,144,190	1
56	OHX	AA	3386	7/7	0.16	-	75,83,104,131	1
55	MG	AA	3056	1/1	0.18	-	55,55,55,55	0
56	OHX	BA	1791	7/7	0.14	-	122,123,136,173	1
56	OHX	AA	3407	7/7	0.16	-	53,82,90,103	2
56	OHX	AA	3387	7/7	0.12	-	110,123,134,164	1
55	MG	AA	3032	1/1	0.27	-	37,37,37,37	0
55	MG	CA	1684	1/1	0.46	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	OHX	AA	3416	7/7	0.15	-	108,113,125,155	1
56	OHX	CA	1766	7/7	0.08	-	116,126,135,171	1
55	MG	DA	3063	1/1	0.55	-	59,59,59,59	0
55	MG	AA	3313	1/1	0.41	-	82,82,82,82	0
55	MG	BA	1681	1/1	0.29	-	64,64,64,64	0
56	OHX	DA	3466	7/7	0.17	-	116,124,134,165	2
56	OHX	AA	3506	7/7	0.14	-	104,115,126,178	1
55	MG	BA	1700	1/1	0.05	-	119,119,119,119	0
55	MG	BA	1661	1/1	0.43	-	61,61,61,61	0
55	MG	DA	3197	1/1	0.27	-	49,49,49,49	0
55	MG	AA	3258	1/1	0.33	-	39,39,39,39	0
55	MG	DA	3164	1/1	0.37	-	63,63,63,63	0
56	OHX	BA	1740	7/7	0.13	-	107,110,122,131	1
55	MG	BB	103	1/1	0.28	-	105,105,105,105	0
55	MG	BC	104	1/1	0.41	-	88,88,88,88	0
56	OHX	CA	1725	7/7	0.10	-	108,111,122,123	1
55	MG	AA	3301	1/1	0.16	-	97,97,97,97	0
55	MG	DA	3315	1/1	0.42	-	78,78,78,78	0
55	MG	CA	1689	1/1	0.17	-	80,80,80,80	0
55	MG	DA	3004	1/1	0.23	-	32,32,32,32	0
56	OHX	CA	1783	7/7	0.21	-	113,117,137,164	1
55	MG	DA	3101	1/1	0.24	-	59,59,59,59	0
55	MG	CA	1675	1/1	0.40	-	94,94,94,94	0
55	MG	DA	3107	1/1	0.24	-	42,42,42,42	0
56	OHX	CA	1781	7/7	0.11	-	153,161,166,239	1
55	MG	CA	1710	1/1	0.13	-	78,78,78,78	0
55	MG	CA	1624	1/1	0.12	-	114,114,114,114	0
55	MG	DA	3312	1/1	0.23	-	81,81,81,81	0
55	MG	DA	3208	1/1	0.46	-	61,61,61,61	0
55	MG	BA	1708	1/1	0.19	-	80,80,80,80	0
55	MG	DA	3032	1/1	0.10	-	38,38,38,38	0
55	MG	DA	3238	1/1	0.35	-	67,67,67,67	0
55	MG	DA	3046	1/1	0.34	-	78,78,78,78	0
55	MG	DA	3332	1/1	0.19	-	78,78,78,78	0
55	MG	AA	3113	1/1	0.22	-	88,88,88,88	0
56	OHX	DA	3446	7/7	0.11	-	118,121,142,162	1
56	OHX	CA	1764	7/7	0.14	-	113,122,135,168	1
55	MG	AA	3026	1/1	0.30	-	43,43,43,43	0
56	OHX	AA	3546	7/7	0.19	-	101,114,120,164	2
56	OHX	DA	3111	7/7	0.21	-	118,129,134,197	1
56	OHX	BA	1754	7/7	0.08	-	136,144,152,183	1
55	MG	AA	3200	1/1	0.32	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	1647	1/1	0.40	-	66,66,66,66	0
55	MG	AA	3037	1/1	0.24	-	55,55,55,55	0
55	MG	CA	1633	1/1	0.55	-	46,46,46,46	0
55	MG	DA	3204	1/1	0.26	-	58,58,58,58	0
56	OHX	DA	3343	7/7	0.16	-	93,113,122,129	0
56	OHX	CA	1746	7/7	0.08	-	112,115,128,150	1
55	MG	DA	3259	1/1	0.34	-	114,114,114,114	0
55	MG	DA	3133	1/1	0.27	-	51,51,51,51	0
55	MG	AA	3084	1/1	0.28	-	104,104,104,104	0
56	OHX	DA	3449	7/7	0.10	-	147,154,162,185	1
56	OHX	AA	3509	7/7	0.22	-	91,109,142,150	3
55	MG	BA	1690	1/1	0.10	-	81,81,81,81	0
56	OHX	AA	3333	7/7	0.13	-	99,103,122,123	0
56	OHX	DA	3419	7/7	0.14	-	82,93,100,126	2
56	OHX	DA	3258	7/7	0.21	-	103,111,118,148	1
56	OHX	DA	3387	7/7	0.07	-	108,115,125,151	1
56	OHX	DA	3065	7/7	0.17	-	55,92,111,137	1
56	OHX	BA	1765	7/7	0.25	-	91,107,120,150	3
55	MG	DA	3286	1/1	0.14	-	77,77,77,77	0
56	OHX	DA	3393	7/7	0.12	-	133,134,150,191	1
55	MG	DA	3321	1/1	0.20	-	56,56,56,56	0
55	MG	AA	3263	1/1	0.27	-	39,39,39,39	0
55	MG	AA	3171	1/1	0.31	-	59,59,59,59	0
55	MG	CA	1700	1/1	0.14	-	97,97,97,97	0
56	OHX	DA	3132	7/7	0.12	-	185,187,192,225	1
55	MG	DA	3033	1/1	0.26	-	82,82,82,82	0
55	MG	CA	1605	1/1	0.23	-	75,75,75,75	0
55	MG	CA	1655	1/1	0.31	-	70,70,70,70	0
56	OHX	DB	218	7/7	0.36	-	134,141,153,171	1
55	MG	DA	3149	1/1	0.23	-	53,53,53,53	0
55	MG	BA	1634	1/1	0.17	-	73,73,73,73	0
56	OHX	BA	1769	7/7	0.11	-	159,168,172,218	1
56	OHX	AA	3374	7/7	0.19	-	32,70,109,140	3
55	MG	DA	3120	1/1	0.31	-	52,52,52,52	0
56	OHX	AF	303	7/7	0.19	-	46,54,72,103	0
55	MG	AA	3194	1/1	0.40	-	56,56,56,56	0
55	MG	BC	103	1/1	0.44	-	70,70,70,70	0
56	OHX	CA	1723	7/7	0.19	-	84,100,111,141	0
56	OHX	CA	1736	7/7	0.10	-	163,166,178,209	0
56	OHX	AA	3373	7/7	0.10	-	84,96,108,141	1
56	OHX	AA	3500	7/7	0.12	-	118,131,153,193	1
55	MG	AF	302	1/1	0.17	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	OHX	AA	3551	7/7	0.25	-	97,115,123,153	1
56	OHX	CA	1809	7/7	0.07	-	150,160,169,213	1
55	MG	AA	3205	1/1	0.14	-	42,42,42,42	0
55	MG	CA	1602	1/1	0.40	-	58,58,58,58	0
56	OHX	BA	1728	7/7	0.07	-	140,147,157,166	1
55	MG	CA	1618	1/1	0.08	-	82,82,82,82	0
55	MG	AA	3252	1/1	0.34	-	52,52,52,52	0
55	MG	DA	3299	1/1	0.20	-	67,67,67,67	0
55	MG	DA	3115	1/1	0.21	-	44,44,44,44	0
55	MG	DA	3152	1/1	0.36	-	57,57,57,57	0
55	MG	AA	3155	1/1	0.11	-	79,79,79,79	0
56	OHX	BA	1716	7/7	0.16	-	73,86,99,116	0
56	OHX	DA	3375	7/7	0.10	-	129,138,149,173	1
56	OHX	DA	3452	7/7	0.17	-	99,118,125,155	1
56	OHX	BA	1768	7/7	0.13	-	87,95,105,130	2
56	OHX	DA	3443	7/7	0.17	-	113,124,137,188	1
56	OHX	BA	1813	7/7	0.17	-	151,161,170,205	1
58	ZN	BQ	101	1/1	0.07	-	135,135,135,135	0
56	OHX	CA	1778	7/7	0.08	-	148,157,164,202	1
55	MG	BA	1608	1/1	0.10	-	89,89,89,89	0
55	MG	DA	3005	1/1	0.25	-	41,41,41,41	0
55	MG	DA	3271	1/1	0.38	-	59,59,59,59	0
55	MG	AA	3186	1/1	0.14	-	57,57,57,57	0
55	MG	AA	3143	1/1	0.35	-	87,87,87,87	0
56	OHX	CA	1786	7/7	0.10	-	163,163,175,198	1
56	OHX	DA	3338	7/7	0.17	-	72,79,93,112	0
55	MG	BA	1649	1/1	0.41	-	92,92,92,92	0
55	MG	AA	3273	1/1	0.40	-	60,60,60,60	0
55	MG	AA	3305	1/1	0.54	-	66,66,66,66	0
55	MG	AA	3281	1/1	0.16	-	93,93,93,93	0
56	OHX	AA	3528	7/7	0.41	-	119,125,142,174	1
56	OHX	AA	3338	7/7	0.12	-	66,87,106,113	2
55	MG	DA	3011	1/1	0.13	-	84,84,84,84	0
55	MG	BA	1629	1/1	0.15	-	79,79,79,79	0
55	MG	CA	1681	1/1	0.27	-	111,111,111,111	0
56	OHX	AA	3405	7/7	0.10	-	100,103,111,158	1
55	MG	CA	1619	1/1	0.23	-	92,92,92,92	0
56	OHX	AA	3404	7/7	0.09	-	108,112,133,175	1
56	OHX	BA	1764	7/7	0.15	-	147,152,158,209	1
56	OHX	DA	3462	7/7	0.12	-	154,157,165,208	1
55	MG	DA	3150	1/1	0.18	-	46,46,46,46	0
56	OHX	CA	1769	7/7	0.10	-	141,144,170,199	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3101	1/1	0.30	-	47,47,47,47	0
55	MG	DA	3139	1/1	0.43	-	54,54,54,54	0
55	MG	DA	3057	1/1	0.32	-	58,58,58,58	0
55	MG	DA	3102	1/1	0.24	-	76,76,76,76	0
55	MG	AA	3125	1/1	0.21	-	63,63,63,63	0
56	OHX	AA	3454	7/7	0.17	-	103,116,132,145	1
56	OHX	BA	1745	7/7	0.12	-	119,123,132,169	1
56	OHX	CA	1803	7/7	0.08	-	137,147,156,198	1
56	OHX	AA	3376	7/7	0.10	-	96,107,117,142	1
56	OHX	DA	3340	7/7	0.13	-	86,102,124,126	1
55	MG	AA	3006	1/1	0.36	-	40,40,40,40	0
56	OHX	BA	1803	7/7	0.08	-	211,214,221,256	1
56	OHX	AA	3326	7/7	0.16	-	75,76,87,119	0
55	MG	AA	3247	1/1	0.47	-	66,66,66,66	0
55	MG	AA	3050	1/1	0.36	-	45,45,45,45	0
56	OHX	BA	1798	7/7	0.10	-	135,136,153,212	1
55	MG	CA	1647	1/1	0.42	-	70,70,70,70	0
55	MG	DA	3240	1/1	0.39	-	64,64,64,64	0
55	MG	BA	1652	1/1	0.38	-	68,68,68,68	0
55	MG	DA	3192	1/1	0.48	-	60,60,60,60	0
55	MG	AA	3178	1/1	0.41	-	76,76,76,76	0
56	OHX	CA	1753	7/7	0.25	-	82,120,146,173	3
55	MG	AA	3097	1/1	0.25	-	50,50,50,50	0
55	MG	DA	3288	1/1	0.26	-	82,82,82,82	0
55	MG	DA	3330	1/1	0.63	-	81,81,81,81	0
56	OHX	DF	301	7/7	0.10	-	53,80,83,83	1
55	MG	AA	3320	1/1	0.19	-	45,45,45,45	0
56	OHX	AA	3515	7/7	0.21	-	93,97,116,159	2
55	MG	AA	3218	1/1	0.34	-	35,35,35,35	0
56	OHX	DA	3103	7/7	0.18	-	94,102,107,128	2
55	MG	AA	3018	1/1	0.24	-	49,49,49,49	0
55	MG	CA	1666	1/1	0.36	-	75,75,75,75	0
55	MG	AA	3081	1/1	0.16	-	81,81,81,81	0
56	OHX	AA	3480	7/7	0.25	-	111,119,135,158	2
55	MG	AA	3238	1/1	0.42	-	47,47,47,47	0
55	MG	CA	1614	1/1	0.20	-	118,118,118,118	0
55	MG	CC	106	1/1	0.54	-	75,75,75,75	0
56	OHX	DA	3455	7/7	0.07	-	139,144,150,194	1
55	MG	CA	1621	1/1	0.34	-	110,110,110,110	0
55	MG	AA	3096	1/1	0.61	-	76,76,76,76	0
55	MG	DA	3135	1/1	0.32	-	42,42,42,42	0
55	MG	AA	3296	1/1	0.41	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	OHX	AA	3561	7/7	0.12	-	86,92,112,144	2
56	OHX	BA	1724	7/7	0.10	-	114,121,136,156	0
55	MG	AA	3288	1/1	0.30	-	55,55,55,55	0
55	MG	BA	1641	1/1	0.24	-	54,54,54,54	0
56	OHX	DA	3447	7/7	0.11	-	122,140,155,176	2
56	OHX	DA	3460	7/7	0.14	-	111,124,134,174	1
55	MG	BA	1713	1/1	0.36	-	81,81,81,81	0
56	OHX	BA	1731	7/7	0.21	-	99,107,129,161	1
56	OHX	DA	3485	7/7	0.13	-	131,137,152,172	1
56	OHX	AA	3335	7/7	0.22	-	62,76,78,127	0
55	MG	DA	3117	1/1	0.28	-	82,82,82,82	0
55	MG	DA	3186	1/1	0.34	-	34,34,34,34	0
55	MG	AA	3245	1/1	0.57	-	70,70,70,70	0
55	MG	BW	201	1/1	0.14	-	92,92,92,92	0
55	MG	DA	3323	1/1	0.52	-	100,100,100,100	0
55	MG	DA	3110	1/1	0.50	-	60,60,60,60	0
56	OHX	CA	1797	7/7	0.46	-	129,132,139,171	1
56	OHX	AA	3516	7/7	0.18	-	90,98,116,166	1
55	MG	DA	3252	1/1	0.57	-	81,81,81,81	0
55	MG	DA	3318	1/1	0.17	-	110,110,110,110	0
56	OHX	DA	3173	7/7	0.11	-	157,163,175,202	1
55	MG	AA	3317	1/1	0.23	-	55,55,55,55	0
55	MG	CA	1664	1/1	0.17	-	57,57,57,57	0
56	OHX	AA	3545	7/7	0.12	-	92,105,127,145	2
55	MG	DA	3195	1/1	0.10	-	46,46,46,46	0
55	MG	AA	3295	1/1	0.40	-	89,89,89,89	0
56	OHX	D1	201	7/7	0.14	-	110,112,135,162	1
