



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 10:35 PM BST

PDB ID : 4V8E  
Title : Crystal structure analysis of ribosomal decoding (near-cognate tRNA-tyr complex).  
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](mailto:validation@mail.wwpdb.org)

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

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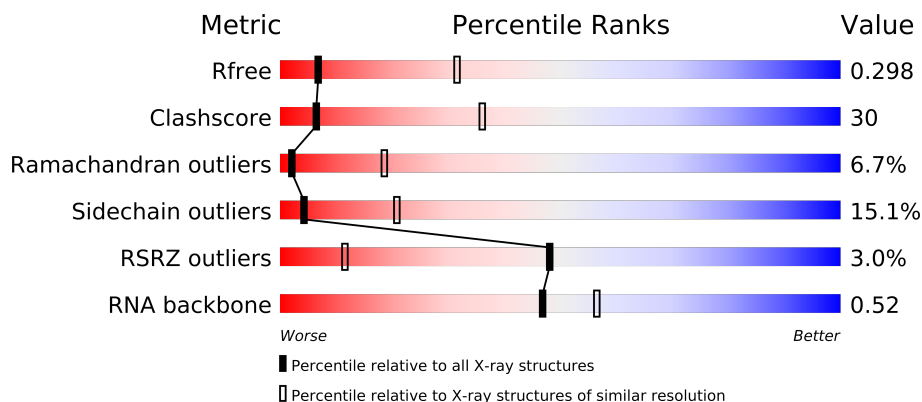
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 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  $\geq 3$ , 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	CA	2912	
2	AB	122	
2	CB	122	
3	AD	276	
3	CD	276	
4	AE	206	
4	CE	206	
5	AF	210	
5	CF	210	
6	AG	182	
6	CG	182	

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Mol	Chain	Length	Quality of chain
7	AH	180	
7	CH	180	
8	AK	148	
8	CK	148	
9	AM	140	
9	CM	140	
10	AN	122	
10	CN	122	
11	AO	150	
11	CO	150	
12	AP	141	
12	CP	141	
13	A0	118	
13	C0	118	
14	AQ	112	
14	CQ	112	
15	AR	146	
15	CR	146	
16	A1	118	
16	C1	118	
17	A2	101	
17	C2	101	
18	AS	113	
18	CS	113	
19	AT	96	
19	CT	96	
20	AU	110	
20	CU	110	
21	AV	206	
21	CV	206	
22	A3	85	
22	C3	85	
23	AZ	98	
23	CZ	98	
24	AW	72	
24	CW	72	
25	AX	60	
25	CX	60	
26	A4	71	
26	C4	71	
27	A5	60	
27	C5	60	

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Mol	Chain	Length	Quality of chain
28	A6	54	
28	C6	54	
29	A7	49	
29	C7	49	
30	A8	65	
30	C8	65	
31	BA	1506	
31	DA	1506	
32	BE	256	
32	DE	256	
33	BF	239	
33	DF	239	
34	BG	208	
34	DG	208	
35	BH	162	
35	DH	162	
36	BI	101	
36	DI	101	
37	BJ	156	
37	DJ	156	
38	BK	138	
38	DK	138	
39	BL	128	
39	DL	128	
40	BM	105	
40	DM	105	
41	BN	129	
41	DN	129	
42	BO	132	
42	DO	132	
43	BP	126	
43	DP	126	
44	BQ	61	
44	DQ	61	
45	BR	89	
45	DR	89	
46	BS	88	
46	DS	88	
47	BT	105	
47	DT	105	
48	BU	88	
48	DU	88	

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Mol	Chain	Length	Quality of chain
49	BV	93	
49	DV	93	
50	BW	106	
50	DW	106	
51	BX	27	
51	DX	27	
52	BB	85	
52	BD	85	
52	DB	85	
52	DD	85	
53	BC	77	
53	DC	77	
54	B1	16	
54	D1	16	

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 303952 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	CA	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
CA	156	U	-	INSERTION	GB AP008226.1
CA	681	A	G	CONFLICT	GB AP008226.1
CA	685	C	G	CONFLICT	GB AP008226.1
CA	696	G	C	CONFLICT	GB AP008226.1
CA	700	A	C	CONFLICT	GB AP008226.1
CA	1105	U	G	CONFLICT	GB AP008226.1
CA	1127	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	CB	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	CD	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	CE	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	CF	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	CG	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	CH	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	CK	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	CM	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	CN	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	CO	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	CP	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	C0	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	CQ	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	CR	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	C1	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	C2	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	CS	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	CT	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	CU	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	CV	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	C3	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	CZ	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	CW	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	CX	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	C4	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	C5	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	C6	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	C7	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	C8	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	DA	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	DE	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	DF	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	DG	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	DH	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	DI	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	DJ	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	DK	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	DL	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	DM	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	DN	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	DO	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	DP	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	DQ	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	DR	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	DS	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	DT	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	DU	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	DV	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	DW	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	DX	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	DB	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
52	DD	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	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	DC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	18	C	U	CONFLICT	GB AP012306.1
DC	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			
54	D1	16	Total	C	N	O	P	0	0	0
			347	156	69	106	16			

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



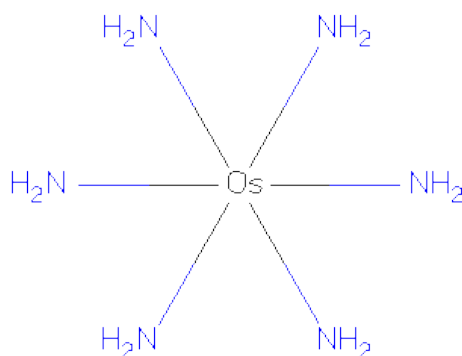
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	BA	115	Total Mg 115 115	0	0
55	CA	274	Total Mg 274 274	0	0
55	C5	1	Total Mg 1 1	0	0
55	AB	6	Total Mg 6 6	0	0
55	B1	1	Total Mg 1 1	0	0
55	DN	1	Total Mg 1 1	0	0
55	DC	6	Total Mg 6 6	0	0
55	BB	5	Total Mg 5 5	0	0
55	AE	3	Total Mg 3 3	0	0
55	DL	1	Total Mg 1 1	0	0
55	C0	1	Total Mg 1 1	0	0
55	AA	331	Total Mg 331 331	0	0
55	BQ	1	Total Mg 1 1	0	0
55	A5	1	Total Mg 1 1	0	0
55	BC	5	Total Mg 5 5	0	0
55	A1	1	Total Mg 1 1	0	0
55	BN	1	Total Mg 1 1	0	0
55	C7	1	Total Mg 1 1	0	0
55	DA	119	Total Mg 119 119	0	0
55	AO	3	Total Mg 3 3	0	0
55	A0	1	Total Mg 1 1	0	0
55	D1	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	CB	7	Total 7	Mg 7	0	0
55	BS	1	Total 1	Mg 1	0	0
55	BD	1	Total 1	Mg 1	0	0
55	CE	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	2	Total 2	Mg 2	0	0

- Molecule 56 is osmium (III) hexammine (three-letter code: OHX) (formula:  $\text{H}_{12}\text{N}_6\text{Os}$ ).



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

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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
			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
			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	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	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	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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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
			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	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
			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		

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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	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	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		

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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
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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
			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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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
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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
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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
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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
			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
			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
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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
			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
			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		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CF	1	Total	N	Os	0	0
			7	6	1		
56	CO	1	Total	N	Os	0	0
			7	6	1		
56	C1	1	Total	N	Os	0	0
			7	6	1		
56	C3	1	Total	N	Os	0	0
			7	6	1		
56	C5	1	Total	N	Os	0	0
			7	6	1		
56	C6	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		
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		
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		
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		
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		
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		
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		
56	DG	1	Total	N	Os	0	0
			7	6	1		
56	DK	1	Total	N	Os	0	0
			7	6	1		
56	DR	1	Total	N	Os	0	0
			7	6	1		
56	DV	1	Total	N	Os	0	0
			7	6	1		
56	DB	1	Total	N	Os	0	0
			7	6	1		
56	DB	1	Total	N	Os	0	0
			7	6	1		
56	DB	1	Total	N	Os	0	0
			7	6	1		
56	DC	1	Total	N	Os	0	0
			7	6	1		
56	DC	1	Total	N	Os	0	0
			7	6	1		
56	DC	1	Total	N	Os	0	0
			7	6	1		
56	DC	1	Total	N	Os	0	0
			7	6	1		
56	DD	1	Total	N	Os	0	0
			7	6	1		

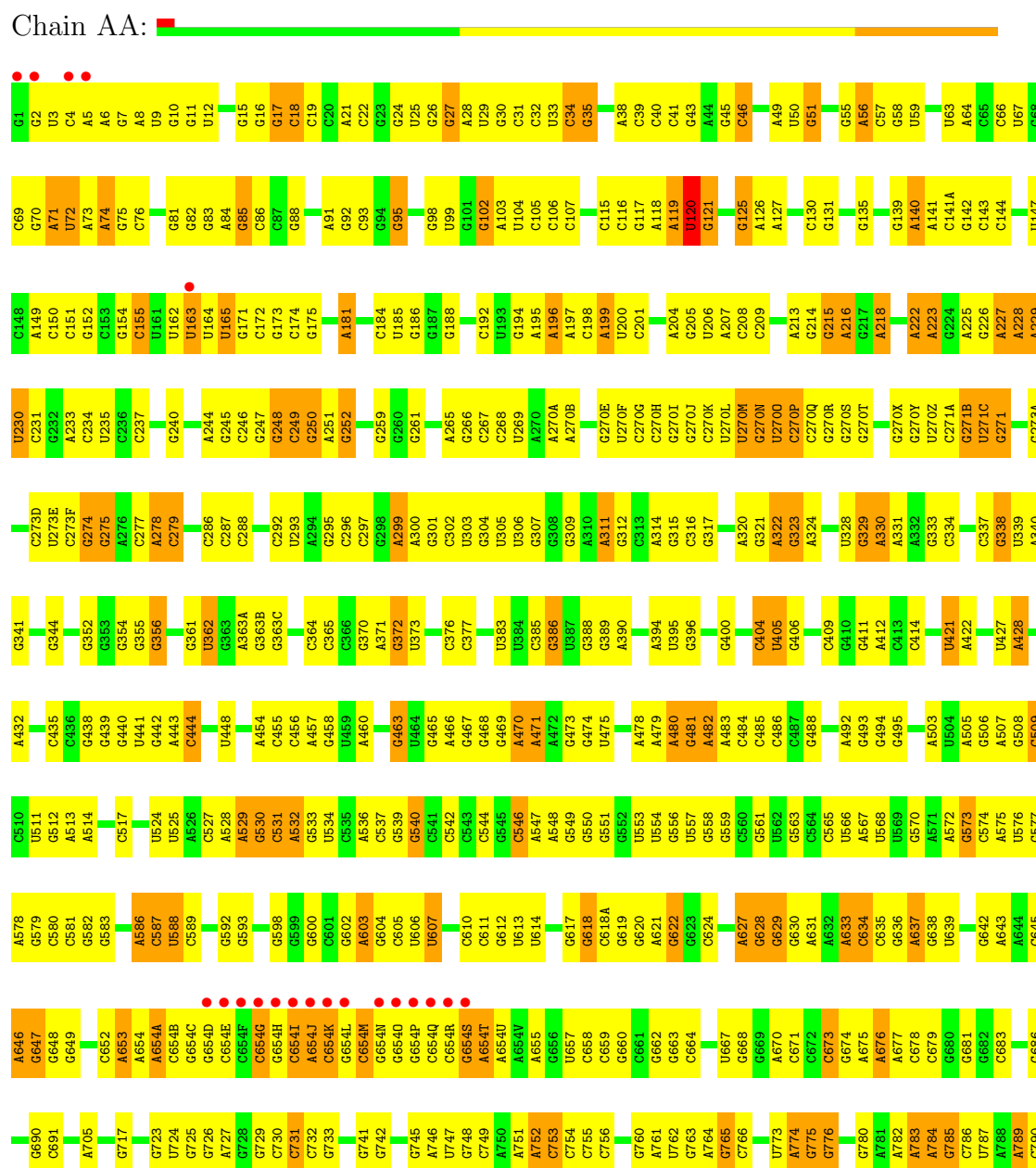
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DG	1	Total	Zn	0	0
			1	1		
57	BG	1	Total	Zn	0	0
			1	1		
57	BQ	1	Total	Zn	0	0
			1	1		
57	DQ	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)