56	OHX	AA	3547	7/7	0.12	-	80,87,107,118	1
55	MG	DA	3334	1/1	0.34	-	75,75,75,75	0
56	OHX	DA	3412	7/7	0.10	-	93,110,113,161	1
55	MG	AA	3206	1/1	0.23	-	37,37,37,37	0
56	OHX	AA	3488	7/7	0.13	-	155,156,163,203	1
56	OHX	DA	3392	7/7	0.13	-	115,117,129,183	1
56	OHX	AA	3370	7/7	0.16	-	74,85,99,119	1
55	MG	AA	3265	1/1	0.16	-	62,62,62,62	0
56	OHX	AA	3459	7/7	0.15	-	91,107,133,162	1
56	OHX	DA	3068	7/7	0.13	-	102,127,131,147	0
56	OHX	CA	1758	7/7	0.07	-	150,162,166,191	1
56	OHX	AA	3419	7/7	0.14	-	102,113,133,143	3
56	OHX	AA	3458	7/7	0.17	-	96,103,139,158	1
55	MG	CA	1649	1/1	0.35	-	92,92,92,92	0
56	OHX	BA	1720	7/7	0.12	-	95,108,133,161	2

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3163	1/1	0.38	-	34,34,34,34	0
56	OHX	DA	3354	7/7	0.14	-	88,99,121,135	1
55	MG	DA	3247	1/1	0.34	-	48,48,48,48	0
55	MG	DA	3202	1/1	0.34	-	65,65,65,65	0
56	OHX	DA	3467	7/7	0.11	-	133,139,156,192	1
55	MG	DA	3145	1/1	0.96	-	82,82,82,82	0
55	MG	BA	1701	1/1	0.38	-	68,68,68,68	0
55	MG	BA	1671	1/1	0.47	-	68,68,68,68	0
56	OHX	BA	1767	7/7	0.08	-	151,158,165,212	1
56	OHX	DA	3370	7/7	0.12	-	94,102,123,149	1
55	MG	BA	1673	1/1	0.45	-	75,75,75,75	0
55	MG	DA	3070	1/1	0.19	-	69,69,69,69	0
55	MG	A0	201	1/1	0.15	-	52,52,52,52	0
56	OHX	DA	3224	7/7	0.35	-	104,110,126,166	1
56	OHX	DA	3438	7/7	0.12	-	120,135,146,170	1
55	MG	DA	3189	1/1	0.63	-	56,56,56,56	0
55	MG	DA	3156	1/1	0.24	-	73,73,73,73	0
55	MG	AA	3217	1/1	0.18	-	66,66,66,66	0
55	MG	CA	1670	1/1	0.18	-	95,95,95,95	0
56	OHX	BA	1755	7/7	0.08	-	123,128,136,161	1
56	OHX	CA	1726	7/7	0.14	-	89,98,100,124	1
55	MG	CA	1631	1/1	0.40	-	74,74,74,74	0
56	OHX	CB	104	7/7	0.45	-	175,181,183,194	1
55	MG	AA	3137	1/1	0.32	-	74,74,74,74	0
56	OHX	DA	3363	7/7	0.12	-	95,105,122,123	2
55	MG	AA	3240	1/1	0.47	-	56,56,56,56	0
55	MG	CA	1688	1/1	0.10	-	79,79,79,79	0
56	OHX	DA	3134	7/7	0.12	-	114,120,126,150	1
56	OHX	AA	3400	7/7	0.14	-	64,77,80,123	1
55	MG	CA	1715	1/1	0.27	-	80,80,80,80	0
55	MG	DA	3302	1/1	0.41	-	98,98,98,98	0
56	OHX	AA	3564	7/7	0.18	-	94,114,124,148	1
56	OHX	AA	3456	7/7	0.17	-	111,115,132,161	3
56	OHX	CA	1815	7/7	0.10	-	158,163,177,221	1
56	OHX	BA	1806	7/7	0.17	-	110,117,124,159	1
55	MG	BB	112	1/1	0.13	-	80,80,80,80	0
56	OHX	CA	1744	7/7	0.09	-	128,134,150,164	1
55	MG	AA	3040	1/1	0.31	-	59,59,59,59	0
56	OHX	AA	3350	7/7	0.12	-	95,103,113,148	1
55	MG	DA	3128	1/1	0.42	-	75,75,75,75	0
56	OHX	DA	3356	7/7	0.13	-	85,97,114,129	2
55	MG	AA	3227	1/1	0.40	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	OHX	DA	3245	7/7	0.12	-	95,128,139,165	1
56	OHX	AA	3381	7/7	0.11	-	127,136,147,180	1
55	MG	AA	3002	1/1	0.40	-	34,34,34,34	0
55	MG	AA	3156	1/1	0.29	-	80,80,80,80	0
56	OHX	AA	3486	7/7	0.13	-	95,110,127,153	1
55	MG	DA	3326	1/1	0.43	-	90,90,90,90	0
55	MG	BA	1644	1/1	0.33	-	62,62,62,62	0
56	OHX	DA	3437	7/7	0.14	-	113,120,134,160	1
55	MG	AA	3223	1/1	0.32	-	43,43,43,43	0
55	MG	AA	3057	1/1	0.18	-	56,56,56,56	0
55	MG	DA	3056	1/1	0.25	-	48,48,48,48	0
55	MG	AA	3181	1/1	0.47	-	71,71,71,71	0
55	MG	AA	3116	1/1	0.26	-	63,63,63,63	0
55	MG	DA	3244	1/1	0.29	-	82,82,82,82	0
55	MG	AA	3215	1/1	0.39	-	69,69,69,69	0
55	MG	AA	3271	1/1	0.42	-	63,63,63,63	0
55	MG	DA	3025	1/1	0.20	-	59,59,59,59	0
56	OHX	DA	3348	7/7	0.11	-	97,115,128,140	1
56	OHX	DA	3172	7/7	0.31	-	95,104,112,142	1
55	MG	AA	3068	1/1	0.13	-	92,92,92,92	0
55	MG	DA	3114	1/1	0.36	-	37,37,37,37	0
56	OHX	AA	3523	7/7	0.14	-	112,123,137,155	1
55	MG	CA	1615	1/1	0.21	-	109,109,109,109	0
56	OHX	AE	304	7/7	0.10	-	73,87,113,116	2
55	MG	BA	1601	1/1	0.31	-	57,57,57,57	0
55	MG	DA	3154	1/1	0.25	-	60,60,60,60	0
55	MG	DA	3035	1/1	0.31	-	95,95,95,95	0
55	MG	DA	3237	1/1	0.28	-	85,85,85,85	0
56	OHX	DA	3410	7/7	0.12	-	107,112,124,146	1
55	MG	CA	1680	1/1	0.38	-	78,78,78,78	0
55	MG	AA	3337	1/1	0.58	-	73,73,73,73	0
55	MG	DA	3280	1/1	0.45	-	63,63,63,63	0
55	MG	AA	3129	1/1	0.19	-	43,43,43,43	0
55	MG	CA	1627	1/1	0.28	-	126,126,126,126	0
55	MG	A1	202	1/1	0.19	-	75,75,75,75	0
55	MG	DA	3121	1/1	0.42	-	78,78,78,78	0
55	MG	BA	1689	1/1	0.14	-	80,80,80,80	0
55	MG	DA	3078	1/1	0.45	-	42,42,42,42	0
56	OHX	AA	3434	7/7	0.17	-	98,102,107,132	1
55	MG	AA	3062	1/1	0.25	-	97,97,97,97	0
56	OHX	BA	1808	7/7	0.17	-	121,129,141,156	1
55	MG	DA	3016	1/1	0.59	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3242	1/1	0.34	-	43,43,43,43	0
55	MG	CA	1654	1/1	0.18	-	89,89,89,89	0
55	MG	AA	3191	1/1	0.11	-	39,39,39,39	0
55	MG	AA	3169	1/1	0.50	-	47,47,47,47	0
56	OHX	CC	110	7/7	0.16	-	103,121,132,150	4
56	OHX	DA	3157	7/7	0.14	-	76,87,96,121	1
55	MG	DA	3095	1/1	0.22	-	58,58,58,58	0
55	MG	DA	3194	1/1	0.37	-	48,48,48,48	0
55	MG	CA	1691	1/1	0.19	-	128,128,128,128	0
55	MG	AA	3267	1/1	0.23	-	37,37,37,37	0
56	OHX	DA	3395	7/7	0.12	-	102,109,124,139	1
55	MG	AA	3174	1/1	0.18	-	91,91,91,91	0
55	MG	AA	3134	1/1	0.40	-	48,48,48,48	0
56	OHX	AA	3428	7/7	0.07	-	114,120,124,169	1
55	MG	BA	1625	1/1	0.33	-	66,66,66,66	0
55	MG	DA	3182	1/1	0.23	-	52,52,52,52	0
56	OHX	DA	3486	7/7	0.22	-	123,132,147,175	1
56	OHX	DA	3371	7/7	0.12	-	119,121,131,160	1
55	MG	DA	3036	1/1	0.12	-	47,47,47,47	0
55	MG	DA	3316	1/1	0.23	-	51,51,51,51	0
55	MG	AA	3310	1/1	0.18	-	71,71,71,71	0
55	MG	AA	3034	1/1	0.32	-	50,50,50,50	0
56	OHX	AA	3517	7/7	0.08	-	125,127,137,177	1
55	MG	CA	1669	1/1	0.36	-	48,48,48,48	0
56	OHX	AA	3342	7/7	0.12	-	65,86,103,114	1
56	OHX	DA	3218	7/7	0.39	-	96,106,121,133	1
55	MG	AA	3259	1/1	0.14	-	60,60,60,60	0
56	OHX	BA	1727	7/7	0.12	-	116,137,148,161	1
55	MG	CA	1607	1/1	0.26	-	86,86,86,86	0
56	OHX	DA	3362	7/7	0.20	-	83,98,103,158	1
55	MG	AA	3235	1/1	0.10	-	57,57,57,57	0
55	MG	CA	1634	1/1	0.60	-	64,64,64,64	0
55	MG	CA	1601	1/1	0.39	-	75,75,75,75	0
56	OHX	AA	3447	7/7	0.10	-	110,120,136,163	1
55	MG	AA	3109	1/1	0.36	-	38,38,38,38	0
56	OHX	BA	1796	7/7	0.26	-	119,126,142,152	1
55	MG	AA	3122	1/1	0.26	-	57,57,57,57	0
55	MG	DA	3042	1/1	0.22	-	74,74,74,74	0
56	OHX	CA	1793	7/7	0.08	-	142,146,153,194	1
55	MG	BA	1643	1/1	0.20	-	67,67,67,67	0
56	OHX	DA	3337	7/7	0.21	-	74,80,86,97	1
56	OHX	DB	214	7/7	0.12	-	145,149,169,184	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3257	1/1	0.29	-	64,64,64,64	0
58	ZN	BG	301	1/1	0.29	-	84,84,84,84	0
55	MG	BA	1612	1/1	0.36	-	100,100,100,100	0
55	MG	BA	1622	1/1	0.18	-	92,92,92,92	0
55	MG	AA	3209	1/1	0.32	-	86,86,86,86	0
56	OHX	BB	114	7/7	0.25	-	176,178,180,206	1
55	MG	DA	3276	1/1	0.40	-	78,78,78,78	0
56	OHX	AA	3513	7/7	0.19	-	120,125,139,159	2
56	OHX	DA	3383	7/7	0.12	-	110,119,138,151	2
55	MG	DA	3006	1/1	0.27	-	63,63,63,63	0
55	MG	DA	3142	1/1	0.42	-	76,76,76,76	0
55	MG	AA	3179	1/1	0.30	-	39,39,39,39	0
55	MG	DA	3113	1/1	0.17	-	73,73,73,73	0
56	OHX	DA	3081	7/7	0.14	-	99,102,113,145	1
55	MG	AA	3297	1/1	0.12	-	80,80,80,80	0
55	MG	AA	3058	1/1	0.11	-	61,61,61,61	0
56	OHX	DA	3350	7/7	0.14	-	90,99,110,132	1
56	OHX	CA	1772	7/7	0.11	-	142,144,153,197	1
55	MG	BA	1679	1/1	0.41	-	60,60,60,60	0
55	MG	DA	3098	1/1	0.19	-	63,63,63,63	0
56	OHX	CA	1773	7/7	0.11	-	123,130,144,181	1
56	OHX	AA	3414	7/7	0.11	-	92,104,120,143	1
55	MG	AA	3300	1/1	0.29	-	81,81,81,81	0
55	MG	B1	101	1/1	0.12	-	96,96,96,96	0
55	MG	CA	1651	1/1	0.18	-	73,73,73,73	0
56	OHX	BA	1802	7/7	0.09	-	100,117,125,149	1
56	OHX	DA	3062	7/7	0.17	-	70,95,103,114	1
55	MG	DA	3143	1/1	0.29	-	38,38,38,38	0
55	MG	AA	3176	1/1	0.42	-	46,46,46,46	0
56	OHX	DA	3349	7/7	0.12	-	103,105,113,143	0
56	OHX	AA	3542	7/7	0.14	-	92,98,124,157	1
55	MG	AA	3028	1/1	0.37	-	35,35,35,35	0
55	MG	BA	1619	1/1	0.39	-	64,64,64,64	0
56	OHX	DA	3405	7/7	0.17	-	129,133,151,175	1
56	OHX	BC	107	7/7	0.12	-	126,137,143,151	1
56	OHX	AA	3382	7/7	0.15	-	65,73,84,93	0
56	OHX	DA	3253	7/7	0.13	-	141,144,160,190	1
55	MG	DA	3076	1/1	0.64	-	54,54,54,54	0
55	MG	CA	1653	1/1	0.23	-	75,75,75,75	0
55	MG	AA	3105	1/1	0.48	-	65,65,65,65	0
56	OHX	DA	3474	7/7	0.22	-	120,126,143,173	1
55	MG	CA	1625	1/1	0.17	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3276	1/1	0.26	-	76,76,76,76	0
56	OHX	DA	3483	7/7	0.12	-	103,116,126,199	1
55	MG	AA	3131	1/1	0.51	-	62,62,62,62	0
56	OHX	CA	1791	7/7	0.10	-	100,118,129,154	1
55	MG	DA	3317	1/1	0.39	-	85,85,85,85	0
55	MG	BA	1688	1/1	0.19	-	79,79,79,79	0
55	MG	DA	3203	1/1	0.53	-	69,69,69,69	0
56	OHX	AA	3535	7/7	0.18	-	94,101,108,146	1
56	OHX	BA	1718	7/7	0.20	-	68,82,103,130	2
56	OHX	DA	3353	7/7	0.13	-	102,117,129,132	1
55	MG	AA	3001	1/1	0.32	-	32,32,32,32	0
56	OHX	DA	3388	7/7	0.14	-	108,118,139,160	1
56	OHX	AA	3378	7/7	0.16	-	77,88,108,118	1
56	OHX	CA	1768	7/7	0.08	-	123,135,145,174	1
56	OHX	AA	3411	7/7	0.08	-	107,117,135,154	0
55	MG	DA	3053	1/1	0.50	-	116,116,116,116	0
55	MG	DA	3231	1/1	0.36	-	50,50,50,50	0
55	MG	AA	3110	1/1	0.39	-	76,76,76,76	0
56	OHX	DA	3472	7/7	0.10	-	162,171,176,223	1
55	MG	AA	3229	1/1	0.28	-	65,65,65,65	0
56	OHX	AA	3366	7/7	0.15	-	79,94,104,141	1
55	MG	AA	3146	1/1	0.36	-	36,36,36,36	0
56	OHX	DA	3470	7/7	0.14	-	152,169,191,193	1
56	OHX	DA	3359	7/7	0.17	-	99,118,131,143	1
56	OHX	AA	3451	7/7	0.18	-	79,96,106,142	1
56	OHX	AA	3377	7/7	0.18	-	77,87,106,151	2
55	MG	CC	101	1/1	0.43	-	79,79,79,79	0
56	OHX	CA	1796	7/7	0.07	-	150,159,170,195	1
56	OHX	DA	3335	7/7	0.17	-	87,96,112,126	0
56	OHX	AA	3476	7/7	0.20	-	88,98,119,157	1
55	MG	CA	1697	1/1	0.13	-	66,66,66,66	0
55	MG	DA	3273	1/1	0.28	-	41,41,41,41	0
56	OHX	CA	1788	7/7	0.17	-	138,144,149,176	1
55	MG	DA	3180	1/1	0.39	-	45,45,45,45	0
56	OHX	AA	3512	7/7	0.16	-	110,115,138,180	2
55	MG	AA	3041	1/1	0.24	-	59,59,59,59	0
56	OHX	DA	3459	7/7	0.20	-	85,104,120,156	1
56	OHX	AA	3396	7/7	0.09	-	93,107,119,142	1
55	MG	DA	3001	1/1	0.33	-	39,39,39,39	0
55	MG	AA	3260	1/1	0.39	-	53,53,53,53	0
55	MG	BA	1705	1/1	0.09	-	109,109,109,109	0
56	OHX	DA	3423	7/7	0.09	-	127,140,151,201	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3334	1/1	0.19	-	90,90,90,90	0
56	OHX	BA	1810	7/7	0.20	-	138,141,150,186	1
55	MG	DA	3264	1/1	0.16	-	78,78,78,78	0
55	MG	DA	3141	1/1	0.25	-	64,64,64,64	0
55	MG	BA	1624	1/1	0.60	-	79,79,79,79	0
56	OHX	BA	1787	7/7	0.13	-	124,129,137,172	1
55	MG	AA	3115	1/1	0.37	-	57,57,57,57	0
55	MG	DA	3313	1/1	0.35	-	88,88,88,88	0
55	MG	AA	3168	1/1	0.41	-	36,36,36,36	0
56	OHX	AA	3352	7/7	0.16	-	80,86,96,122	1
56	OHX	AA	3439	7/7	0.14	-	114,122,140,194	1
56	OHX	BA	1807	7/7	0.12	-	133,136,150,177	1
55	MG	AA	3079	1/1	0.39	-	67,67,67,67	0
56	OHX	AA	3332	7/7	0.16	-	40,73,95,99	2
55	MG	BA	1663	1/1	0.69	-	80,80,80,80	0
55	MG	CA	1692	1/1	0.18	-	104,104,104,104	0
55	MG	AA	3324	1/1	0.20	-	84,84,84,84	0
56	OHX	DA	3436	7/7	0.12	-	121,133,143,171	1
55	MG	CA	1652	1/1	0.10	-	69,69,69,69	0
55	MG	AA	3093	1/1	0.40	-	35,35,35,35	0
56	OHX	CA	1745	7/7	0.13	-	117,120,127,165	1
56	OHX	AA	3368	7/7	0.07	-	104,115,121,140	1
55	MG	BA	1653	1/1	0.29	-	64,64,64,64	0
55	MG	AA	3322	1/1	0.22	-	81,81,81,81	0
56	OHX	AA	3473	7/7	0.22	-	104,114,132,167	1
56	OHX	AA	3548	7/7	0.15	-	125,128,143,177	1
56	OHX	BA	1776	7/7	0.28	-	119,138,152,176	2
55	MG	AA	3185	1/1	0.36	-	35,35,35,35	0
55	MG	BA	1666	1/1	0.40	-	81,81,81,81	0
55	MG	CA	1632	1/1	0.49	-	56,56,56,56	0
55	MG	BA	1610	1/1	0.10	-	75,75,75,75	0
55	MG	AA	3065	1/1	0.22	-	46,46,46,46	0
55	MG	DA	3291	1/1	0.22	-	66,66,66,66	0
56	OHX	AA	3354	7/7	0.14	-	96,105,128,164	0
56	OHX	DA	3347	7/7	0.12	-	89,99,108,134	0
55	MG	AA	3224	1/1	0.28	-	79,79,79,79	0
56	OHX	CA	1730	7/7	0.12	-	132,134,143,167	0
56	OHX	AA	3345	7/7	0.09	-	87,112,122,135	0
55	MG	BA	1683	1/1	0.30	-	85,85,85,85	0
55	MG	DA	3234	1/1	0.28	-	41,41,41,41	0
55	MG	BD	101	1/1	0.14	-	103,103,103,103	0
55	MG	BB	105	1/1	0.15	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	OHX	CA	1738	7/7	0.09	-	120,123,126,168	1
56	OHX	AA	3568	7/7	0.15	-	101,109,114,153	1
55	MG	DA	3266	1/1	0.46	-	88,88,88,88	0
56	OHX	DA	3136	7/7	0.14	-	95,108,117,144	1
56	OHX	AA	3393	7/7	0.15	-	50,81,89,115	2
56	OHX	DA	3248	7/7	0.12	-	110,118,139,156	1
55	MG	AA	3160	1/1	0.33	-	69,69,69,69	0
55	MG	CA	1638	1/1	0.35	-	59,59,59,59	0
56	OHX	CC	109	7/7	0.21	-	112,114,129,153	3
56	OHX	AA	3432	7/7	0.10	-	129,136,142,160	1
56	OHX	CA	1779	7/7	0.05	-	125,132,137,172	1
56	OHX	DA	3413	7/7	0.28	-	103,122,138,176	1
55	MG	DB	203	1/1	0.12	-	121,121,121,121	0
55	MG	DA	3287	1/1	0.26	-	102,102,102,102	0
56	OHX	AA	3346	7/7	0.17	-	73,81,101,124	2
56	OHX	DA	3071	7/7	0.13	-	107,121,146,184	0
56	OHX	DA	3430	7/7	0.06	-	176,181,185,214	1
56	OHX	CR	101	7/7	0.41	-	143,150,160,179	1
55	MG	AA	3222	1/1	0.39	-	85,85,85,85	0
56	OHX	CA	1811	7/7	0.18	-	126,129,137,159	1
55	MG	AA	3211	1/1	0.21	-	58,58,58,58	0
56	OHX	AA	3455	7/7	0.13	-	173,192,201,215	1
55	MG	BA	1655	1/1	0.32	-	84,84,84,84	0
55	MG	AA	3282	1/1	0.09	-	103,103,103,103	0
56	OHX	DA	3444	7/7	0.12	-	123,132,145,175	1
55	MG	AA	3195	1/1	0.35	-	58,58,58,58	0
55	MG	CA	1660	1/1	0.23	-	97,97,97,97	0
55	MG	BA	1704	1/1	0.11	-	127,127,127,127	0
55	MG	CA	1611	1/1	0.18	-	81,81,81,81	0
55	MG	CA	1616	1/1	0.42	-	100,100,100,100	0
56	OHX	BA	1758	7/7	0.06	-	153,155,160,202	1
56	OHX	AA	3369	7/7	0.11	-	76,100,116,143	1
56	OHX	DA	3366	7/7	0.14	-	87,100,130,154	2
56	OHX	AA	3360	7/7	0.14	-	88,94,111,129	2
55	MG	AA	3048	1/1	0.23	-	91,91,91,91	0
55	MG	AA	3285	1/1	0.27	-	77,77,77,77	0
55	MG	CA	1676	1/1	0.32	-	78,78,78,78	0
55	MG	BA	1656	1/1	0.37	-	73,73,73,73	0
55	MG	AA	3139	1/1	0.24	-	47,47,47,47	0
56	OHX	AA	3330	7/7	0.17	-	81,85,101,147	0
55	MG	AA	3261	1/1	0.21	-	53,53,53,53	0
55	MG	DA	3009	1/1	0.28	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	OHX	DA	3477	7/7	0.07	-	153,157,164,211	1
55	MG	AA	3033	1/1	0.31	-	39,39,39,39	0
55	MG	DA	3086	1/1	0.39	-	51,51,51,51	0
55	MG	DA	3017	1/1	0.48	-	66,66,66,66	0
55	MG	CA	1721	1/1	0.22	-	80,80,80,80	0
55	MG	AA	3108	1/1	0.14	-	54,54,54,54	0
55	MG	DA	3034	1/1	0.19	-	69,69,69,69	0
55	MG	AA	3061	1/1	0.22	-	59,59,59,59	0
56	OHX	AA	3375	7/7	0.11	-	83,101,103,143	1
55	MG	AA	3190	1/1	0.21	-	43,43,43,43	0
55	MG	AA	3237	1/1	0.44	-	62,62,62,62	0
55	MG	AA	3184	1/1	0.34	-	35,35,35,35	0
55	MG	DA	3020	1/1	0.60	-	60,60,60,60	0
56	OHX	AA	3507	7/7	0.48	-	120,135,161,172	2
55	MG	AA	3080	1/1	0.18	-	63,63,63,63	0
56	OHX	DA	3246	7/7	0.14	-	89,97,107,138	1
55	MG	CA	1711	1/1	0.39	-	57,57,57,57	0
56	OHX	AA	3471	7/7	0.13	-	80,105,117,155	1
55	MG	AA	3039	1/1	0.38	-	50,50,50,50	0
55	MG	DB	206	1/1	0.48	-	81,81,81,81	0
55	MG	BA	1682	1/1	0.10	-	68,68,68,68	0
56	OHX	AA	3562	7/7	0.14	-	100,110,119,157	1
55	MG	AB	202	1/1	0.22	-	80,80,80,80	0
56	OHX	AA	3364	7/7	0.15	-	72,81,97,125	1
56	OHX	AA	3477	7/7	0.13	-	81,92,107,133	2
56	OHX	CA	1780	7/7	0.09	-	138,146,156,182	1
56	OHX	DA	3358	7/7	0.10	-	107,117,135,165	2
55	MG	AA	3094	1/1	0.53	-	48,48,48,48	0
55	MG	DA	3274	1/1	0.37	-	69,69,69,69	0
55	MG	DA	3167	1/1	0.25	-	61,61,61,61	0
55	MG	DA	3089	1/1	0.41	-	54,54,54,54	0
56	OHX	CA	1790	7/7	0.18	-	99,111,123,147	2
55	MG	AA	3214	1/1	0.35	-	41,41,41,41	0
56	OHX	AA	3491	7/7	0.15	-	96,99,117,169	1
56	OHX	DA	3243	7/7	0.19	-	74,100,112,145	2
55	MG	AA	3154	1/1	0.22	-	52,52,52,52	0
56	OHX	AA	3539	7/7	0.09	-	130,133,143,179	1
55	MG	DA	3052	1/1	0.44	-	42,42,42,42	0
56	OHX	AB	213	7/7	0.15	-	88,108,129,159	3
55	MG	BA	1630	1/1	0.21	-	109,109,109,109	0
55	MG	DA	3201	1/1	0.39	-	86,86,86,86	0
55	MG	BA	1697	1/1	0.43	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	OHX	AA	3449	7/7	0.14	-	102,118,124,165	1
55	MG	DA	3281	1/1	0.22	-	65,65,65,65	0
56	OHX	BA	1809	7/7	0.07	-	159,162,164,206	1
55	MG	DA	3055	1/1	0.40	-	54,54,54,54	0
55	MG	AA	3339	1/1	0.52	-	58,58,58,58	0
55	MG	DA	3275	1/1	0.46	-	53,53,53,53	0
55	MG	AA	3280	1/1	0.37	-	61,61,61,61	0
56	OHX	DA	3406	7/7	0.12	-	88,107,111,147	3
56	OHX	AA	3371	7/7	0.17	-	65,79,88,136	2
55	MG	DA	3161	1/1	0.35	-	41,41,41,41	0
56	OHX	DA	3379	7/7	0.13	-	116,134,147,164	1
55	MG	AA	3232	1/1	0.10	-	62,62,62,62	0
55	MG	DA	3069	1/1	0.11	-	63,63,63,63	0
55	MG	DA	3210	1/1	0.74	-	73,73,73,73	0
55	MG	CA	1623	1/1	0.24	-	96,96,96,96	0
56	OHX	DA	3427	7/7	0.12	-	134,147,151,184	1
56	OHX	DA	3163	7/7	0.18	-	124,127,154,166	1
56	OHX	DA	3386	7/7	0.11	-	108,110,132,139	1
55	MG	AA	3162	1/1	0.23	-	48,48,48,48	0
55	MG	AA	3036	1/1	0.44	-	48,48,48,48	0
55	MG	DA	3175	1/1	0.41	-	53,53,53,53	0
56	OHX	AA	3424	7/7	0.16	-	84,93,116,147	1
56	OHX	DB	211	7/7	0.12	-	105,121,145,156	2
56	OHX	DA	3440	7/7	0.15	-	142,144,161,189	1
55	MG	BA	1707	1/1	0.10	-	63,63,63,63	0
55	MG	DA	3104	1/1	0.35	-	64,64,64,64	0
55	MG	DA	3072	1/1	0.08	-	93,93,93,93	0
56	OHX	DA	3257	7/7	0.22	-	107,112,124,148	1
55	MG	DA	3181	1/1	0.31	-	98,98,98,98	0
56	OHX	CA	1732	7/7	0.12	-	112,117,126,152	1
55	MG	DB	204	1/1	0.24	-	76,76,76,76	0
55	MG	BS	101	1/1	0.27	-	81,81,81,81	0
55	MG	DA	3040	1/1	0.21	-	66,66,66,66	0
55	MG	AA	3298	1/1	0.24	-	45,45,45,45	0
55	MG	DA	3012	1/1	0.30	-	44,44,44,44	0
55	MG	AA	3007	1/1	0.36	-	43,43,43,43	0
56	OHX	AA	3421	7/7	0.13	-	78,84,91,130	1
56	OHX	AA	3327	7/7	0.21	-	38,70,106,113	0
55	MG	BA	1631	1/1	0.09	-	85,85,85,85	0
55	MG	CA	1620	1/1	0.22	-	63,63,63,63	0
56	OHX	CA	1739	7/7	0.09	-	140,150,165,188	1
56	OHX	AA	3426	7/7	0.11	-	104,117,127,168	3

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	OHX	DA	3445	7/7	0.10	-	121,130,142,174	1
55	MG	AA	3219	1/1	0.27	-	65,65,65,65	0
55	MG	CA	1613	1/1	0.26	-	73,73,73,73	0
56	OHX	DB	209	7/7	0.15	-	130,143,158,186	1
56	OHX	AA	3418	7/7	0.15	-	96,110,119,135	1
55	MG	BA	1621	1/1	0.26	-	77,77,77,77	0
55	MG	CA	1686	1/1	0.57	-	110,110,110,110	0
55	MG	AA	3270	1/1	0.35	-	90,90,90,90	0
56	OHX	AA	3556	7/7	0.12	-	82,96,111,154	1
55	MG	AA	3319	1/1	0.09	-	63,63,63,63	0
55	MG	AA	3226	1/1	0.51	-	68,68,68,68	0