G1062	G1063	G1064	G1065	G1066	G1067	G1068	G1069	G1070	G1071	G1072	G1073	G1074	G1075	G1076	G1077	G1078	G1079	G1080	G1081	G1082	G1083	G1084	G1085	G1086	G1087	G1088	G1089	G1090	G1091	G1092	G1093	G1094	G1095	G1096	G1097	G1098	G1099	G1100	G1101	G1102	G1103	G1104	G1105	G1106	G1107	G1108	G1109	G1110	G1111	G1112	G1113	G1114	G1115	G1116	G1117	G1118	G1119	G1120	G1121	G1122	G1123	G1124																																																																																																																																																																																																																																																																																																																																																																																																																																																		
A1127	A1128	C1065	C1066	C1067	C1068	C1069	C1070	C1071	C1072	C1073	C1074	C1075	C1076	C1077	C1078	C1079	C1080	C1081	C1082	C1083	C1084	C1085	C1086	C1087	C1088	C1089	C1090	C1091	C1092	C1093	C1094	C1095	C1096	C1097	C1098	C1099	C1100	C1101	C1102	C1103	C1104	C1105	C1106	C1107	C1108	C1109	C1110	C1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	C1120	C1121	C1122	C1123	C1124																																																																																																																																																																																																																																																																																																																																																																																																																																																			
G1000	G1001	G1002	G1003	G1004	G1005	G1006	G1007	G1008	G1009	G1010	G1011	G1012	G1013	G1014	G1015	G1016	G1017	G1018	G1019	G1020	G1021	G1022	G1023	G1024	G1025	G1026	G1027	G1028	G1029	G1030	G1031	G1032	G1033	G1034	G1035	G1036	G1037	G1038	G1039	G1040	G1041	G1042	G1043	G1044	G1045	G1046	G1047	G1048	G1049	G1050	G1051	G1052	G1053	G1054	G1055	G1056	G1057	G1058	G1059	G1060	G1061																																																																																																																																																																																																																																																																																																																																																																																																																																																			
G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999																																																																																																																																																																																																																																																																																																																																																																																																																																																				
C801	C802	U810	G811	G812	G813	G814	U821	U822	U823	U824	G825	G826	U827	G828	G829	G830	G831	G832	G833	G834	G835	G836	G837	G838	G839	G840	G841	G842	G843	G844	G845	G846	G847	G848	G849	G850	U851	G852	G853	G854	G855	G856	U859	G860	G861	G862	G863	G864	G865	G866	G867	G868	G869	G870	G871	G872	G873	G874	G875	G876	G877	G878	G879	G880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999																																																																																																																																																																																																																																																																																																																									
U423	U424	A429	U433	U434	U435	U436	U437	U438	U439	U440	U441	U442	U443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U468	U469	U470	U471	U472	U473	U474	U475	U476	U477	U478	U479	U480	U481	U482	U483	U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554	U555	U556	U557	U558	U559	U560	U561	U562	U563	U564	U565	U566	U567	U568	U569	U570	U571	U572	U573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583	U584	U585	U586	U587	U588	U589	U590	U591	U592	U593	U594	U595	U596	U597	U598	U599	U600	U601	U602	U603	U604	U605	U606	U607	U608	U609	U610	U611	U612	U613	U614	U615	U616	U617	U618	U619	U620	U621	U622	U623	U624	U625	U626	U627	U628	U629	U630	U631	U632	U633	U634	U635	U636	U637	U638	U639	U640	U641	U642	U643	U644	U645	U646	U647	U648	U649	U650	U651	U652	U653	U654	U655	U656	U657	U658	U659	U660	U661	U662	U663	U664	U665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732	U733	U734	U735	U736	U737	U738	U739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792	U793	U794	U795	U796	U797	U798	U799	U800																																																																																																																														
G216	A217	A218	A219	U220	A223	C224	U225	C226	C227	C228	A231	G232	U233	G234	G235	C236	G237	G238	C239	G240	A241	G242	A245	G248	G249	G250	G251	G252	G253	G254	G255	G256	G257	G258	G259	G260	G261	G262	G263	G264	G265	G266	G267	G268	G269	G270	G271	G272	G273	G274	G275	G276	G277	G278	G279	G280	G281	G282	G283	U286	C287																																																																																																																																																																																																																																																																																																																																																																																																																																																			
G290	G291	G292	C295	C296	C297	C298	C299	C300	C301	C302	A303	C304	C305	C306	C307	C308	C309	C310	C311	C312	C313	C314	C315	U328	C329	U330	U331	U332	U333	U334	U335	U336	U337	U338	U339	U340	U341	U342	U343	U344	U345	U346	U347	U348	U349	U350	U351	U352	U353	U354	U355	U356	U357	U358	U359	U360	U361	U362	U363	U364	U365	U366	U367	U368	U369	U370	U371	U372	U373	U374	U375	U376	U377	U378	U379	U380	U381	U382	U383	U384	U385	U386	U387	U388	U389	U390	U391	U392	U393	U394	U395	U396	U397	U398	U399	U400	U401	U402	U403	U404	U405	U406	U407	U408	U409	U410	U411	U412	U413	U414	U415	U416	U417	U418	U419	U420	U421	U422	U423	U424	U425	U426	U427	U428	U429	U430	U431	U432	U433	U434	U435	U436	U437	U438	U439	U440	U441	U442	U443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U468	U469	U470	U471	U472	U473	U474	U475	U476	U477	U478	U479	U480	U481	U482	U483	U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554	U555	U556	U557	U558	U559	U560	U561	U562	U563	U564	U565	U566	U567	U568	U569	U570	U571	U572	U573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583	U584	U585	U586	U587	U588	U589	U590	U591	U592	U593	U594	U595	U596	U597	U598	U599	U600	U601	U602	U603	U604	U605	U606	U607	U608	U609	U610	U611	U612	U613	U614	U615	U616	U617	U618	U619	U620	U621	U622	U623	U624	U625	U626	U627	U628	U629	U630	U631	U632	U633	U634	U635	U636	U637	U638	U639	U640	U641	U642	U643	U644	U645	U646	U647	U648	U649	U650	U651	U652	U653	U654	U655	U656	U657	U658	U659	U660	U661	U662	U663	U664	U665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732	U733	U734	U735	U736	U737	U738	U739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792	U793	U794	U795	U796	U797	U798	U799	U800
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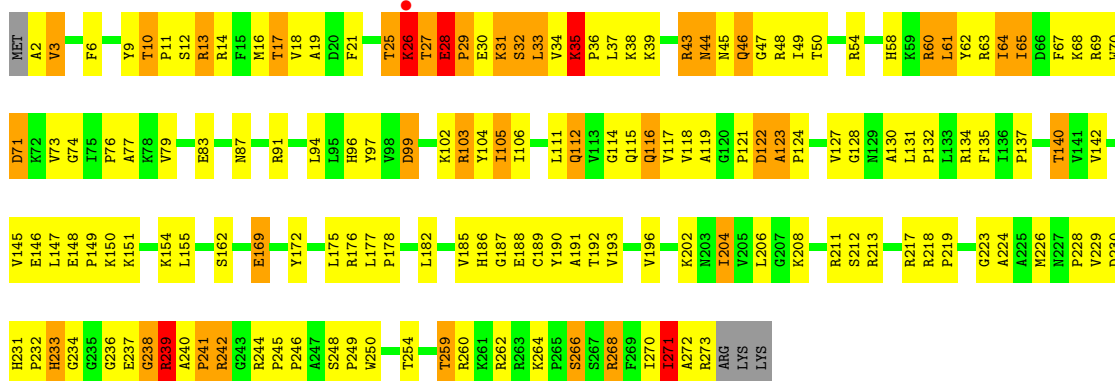






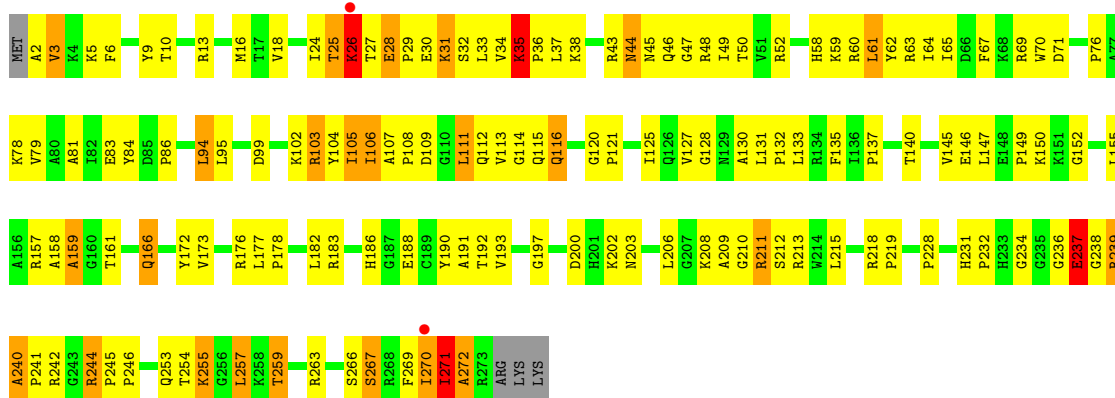
• Molecule 3: 50S ribosomal protein L2

Chain AD:



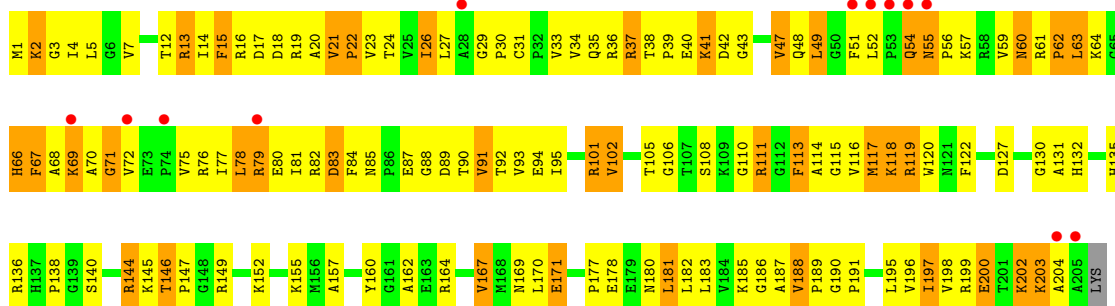
• Molecule 3: 50S ribosomal protein L2

Chain CD:



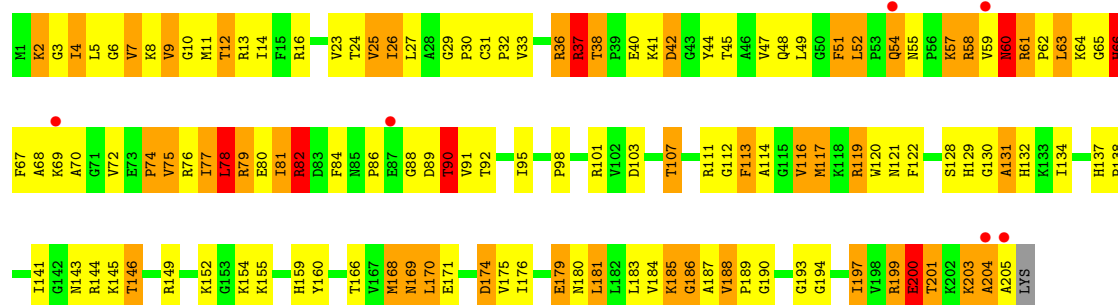
• Molecule 4: 50S ribosomal protein L3

Chain AE:



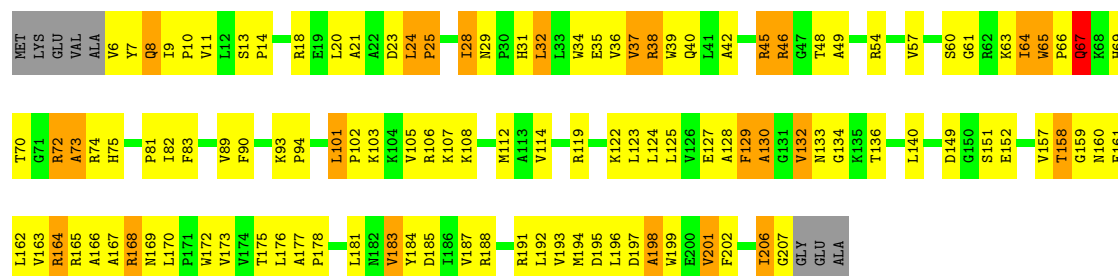
• Molecule 4: 50S ribosomal protein L3

Chain CE:



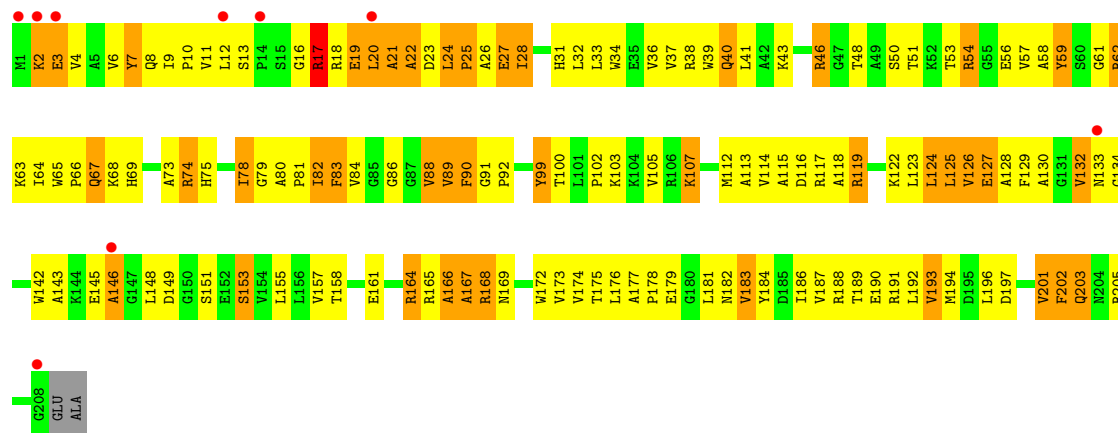
• Molecule 5: 50S ribosomal protein L4

Chain AF:



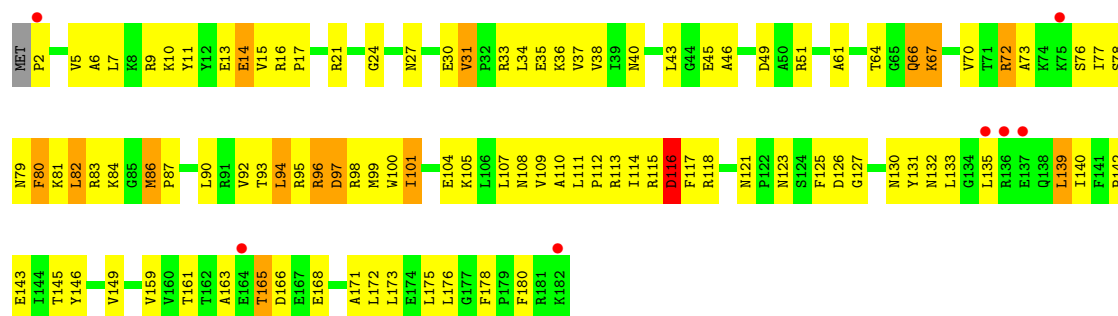
• Molecule 5: 50S ribosomal protein L4

Chain CF:



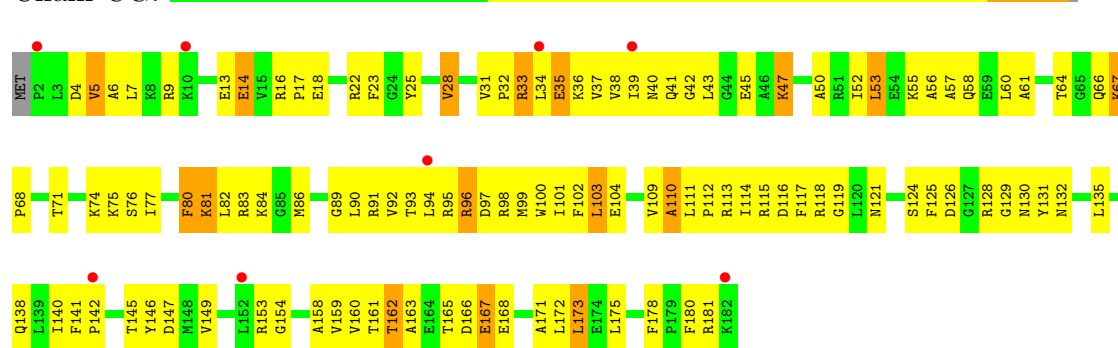
• Molecule 6: 50S ribosomal protein L5

Chain AG:



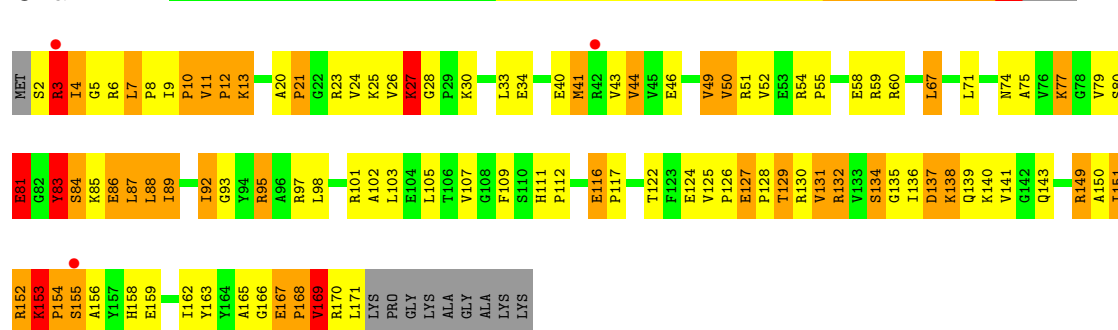
- Molecule 6: 50S ribosomal protein L5

Chain CG:



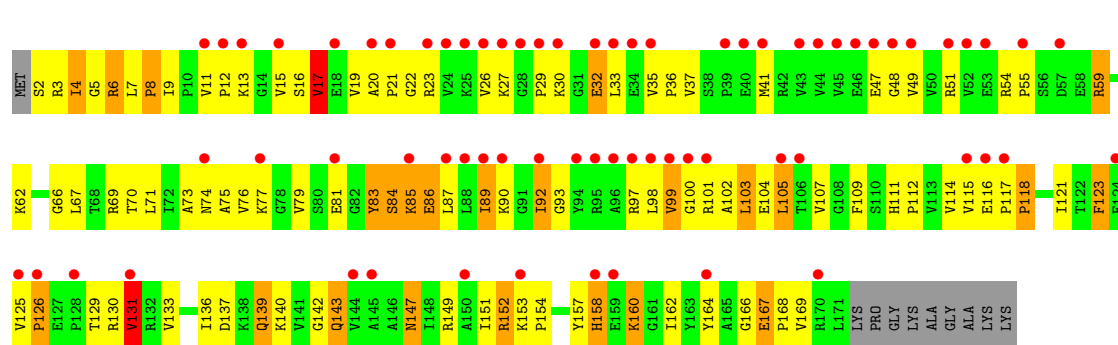
- Molecule 7: 50S ribosomal protein L6

Chain AH:



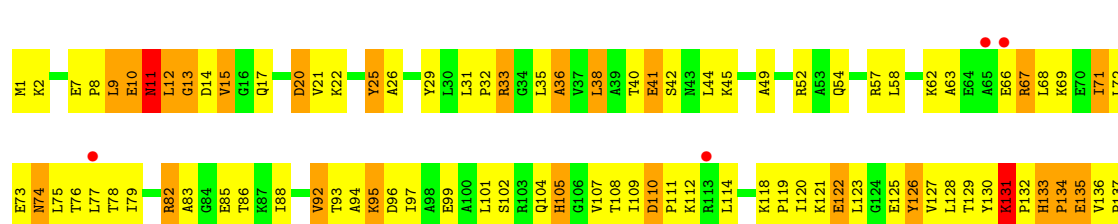
- Molecule 7: 50S ribosomal protein L6

Chain CH:



- Molecule 8: 50S ribosomal protein L9

Chain AK:





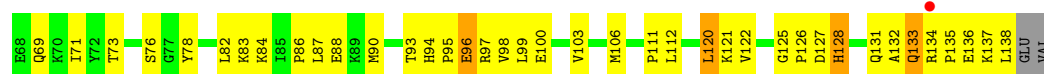
• Molecule 8: 50S ribosomal protein L9

Chain CK:



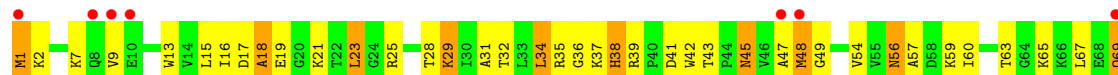
• Molecule 9: 50S ribosomal protein L13

Chain AM:



• Molecule 9: 50S ribosomal protein L13

Chain CM:



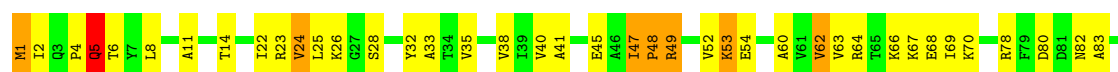
• Molecule 10: 50S ribosomal protein L14

Chain AN:

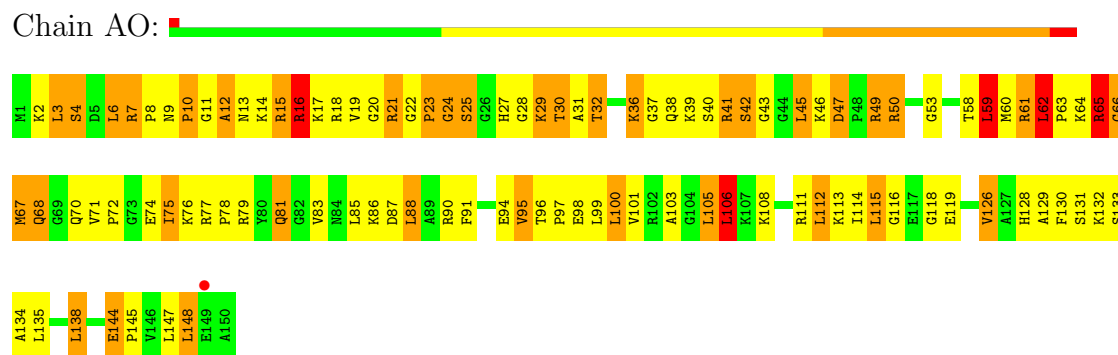


• Molecule 10: 50S ribosomal protein L14

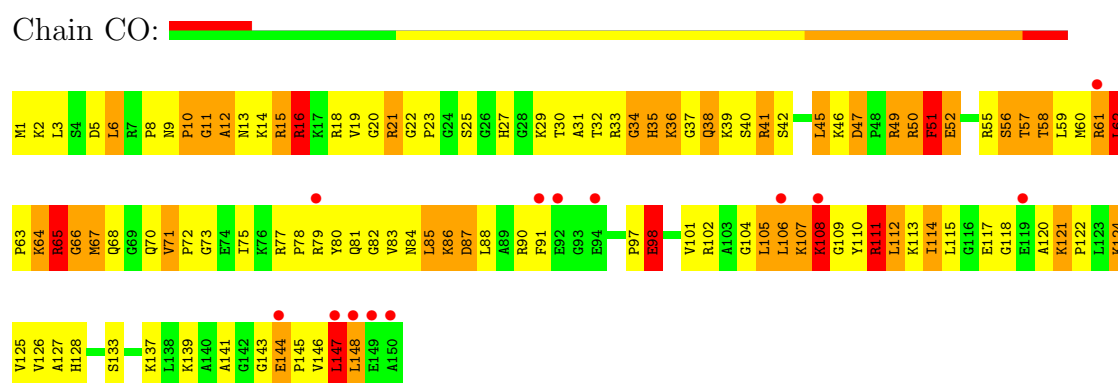
Chain CN:



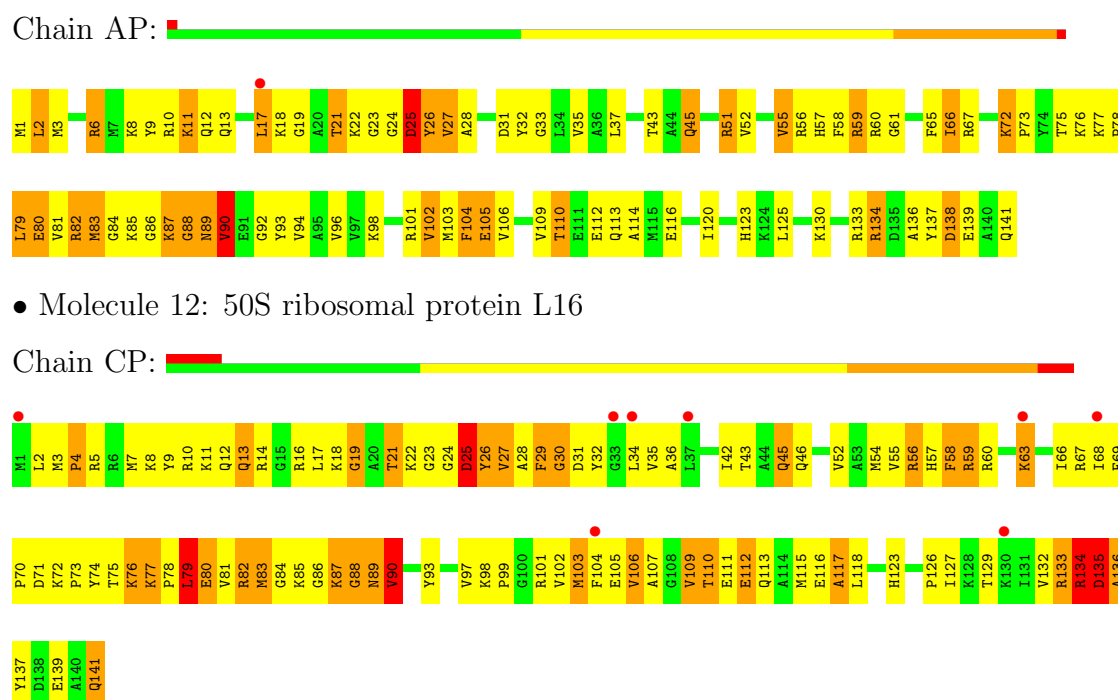
- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15

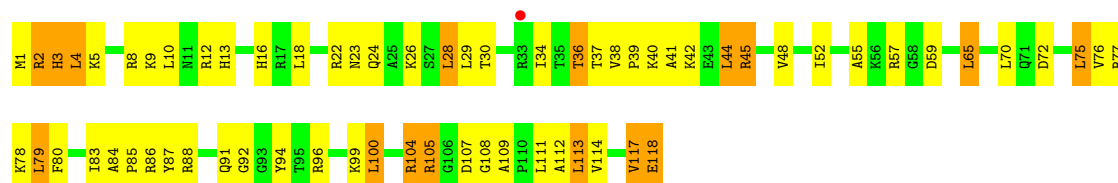


- Molecule 12: 50S ribosomal protein L16



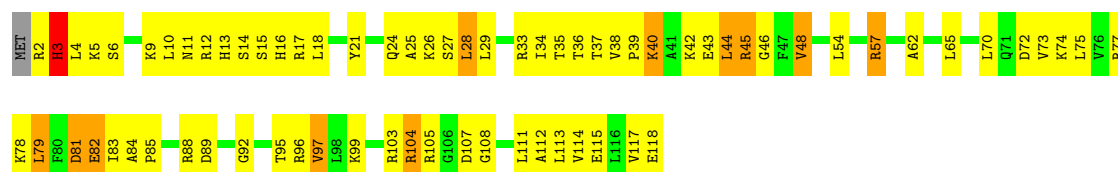
- Molecule 13: 50S ribosomal protein L17





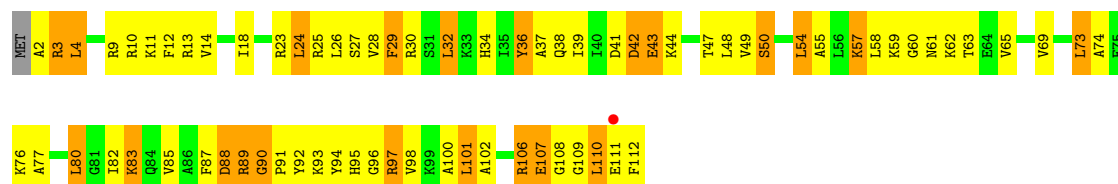
• Molecule 13: 50S ribosomal protein L17

Chain C0:



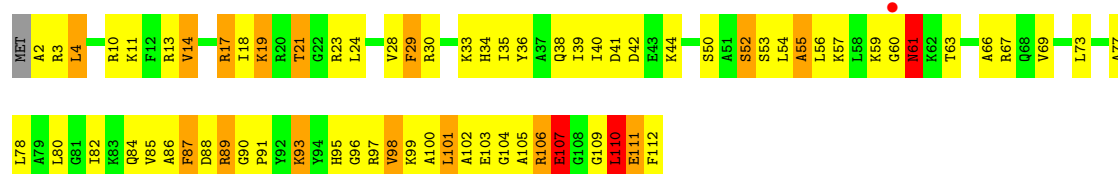
• Molecule 14: 50S ribosomal protein L18

Chain AQ:



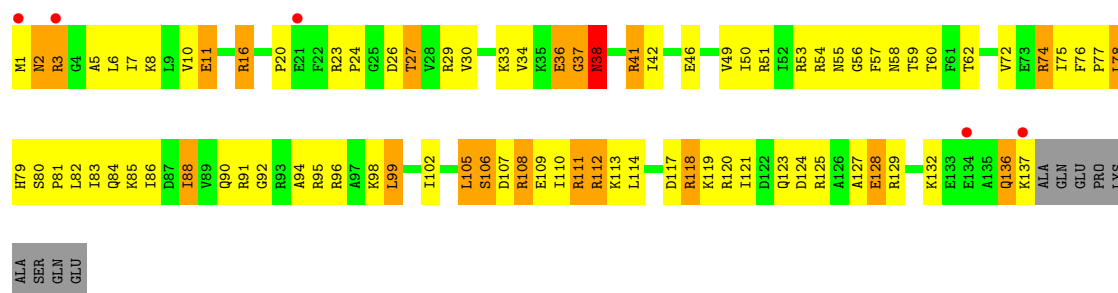
• Molecule 14: 50S ribosomal protein L18

Chain CQ:



• Molecule 15: 50S ribosomal protein L19

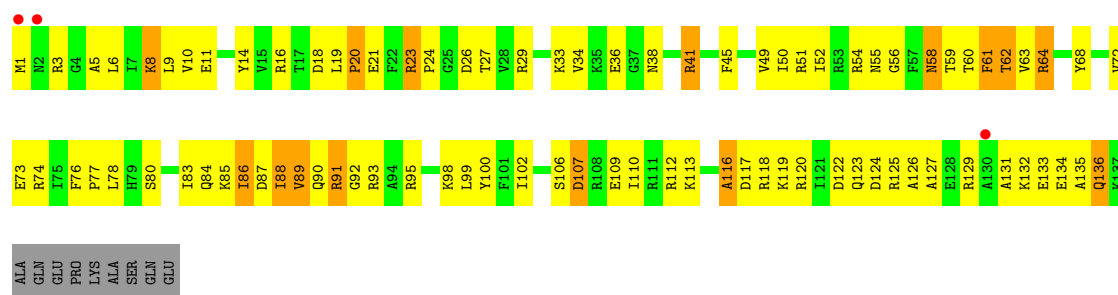
Chain AR:



• Molecule 15: 50S ribosomal protein L19

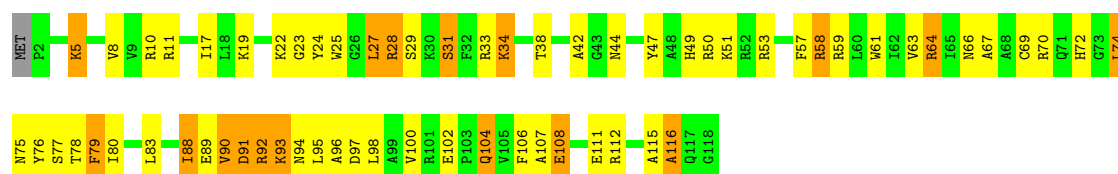
Chain CR:





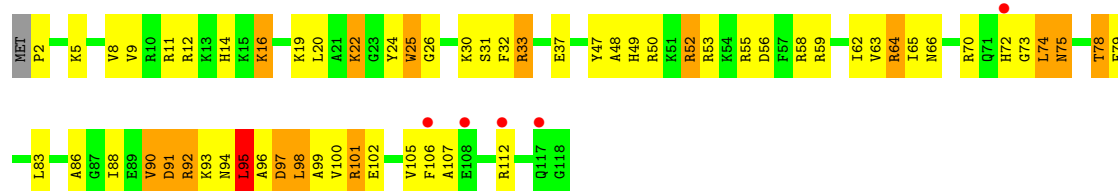
- Molecule 16: 50S ribosomal protein L20

Chain A1:



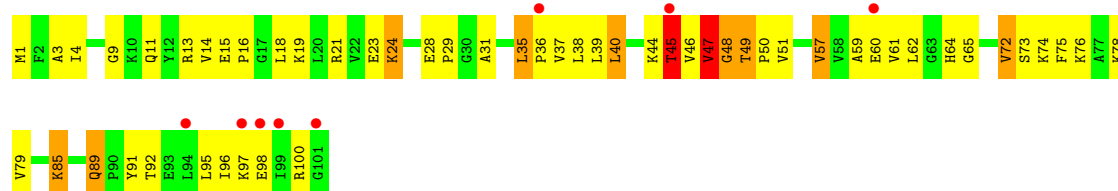
- Molecule 16: 50S ribosomal protein L20

Chain C1:



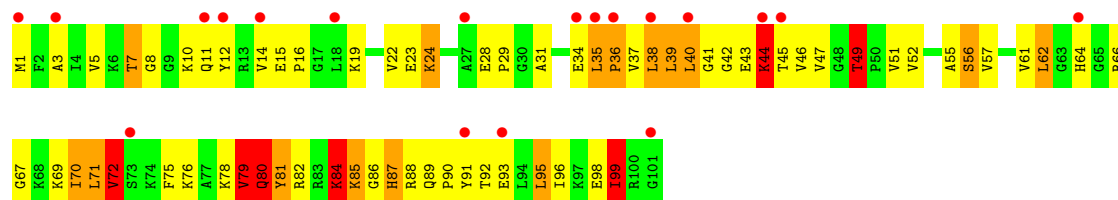
- Molecule 17: 50S ribosomal protein L21

Chain A2:



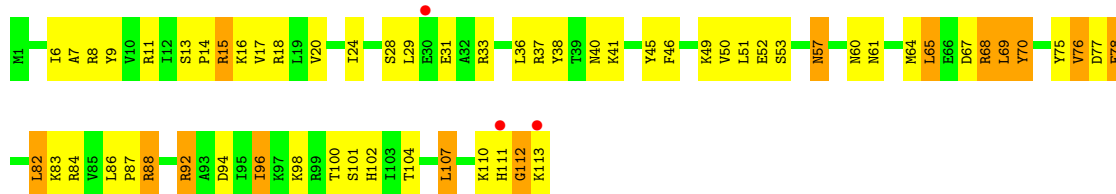
- Molecule 17: 50S ribosomal protein L21

Chain C2:



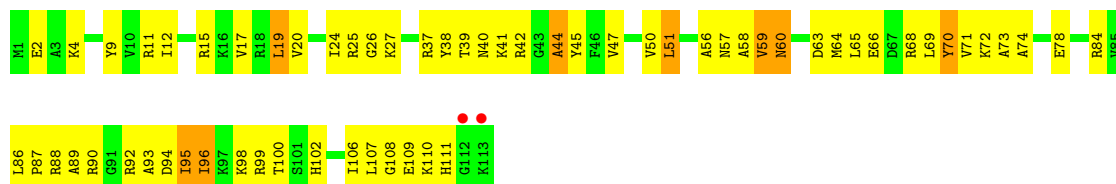
- Molecule 18: 50S ribosomal protein L22

Chain AS:



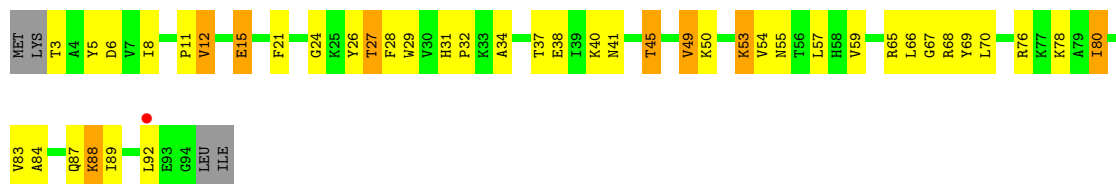
• Molecule 18: 50S ribosomal protein L22

Chain CS:



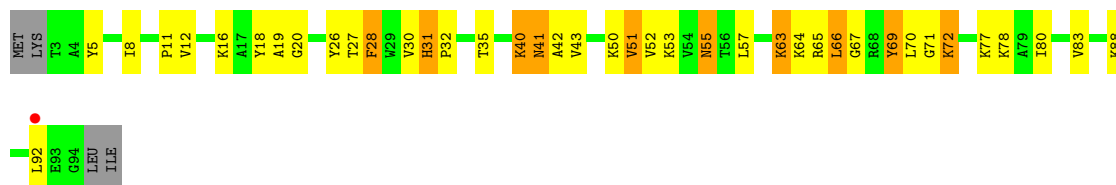
• Molecule 19: 50S ribosomal protein L23

Chain AT:



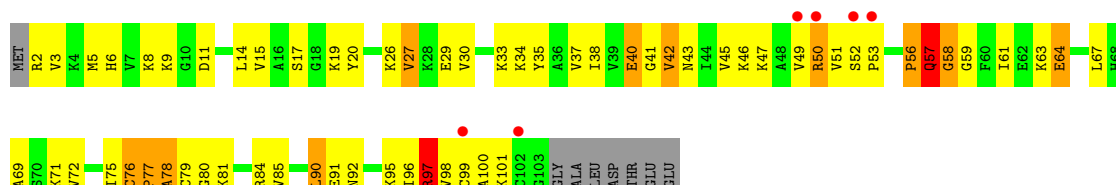
• Molecule 19: 50S ribosomal protein L23

Chain CT:



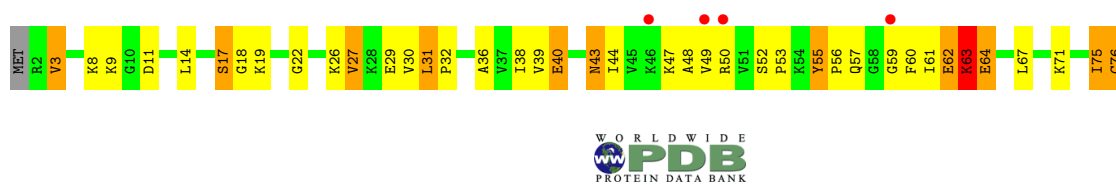
• Molecule 20: 50S ribosomal protein L24

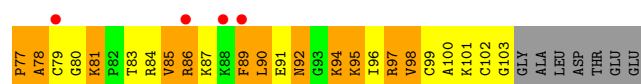
Chain AU:



• Molecule 20: 50S ribosomal protein L24

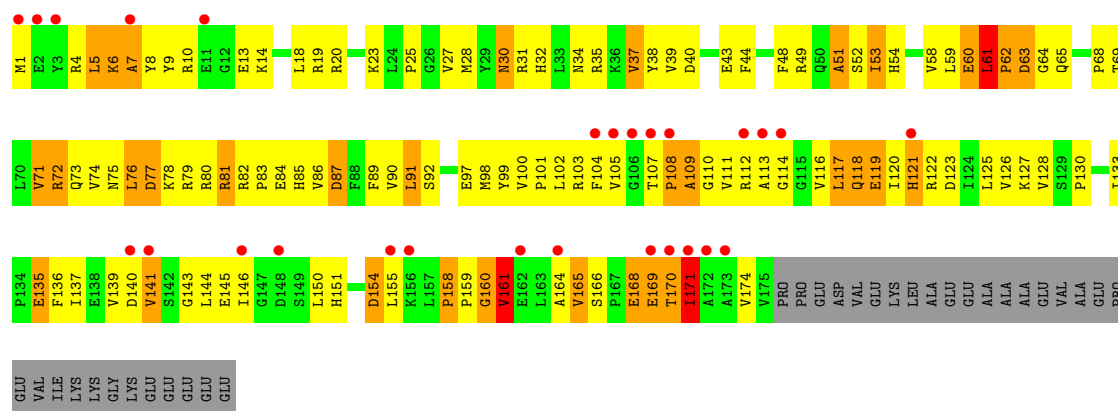
Chain CU:





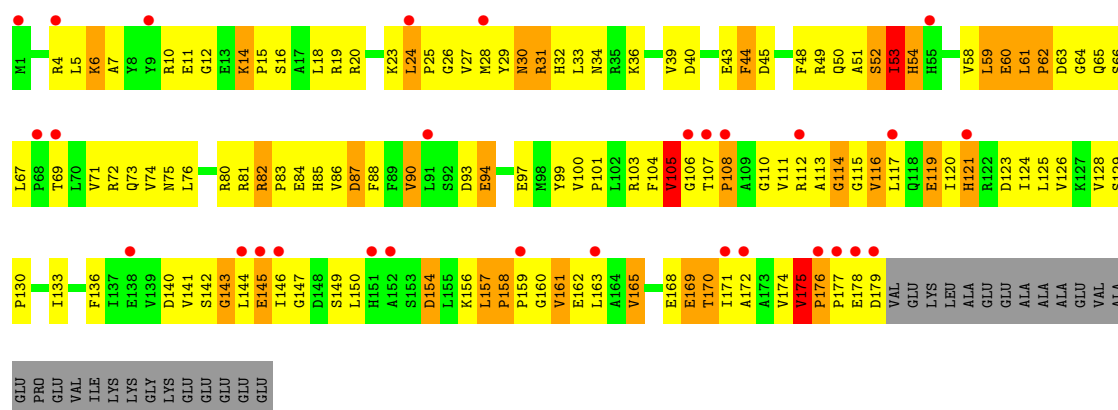
• Molecule 21: 50S ribosomal protein L25

Chain AV:



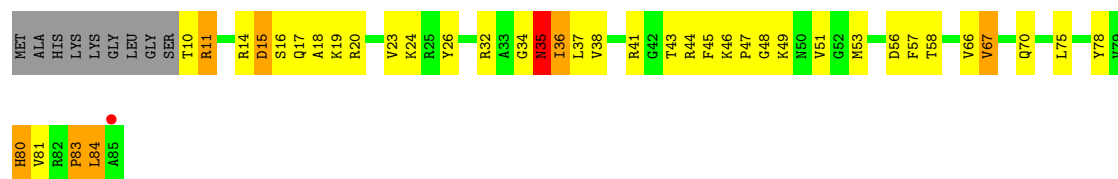
• Molecule 21: 50S ribosomal protein L25

Chain CV:



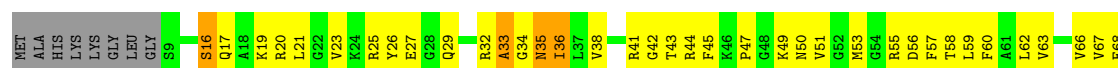
• Molecule 22: 50S ribosomal protein L27

Chain A3:



• Molecule 22: 50S ribosomal protein L27

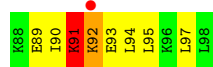
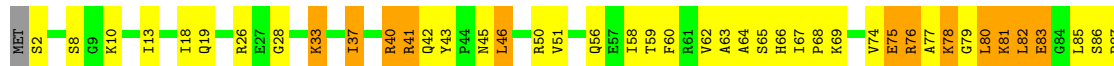
Chain C3:





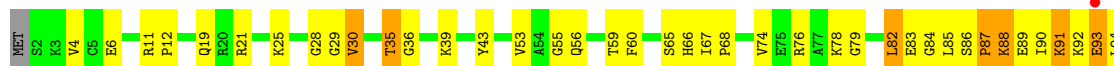
- Molecule 23: 50S ribosomal protein L28

Chain AZ:



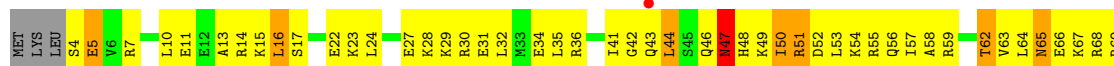
- Molecule 23: 50S ribosomal protein L28

Chain CZ:



- Molecule 24: 50S ribosomal protein L29

Chain AW:



- Molecule 24: 50S ribosomal protein L29

Chain CW:



- Molecule 25: 50S ribosomal protein L30

Chain AX:



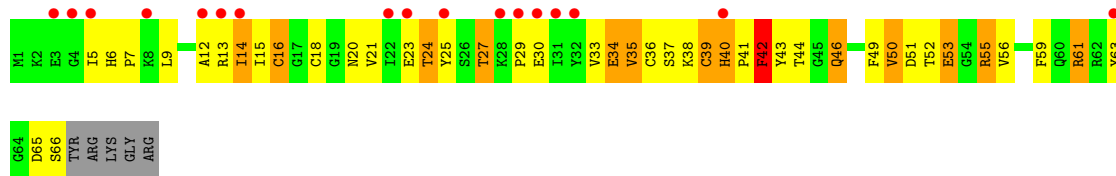
- Molecule 25: 50S ribosomal protein L30