55	MG	BA	1677	1/1	0.42	-	101,101,101,101	0
56	OHX	BB	115	7/7	0.20	-	90,109,116,116	3
55	MG	BA	1620	1/1	0.24	-	73,73,73,73	0
56	OHX	CA	1760	7/7	0.07	-	145,148,151,188	1
55	MG	AA	3220	1/1	0.25	-	38,38,38,38	0
56	OHX	CA	1728	7/7	0.14	-	104,119,138,150	2
56	OHX	BA	1719	7/7	0.14	-	85,102,114,124	1
56	OHX	AA	3384	7/7	0.10	-	96,100,107,136	1
55	MG	DB	202	1/1	0.17	-	98,98,98,98	0
56	OHX	CA	1787	7/7	0.16	-	117,122,135,155	1
55	MG	CC	107	1/1	0.26	-	80,80,80,80	0
56	OHX	AA	3529	7/7	0.17	-	114,130,134,179	1
56	OHX	DB	220	7/7	0.20	-	159,162,171,208	1
55	MG	DA	3282	1/1	0.35	-	69,69,69,69	0
55	MG	DA	3200	1/1	1.01	-	86,86,86,86	0
56	OHX	CA	1749	7/7	0.14	-	124,137,161,188	2
56	OHX	AA	3482	7/7	0.21	-	85,96,105,135	1
55	MG	DA	3298	1/1	0.30	-	102,102,102,102	0
55	MG	CA	1718	1/1	0.30	-	84,84,84,84	0
56	OHX	AA	3569	7/7	0.11	-	134,142,144,168	1
55	MG	DA	3206	1/1	0.12	-	52,52,52,52	0
56	OHX	BA	1743	7/7	0.20	-	79,96,129,159	2
55	MG	BA	1698	1/1	0.37	-	54,54,54,54	0
56	OHX	AA	3438	7/7	0.10	-	113,130,139,188	1
55	MG	AA	3277	1/1	0.48	-	94,94,94,94	0
56	OHX	DA	3415	7/7	0.16	-	128,140,160,189	1
56	OHX	DA	3357	7/7	0.12	-	100,118,130,150	1
56	OHX	BA	1733	7/7	0.09	-	98,108,118,146	1
56	OHX	AA	3425	7/7	0.09	-	158,168,177,207	1
56	OHX	AA	3420	7/7	0.21	-	112,125,135,178	2
58	ZN	CQ	101	1/1	0.12	-	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3043	1/1	0.42	-	73,73,73,73	0
56	OHX	BA	1811	7/7	0.13	-	110,118,135,147	1
55	MG	DA	3153	1/1	0.42	-	69,69,69,69	0
56	OHX	AA	3445	7/7	0.12	-	118,124,140,177	1
56	OHX	AA	3464	7/7	0.12	-	105,115,140,175	1
56	OHX	D5	102	7/7	0.32	-	114,129,141,158	1
55	MG	AA	3182	1/1	0.37	-	66,66,66,66	0
56	OHX	DA	3465	7/7	0.13	-	123,136,143,165	1
56	OHX	AA	3501	7/7	0.10	-	104,117,124,169	1
56	OHX	BA	1752	7/7	0.07	-	168,174,177,207	1
56	OHX	BD	103	7/7	0.14	-	108,110,116,155	1
56	OHX	CA	1724	7/7	0.11	-	88,111,121,131	0
56	OHX	DA	3401	7/7	0.11	-	108,115,120,150	1
56	OHX	DA	3364	7/7	0.13	-	75,93,104,118	1
55	MG	DA	3039	1/1	0.20	-	102,102,102,102	0
55	MG	AA	3017	1/1	0.37	-	26,26,26,26	0
56	OHX	AA	3525	7/7	0.11	-	118,124,140,179	1
55	MG	AA	3144	1/1	0.34	-	43,43,43,43	0
56	OHX	AA	3446	7/7	0.15	-	148,150,154,190	1
55	MG	AB	206	1/1	0.48	-	77,77,77,77	0
55	MG	AA	3239	1/1	0.52	-	52,52,52,52	0
56	OHX	CA	1814	7/7	0.07	-	149,152,161,212	1
55	MG	AA	3201	1/1	0.41	-	35,35,35,35	0
55	MG	DA	3268	1/1	0.32	-	44,44,44,44	0
56	OHX	AA	3388	7/7	0.11	-	106,112,125,156	1
55	MG	BB	111	1/1	0.23	-	80,80,80,80	0
56	OHX	CA	1759	7/7	0.16	-	125,133,140,148	1
56	OHX	AA	3550	7/7	0.10	-	118,128,136,169	1
56	OHX	AA	3481	7/7	0.14	-	88,92,119,127	2
56	OHX	AA	3533	7/7	0.09	-	79,94,100,134	1
56	OHX	AA	3340	7/7	0.14	-	84,93,95,126	0
56	OHX	BG	302	7/7	0.10	-	138,141,145,177	1
56	OHX	CA	1808	7/7	0.15	-	163,164,177,210	1
55	MG	DA	3002	1/1	0.51	-	46,46,46,46	0
56	OHX	CA	1751	7/7	0.18	-	102,126,129,174	1
56	OHX	DA	3342	7/7	0.13	-	79,85,102,102	2
55	MG	AA	3051	1/1	0.40	-	69,69,69,69	0
55	MG	DA	3228	1/1	0.40	-	58,58,58,58	0
55	MG	AA	3372	1/1	0.27	-	80,80,80,80	0
56	OHX	AA	3494	7/7	0.12	-	112,122,130,153	1
56	OHX	AA	3450	7/7	0.11	-	97,112,128,161	2
56	OHX	AA	3379	7/7	0.23	-	20,47,62,138	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CB	103	1/1	0.13	-	80,80,80,80	0
56	OHX	CA	1799	7/7	0.38	-	142,145,160,170	1
56	OHX	CA	1776	7/7	0.16	-	112,115,132,151	1
55	MG	CA	1637	1/1	0.49	-	69,69,69,69	0
55	MG	AA	3119	1/1	0.24	-	86,86,86,86	0
55	MG	DA	3305	1/1	0.22	-	48,48,48,48	0
56	OHX	DA	3376	7/7	0.18	-	38,106,133,165	3
56	OHX	AA	3497	7/7	0.25	-	105,127,139,145	1
55	MG	BA	1626	1/1	0.54	-	47,47,47,47	0
55	MG	AA	3262	1/1	0.28	-	62,62,62,62	0
55	MG	BA	1602	1/1	0.23	-	66,66,66,66	0
56	OHX	AA	3415	7/7	0.07	-	90,93,100,146	1
55	MG	AA	3005	1/1	0.36	-	48,48,48,48	0
56	OHX	CD	101	7/7	0.09	-	166,174,199,220	1
55	MG	BA	1703	1/1	0.19	-	90,90,90,90	0
55	MG	DA	3285	1/1	0.40	-	57,57,57,57	0
56	OHX	AB	218	7/7	0.13	-	138,141,157,181	1
55	MG	AA	3308	1/1	0.34	-	63,63,63,63	0
56	OHX	AB	211	7/7	0.11	-	124,127,142,178	1
56	OHX	CA	1767	7/7	0.28	-	110,139,162,203	1
56	OHX	DB	212	7/7	0.11	-	144,152,161,194	1
55	MG	DA	3147	1/1	0.30	-	55,55,55,55	0
56	OHX	DA	3491	7/7	0.09	-	104,107,129,176	1
56	OHX	BC	106	7/7	0.15	-	119,120,134,160	1
55	MG	CA	1719	1/1	0.32	-	94,94,94,94	0
55	MG	DA	3290	1/1	0.15	-	37,37,37,37	0
56	OHX	DA	3385	7/7	0.15	-	78,128,134,201	1
55	MG	BA	1609	1/1	0.26	-	65,65,65,65	0
55	MG	C1	101	1/1	0.28	-	102,102,102,102	0
55	MG	AA	3221	1/1	0.30	-	41,41,41,41	0
55	MG	AA	3145	1/1	0.31	-	27,27,27,27	0
55	MG	CA	1702	1/1	0.45	-	59,59,59,59	0
56	OHX	BA	1762	7/7	0.17	-	121,131,144,180	1
55	MG	BA	1712	1/1	0.06	-	74,74,74,74	0
56	OHX	BA	1814	7/7	0.10	-	88,100,109,173	0
56	OHX	AA	3417	7/7	0.21	-	90,102,131,147	3
56	OHX	AA	3328	7/7	0.17	-	67,76,86,89	1
55	MG	DA	3331	1/1	0.37	-	69,69,69,69	0
55	MG	DA	3227	1/1	0.27	-	44,44,44,44	0
55	MG	DA	3193	1/1	0.31	-	43,43,43,43	0
55	MG	AA	3047	1/1	0.31	-	65,65,65,65	0
55	MG	DA	3050	1/1	0.79	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	OHX	CB	105	7/7	0.33	-	139,142,156,183	2
56	OHX	AA	3444	7/7	0.13	-	79,89,101,122	2
56	OHX	CA	1741	7/7	0.11	-	101,122,129,156	2
56	OHX	DA	3367	7/7	0.20	-	100,113,133,149	1
55	MG	CA	1671	1/1	0.30	-	78,78,78,78	0
56	OHX	AB	215	7/7	0.17	-	110,123,130,165	1
56	OHX	AA	3385	7/7	0.16	-	73,87,109,139	2
55	MG	BA	1618	1/1	0.25	-	71,71,71,71	0
55	MG	AA	3316	1/1	0.18	-	79,79,79,79	0
56	OHX	CA	1782	7/7	0.19	-	134,137,147,160	1
56	OHX	BA	1794	7/7	0.10	-	156,163,165,204	1
55	MG	CA	1622	1/1	0.43	-	89,89,89,89	0
55	MG	DA	3225	1/1	0.40	-	55,55,55,55	0
56	OHX	AA	3508	7/7	0.11	-	192,206,214,236	1
55	MG	CA	1612	1/1	0.22	-	95,95,95,95	0
55	MG	DA	3037	1/1	0.43	-	73,73,73,73	0
56	OHX	DA	3424	7/7	0.21	-	124,129,137,157	2
56	OHX	DA	3162	7/7	0.18	-	128,132,141,207	0
55	MG	AA	3027	1/1	0.26	-	35,35,35,35	0
55	MG	CA	1645	1/1	0.49	-	58,58,58,58	0
55	MG	DA	3077	1/1	0.54	-	52,52,52,52	0
55	MG	AA	3099	1/1	0.34	-	60,60,60,60	0
55	MG	BA	1710	1/1	0.29	-	113,113,113,113	0
55	MG	AA	3090	1/1	0.34	-	78,78,78,78	0
56	OHX	DA	3373	7/7	0.17	-	93,104,119,171	1
55	MG	CA	1643	1/1	0.47	-	68,68,68,68	0
55	MG	AA	3266	1/1	0.41	-	62,62,62,62	0
55	MG	AA	3189	1/1	0.31	-	63,63,63,63	0
55	MG	DA	3019	1/1	0.28	-	41,41,41,41	0
55	MG	DA	3049	1/1	0.42	-	104,104,104,104	0
55	MG	DA	3205	1/1	0.13	-	106,106,106,106	0
55	MG	CA	1635	1/1	0.34	-	51,51,51,51	0
56	OHX	DA	3254	7/7	0.27	-	126,129,138,165	1
55	MG	DA	3191	1/1	0.40	-	66,66,66,66	0
55	MG	CC	105	1/1	0.49	-	66,66,66,66	0
55	MG	DA	3322	1/1	0.16	-	152,152,152,152	0
56	OHX	AA	3353	7/7	0.18	-	71,99,117,132	1
55	MG	DA	3293	1/1	0.45	-	88,88,88,88	0
55	MG	BA	1623	1/1	0.42	-	39,39,39,39	0
55	MG	AF	301	1/1	0.07	-	74,74,74,74	0
55	MG	AA	3066	1/1	0.24	-	62,62,62,62	0
56	OHX	AA	3403	7/7	0.16	-	59,89,94,139	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3138	1/1	0.35	-	43,43,43,43	0
56	OHX	BR	101	7/7	0.17	-	132,137,152,164	1
55	MG	DA	3328	1/1	0.25	-	99,99,99,99	0
55	MG	AA	3314	1/1	0.14	-	63,63,63,63	0
55	MG	DA	3230	1/1	0.19	-	51,51,51,51	0
55	MG	AA	3136	1/1	0.21	-	42,42,42,42	0
55	MG	AA	3077	1/1	0.40	-	39,39,39,39	0
55	MG	AA	3241	1/1	0.29	-	52,52,52,52	0
55	MG	DA	3088	1/1	0.28	-	47,47,47,47	0
55	MG	AA	3183	1/1	0.27	-	59,59,59,59	0
55	MG	DA	3284	1/1	0.26	-	89,89,89,89	0
56	OHX	AA	3527	7/7	0.09	-	147,148,161,187	1
56	OHX	AA	3349	7/7	0.09	-	94,104,124,143	0
56	OHX	AA	3347	7/7	0.15	-	74,77,98,102	2
55	MG	BA	1611	1/1	0.32	-	47,47,47,47	0
56	OHX	AA	3469	7/7	0.08	-	103,113,128,153	1
56	OHX	AA	3503	7/7	0.25	-	99,108,119,150	1
56	OHX	A1	204	7/7	0.15	-	107,117,147,182	3
55	MG	AA	3188	1/1	0.15	-	29,29,29,29	0
55	MG	BA	1659	1/1	0.48	-	43,43,43,43	0
55	MG	AA	3167	1/1	0.17	-	51,51,51,51	0
55	MG	AA	3069	1/1	0.17	-	54,54,54,54	0
56	OHX	BA	1742	7/7	0.12	-	149,155,172,201	1
55	MG	AA	3251	1/1	0.57	-	75,75,75,75	0
56	OHX	D8	101	7/7	0.20	-	140,149,164,175	1
56	OHX	DA	3464	7/7	0.26	-	117,129,143,171	1
56	OHX	AA	3442	7/7	0.13	-	97,106,127,148	1
55	MG	AA	3157	1/1	0.40	-	86,86,86,86	0
55	MG	AA	3126	1/1	0.29	-	54,54,54,54	0
56	OHX	BA	1774	7/7	0.12	-	104,121,130,163	1
56	OHX	AA	3406	7/7	0.11	-	93,96,102,133	1
55	MG	AA	3228	1/1	0.40	-	53,53,53,53	0
56	OHX	DA	3170	7/7	0.13	-	114,125,135,172	1
55	MG	DB	205	1/1	0.19	-	64,64,64,64	0
55	MG	BB	102	1/1	0.32	-	92,92,92,92	0
56	OHX	AA	3530	7/7	0.28	-	117,123,125,163	1
55	MG	DA	3309	1/1	0.17	-	68,68,68,68	0
55	MG	DA	3030	1/1	0.24	-	94,94,94,94	0
56	OHX	DA	3365	7/7	0.11	-	100,119,136,159	2
56	OHX	DA	3360	7/7	0.14	-	72,81,91,113	1
56	OHX	BA	1789	7/7	0.05	-	132,137,146,191	1
56	OHX	BA	1732	7/7	0.11	-	128,131,145,175	2

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1699	1/1	0.44	-	86,86,86,86	0
55	MG	A3	101	1/1	0.39	-	71,71,71,71	0
55	MG	CA	1674	1/1	0.60	-	97,97,97,97	0
56	OHX	DA	3479	7/7	0.12	-	150,159,164,201	1
56	OHX	BA	1726	7/7	0.08	-	134,139,145,195	0
55	MG	CA	1644	1/1	0.34	-	89,89,89,89	0
56	OHX	AB	214	7/7	0.14	-	125,133,135,173	1
56	OHX	CA	1774	7/7	0.20	-	137,150,161,190	1
55	MG	AA	3289	1/1	0.39	-	61,61,61,61	0
56	OHX	BA	1766	7/7	0.19	-	108,139,151,181	2
56	OHX	DA	3442	7/7	0.11	-	135,142,161,190	1
55	MG	CB	102	1/1	0.40	-	80,80,80,80	0
55	MG	AA	3161	1/1	0.21	-	57,57,57,57	0
55	MG	AA	3045	1/1	0.17	-	33,33,33,33	0
55	MG	AA	3063	1/1	0.33	-	45,45,45,45	0
55	MG	AA	3074	1/1	0.13	-	90,90,90,90	0
57	PAR	BA	1715	42/42	0.17	-	61,73,83,89	0
55	MG	DA	3119	1/1	0.31	-	38,38,38,38	0
55	MG	AA	3130	1/1	0.34	-	43,43,43,43	0
55	MG	AA	3284	1/1	0.31	-	68,68,68,68	0
55	MG	AA	3038	1/1	0.41	-	68,68,68,68	0
55	MG	AA	3311	1/1	0.32	-	90,90,90,90	0
55	MG	DA	3270	1/1	0.63	-	73,73,73,73	0
56	OHX	CA	1748	7/7	0.08	-	137,145,152,186	1
56	OHX	AA	3478	7/7	0.17	-	147,161,167,217	1
56	OHX	DA	3428	7/7	0.15	-	93,108,120,163	1
55	MG	AA	3086	1/1	0.34	-	73,73,73,73	0
55	MG	CA	1716	1/1	0.34	-	79,79,79,79	0
55	MG	AA	3246	1/1	0.29	-	44,44,44,44	0
55	MG	BA	1670	1/1	0.33	-	100,100,100,100	0
56	OHX	AA	3409	7/7	0.13	-	99,110,115,152	1
56	OHX	AA	3492	7/7	0.10	-	139,142,151,196	1
55	MG	DB	201	1/1	0.12	-	95,95,95,95	0
56	OHX	AA	3466	7/7	0.10	-	98,120,132,157	1
55	MG	DA	3314	1/1	0.18	-	70,70,70,70	0
55	MG	AA	3216	1/1	0.45	-	33,33,33,33	0
55	MG	DA	3261	1/1	0.38	-	53,53,53,53	0
55	MG	AA	3304	1/1	0.15	-	55,55,55,55	0
56	OHX	AA	3392	7/7	0.18	-	81,92,124,181	2
55	MG	DA	3125	1/1	0.27	-	54,54,54,54	0
55	MG	AA	3302	1/1	0.42	-	72,72,72,72	0
55	MG	DA	3080	1/1	0.34	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3051	1/1	0.46	-	39,39,39,39	0
56	OHX	CA	1794	7/7	0.17	-	102,115,122,149	1
55	MG	DA	3048	1/1	0.47	-	93,93,93,93	0
55	MG	AA	3278	1/1	0.51	-	73,73,73,73	0
56	OHX	A6	101	7/7	0.14	-	112,127,141,158	2
55	MG	CA	1682	1/1	0.25	-	107,107,107,107	0
56	OHX	AA	3398	7/7	0.14	-	90,95,125,158	1
55	MG	AA	3078	1/1	0.24	-	97,97,97,97	0
55	MG	BA	1667	1/1	0.51	-	73,73,73,73	0
55	MG	AA	3111	1/1	0.33	-	69,69,69,69	0
56	OHX	BA	1785	7/7	0.12	-	117,124,136,144	2
55	MG	CA	1657	1/1	0.16	-	81,81,81,81	0
55	MG	BA	1638	1/1	0.29	-	104,104,104,104	0
56	OHX	DA	3369	7/7	0.13	-	89,100,105,125	1
55	MG	DA	3233	1/1	0.27	-	65,65,65,65	0
55	MG	AA	3147	1/1	0.37	-	49,49,49,49	0
56	OHX	DB	215	7/7	0.16	-	147,149,158,191	1
55	MG	AA	3272	1/1	0.38	-	29,29,29,29	0
56	OHX	DA	3124	7/7	0.16	-	144,164,170,220	1
56	OHX	BA	1790	7/7	0.08	-	163,166,178,211	1
55	MG	CA	1694	1/1	0.29	-	89,89,89,89	0
55	MG	CA	1608	1/1	0.27	-	76,76,76,76	0
55	MG	AA	3274	1/1	0.10	-	36,36,36,36	0
56	OHX	DA	3422	7/7	0.13	-	92,100,111,154	1
56	OHX	DA	3489	7/7	0.13	-	117,121,134,153	1
56	OHX	AA	3410	7/7	0.13	-	91,99,106,125	1
56	OHX	AA	3563	7/7	0.13	-	128,136,143,179	1
56	OHX	AA	3522	7/7	0.21	-	74,93,104,150	2
55	MG	CA	1646	1/1	0.17	-	79,79,79,79	0
55	MG	CA	1714	1/1	0.38	-	84,84,84,84	0
55	MG	DA	3100	1/1	0.32	-	87,87,87,87	0
56	OHX	AA	3359	7/7	0.12	-	91,110,118,137	1
56	OHX	DA	3215	7/7	0.14	-	97,115,127,150	3
55	MG	BC	101	1/1	0.32	-	62,62,62,62	0
56	OHX	DA	3469	7/7	0.17	-	116,119,133,163	1
55	MG	AA	3132	1/1	0.49	-	48,48,48,48	0
55	MG	AA	3098	1/1	0.28	-	29,29,29,29	0
55	MG	AA	3072	1/1	0.37	-	73,73,73,73	0
55	MG	DA	3207	1/1	0.25	-	37,37,37,37	0
55	MG	DA	3303	1/1	0.21	-	97,97,97,97	0
55	MG	AA	3202	1/1	0.20	-	30,30,30,30	0
55	MG	DA	3028	1/1	0.44	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	OHX	DB	216	7/7	0.12	-	123,138,155,204	1
55	MG	CA	1713	1/1	0.20	-	114,114,114,114	0
56	OHX	DA	3109	7/7	0.33	-	99,116,138,153	1
55	MG	AA	3035	1/1	0.18	-	38,38,38,38	0
55	MG	CA	1663	1/1	0.17	-	65,65,65,65	0
56	OHX	DA	3176	7/7	0.22	-	162,165,176,192	1
56	OHX	DA	3091	7/7	0.15	-	103,121,134,170	1
56	OHX	AA	3431	7/7	0.11	-	101,115,120,168	1
56	OHX	AA	3544	7/7	0.21	-	118,127,137,169	1
56	OHX	AA	3541	7/7	0.39	-	131,134,141,173	1
55	MG	BA	1603	1/1	0.17	-	40,40,40,40	0
56	OHX	DA	3463	7/7	0.18	-	142,149,156,188	1
55	MG	AA	3253	1/1	0.35	-	49,49,49,49	0
56	OHX	BA	1792	7/7	0.14	-	118,131,146,181	1
55	MG	AA	3128	1/1	0.30	-	53,53,53,53	0
55	MG	AE	301	1/1	0.32	-	51,51,51,51	0
55	MG	AA	3192	1/1	0.37	-	34,34,34,34	0
56	OHX	CK	201	7/7	0.28	-	143,148,155,179	1
56	OHX	DA	3439	7/7	0.13	-	127,146,152,174	1
56	OHX	BA	1759	7/7	0.07	-	173,177,187,214	1
55	MG	BA	1672	1/1	0.24	-	82,82,82,82	0
56	OHX	CA	1761	7/7	0.08	-	133,143,154,174	1
56	OHX	AA	3566	7/7	0.14	-	171,177,185,204	1
56	OHX	AA	3422	7/7	0.20	-	63,104,126,147	2
55	MG	AA	3357	1/1	0.24	-	69,69,69,69	0
55	MG	DA	3044	1/1	0.32	-	100,100,100,100	0
55	MG	AA	3089	1/1	0.26	-	130,130,130,130	0
56	OHX	AA	3531	7/7	0.12	-	225,229,234,256	1
56	OHX	CA	1740	7/7	0.08	-	125,134,139,166	1
56	OHX	AA	3430	7/7	0.08	-	119,125,132,176	1
55	MG	BA	1635	1/1	0.08	-	86,86,86,86	0
55	MG	CA	1658	1/1	0.31	-	65,65,65,65	0
55	MG	BA	1645	1/1	0.12	-	76,76,76,76	0
56	OHX	AA	3460	7/7	0.10	-	131,133,148,193	1
56	OHX	CA	1731	7/7	0.17	-	90,118,129,156	1
55	MG	DA	3300	1/1	0.25	-	63,63,63,63	0
55	MG	A1	201	1/1	0.32	-	62,62,62,62	0
55	MG	DA	3294	1/1	0.15	-	74,74,74,74	0
55	MG	AA	3318	1/1	0.23	-	75,75,75,75	0
55	MG	DA	3059	1/1	0.27	-	40,40,40,40	0
55	MG	CA	1661	1/1	0.48	-	83,83,83,83	0
55	MG	C1	102	1/1	0.42	-	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	1640	1/1	0.19	-	71,71,71,71	0
56	OHX	CA	1754	7/7	0.15	-	116,125,134,168	1
56	OHX	AA	3429	7/7	0.14	-	84,97,102,156	1
56	OHX	BA	1730	7/7	0.12	-	106,118,135,150	1
56	OHX	DA	3425	7/7	0.09	-	125,134,139,188	1
56	OHX	DA	3118	7/7	0.18	-	99,101,123,146	3
56	OHX	DA	3249	7/7	0.12	-	93,103,118,149	1
55	MG	DA	3184	1/1	0.51	-	37,37,37,37	0
56	OHX	AA	3520	7/7	0.24	-	88,95,98,151	2
56	OHX	AW	101	7/7	0.16	-	112,118,129,149	1
56	OHX	AA	3329	7/7	0.16	-	73,97,104,113	0
55	MG	DA	3140	1/1	0.39	-	55,55,55,55	0
55	MG	BA	1616	1/1	0.07	-	101,101,101,101	0
56	OHX	DA	3471	7/7	0.12	-	112,124,129,160	1
56	OHX	DA	3434	7/7	0.12	-	127,134,154,190	1
56	OHX	CA	1743	7/7	0.10	-	101,120,132,162	1
56	OHX	CA	1777	7/7	0.08	-	157,162,168,202	1
55	MG	CA	1673	1/1	0.35	-	76,76,76,76	0
56	OHX	DA	3451	7/7	0.11	-	103,107,114,153	1
56	OHX	AA	3558	7/7	0.14	-	92,100,110,168	1
55	MG	AA	3015	1/1	0.29	-	44,44,44,44	0
56	OHX	BA	1723	7/7	0.15	-	93,106,124,143	1
55	MG	BA	1650	1/1	0.20	-	85,85,85,85	0
55	MG	DA	3031	1/1	0.20	-	77,77,77,77	0
56	OHX	DA	3351	7/7	0.12	-	87,96,108,109	1
55	MG	AA	3165	1/1	0.54	-	79,79,79,79	0
56	OHX	AA	3391	7/7	0.14	-	69,80,102,109	3
56	OHX	AA	3462	7/7	0.17	-	105,108,119,142	2
56	OHX	BA	1783	7/7	0.09	-	121,130,148,178	1
55	MG	BA	1695	1/1	0.16	-	132,132,132,132	0
56	OHX	D3	101	7/7	0.13	-	129,139,156,171	2
55	MG	BA	1664	1/1	0.27	-	54,54,54,54	0
55	MG	AA	3071	1/1	0.42	-	84,84,84,84	0
56	OHX	A1	203	7/7	0.16	-	97,103,123,154	1
56	OHX	AA	3505	7/7	0.14	-	143,150,161,212	1
55	MG	DA	3013	1/1	0.37	-	40,40,40,40	0
55	MG	BA	1692	1/1	0.12	-	73,73,73,73	0
56	OHX	AA	3489	7/7	0.10	-	136,140,156,178	1
55	MG	BA	1709	1/1	0.16	-	68,68,68,68	0
55	MG	CA	1617	1/1	0.13	-	126,126,126,126	0
55	MG	AA	3049	1/1	0.17	-	66,66,66,66	0
55	MG	BA	1627	1/1	0.16	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1656	1/1	0.29	-	94,94,94,94	0
56	OHX	AA	3380	7/7	0.14	-	86,90,110,143	1
55	MG	BA	1693	1/1	0.14	-	68,68,68,68	0
55	MG	BA	1702	1/1	0.38	-	84,84,84,84	0
56	OHX	AA	3521	7/7	0.12	-	103,107,119,167	2
55	MG	AA	3197	1/1	0.27	-	57,57,57,57	0
56	OHX	AA	3412	7/7	0.13	-	119,122,141,174	1
55	MG	CA	1707	1/1	0.17	-	97,97,97,97	0
55	MG	AA	3234	1/1	0.13	-	68,68,68,68	0
56	OHX	AA	3554	7/7	0.18	-	138,143,153,173	1
56	OHX	DA	3377	7/7	0.14	-	91,105,111,146	2
55	MG	CA	1672	1/1	0.80	-	125,125,125,125	0
55	MG	AA	3060	1/1	0.21	-	89,89,89,89	0
55	MG	AE	303	1/1	0.19	-	36,36,36,36	0
56	OHX	BA	1747	7/7	0.21	-	117,129,140,148	1
56	OHX	AA	3331	7/7	0.17	-	93,94,108,145	0
56	OHX	AA	3470	7/7	0.08	-	116,126,152,171	1
56	OHX	AA	3567	7/7	0.13	-	125,135,148,181	2
56	OHX	BA	1770	7/7	0.10	-	114,115,121,163	1
55	MG	AA	3307	1/1	0.31	-	72,72,72,72	0
55	MG	CA	1705	1/1	0.40	-	73,73,73,73	0
55	MG	BA	1606	1/1	0.20	-	70,70,70,70	0
55	MG	AA	3022	1/1	0.34	-	28,28,28,28	0
56	OHX	AB	208	7/7	0.14	-	95,117,137,155	2
56	OHX	BA	1756	7/7	0.08	-	153,171,174,206	1
55	MG	AA	3100	1/1	0.33	-	58,58,58,58	0
55	MG	AA	3207	1/1	0.50	-	44,44,44,44	0
56	OHX	AA	3463	7/7	0.13	-	94,102,127,154	1
55	MG	AA	3203	1/1	0.40	-	72,72,72,72	0
55	MG	DA	3054	1/1	0.15	-	56,56,56,56	0
56	OHX	DA	3390	7/7	0.08	-	117,127,135,170	1
55	MG	BB	109	1/1	0.19	-	80,80,80,80	0
56	OHX	BA	1750	7/7	0.15	-	112,129,139,168	1
56	OHX	AA	3514	7/7	0.12	-	126,137,144,183	1
55	MG	DA	3301	1/1	0.34	-	60,60,60,60	0
55	MG	BA	1657	1/1	0.34	-	87,87,87,87	0