Chain CX:



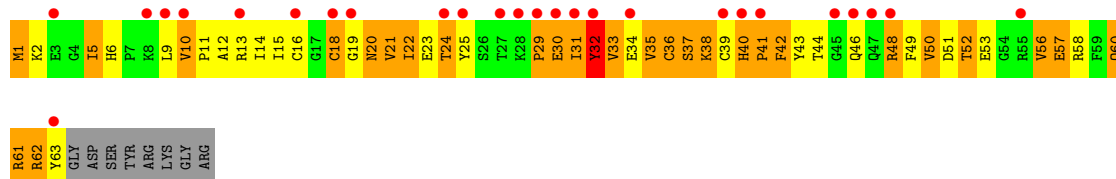
- Molecule 26: 50S ribosomal protein L31

Chain A4:



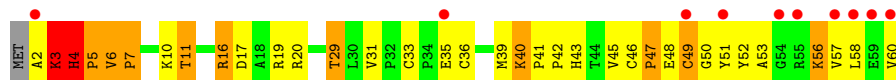
- Molecule 26: 50S ribosomal protein L31

Chain C4:



- Molecule 27: 50S ribosomal protein L32

Chain A5:



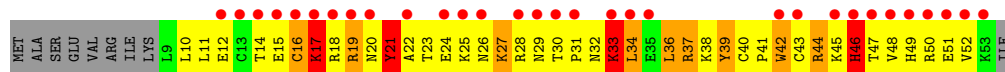
- Molecule 27: 50S ribosomal protein L32

Chain C5:



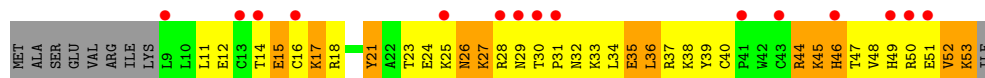
- Molecule 28: 50S ribosomal protein L33

Chain A6:



- Molecule 28: 50S ribosomal protein L33

Chain C6:



- Molecule 29: 50S ribosomal protein L34

Chain A7:



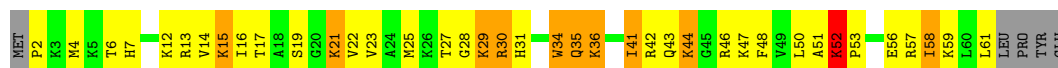
- Molecule 29: 50S ribosomal protein L34

Chain C7:



- Molecule 30: 50S ribosomal protein L35

Chain A8:



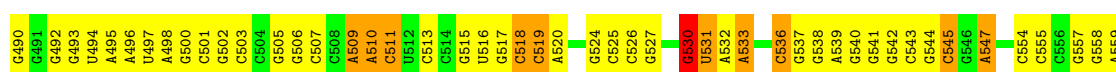
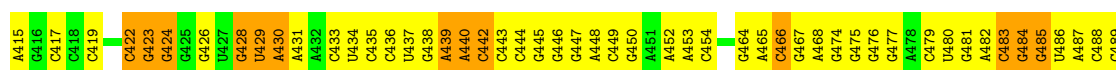
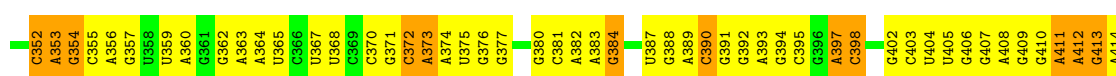
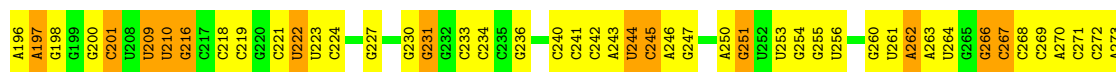
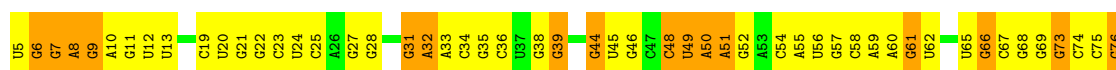
- Molecule 30: 50S ribosomal protein L35

Chain C8:



- Molecule 31: 16S ribosomal RNA

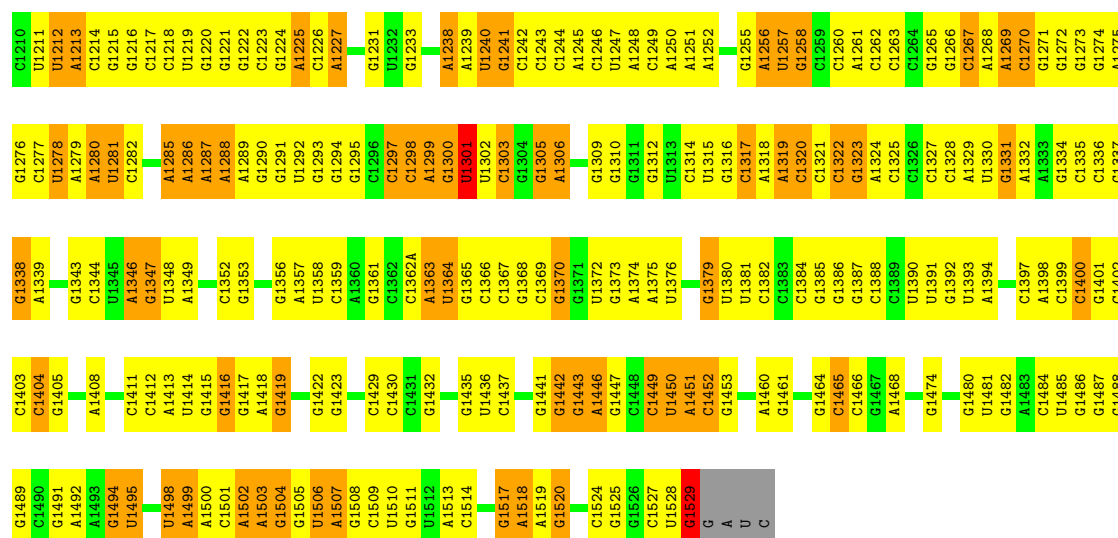
Chain BA:





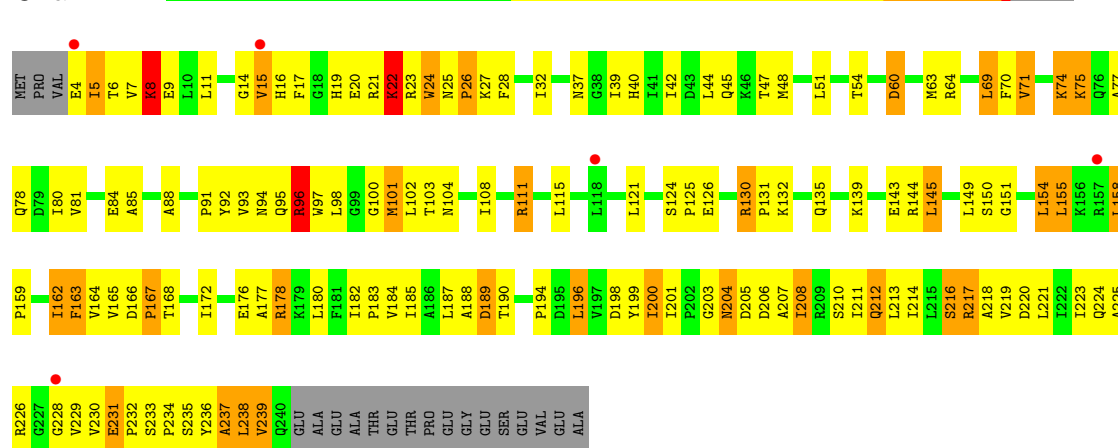
C1145	A1080	G1022	U961	G886	C808	U740	G674	C601	A533	A452	G302	C221	G153	G81
A1146	G1081	G1023	C962	G887	C812	G741	U677	G604	U534	A453	A303	U222	C154	U82
U1147	U1082	G1024	G963	G890	U813	G742	U678	U605	A535	C454	U304	U223	C155	U84
U1148	U1083	U1025	A964	U891	U814	U743	U679	U606	C536	C455	G305	G306	G156	U85
C1149	G1084	G1026	A965	U892	A815	C744	C680	A607	G537	C456	G306	C224	G157	U86
U1150	U1085	C1027	G966	C893	A816	C745	C681		G538	C457	C312	C225	A160	A87
A1151	U1086	C1028	C967		C817	G746	G682	C615	A539	C458	C313	G226	A161	C88
A1152	G1087	U1029	A968	C897	C818	G747	G683	G616	G540	A464	A313		A161	U89
C1153		C1028B	A969	C898	A819	G748	G684	G617	G541	A465	G316	G230	C165	C90
G1154	A1092	G1029	C970	C899	A820	U751	A684	C618	G542	C466	G316	G231	G166	C91
G1155	A1093	C1030	G971	C899	A821	G752	A685	C619	C543	C467	C390	G232	G167	G92
A1156	G1094	G1031	C972	A901	A753	G753	A686	U619	G544	A468	G391	C235	G168	U93
U1157	U1095	A1032	C973	A901	C754	G754	A687	C620	G545	A469	C392	G236	G169	G95
C1158	C1096	G1032A	A974	G902	G755	G755	G688	A621	G546	A474	G392	C237	C170	G96
U1159	C1097	U1032B	A975		C756	C756	G689	A622	A547	A476	A397		U170	U97
G1160	C1098	G1033	C976	A907	U827	U757	G690	A623	G548	A477	C398	A243		C99
C1161	G1099	G1034	A977	A908	A828	G758	G691	C624	C549	A478	A325	U244	U173	A101
C1162	C1100	A1035	A978	A909	U833	G759	U692	G625	G550	C479	G326	C245	C174	G102
C1163	A1101	G1036	C979	C910	C834	G760	G693	U626	U551	U480	C328	A246	C175	C103
C1164	A1102	C1037	C980		U835		A694	G627	U552		A329	G247	C176	
		C1038	U981	A913	G836	G763	A695	G628	A553	A484	G108		C177	G108
		C1039	U982	A914	G837	C764	A696	G629	C554	A485	A109	A250	C178	A109
		U1040	A983	A915	G838	G765	U697	G630	C555	U486	C110	G251	A179	C110
		A1041	C984		U841		G698	G631	C557		A408		U180	G111
		C1042	C985	A918	C842	G769	C699	A632	G557	G491	G337	G255	G181	G112
		C1043	A986	A919	U843			G633	G558	G492	A338		U182	G113
		A1044	G987	U920	C848	G773	A702	C634	A559	G493	C339	G259	G183	U114
		C1045	G988	U921	C849	G774	G703	C635	U560	G494	U340	G260	G184	
		A1046	C989	G922	U850	G775	A704	U636	U561	A495	C341	A262	C186	G115
		G1047	C990	A923	G851	G776	U705	C637	C562	A496	A414	U261	C186	A116
		U1048	U991	C924	G852	A777	A706		A563	U497	A344	A263	C186C	G121
		C1049	U992	G925	G853	G778	C707	C643	C564	A498	A345	U264	C186E	G122
		G1050	G993	G926	G854	G779	C708	C644	G570	C501	G346	G265	C186F	C123
		U1051	A994	G927	G855	A780	G709	U646	U571	G502	G347	G267	C187	G127
		U1052	C995		G855	A781	G710	C647	A573	C503	A349	C268	U188	G128
		G1053		C934	G858	A782	G715		A574	C504	G350	C269	U189	U129
		C1054	G938	A935	A859	C783	A716		A574	C505	G351	A270	U129A	
		A1055			A860	C784	G717	C651	G575		C352	C271	A130	G130
		U1056		G939	G861	G785	G718	U652	G576	C508	A353	C272	G191A	C131
		G1057	G1001	C940	C862	G786	G719	A654	A509	A510	G354	A273	G191B	C132
		U1058	G1002	G941	C862	A787	C719	A655	A510	U429	C355		G191C	U133
		C1059	G1003	G942	A865	U788	C720	A656	C511				U191D	U134
		C1060	A1004	U943	A866	U789	G721	C656					G191E	A134
			A1005	C944	G867	A790		G657	G580		U359	C277	U191F	C135
		G1064	C1006	G945	C868	G791	G724	C658	U582	U516	A360	A279	G191	C136
		U1065	C1007	G946	G869	A792	G725	U659	U583	G517	G361	C280	U192	C137
		C1066	C1008	G947	U870	U793	C726	G660	G584	C518	G362	G281	C193	G138
		A1067	G1009	C948	U871	A794	G727	G661	G585	C519	A363	A282	C194	G139
		G1068	G1010	A949	A872	C795	A728	G662	C586	A520	A364	C283	C195	A140
		C1069	G1011	U950	A873	C796	A729	A663	G587	G521	U437	G284	A196	A141
		U1070	U1012	G951	A874	C797	G730	C664	G588	C522	C366	G285	A197	G142
		C1071	G1013	U952	C875	G798	G731	A665	G592	A523	U367		A198	A143
		G1072	A1014	G953	C879	G799	C732	G666	G593	C526	C372	G289	G199	A144
		U1073	A1015	G954	C879	C800	A733	G667	G594	G527	A373	U296	G200	G145
		G1074	A1016	G955	C880	G735	C734	G668	C595	C528	A374	G297	C201	G146
		C1075	G1017	U956	G881	G736	G735	U669	G597	G529	U375	A298	U208	G148
		G1076	G1018	U957	C882	U804	C738	G670	G598	G530	G376	A299	U209	G149
		U1077	C1019	A958	C883	C805	A737	G671	U599	U531	G377	A300	G210	A149
		U1078	U1020	A959	U884	C806	A738	U672	C599		G377	A300	G216	C217
		G1079	G1021	U960	G885	A807	C739	G673	C600	A532	G378	G301	C217	





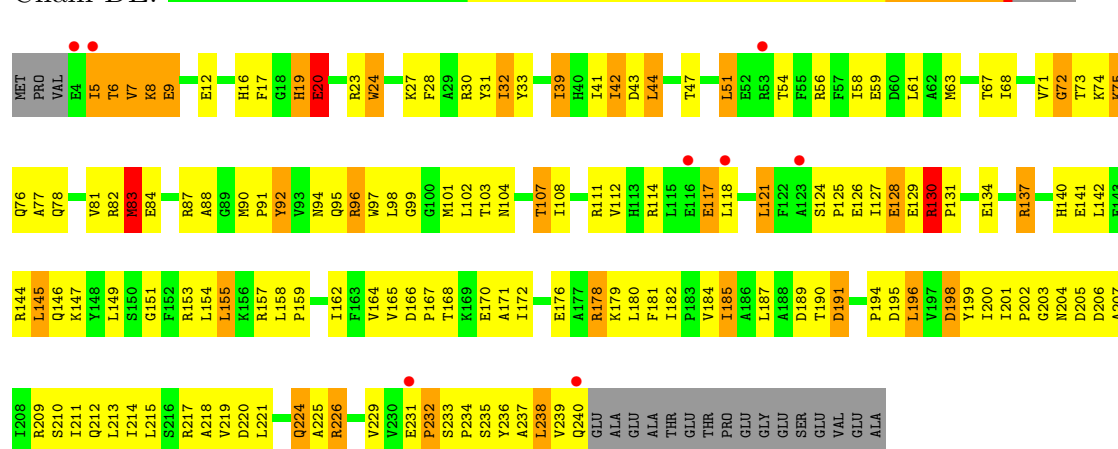
### • Molecule 32: 30S RIBOSOMAL PROTEIN S2