55	MG	AA	3042	1/1	0.23	-	42,42,42,42	0
55	MG	CA	1695	1/1	0.12	-	94,94,94,94	0
55	MG	AA	3210	1/1	0.53	-	43,43,43,43	0
55	MG	DA	3296	1/1	0.43	-	103,103,103,103	0
55	MG	DA	3155	1/1	0.34	-	58,58,58,58	0
56	OHX	AA	3537	7/7	0.08	-	164,173,184,214	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3232	1/1	0.59	-	63,63,63,63	0
56	OHX	DA	3171	7/7	0.18	-	95,116,127,171	1
56	OHX	BA	1793	7/7	0.18	-	129,132,141,164	1
56	OHX	AA	3351	7/7	0.13	-	60,68,78,99	3
56	OHX	BA	1784	7/7	0.14	-	94,101,111,137	1
55	MG	DA	3216	1/1	0.36	-	71,71,71,71	0
55	MG	DA	3211	1/1	0.40	-	57,57,57,57	0
55	MG	BA	1696	1/1	0.28	-	94,94,94,94	0
56	OHX	CA	1795	7/7	0.11	-	115,125,132,165	1
56	OHX	AA	3510	7/7	0.12	-	98,106,123,159	1
56	OHX	DA	3426	7/7	0.07	-	118,125,141,168	1
55	MG	AA	3254	1/1	0.32	-	43,43,43,43	0
56	OHX	BA	1722	7/7	0.07	-	114,116,123,159	0
55	MG	AA	3198	1/1	0.27	-	34,34,34,34	0
56	OHX	AA	3511	7/7	0.14	-	133,137,167,178	2
56	OHX	BA	1757	7/7	0.18	-	86,113,131,156	4
55	MG	DA	3003	1/1	0.25	-	43,43,43,43	0
55	MG	DA	3239	1/1	0.19	-	79,79,79,79	0
55	MG	AB	204	1/1	0.44	-	80,80,80,80	0
55	MG	DA	3269	1/1	0.41	-	52,52,52,52	0
55	MG	AA	3008	1/1	0.37	-	32,32,32,32	0
55	MG	AA	3029	1/1	0.29	-	59,59,59,59	0
56	OHX	BA	1797	7/7	0.15	-	117,130,138,173	1
56	OHX	AA	3361	7/7	0.12	-	76,81,111,125	3
55	MG	AA	3199	1/1	0.51	-	75,75,75,75	0
55	MG	DA	3060	1/1	0.46	-	77,77,77,77	0
56	OHX	CA	1765	7/7	0.07	-	169,177,182,233	1
56	OHX	DA	3407	7/7	0.14	-	124,134,145,191	1
56	OHX	DA	3476	7/7	0.12	-	126,136,143,174	1
56	OHX	AA	3461	7/7	0.12	-	102,110,120,148	1
56	OHX	CA	1762	7/7	0.08	-	148,151,154,182	1
55	MG	CA	1693	1/1	0.13	-	55,55,55,55	0
55	MG	AA	3152	1/1	0.39	-	50,50,50,50	0
55	MG	DA	3179	1/1	0.37	-	46,46,46,46	0
55	MG	AA	3043	1/1	0.38	-	75,75,75,75	0
55	MG	AA	3293	1/1	0.23	-	72,72,72,72	0
55	MG	CA	1639	1/1	0.41	-	69,69,69,69	0
55	MG	BC	102	1/1	0.35	-	65,65,65,65	0
55	MG	DA	3137	1/1	0.40	-	51,51,51,51	0
55	MG	CA	1667	1/1	0.46	-	78,78,78,78	0
55	MG	CA	1704	1/1	0.08	-	135,135,135,135	0
55	MG	DA	3038	1/1	0.25	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BB	106	1/1	0.59	-	102,102,102,102	0
56	OHX	DA	3456	7/7	0.11	-	133,142,150,207	1
55	MG	DA	3235	1/1	0.42	-	66,66,66,66	0
55	MG	AA	3212	1/1	0.38	-	33,33,33,33	0
55	MG	AA	3088	1/1	0.28	-	66,66,66,66	0
55	MG	DA	3026	1/1	0.27	-	55,55,55,55	0
55	MG	CA	1698	1/1	0.68	-	86,86,86,86	0
56	OHX	BA	1801	7/7	0.08	-	129,138,143,174	1
55	MG	DA	3015	1/1	0.21	-	56,56,56,56	0
56	OHX	DA	3217	7/7	0.09	-	144,149,153,189	1
56	OHX	DA	3450	7/7	0.14	-	133,139,150,199	1
55	MG	DA	3092	1/1	0.23	-	74,74,74,74	0
55	MG	DA	3190	1/1	0.61	-	44,44,44,44	0
55	MG	DA	3108	1/1	0.48	-	56,56,56,56	0
56	OHX	AA	3485	7/7	0.17	-	103,114,131,163	1
56	OHX	AA	3390	7/7	0.16	-	48,74,93,125	2
55	MG	DA	3090	1/1	0.30	-	54,54,54,54	0
56	OHX	BC	105	7/7	0.12	-	129,141,151,159	1
56	OHX	CA	1789	7/7	0.11	-	152,164,170,204	1
55	MG	AA	3127	1/1	0.34	-	45,45,45,45	0
56	OHX	AA	3483	7/7	0.16	-	106,109,118,158	2
56	OHX	CA	1784	7/7	0.17	-	127,135,151,190	1
56	OHX	BA	1771	7/7	0.18	-	101,104,120,152	2
55	MG	DA	3022	1/1	0.69	-	63,63,63,63	0
55	MG	BA	1662	1/1	0.25	-	56,56,56,56	0
55	MG	AA	3055	1/1	0.31	-	88,88,88,88	0
55	MG	CA	1641	1/1	0.41	-	85,85,85,85	0
55	MG	AA	3287	1/1	0.29	-	66,66,66,66	0
56	OHX	BA	1738	7/7	0.17	-	112,124,136,189	1
55	MG	DA	3122	1/1	0.34	-	30,30,30,30	0
55	MG	DA	3008	1/1	0.18	-	43,43,43,43	0
55	MG	AA	3135	1/1	0.39	-	66,66,66,66	0
56	OHX	DA	3166	7/7	0.10	-	159,166,176,197	1
56	OHX	DA	3408	7/7	0.14	-	122,131,146,182	1
55	MG	AA	3044	1/1	0.45	-	42,42,42,42	0
56	OHX	AA	3413	7/7	0.12	-	94,104,121,143	1
56	OHX	DA	3382	7/7	0.15	-	67,85,95,136	2
56	OHX	AA	3437	7/7	0.18	-	76,82,94,136	1
55	MG	AA	3208	1/1	0.37	-	62,62,62,62	0
55	MG	DA	3066	1/1	0.32	-	77,77,77,77	0
56	OHX	BA	1746	7/7	0.12	-	95,103,110,146	1
56	OHX	BA	1782	7/7	0.10	-	137,145,154,180	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3149	1/1	0.34	-	58,58,58,58	0
55	MG	BA	1680	1/1	0.15	-	64,64,64,64	0
55	MG	DA	3324	1/1	0.49	-	66,66,66,66	0
56	OHX	AA	3399	7/7	0.14	-	97,111,117,147	1
55	MG	CA	1665	1/1	0.33	-	114,114,114,114	0
56	OHX	DA	3398	7/7	0.11	-	119,127,142,162	1
55	MG	AA	3046	1/1	0.31	-	50,50,50,50	0
56	OHX	DA	3169	7/7	0.18	-	110,124,136,172	1
56	OHX	AA	3465	7/7	0.19	-	82,99,109,148	1
56	OHX	CA	1798	7/7	0.11	-	116,126,129,163	1
55	MG	AA	3075	1/1	0.22	-	78,78,78,78	0
56	OHX	AA	3484	7/7	0.13	-	123,137,150,203	1
56	OHX	DB	210	7/7	0.11	-	119,127,150,173	2
55	MG	AA	3303	1/1	0.16	-	77,77,77,77	0
55	MG	CA	1687	1/1	0.32	-	104,104,104,104	0
55	MG	DA	3018	1/1	0.33	-	47,47,47,47	0
56	OHX	DA	3478	7/7	0.17	-	106,110,128,170	1
56	OHX	CA	1747	7/7	0.17	-	129,134,147,212	1
55	MG	DA	3085	1/1	0.37	-	53,53,53,53	0
55	MG	DA	3260	1/1	0.29	-	68,68,68,68	0
56	OHX	CA	1792	7/7	0.07	-	189,191,192,232	1
56	OHX	BA	1739	7/7	0.09	-	109,119,131,155	1
55	MG	AA	3279	1/1	0.50	-	90,90,90,90	0
56	OHX	BA	1773	7/7	0.08	-	135,139,146,167	1
56	OHX	DA	3061	7/7	0.12	-	81,86,92,106	0
56	OHX	CV	101	7/7	0.10	-	174,182,196,223	1
56	OHX	BA	1734	7/7	0.15	-	92,99,114,146	1
56	OHX	DA	3220	7/7	0.11	-	141,154,156,201	1
56	OHX	CA	1802	7/7	0.09	-	130,138,148,200	1
56	OHX	AA	3457	7/7	0.10	-	86,94,124,185	1
56	OHX	AA	3504	7/7	0.17	-	101,103,116,145	2
56	OHX	DA	3458	7/7	0.08	-	173,175,178,215	1
56	OHX	DA	3417	7/7	0.07	-	145,152,156,188	1
55	MG	DA	3158	1/1	0.62	-	88,88,88,88	0
55	MG	AA	3173	1/1	0.44	-	65,65,65,65	0
56	OHX	BA	1751	7/7	0.15	-	101,112,132,168	2
55	MG	AA	3275	1/1	0.57	-	71,71,71,71	0
56	OHX	AA	3402	7/7	0.10	-	73,86,98,123	1
55	MG	AA	3153	1/1	0.41	-	40,40,40,40	0
55	MG	DA	3116	1/1	0.20	-	62,62,62,62	0
55	MG	BA	1714	1/1	0.58	-	83,83,83,83	0
56	OHX	AA	3524	7/7	0.13	-	115,120,140,187	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	MG	CA	1640	1/1	0.27	-	77,77,77,77	0
56	OHX	DA	3075	7/7	0.15	-	89,91,114,123	1
55	MG	AA	3193	1/1	0.34	-	86,86,86,86	0
56	OHX	AA	3336	7/7	0.18	-	67,91,105,145	0
56	OHX	DA	3394	7/7	0.12	-	127,139,150,223	0
56	OHX	AA	3440	7/7	0.10	-	83,91,111,141	1
55	MG	DA	3262	1/1	0.24	-	59,59,59,59	0
56	OHX	DA	3411	7/7	0.13	-	104,112,132,163	1
56	OHX	AA	3532	7/7	0.14	-	136,144,160,202	1
56	OHX	CA	1756	7/7	0.11	-	99,109,123,147	2
56	OHX	AA	3540	7/7	0.22	-	104,109,137,150	2
55	MG	CA	1668	1/1	0.35	-	80,80,80,80	0
55	MG	AA	3269	1/1	0.33	-	59,59,59,59	0
55	MG	DA	3263	1/1	0.27	-	55,55,55,55	0
55	MG	DA	3308	1/1	0.22	-	60,60,60,60	0
56	OHX	AA	3560	7/7	0.17	-	132,136,153,192	1
56	OHX	BA	1781	7/7	0.16	-	115,133,141,174	1
55	MG	AA	3249	1/1	0.25	-	81,81,81,81	0
56	OHX	BA	1780	7/7	0.21	-	115,123,136,153	1
55	MG	AA	3054	1/1	0.24	-	83,83,83,83	0
56	OHX	DA	3346	7/7	0.10	-	107,113,126,132	0
55	MG	AA	3070	1/1	0.12	-	56,56,56,56	0
56	OHX	DA	3084	7/7	0.13	-	132,139,149,176	1
56	OHX	DA	3473	7/7	0.10	-	138,151,163,196	1
56	OHX	DA	3461	7/7	0.10	-	171,173,180,211	1
55	MG	CA	1708	1/1	0.12	-	95,95,95,95	0
55	MG	AA	3148	1/1	0.24	-	69,69,69,69	0
56	OHX	AA	3394	7/7	0.14	-	113,123,125,181	1
55	MG	A5	101	1/1	0.31	-	43,43,43,43	0
55	MG	A7	101	1/1	0.36	-	56,56,56,56	0
56	OHX	CA	1775	7/7	0.12	-	139,154,159,200	1
55	MG	CA	1685	1/1	0.43	-	104,104,104,104	0
56	OHX	AA	3362	7/7	0.14	-	104,116,120,168	1
55	MG	DE	301	1/1	0.33	-	52,52,52,52	0
55	MG	DA	3177	1/1	0.46	-	61,61,61,61	0
55	MG	DA	3250	1/1	0.34	-	64,64,64,64	0
56	OHX	AA	3452	7/7	0.10	-	92,103,111,136	1
55	MG	DA	3229	1/1	0.41	-	45,45,45,45	0
55	MG	BA	1614	1/1	0.11	-	73,73,73,73	0
55	MG	AB	201	1/1	0.28	-	85,85,85,85	0
55	MG	BA	1660	1/1	0.52	-	52,52,52,52	0
56	OHX	CC	108	7/7	0.16	-	130,137,148,169	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3265	1/1	0.14	-	73,73,73,73	0
56	OHX	DA	3099	7/7	0.24	-	104,109,114,163	1
56	OHX	CA	1801	7/7	0.10	-	137,140,148,200	1
55	MG	CC	104	1/1	0.46	-	89,89,89,89	0
55	MG	AA	3175	1/1	0.23	-	46,46,46,46	0
56	OHX	AA	3443	7/7	0.13	-	110,114,126,149	2
56	OHX	BA	1800	7/7	0.08	-	127,133,145,177	1
55	MG	AA	3248	1/1	0.31	-	28,28,28,28	0
55	MG	AA	3016	1/1	0.35	-	29,29,29,29	0
56	OHX	BA	1735	7/7	0.09	-	120,129,137,168	1
56	OHX	DA	3159	7/7	0.16	-	75,86,105,131	3
55	MG	BA	1675	1/1	0.46	-	87,87,87,87	0
55	MG	BA	1632	1/1	0.19	-	73,73,73,73	0
55	MG	AA	3166	1/1	0.33	-	41,41,41,41	0
56	OHX	DA	3073	7/7	0.17	-	89,101,109,132	1
55	MG	DA	3198	1/1	0.38	-	44,44,44,44	0
55	MG	AE	302	1/1	0.23	-	74,74,74,74	0
56	OHX	DA	3399	7/7	0.21	-	104,107,123,144	2
56	OHX	CA	1755	7/7	0.11	-	119,128,149,178	1
56	OHX	DA	3453	7/7	0.18	-	145,153,160,191	1
56	OHX	CA	1729	7/7	0.14	-	104,115,126,154	1
56	OHX	DA	3396	7/7	0.17	-	96,99,105,140	1
55	MG	DA	3010	1/1	0.34	-	47,47,47,47	0
55	MG	DA	3096	1/1	0.20	-	85,85,85,85	0
56	OHX	AA	3395	7/7	0.18	-	100,109,130,162	1
56	OHX	DA	3420	7/7	0.10	-	116,120,125,152	1
55	MG	AA	3140	1/1	0.34	-	70,70,70,70	0
55	MG	AA	3117	1/1	0.21	-	90,90,90,90	0
55	MG	DA	3093	1/1	0.15	-	46,46,46,46	0
56	OHX	DB	219	7/7	0.16	-	147,161,178,209	1
56	OHX	DB	217	7/7	0.16	-	135,139,157,196	1
56	OHX	DA	3160	7/7	0.17	-	79,114,122,124	0
55	MG	DA	3222	1/1	0.27	-	83,83,83,83	0
55	MG	AA	3323	1/1	0.26	-	58,58,58,58	0
55	MG	AA	3233	1/1	0.28	-	82,82,82,82	0
56	OHX	BA	1795	7/7	0.12	-	152,159,163,204	1
55	MG	BB	107	1/1	0.16	-	80,80,80,80	0
56	OHX	AA	3363	7/7	0.12	-	89,101,119,137	1
56	OHX	DA	3127	7/7	0.25	-	118,132,150,170	2
56	OHX	AA	3341	7/7	0.18	-	77,80,88,124	1
55	MG	AA	3196	1/1	0.34	-	43,43,43,43	0
55	MG	BA	1637	1/1	0.22	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3325	1/1	0.37	-	75,75,75,75	0
56	OHX	AA	3553	7/7	0.12	-	160,165,172,209	1
55	MG	BA	1711	1/1	0.28	-	90,90,90,90	0
55	MG	DA	3267	1/1	0.31	-	82,82,82,82	0
55	MG	AA	3124	1/1	0.34	-	88,88,88,88	0
56	OHX	AA	3487	7/7	0.11	-	73,82,95,140	2
56	OHX	CA	1733	7/7	0.13	-	109,120,127,147	1
56	OHX	AA	3367	7/7	0.24	-	69,72,90,147	3
56	OHX	DA	3389	7/7	0.10	-	82,85,99,113	1
55	MG	AA	3092	1/1	0.19	-	92,92,92,92	0
55	MG	AA	3114	1/1	0.35	-	62,62,62,62	0
55	MG	BA	1617	1/1	0.47	-	60,60,60,60	0
55	MG	AA	3291	1/1	0.41	-	99,99,99,99	0
55	MG	BB	110	1/1	0.24	-	80,80,80,80	0
56	OHX	AA	3518	7/7	0.09	-	106,114,121,148	1
56	OHX	AB	210	7/7	0.10	-	101,108,128,154	1
55	MG	AB	203	1/1	0.23	-	58,58,58,58	0
55	MG	BB	108	1/1	0.26	-	80,80,80,80	0
55	MG	AA	3112	1/1	0.21	-	87,87,87,87	0
55	MG	D5	101	1/1	0.18	-	43,43,43,43	0
56	OHX	DA	3391	7/7	0.10	-	117,125,144,183	1
55	MG	AA	3025	1/1	0.33	-	37,37,37,37	0
55	MG	BA	1706	1/1	0.36	-	111,111,111,111	0
56	OHX	DA	3384	7/7	0.13	-	89,92,105,143	2
56	OHX	AA	3397	7/7	0.11	-	96,102,109,143	1
56	OHX	CA	1763	7/7	0.07	-	142,143,157,189	1
56	OHX	DA	3421	7/7	0.16	-	96,112,124,166	1
55	MG	BA	1678	1/1	0.28	-	44,44,44,44	0
55	MG	BA	1615	1/1	0.45	-	78,78,78,78	0
56	OHX	DA	3168	7/7	0.16	-	129,143,154,181	1
55	MG	AA	3023	1/1	0.29	-	35,35,35,35	0
56	OHX	DA	3212	7/7	0.14	-	64,77,91,94	1
56	OHX	BD	104	7/7	0.33	-	94,101,103,107	3
55	MG	DA	3027	1/1	0.12	-	78,78,78,78	0
55	MG	AA	3003	1/1	0.31	-	39,39,39,39	0
55	MG	CA	1677	1/1	0.45	-	73,73,73,73	0
56	OHX	DA	3368	7/7	0.10	-	86,101,103,132	2
55	MG	AA	3170	1/1	0.60	-	69,69,69,69	0
55	MG	AA	3141	1/1	0.34	-	80,80,80,80	0
55	MG	BA	1685	1/1	0.17	-	93,93,93,93	0
56	OHX	DA	3418	7/7	0.10	-	87,98,117,139	3
55	MG	BA	1691	1/1	0.17	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	OHX	AA	3555	7/7	0.17	-	82,85,105,128	1
56	OHX	AA	3358	7/7	0.10	-	79,81,92,113	1
56	OHX	BA	1778	7/7	0.22	-	125,131,152,191	1
55	MG	AB	205	1/1	0.27	-	68,68,68,68	0
56	OHX	DA	3361	7/7	0.13	-	68,94,122,134	3
56	OHX	DA	3339	7/7	0.14	-	91,96,120,132	0
55	MG	CA	1659	1/1	0.07	-	116,116,116,116	0
55	MG	DA	3236	1/1	0.38	-	62,62,62,62	0
56	OHX	BA	1775	7/7	0.15	-	113,130,145,176	1
56	OHX	DA	3409	7/7	0.16	-	103,117,129,162	1
55	MG	DA	3306	1/1	0.47	-	86,86,86,86	0
55	MG	BA	1699	1/1	0.52	-	84,84,84,84	0
55	MG	AA	3138	1/1	0.20	-	78,78,78,78	0
55	MG	DA	3144	1/1	0.49	-	44,44,44,44	0
55	MG	AA	3085	1/1	0.28	-	74,74,74,74	0
55	MG	DA	3126	1/1	0.41	-	63,63,63,63	0
55	MG	AA	3255	1/1	0.23	-	47,47,47,47	0
56	OHX	BA	1725	7/7	0.14	-	95,114,126,182	1
55	MG	CA	1610	1/1	0.38	-	87,87,87,87	0
55	MG	DA	3130	1/1	0.16	-	48,48,48,48	0
55	MG	AA	3264	1/1	0.23	-	51,51,51,51	0
56	OHX	DA	3374	7/7	0.09	-	127,131,139,156	1
56	OHX	AA	3453	7/7	0.13	-	72,88,95,134	2
56	OHX	DA	3345	7/7	0.12	-	89,96,107,130	0
55	MG	AA	3011	1/1	0.26	-	44,44,44,44	0
55	MG	BA	1684	1/1	0.19	-	67,67,67,67	0
55	MG	CA	1628	1/1	0.23	-	137,137,137,137	0
55	MG	BF	301	1/1	0.19	-	79,79,79,79	0
56	OHX	AA	3552	7/7	0.17	-	96,106,128,164	1
55	MG	D7	101	1/1	0.44	-	69,69,69,69	0
56	OHX	AA	3348	7/7	0.13	-	75,81,98,100	3
55	MG	CA	1720	1/1	0.86	-	110,110,110,110	0
56	OHX	AA	3543	7/7	0.09	-	145,150,162,204	1
55	MG	AA	3087	1/1	0.26	-	82,82,82,82	0
56	OHX	DA	3255	7/7	0.19	-	93,104,107,143	1
55	MG	AA	3107	1/1	0.42	-	51,51,51,51	0
55	MG	AA	3102	1/1	0.35	-	52,52,52,52	0
56	OHX	DA	3490	7/7	0.14	-	103,106,122,159	3
55	MG	DA	3297	1/1	0.35	-	70,70,70,70	0
55	MG	DA	3242	1/1	0.45	-	99,99,99,99	0
56	OHX	BA	1812	7/7	0.06	-	170,174,180,213	1
56	OHX	CA	1727	7/7	0.09	-	114,118,131,143	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CC	102	1/1	0.77	-	69,69,69,69	0
55	MG	BA	1694	1/1	0.25	-	60,60,60,60	0
56	OHX	DA	3484	7/7	0.14	-	109,123,139,168	1
56	OHX	DA	3481	7/7	0.12	-	136,140,149,177	1
56	OHX	DA	3226	7/7	0.15	-	120,131,144,175	1
55	MG	BA	1648	1/1	0.41	-	86,86,86,86	0
55	MG	DA	3188	1/1	0.35	-	38,38,38,38	0
55	MG	DA	3131	1/1	0.34	-	72,72,72,72	0
55	MG	AA	3159	1/1	0.39	-	81,81,81,81	0
55	MG	AA	3052	1/1	0.27	-	71,71,71,71	0
55	MG	CA	1701	1/1	0.27	-	109,109,109,109	0
55	MG	DA	3292	1/1	0.22	-	51,51,51,51	0
56	OHX	DA	3468	7/7	0.17	-	143,146,150,189	1
55	MG	DA	3067	1/1	0.12	-	82,82,82,82	0
56	OHX	AA	3549	7/7	0.32	-	96,102,109,128	2
56	OHX	AB	209	7/7	0.13	-	98,103,137,147	3
55	MG	AA	3150	1/1	0.23	-	53,53,53,53	0
55	MG	AA	3010	1/1	0.25	-	39,39,39,39	0
55	MG	DA	3151	1/1	0.28	-	62,62,62,62	0
55	MG	CA	1629	1/1	0.41	-	166,166,166,166	0
56	OHX	AA	3559	7/7	0.15	-	123,137,143,179	1
56	OHX	DA	3378	7/7	0.10	-	153,156,169,185	0
55	MG	DA	3241	1/1	0.13	-	47,47,47,47	0
55	MG	AA	3312	1/1	0.20	-	71,71,71,71	0
56	OHX	AA	3557	7/7	0.22	-	89,102,113,146	1
58	ZN	CG	301	1/1	0.27	-	116,116,116,116	0
55	MG	DA	3311	1/1	0.39	-	63,63,63,63	0
55	MG	AA	3243	1/1	0.40	-	62,62,62,62	0
55	MG	AA	3321	1/1	0.32	-	41,41,41,41	0
55	MG	AA	3013	1/1	0.32	-	27,27,27,27	0
56	OHX	DA	3174	7/7	0.16	-	100,112,120,180	1
57	PAR	CA	1722	42/42	0.15	-	72,88,95,97	0
55	MG	CA	1604	1/1	0.16	-	72,72,72,72	0
55	MG	DA	3007	1/1	0.27	-	43,43,43,43	0
55	MG	AA	3067	1/1	0.13	-	50,50,50,50	0
55	MG	DA	3029	1/1	0.34	-	70,70,70,70	0
56	OHX	BA	1779	7/7	0.14	-	129,134,141,170	1
55	MG	AA	3091	1/1	0.45	-	85,85,85,85	0
56	OHX	AA	3536	7/7	0.14	-	99,110,129,173	2
56	OHX	BA	1737	7/7	0.12	-	120,131,149,172	1
55	MG	AA	3024	1/1	0.39	-	45,45,45,45	0
56	OHX	DA	3064	7/7	0.15	-	87,100,123,131	3

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	OHX	DA	3432	7/7	0.09	-	116,131,140,173	1
55	MG	AA	3053	1/1	0.26	-	77,77,77,77	0
55	MG	AA	3250	1/1	0.38	-	55,55,55,55	0
56	OHX	AA	3423	7/7	0.10	-	100,115,121,157	1
55	MG	BB	113	1/1	0.23	-	80,80,80,80	0
55	MG	BA	1633	1/1	0.25	-	77,77,77,77	0
55	MG	DA	3112	1/1	0.52	-	85,85,85,85	0
56	OHX	DA	3414	7/7	0.14	-	126,128,140,174	1
56	OHX	CB	106	7/7	0.31	-	97,107,117,126	6
56	OHX	AA	3468	7/7	0.09	-	110,120,137,165	1
56	OHX	AA	3436	7/7	0.17	-	90,93,119,164	1
55	MG	BA	1658	1/1	0.40	-	47,47,47,47	0
56	OHX	BA	1772	7/7	0.10	-	165,176,177,219	1
55	MG	AA	3059	1/1	0.34	-	77,77,77,77	0
55	MG	DA	3219	1/1	0.15	-	62,62,62,62	0
55	MG	BA	1604	1/1	0.19	-	69,69,69,69	0
56	OHX	DA	3355	7/7	0.11	-	109,111,119,148	2
55	MG	BA	1639	1/1	0.20	-	101,101,101,101	0
55	MG	DA	3074	1/1	0.43	-	40,40,40,40	0
55	MG	DA	3327	1/1	0.22	-	73,73,73,73	0
56	OHX	AA	3479	7/7	0.15	-	94,103,125,176	3
56	OHX	DA	3105	7/7	0.18	-	134,136,144,206	1
56	OHX	DA	3352	7/7	0.11	-	105,120,129,149	0
55	MG	AA	3315	1/1	0.12	-	50,50,50,50	0
56	OHX	CA	1813	7/7	0.28	-	138,144,151,179	1
56	OHX	DA	3381	7/7	0.13	-	111,118,134,167	1
56	OHX	AA	3565	7/7	0.11	-	97,104,114,159	1
56	OHX	DA	3397	7/7	0.08	-	104,119,125,149	1
55	MG	AA	3299	1/1	0.30	-	41,41,41,41	0
55	MG	AA	3082	1/1	0.27	-	57,57,57,57	0
56	OHX	AA	3502	7/7	0.11	-	128,135,148,184	1
56	OHX	DA	3433	7/7	0.20	-	104,114,132,147	1
55	MG	CA	1703	1/1	0.55	-	84,84,84,84	0
55	MG	CA	1679	1/1	0.11	-	87,87,87,87	0
56	OHX	AA	3427	7/7	0.12	-	131,132,136,155	1
55	MG	BA	1665	1/1	0.23	-	53,53,53,53	0
56	OHX	CA	1742	7/7	0.12	-	153,166,169,174	1
56	OHX	BA	1777	7/7	0.07	-	176,178,192,246	1
56	OHX	DA	3441	7/7	0.11	-	114,122,135,176	1
55	MG	AA	3356	1/1	0.51	-	70,70,70,70	0
56	OHX	BD	102	7/7	0.07	-	170,180,207,224	1
55	MG	AA	3158	1/1	0.42	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3118	1/1	0.22	-	69,69,69,69	0
56	OHX	BL	201	7/7	0.09	-	145,153,159,202	1
56	OHX	DO	201	7/7	0.16	-	112,117,125,146	1
56	OHX	DA	3083	7/7	0.11	-	104,111,120,146	1
55	MG	CA	1696	1/1	0.58	-	74,74,74,74	0
56	OHX	AA	3495	7/7	0.18	-	106,114,133,188	1
56	OHX	AA	3498	7/7	0.28	-	120,126,136,160	2
56	OHX	DA	3403	7/7	0.11	-	99,105,122,140	1
55	MG	AA	3283	1/1	0.10	-	21,21,21,21	0
55	MG	DA	3045	1/1	0.16	-	61,61,61,61	0
55	MG	DA	3307	1/1	0.50	-	119,119,119,119	0
56	OHX	AA	3496	7/7	0.11	-	107,119,130,176	1
55	MG	CA	1606	1/1	0.15	-	70,70,70,70	0
56	OHX	AA	3493	7/7	0.11	-	102,115,123,140	1
56	OHX	CA	1770	7/7	0.08	-	143,153,167,200	1
55	MG	AA	3294	1/1	0.31	-	36,36,36,36	0
55	MG	DA	3289	1/1	0.21	-	84,84,84,84	0
55	MG	BA	1674	1/1	0.22	-	67,67,67,67	0