Chain BE:



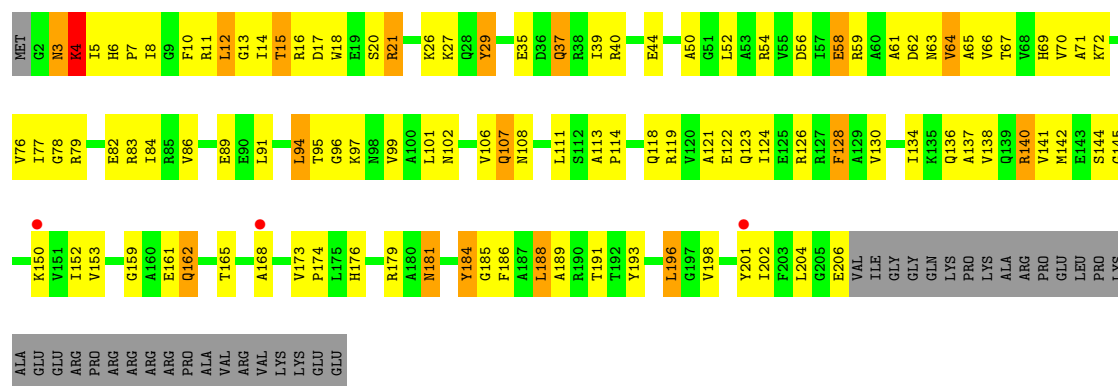
### • Molecule 32: 30S RIBOSOMAL PROTEIN S2

Chain DE:



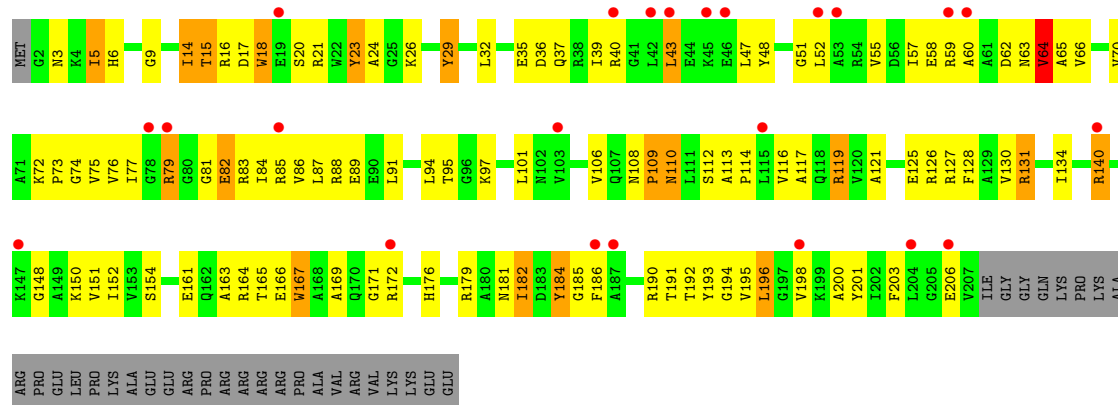
### • Molecule 33: 30S RIBOSOMAL PROTEIN S3

Chain BF:



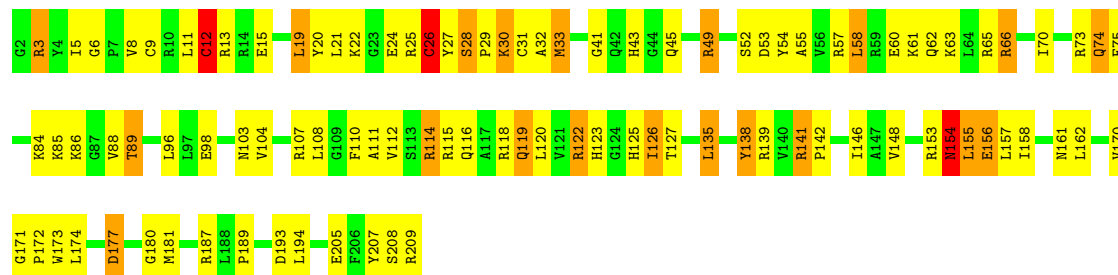
• Molecule 33: 30S RIBOSOMAL PROTEIN S3

Chain DF:



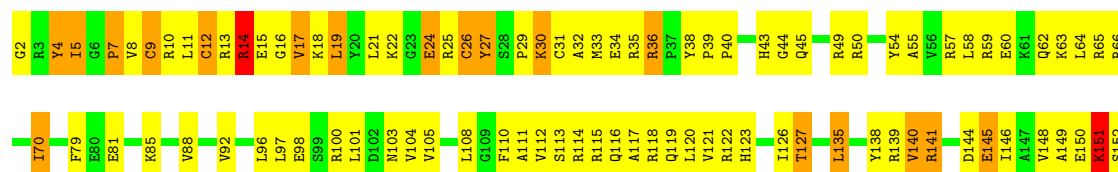
• Molecule 34: 30S RIBOSOMAL PROTEIN S4

Chain BG:



• Molecule 34: 30S RIBOSOMAL PROTEIN S4

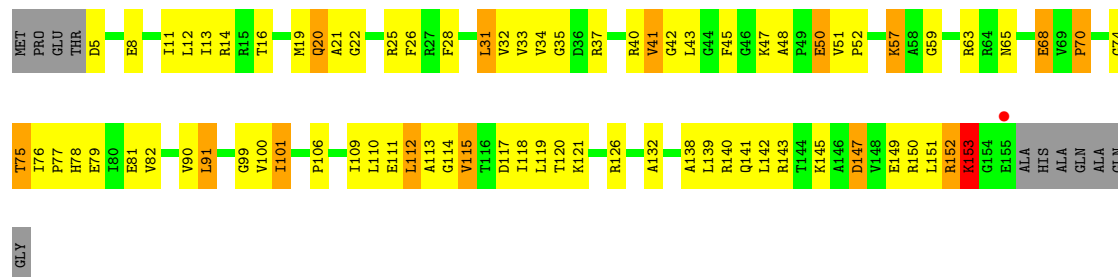
Chain DG:





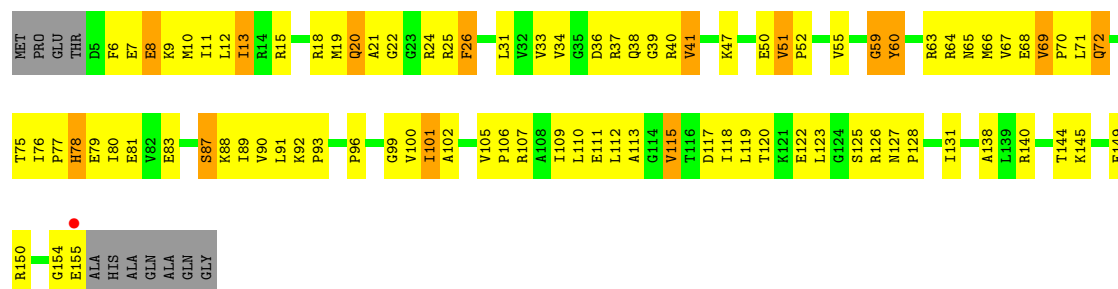
• Molecule 35: 30S RIBOSOMAL PROTEIN S5

Chain BH:



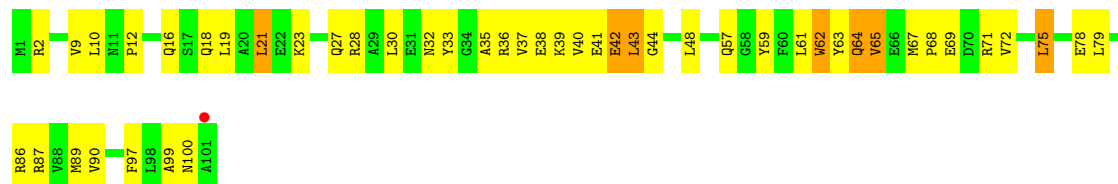
• Molecule 35: 30S RIBOSOMAL PROTEIN S5

Chain DH:



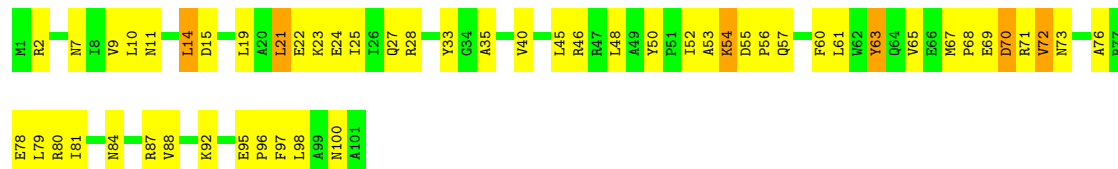
• Molecule 36: 30S RIBOSOMAL PROTEIN S6

Chain BI:



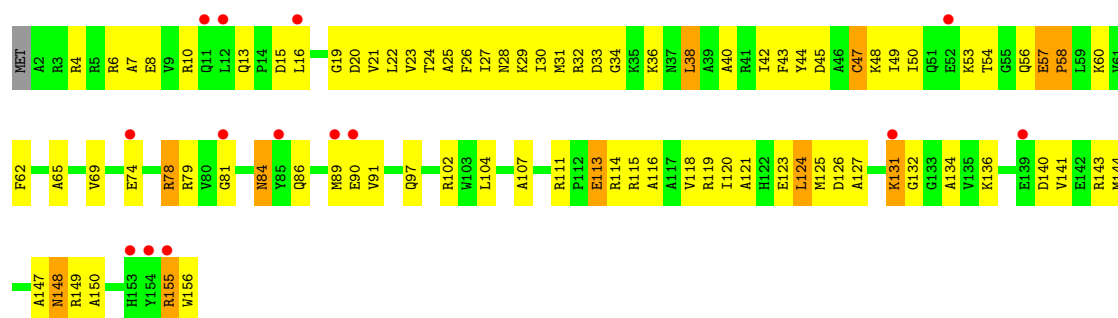
• Molecule 36: 30S RIBOSOMAL PROTEIN S6

Chain DI:



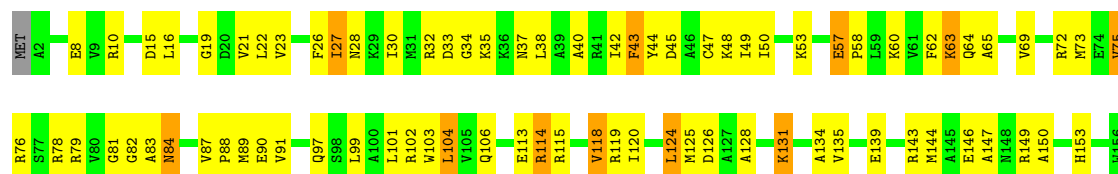
• Molecule 37: 30S RIBOSOMAL PROTEIN S7

Chain BJ:



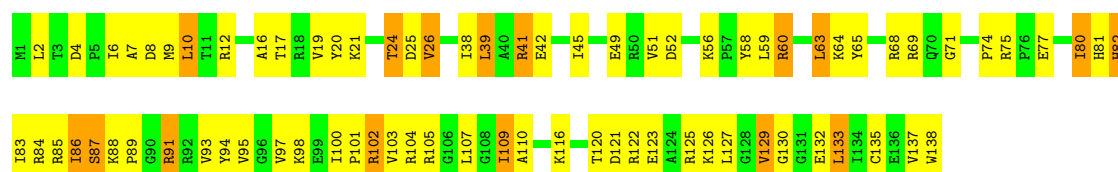
• Molecule 37: 30S RIBOSOMAL PROTEIN S7

Chain DJ:



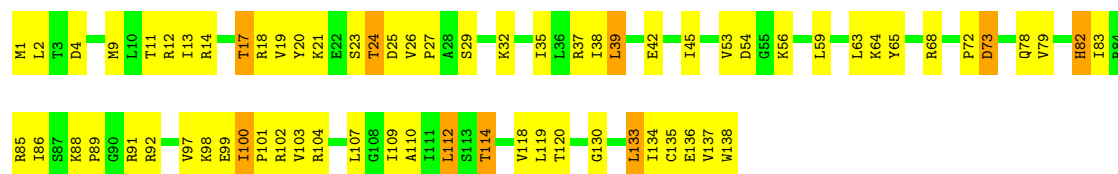
• Molecule 38: 30S RIBOSOMAL PROTEIN S8

Chain BK:



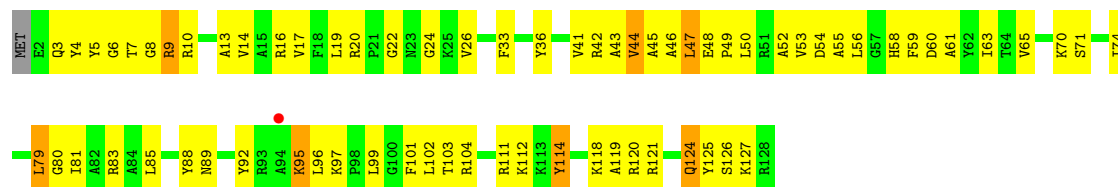
• Molecule 38: 30S RIBOSOMAL PROTEIN S8

Chain DK:



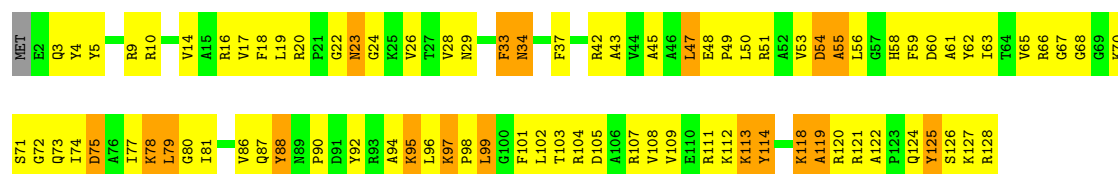
• Molecule 39: 30S RIBOSOMAL PROTEIN S9

Chain BL:



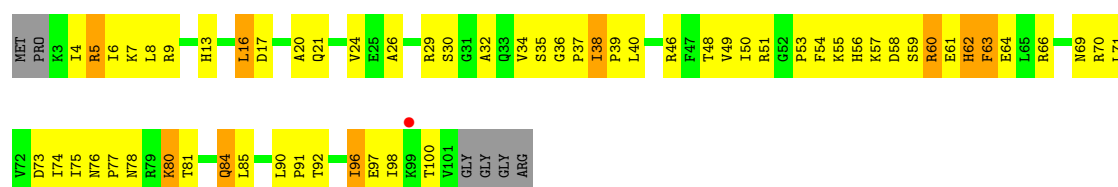
• Molecule 39: 30S RIBOSOMAL PROTEIN S9

Chain DL:



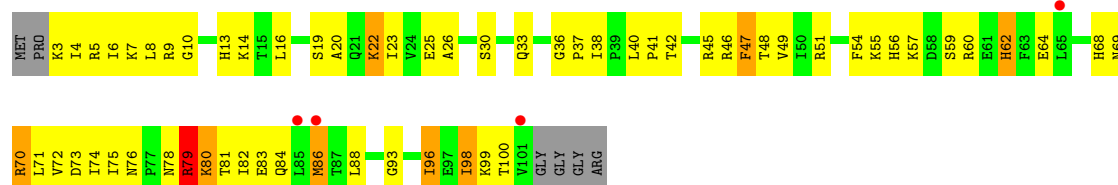
• Molecule 40: 30S RIBOSOMAL PROTEIN S10

Chain BM:



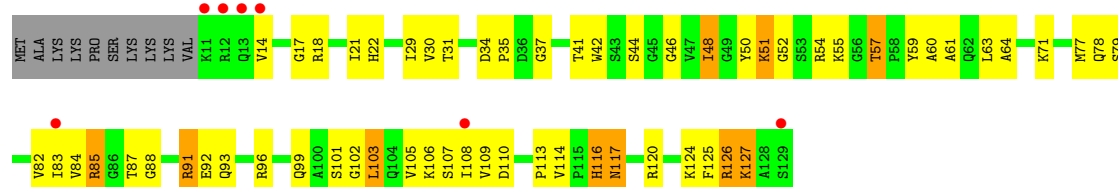
• Molecule 40: 30S RIBOSOMAL PROTEIN S10

Chain DM:



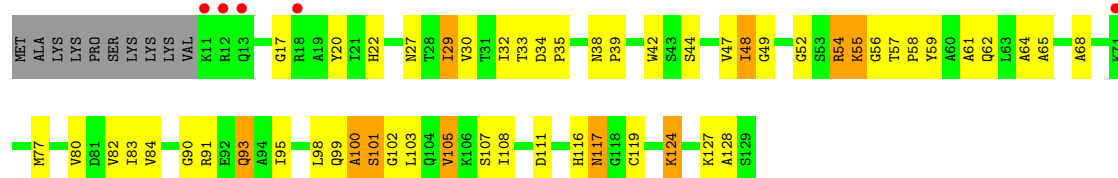
• Molecule 41: 30S RIBOSOMAL PROTEIN S11

Chain BN:



• Molecule 41: 30S RIBOSOMAL PROTEIN S11

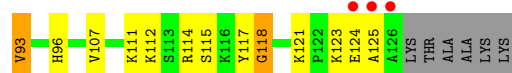
Chain DN:



• Molecule 42: 30S RIBOSOMAL PROTEIN S12

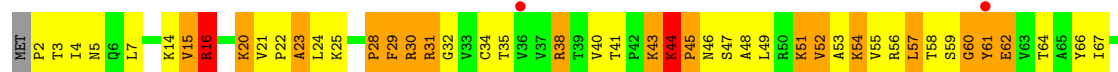
Chain BO:





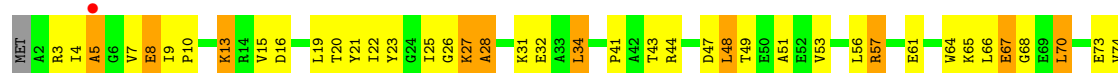
• Molecule 42: 30S RIBOSOMAL PROTEIN S12

Chain DO:



• Molecule 43: 30S RIBOSOMAL PROTEIN S13

Chain BP:



• Molecule 43: 30S RIBOSOMAL PROTEIN S13

Chain DP:



• Molecule 44: 30S RIBOSOMAL PROTEIN S14

Chain BQ:



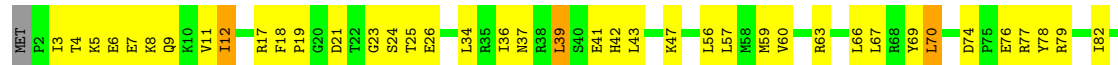
• Molecule 44: 30S RIBOSOMAL PROTEIN S14

Chain DQ:



• Molecule 45: 30S RIBOSOMAL PROTEIN S15

Chain BR:





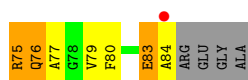
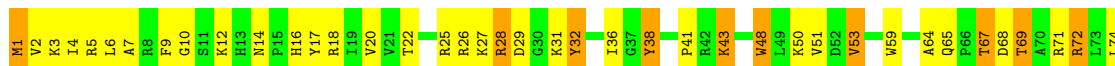
- Molecule 45: 30S RIBOSOMAL PROTEIN S15

Chain DR:



- Molecule 46: 30S RIBOSOMAL PROTEIN S16

Chain BS:



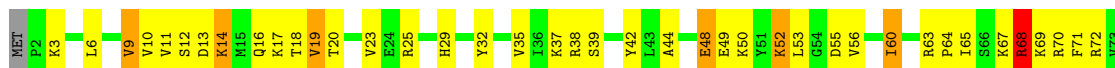
- Molecule 46: 30S RIBOSOMAL PROTEIN S16

Chain DS:



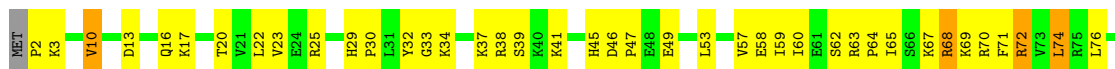
- Molecule 47: 30S RIBOSOMAL PROTEIN S17

Chain BT:



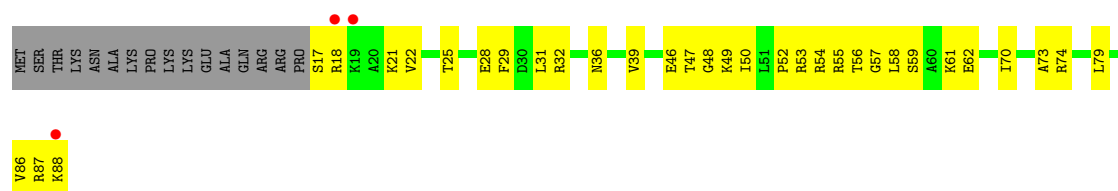
- Molecule 47: 30S RIBOSOMAL PROTEIN S17

Chain DT:



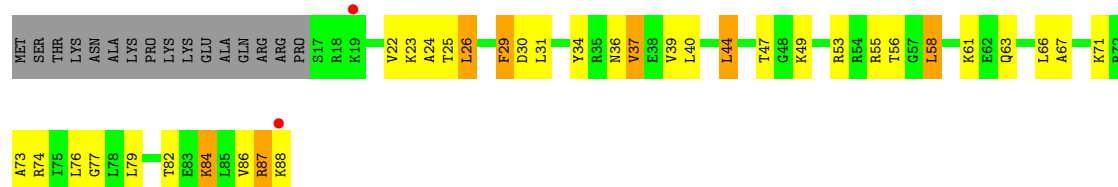
- Molecule 48: 30S RIBOSOMAL PROTEIN S18

Chain BU:



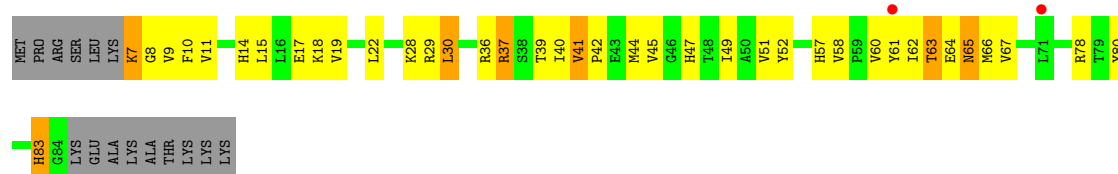
• Molecule 48: 30S RIBOSOMAL PROTEIN S18

Chain DU:



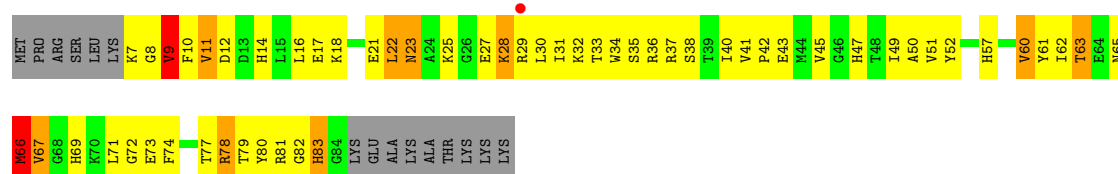
• Molecule 49: 30S RIBOSOMAL PROTEIN S19

Chain BV:



• Molecule 49: 30S RIBOSOMAL PROTEIN S19

Chain DV:



• Molecule 50: 30S RIBOSOMAL PROTEIN S20

Chain BW:



• Molecule 50: 30S RIBOSOMAL PROTEIN S20

Chain DW:

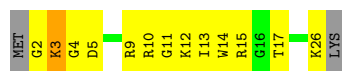






- Molecule 51: 30S RIBOSOMAL PROTEIN THX

Chain BX:



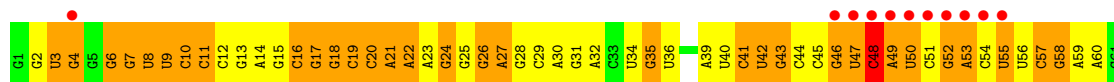
- Molecule 51: 30S RIBOSOMAL PROTEIN THX

Chain DX:



- Molecule 52: TRNA-TYR

Chain BB:



- Molecule 52: TRNA-TYR

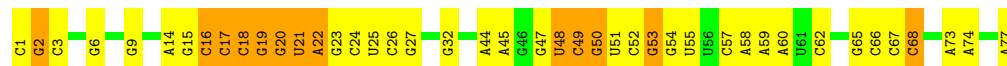
Chain BD:





- Molecule 53: TRNA-FMET

Chain BC:



- Molecule 53: TRNA-FMET

Chain DC:



- Molecule 54: MRNA

Chain B1:



- Molecule 54: MRNA

Chain D1:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.25Å 450.87Å 622.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	256.19 – 3.30 256.19 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (256.19-3.30) 92.8 (256.19-3.20)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_810)	Depositor
R, $R_{free}$	0.206 , 0.259 0.258 , 0.298	Depositor DCC
$R_{free}$ test set	888 reflections (0.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	90.6	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 61.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 962434 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	303952	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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, OHX, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	AA	0.34	0/70233	0.73	38/109643 (0.0%)
1	CA	0.30	1/70122 (0.0%)	0.70	35/109469 (0.0%)
2	AB	0.32	0/2928	0.79	11/4568 (0.2%)
2	CB	0.27	0/2928	0.70	1/4568 (0.0%)
3	AD	0.30	0/2165	0.56	0/2919
3	CD	0.28	0/2165	0.50	0/2919
4	AE	0.27	0/1601	0.53	0/2160
4	CE	0.26	0/1601	0.51	0/2160
5	AF	0.27	0/1620	0.49	0/2194
5	CF	0.25	0/1662	0.54	0/2249
6	AG	0.23	0/1499	0.45	0/2016
6	CG	0.21	0/1499	0.42	0/2016
7	AH	0.27	0/1332	0.51	0/1802
7	CH	0.23	0/1332	0.47	0/1802
8	AK	0.24	0/1151	0.50	0/1558
8	CK	0.22	0/1151	0.50	0/1558
9	AM	0.26	0/1131	0.48	0/1525
9	CM	0.23	0/1131	0.45	0/1525
10	AN	0.26	0/943	0.47	0/1269
10	CN	0.25	0/943	0.45	0/1269
11	AO	0.27	0/1162	0.60	1/1544 (0.1%)
11	CO	0.24	0/1162	0.47	0/1544
12	AP	0.27	0/1143	0.45	0/1527
12	CP	0.23	0/1143	0.43	0/1527
13	A0	0.25	0/982	0.48	0/1312
13	C0	0.24	0/974	0.44	0/1302
14	AQ	0.25	0/892	0.47	0/1187
14	CQ	0.24	0/892	0.47	0/1187
15	AR	0.27	0/1155	0.50	0/1542
15	CR	0.24	0/1155	0.44	0/1542
16	A1	0.27	0/982	0.50	0/1306
16	C1	0.24	0/982	0.41	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	A2	0.26	0/790	0.50	0/1057
17	C2	0.26	0/790	0.53	0/1057
18	AS	0.26	0/911	0.46	0/1220
18	CS	0.25	0/911	0.46	0/1220
19	AT	0.31	0/739	0.49	0/993
19	CT	0.28	0/739	0.47	0/993
20	AU	0.27	0/798	0.49	0/1064
20	CU	0.25	0/798	0.48	0/1064
21	AV	0.25	0/1427	0.50	1/1935 (0.1%)
21	CV	0.22	0/1460	0.45	0/1982
22	A3	0.27	0/615	0.50	0/819
22	C3	0.25	0/621	0.48	0/827
23	AZ	0.26	0/770	0.50	0/1022
23	CZ	0.26	0/770	0.51	0/1022
24	AW	0.29	0/560	0.54	0/741
24	CW	0.24	0/560	0.45	0/741
25	AX	0.24	0/474	0.40	0/635
25	CX	0.21	0/474	0.40	0/635
26	A4	0.25	0/545	0.58	0/733
26	C4	0.26	0/527	0.55	0/709
27	A5	0.24	0/473	0.49	0/639
27	C5	0.25	0/473	0.51	0/639
28	A6	0.28	0/396	0.54	0/529
28	C6	0.25	0/396	0.58	0/529
29	A7	0.31	0/399	0.48	0/526
29	C7	0.25	0/399	0.45	0/526
30	A8	0.34	0/486	0.61	0/638
30	C8	0.27	0/486	0.51	0/638
31	BA	0.28	0/36139	0.68	22/56406 (0.0%)
31	DA	0.26	0/36142	0.65	20/56410 (0.0%)
32	BE	0.22	0/1959	0.43	0/2642
32	DE	0.22	0/1959	0.43	0/2642
33	BF	0.23	0/1629	0.41	0/2195
33	DF	0.21	0/1636	0.40	0/2205
34	BG	0.26	0/1733	0.45	0/2318
34	DG	0.24	0/1733	0.45	0/2318
35	BH	0.24	0/1171	0.44	0/1576
35	DH	0.22	0/1171	0.43	0/1576
36	BI	0.24	0/856	0.43	0/1154
36	DI	0.23	0/856	0.44	0/1154
37	BJ	0.23	0/1276	0.38	0/1709
37	DJ	0.21	0/1276	0.37	0/1709
38	BK	0.23	0/1136	0.47	0/1527