56	OHX	DA	3404	7/7	0.11	-	107,121,131,166	1
56	OHX	DA	3416	7/7	0.14	-	112,112,142,167	1
55	MG	CA	1690	1/1	0.11	-	93,93,93,93	0
56	OHX	DA	3402	7/7	0.11	-	122,136,148,204	1
56	OHX	CA	1812	7/7	0.12	-	134,141,149,203	1
55	MG	AA	3009	1/1	0.23	-	29,29,29,29	0
56	OHX	BA	1788	7/7	0.26	-	123,136,147,176	1
55	MG	DA	3310	1/1	0.20	-	73,73,73,73	0
55	MG	DA	3021	1/1	0.28	-	62,62,62,62	0
55	MG	CA	1683	1/1	0.34	-	79,79,79,79	0
56	OHX	DA	3165	7/7	0.18	-	123,135,143,168	1
55	MG	DA	3047	1/1	0.14	-	79,79,79,79	0
56	OHX	AA	3474	7/7	0.12	-	113,120,132,160	1
56	OHX	AA	3475	7/7	0.08	-	132,134,145,192	1
55	MG	BA	1687	1/1	0.23	-	96,96,96,96	0
55	MG	CA	1642	1/1	0.60	-	69,69,69,69	0
55	MG	AA	3225	1/1	0.50	-	52,52,52,52	0
56	OHX	AA	3534	7/7	0.10	-	103,124,138,161	2
56	OHX	AA	3435	7/7	0.14	-	83,103,126,156	2
56	OHX	BA	1805	7/7	0.18	-	98,103,107,150	1
56	OHX	BA	1717	7/7	0.16	-	81,90,105,119	0
55	MG	DA	3329	1/1	0.39	-	60,60,60,60	0
56	OHX	AB	212	7/7	0.11	-	91,105,122,151	3
56	OHX	DA	3488	7/7	0.27	-	87,112,131,159	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3019	1/1	0.30	-	42,42,42,42	0
56	OHX	BA	1761	7/7	0.08	-	136,147,154,197	1
55	MG	AA	3256	1/1	0.41	-	52,52,52,52	0
56	OHX	AA	3408	7/7	0.14	-	107,111,135,163	1
56	OHX	AA	3526	7/7	0.23	-	87,90,101,128	1
55	MG	CA	1609	1/1	0.37	-	112,112,112,112	0
55	MG	AA	3123	1/1	0.20	-	65,65,65,65	0
56	OHX	DA	3214	7/7	0.20	-	82,92,98,133	2
55	MG	AA	3103	1/1	0.32	-	50,50,50,50	0
56	OHX	AB	216	7/7	0.19	-	106,124,147,185	1
56	OHX	DA	3380	7/7	0.08	-	108,123,139,150	1
55	MG	CA	1712	1/1	0.20	-	83,83,83,83	0
56	OHX	BA	1748	7/7	0.13	-	124,127,141,171	1
56	OHX	AB	217	7/7	0.23	-	100,108,115,151	1
55	MG	AA	3268	1/1	0.15	-	38,38,38,38	0
56	OHX	DA	3487	7/7	0.16	-	106,108,129,150	1
56	OHX	CA	1807	7/7	0.24	-	109,119,124,150	1
56	OHX	DA	3482	7/7	0.15	-	128,142,154,190	1
56	OHX	DA	3448	7/7	0.12	-	134,147,163,206	1
55	MG	D0	201	1/1	0.13	-	51,51,51,51	0
56	OHX	AA	3389	7/7	0.18	-	80,93,103,143	0
55	MG	DA	3106	1/1	0.22	-	80,80,80,80	0
56	OHX	BA	1729	7/7	0.11	-	110,115,135,137	1
55	MG	DA	3278	1/1	0.40	-	84,84,84,84	0
56	OHX	AA	3365	7/7	0.11	-	86,102,111,118	3
55	MG	DA	3304	1/1	0.17	-	89,89,89,89	0
56	OHX	AA	3448	7/7	0.12	-	141,143,155,200	1
55	MG	AA	3076	1/1	0.22	-	81,81,81,81	0
56	OHX	CA	1752	7/7	0.16	-	139,147,150,191	1
56	OHX	BA	1749	7/7	0.16	-	112,116,136,168	1
55	MG	CA	1626	1/1	0.35	-	124,124,124,124	0
55	MG	AA	3073	1/1	0.32	-	68,68,68,68	0
55	MG	CA	1603	1/1	0.31	-	62,62,62,62	0
56	OHX	DA	3223	7/7	0.20	-	126,133,144,169	1
55	MG	DA	3277	1/1	0.09	-	89,89,89,89	0
55	MG	AA	3172	1/1	0.55	-	71,71,71,71	0
55	MG	DA	3146	1/1	0.23	-	33,33,33,33	0
55	MG	AA	3286	1/1	0.34	-	83,83,83,83	0
55	MG	AA	3012	1/1	0.29	-	45,45,45,45	0
55	MG	CA	1650	1/1	0.27	-	66,66,66,66	0
55	MG	BA	1646	1/1	0.28	-	48,48,48,48	0
56	OHX	DA	3431	7/7	0.17	-	139,144,155,180	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3031	1/1	0.32	-	40,40,40,40	0
56	OHX	DA	3344	7/7	0.15	-	93,104,111,114	1
56	OHX	AB	219	7/7	0.47	-	112,116,126,139	1
55	MG	AA	3306	1/1	0.44	-	100,100,100,100	0
55	MG	DA	3058	1/1	0.34	-	70,70,70,70	0
56	OHX	AA	3401	7/7	0.13	-	101,105,125,153	1
55	MG	DA	3272	1/1	0.09	-	57,57,57,57	0
55	MG	CA	1662	1/1	0.37	-	92,92,92,92	0
55	MG	DA	3199	1/1	0.44	-	77,77,77,77	0
56	OHX	DA	3475	7/7	0.17	-	126,139,148,175	1
56	OHX	CA	1805	7/7	0.14	-	128,130,148,187	1
55	MG	DA	3079	1/1	0.24	-	49,49,49,49	0
55	MG	AA	3020	1/1	0.39	-	42,42,42,42	0
55	MG	AA	3231	1/1	0.42	-	57,57,57,57	0
55	MG	DA	3097	1/1	0.42	-	67,67,67,67	0
55	MG	BA	1642	1/1	0.41	-	69,69,69,69	0
56	OHX	BA	1763	7/7	0.13	-	123,136,140,184	1
55	MG	AA	3151	1/1	0.30	-	46,46,46,46	0
55	MG	DA	3024	1/1	0.27	-	63,63,63,63	0
55	MG	DA	3213	1/1	0.35	-	57,57,57,57	0
55	MG	BA	1669	1/1	0.30	-	68,68,68,68	0
56	OHX	AA	3538	7/7	0.20	-	95,101,128,162	1
55	MG	AA	3004	1/1	0.34	-	32,32,32,32	0
56	OHX	DA	3457	7/7	0.08	-	149,156,166,200	1
55	MG	BA	1636	1/1	0.15	-	111,111,111,111	0
56	OHX	DA	3082	7/7	0.13	-	92,102,108,132	1
55	MG	CA	1648	1/1	0.40	-	70,70,70,70	0
55	MG	CA	1678	1/1	0.09	-	97,97,97,97	0
56	OHX	DA	3435	7/7	0.21	-	86,99,124,155	1
56	OHX	CA	1771	7/7	0.13	-	105,107,134,145	1
55	MG	AA	3142	1/1	0.47	-	75,75,75,75	0
56	OHX	DB	208	7/7	0.10	-	120,124,144,144	2
56	OHX	CA	1737	7/7	0.08	-	103,118,125,148	1
55	MG	DA	3129	1/1	0.30	-	68,68,68,68	0
56	OHX	AA	3441	7/7	0.15	-	113,135,152,175	1
55	MG	DA	3333	1/1	0.31	-	84,84,84,84	0
55	MG	AA	3343	1/1	0.27	-	92,92,92,92	0
56	OHX	DA	3221	7/7	0.10	-	120,130,140,174	1
55	MG	DB	207	1/1	0.17	-	70,70,70,70	0
56	OHX	BA	1786	7/7	0.20	-	133,136,154,188	1
55	MG	BA	1654	1/1	0.26	-	64,64,64,64	0
55	MG	DA	3183	1/1	0.29	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3292	1/1	0.42	-	62,62,62,62	0
55	MG	DA	3187	1/1	0.28	-	55,55,55,55	0
55	MG	AA	3187	1/1	0.24	-	40,40,40,40	0
56	OHX	AA	3490	7/7	0.10	-	85,93,105,125	1
55	MG	BA	1651	1/1	0.40	-	76,76,76,76	0
56	OHX	AA	3499	7/7	0.15	-	107,112,120,152	1
55	MG	CA	1709	1/1	0.22	-	76,76,76,76	0
55	MG	BA	1628	1/1	0.28	-	95,95,95,95	0
55	MG	AA	3120	1/1	0.49	-	74,74,74,74	0
56	OHX	AA	3519	7/7	0.20	-	103,114,126,154	1
55	MG	DA	3014	1/1	0.28	-	55,55,55,55	0
55	MG	DA	3279	1/1	0.33	-	68,68,68,68	0
56	OHX	BA	1760	7/7	0.12	-	109,109,121,147	1
55	MG	AA	3213	1/1	0.18	-	60,60,60,60	0
55	MG	CA	1717	1/1	0.28	-	64,64,64,64	0
56	OHX	CA	1810	7/7	0.11	-	113,132,142,167	1
56	OHX	DB	213	7/7	0.15	-	125,144,157,169	2
56	OHX	BA	1741	7/7	0.12	-	95,110,126,148	1
56	OHX	BA	1744	7/7	0.12	-	134,144,157,183	1
55	MG	BA	1613	1/1	0.14	-	116,116,116,116	0
55	MG	AA	3121	1/1	0.35	-	65,65,65,65	0
55	MG	AA	3104	1/1	0.23	-	62,62,62,62	0
55	MG	CB	101	1/1	0.40	-	105,105,105,105	0
56	OHX	DA	3087	7/7	0.14	-	102,119,134,177	1
55	MG	AA	3083	1/1	0.37	-	94,94,94,94	0
55	MG	BA	1668	1/1	0.30	-	64,64,64,64	0
55	MG	DA	3256	1/1	0.30	-	89,89,89,89	0
56	OHX	DA	3429	7/7	0.10	-	118,130,143,180	1
55	MG	AA	3309	1/1	0.34	-	77,77,77,77	0
56	OHX	DA	3094	7/7	0.17	-	110,121,124,149	1
55	MG	AA	3014	1/1	0.34	-	33,33,33,33	0
55	MG	CA	1630	1/1	0.45	-	86,86,86,86	0
55	MG	AA	3064	1/1	0.23	-	52,52,52,52	0
55	MG	AA	3244	1/1	0.31	-	41,41,41,41	0
55	MG	AA	3204	1/1	0.38	-	45,45,45,45	0
55	MG	AA	3177	1/1	0.28	-	46,46,46,46	0
55	MG	AA	3236	1/1	0.47	-	66,66,66,66	0
55	MG	AA	3021	1/1	0.28	-	35,35,35,35	0
55	MG	DA	3023	1/1	0.56	-	70,70,70,70	0
55	MG	CA	1706	1/1	0.62	-	85,85,85,85	0
55	MG	BA	1686	1/1	0.11	-	100,100,100,100	0
56	OHX	CA	1800	7/7	0.07	-	165,167,172,220	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	OHX	AA	3344	7/7	0.10	-	86,92,112,118	1
56	OHX	A3	102	7/7	0.20	-	106,109,134,147	2
56	OHX	DA	3454	7/7	0.17	-	136,143,163,191	1
56	OHX	CA	1806	7/7	0.10	-	138,150,153,181	1
56	OHX	AA	3383	7/7	0.12	-	91,96,109,133	1
56	OHX	CA	1735	7/7	0.10	-	146,153,168,212	0
56	OHX	CA	1757	7/7	0.14	-	117,123,150,175	1
55	MG	AA	3180	1/1	0.45	-	42,42,42,42	0
55	MG	DA	3196	1/1	0.40	-	54,54,54,54	0
55	MG	CC	103	1/1	0.73	-	97,97,97,97	0
56	OHX	DA	3400	7/7	0.13	-	113,116,126,149	1
56	OHX	BA	1721	7/7	0.10	-	109,115,141,157	1
56	OHX	BA	1804	7/7	0.15	-	147,154,164,208	1
56	OHX	AO	202	7/7	0.11	-	93,104,115,140	1
55	MG	DA	3295	1/1	0.42	-	77,77,77,77	0
55	MG	DA	3325	1/1	0.45	-	91,91,91,91	0
55	MG	BB	104	1/1	0.81	-	100,100,100,100	0
55	MG	AA	3030	1/1	0.34	-	36,36,36,36	0
56	OHX	BA	1799	7/7	0.08	-	170,176,182,227	1
56	OHX	AA	3467	7/7	0.12	-	72,88,95,139	1
55	MG	BA	1607	1/1	0.11	-	102,102,102,102	0
56	OHX	DA	3341	7/7	0.15	-	87,105,126,140	0
55	MG	DA	3148	1/1	0.41	-	50,50,50,50	0
55	MG	DA	3319	1/1	0.47	-	69,69,69,69	0
56	OHX	BA	1736	7/7	0.12	-	112,121,128,152	1
55	MG	AA	3230	1/1	0.47	-	72,72,72,72	0
56	OHX	AA	3472	7/7	0.21	-	95,115,124,169	1
56	OHX	CA	1734	7/7	0.09	-	145,147,151,167	1
56	OHX	BA	1753	7/7	0.16	-	103,110,125,169	1
56	OHX	CA	1804	7/7	0.23	-	145,149,162,192	1
55	MG	CN	201	1/1	0.12	-	79,79,79,79	0
55	MG	DA	3320	1/1	0.50	-	132,132,132,132	0
55	MG	DA	3123	1/1	0.29	-	38,38,38,38	0
56	OHX	DA	3251	7/7	0.25	-	102,112,141,176	3
55	MG	CA	1636	1/1	0.19	-	82,82,82,82	0
56	OHX	AB	207	7/7	0.11	-	89,93,105,113	1
55	MG	AA	3106	1/1	0.25	-	72,72,72,72	0
55	MG	DA	3209	1/1	0.30	-	64,64,64,64	0
55	MG	DA	3178	1/1	0.56	-	58,58,58,58	0
55	MG	BA	1605	1/1	0.11	-	81,81,81,81	0
55	MG	BA	1676	1/1	0.41	-	78,78,78,78	0
55	MG	BB	101	1/1	0.12	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3133	1/1	0.32	-	45,45,45,45	0
55	MG	AA	3095	1/1	0.34	-	42,42,42,42	0
56	OHX	DA	3336	7/7	0.18	-	86,95,105,106	0
55	MG	DA	3041	1/1	0.34	-	79,79,79,79	0
56	OHX	AA	3355	7/7	0.15	-	88,95,127,131	3
55	MG	DA	3185	1/1	0.40	-	49,49,49,49	0
55	MG	AA	3164	1/1	0.30	-	45,45,45,45	0
56	OHX	CA	1750	7/7	0.14	-	110,113,130,151	1

6.5 Other polymers

There are no such residues in this entry.