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DK	0.21	0/1136	0.42	0/1527
39	BL	0.22	0/1029	0.41	0/1379
39	DL	0.23	0/1029	0.44	0/1379
40	BM	0.22	0/814	0.45	0/1095
40	DM	0.21	0/814	0.44	0/1095
41	BN	0.24	0/900	0.47	0/1213
41	DN	0.23	0/900	0.45	0/1213
42	BO	0.26	0/991	0.47	0/1327
42	DO	0.24	0/991	0.47	0/1327
43	BP	0.22	0/938	0.47	0/1258
43	DP	0.21	0/943	0.43	0/1265
44	BQ	0.26	0/485	0.45	0/643
44	DQ	0.23	0/485	0.46	0/643
45	BR	0.24	0/745	0.41	0/992
45	DR	0.22	0/745	0.40	0/992
46	BS	0.22	0/721	0.43	0/970
46	DS	0.22	0/721	0.43	0/970
47	BT	0.24	0/847	0.41	0/1131
47	DT	0.23	0/847	0.40	0/1131
48	BU	0.24	0/596	0.45	0/790
48	DU	0.24	0/596	0.43	0/790
49	BV	0.22	0/638	0.44	0/860
49	DV	0.23	0/638	0.46	0/860
50	BW	0.22	0/765	0.42	0/1007
50	DW	0.23	0/765	0.47	0/1007
51	BX	0.22	0/221	0.39	0/288
51	DX	0.21	0/221	0.41	0/288
52	BB	0.35	0/1992	0.71	2/3099 (0.1%)
52	BD	0.32	0/1992	0.66	2/3099 (0.1%)
52	DB	0.35	0/1992	0.68	1/3099 (0.0%)
52	DD	0.32	0/1992	0.64	2/3099 (0.1%)
53	BC	0.26	0/1835	0.61	0/2859
53	DC	0.24	0/1835	0.56	0/2859
54	B1	0.33	0/390	0.59	1/606 (0.2%)
54	D1	0.34	0/390	0.63	1/606 (0.2%)
All	All	0.29	1/324159 (0.0%)	0.65	138/485455 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	2884	A	N7-C5	-5.57	1.35	1.39

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BA	1495	U	N1-C2-O2	9.65	129.55	122.80
1	AA	673	C	C2-N3-C4	-8.89	115.45	119.90
2	AB	81	G	C5-C6-O6	-8.73	123.36	128.60
1	CA	979	A	C4-N9-C1'	8.38	141.38	126.30
1	CA	1922	G	N3-C4-N9	-8.15	121.11	126.00

There are no chirality outliers.

There are no planarity outliers.

## 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	31613	2349	0
1	CA	62607	0	31564	2395	0
2	AB	2617	0	1328	88	0
2	CB	2617	0	1328	126	0
3	AD	2115	0	2195	232	0
3	CD	2115	0	2195	198	0
4	AE	1568	0	1634	155	0
4	CE	1568	0	1634	162	0
5	AF	1585	0	1632	122	0
5	CF	1627	0	1680	182	0
6	AG	1474	0	1535	112	0
6	CG	1474	0	1535	112	0
7	AH	1307	0	1382	129	0
7	CH	1307	0	1382	110	1
8	AK	1136	0	1223	92	0
8	CK	1136	0	1223	77	0
9	AM	1104	0	1180	81	0
9	CM	1104	0	1180	64	0
10	AN	933	0	996	64	0
10	CN	933	0	996	53	0
11	AO	1145	0	1228	178	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	CO	1145	0	1228	265	0
12	AP	1122	0	1179	168	0
12	CP	1122	0	1179	189	0
13	A0	968	0	1033	74	0
13	C0	960	0	1021	70	0
14	AQ	882	0	943	83	0
14	CQ	882	0	943	89	0
15	AR	1141	0	1202	107	0
15	CR	1141	0	1202	94	0
16	A1	964	0	1022	87	0
16	C1	964	0	1022	83	0
17	A2	779	0	852	63	0
17	C2	779	0	852	99	0
18	AS	900	0	964	55	0
18	CS	900	0	964	54	0
19	AT	725	0	778	43	0
19	CT	725	0	778	39	0
20	AU	785	0	878	75	0
20	CU	785	0	878	80	0
21	AV	1397	0	1430	140	0
21	CV	1428	0	1454	149	0
22	A3	607	0	628	42	0
22	C3	613	0	633	47	0
23	AZ	763	0	848	49	0
23	CZ	763	0	848	44	0
24	AW	558	0	610	45	0
24	CW	558	0	610	51	0
25	AX	469	0	518	28	0
25	CX	469	0	518	27	0
26	A4	533	0	522	72	0
26	C4	515	0	510	96	0
27	A5	459	0	480	88	0
27	C5	459	0	478	33	0
28	A6	389	0	404	59	0
28	C6	389	0	404	51	0
29	A7	391	0	432	21	0
29	C7	391	0	432	33	0
30	A8	480	0	549	67	0
30	C8	480	0	549	114	0
31	BA	32284	0	16296	1465	1
31	DA	32287	0	16295	1435	0
32	BE	1924	0	1975	137	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	DE	1924	0	1975	162	0
33	BF	1605	0	1668	95	0
33	DF	1612	0	1677	110	0
34	BG	1703	0	1763	120	0
34	DG	1703	0	1763	129	0
35	BH	1155	0	1213	71	0
35	DH	1155	0	1213	79	0
36	BI	843	0	857	36	0
36	DI	843	0	857	46	0
37	BJ	1257	0	1296	70	0
37	DJ	1257	0	1296	91	0
38	BK	1116	0	1177	83	0
38	DK	1116	0	1177	56	0
39	BL	1010	0	1037	72	0
39	DL	1010	0	1037	112	0
40	BM	801	0	849	79	0
40	DM	801	0	849	87	0
41	BN	885	0	904	54	0
41	DN	885	0	904	58	0
42	BO	975	0	1062	53	0
42	DO	975	0	1062	89	0
43	BP	928	0	987	74	0
43	DP	933	0	992	81	0
44	BQ	476	0	511	43	0
44	DQ	476	0	511	53	0
45	BR	734	0	771	34	0
45	DR	734	0	771	38	0
46	BS	705	0	725	54	0
46	DS	705	0	725	35	0
47	BT	834	0	904	53	0
47	DT	834	0	904	41	0
48	BU	591	0	662	38	0
48	DU	591	0	662	40	0
49	BV	624	0	636	50	0
49	DV	624	0	636	77	0
50	BW	763	0	861	59	0
50	DW	763	0	861	48	0
51	BX	217	0	234	12	0
51	DX	217	0	234	21	0
52	BB	1814	0	932	159	0
52	BD	1814	0	932	154	0
52	DB	1814	0	932	174	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	DD	1814	0	932	173	0
53	BC	1643	0	837	47	0
53	DC	1643	0	837	51	0
54	B1	347	0	174	24	0
54	D1	347	0	174	25	0
55	A0	1	0	0	0	0
55	A1	1	0	0	0	0
55	A3	1	0	0	0	0
55	A5	1	0	0	0	0
55	AA	331	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	3	0	0	0	0
55	B1	1	0	0	0	0
55	BA	115	0	0	0	0
55	BB	5	0	0	0	0
55	BC	5	0	0	0	0
55	BD	1	0	0	0	0
55	BN	1	0	0	0	0
55	BQ	1	0	0	0	0
55	BS	1	0	0	0	0
55	C0	1	0	0	0	0
55	C5	1	0	0	0	0
55	C7	1	0	0	0	0
55	CA	274	0	0	0	0
55	CB	7	0	0	0	0
55	CE	1	0	0	0	0
55	D1	1	0	0	0	0
55	DA	119	0	0	0	0
55	DB	2	0	0	0	0
55	DC	6	0	0	0	0
55	DL	1	0	0	0	0
55	DN	1	0	0	0	0
56	A1	14	0	0	0	0
56	A3	7	0	0	0	0
56	A6	7	0	0	3	0
56	AA	1666	0	0	98	0
56	AB	91	0	0	4	0
56	AE	7	0	0	0	0
56	AF	7	0	0	1	0
56	AO	14	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	AW	7	0	0	0	0
56	BA	707	0	0	51	0
56	BB	14	0	0	1	0
56	BC	14	0	0	2	0
56	BD	21	0	0	1	0
56	BG	7	0	0	2	0
56	BR	7	0	0	0	0
56	C1	7	0	0	0	0
56	C3	7	0	0	0	0
56	C5	7	0	0	1	0
56	C6	7	0	0	4	0
56	CA	1526	0	0	72	0
56	CB	91	0	0	4	0
56	CF	7	0	0	0	0
56	CO	7	0	0	0	0
56	DA	651	0	0	55	0
56	DB	21	0	0	1	0
56	DC	28	0	0	10	0
56	DD	7	0	0	1	0
56	DG	7	0	0	2	0
56	DK	7	0	0	1	0
56	DR	7	0	0	0	0
56	DV	7	0	0	1	0
57	BG	1	0	0	0	0
57	BQ	1	0	0	0	0
57	DG	1	0	0	0	0
57	DQ	1	0	0	0	0
All	All	303952	0	200977	14995	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 30.

The worst 5 of 14995 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:CA:2320:G:C8	1:CA:2324:A:C2	1.85	1.64
1:CA:216:G:N2	1:CA:218:A:H61	1.09	1.47
1:AA:2308:G:N1	1:AA:2311:A:N1	1.63	1.43
1:CA:216:G:H21	1:CA:218:A:N6	0.92	1.42
1:AA:2308:G:N2	1:AA:2311:A:H2	1.02	1.42

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:CH:100:GLY:O[3_555]	1.93	0.27

## 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%)	218 (81%)	35 (13%)	17 (6%)	2	20
3	CD	270/276 (98%)	218 (81%)	40 (15%)	12 (4%)	4	32
4	AE	203/206 (98%)	141 (70%)	39 (19%)	23 (11%)	1	5
4	CE	203/206 (98%)	131 (64%)	46 (23%)	26 (13%)	0	3
5	AF	200/210 (95%)	168 (84%)	23 (12%)	9 (4%)	4	32
5	CF	206/210 (98%)	144 (70%)	35 (17%)	27 (13%)	0	3
6	AG	179/182 (98%)	147 (82%)	25 (14%)	7 (4%)	5	37
6	CG	179/182 (98%)	144 (80%)	27 (15%)	8 (4%)	4	32
7	AH	168/180 (93%)	123 (73%)	20 (12%)	25 (15%)	0	2
7	CH	168/180 (93%)	111 (66%)	41 (24%)	16 (10%)	1	9
8	AK	144/148 (97%)	99 (69%)	31 (22%)	14 (10%)	1	8
8	CK	144/148 (97%)	104 (72%)	32 (22%)	8 (6%)	3	25
9	AM	136/140 (97%)	108 (79%)	17 (12%)	11 (8%)	1	13
9	CM	136/140 (97%)	106 (78%)	23 (17%)	7 (5%)	3	28
10	AN	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	14	62
10	CN	120/122 (98%)	107 (89%)	9 (8%)	4 (3%)	6	43
11	AO	148/150 (99%)	93 (63%)	35 (24%)	20 (14%)	0	3
11	CO	148/150 (99%)	91 (62%)	32 (22%)	25 (17%)	0	1
12	AP	139/141 (99%)	101 (73%)	21 (15%)	17 (12%)	1	4
12	CP	139/141 (99%)	95 (68%)	24 (17%)	20 (14%)	0	2
13	A0	116/118 (98%)	96 (83%)	15 (13%)	5 (4%)	4	34
13	C0	115/118 (98%)	97 (84%)	12 (10%)	6 (5%)	3	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	AQ	109/112 (97%)	86 (79%)	14 (13%)	9 (8%)	1	12
14	CQ	109/112 (97%)	72 (66%)	24 (22%)	13 (12%)	1	4
15	AR	135/146 (92%)	107 (79%)	22 (16%)	6 (4%)	4	32
15	CR	135/146 (92%)	112 (83%)	15 (11%)	8 (6%)	2	23
16	A1	115/118 (98%)	96 (84%)	13 (11%)	6 (5%)	3	27
16	C1	115/118 (98%)	89 (77%)	16 (14%)	10 (9%)	1	11
17	A2	99/101 (98%)	85 (86%)	9 (9%)	5 (5%)	3	28
17	C2	99/101 (98%)	73 (74%)	14 (14%)	12 (12%)	1	4
18	AS	111/113 (98%)	97 (87%)	13 (12%)	1 (1%)	25	76
18	CS	111/113 (98%)	99 (89%)	9 (8%)	3 (3%)	8	49
19	AT	90/96 (94%)	84 (93%)	5 (6%)	1 (1%)	21	73
19	CT	90/96 (94%)	73 (81%)	14 (16%)	3 (3%)	6	43
20	AU	100/110 (91%)	76 (76%)	13 (13%)	11 (11%)	1	6
20	CU	100/110 (91%)	62 (62%)	27 (27%)	11 (11%)	1	6
21	AV	173/206 (84%)	113 (65%)	40 (23%)	20 (12%)	1	5
21	CV	177/206 (86%)	112 (63%)	40 (23%)	25 (14%)	0	2
22	A3	74/85 (87%)	62 (84%)	7 (10%)	5 (7%)	2	18
22	C3	75/85 (88%)	59 (79%)	13 (17%)	3 (4%)	5	36
23	AZ	95/98 (97%)	76 (80%)	13 (14%)	6 (6%)	2	20
23	CZ	95/98 (97%)	76 (80%)	9 (10%)	10 (10%)	1	6
24	AW	64/72 (89%)	57 (89%)	4 (6%)	3 (5%)	4	30
24	CW	64/72 (89%)	52 (81%)	7 (11%)	5 (8%)	1	14
25	AX	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
25	CX	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
26	A4	64/71 (90%)	39 (61%)	13 (20%)	12 (19%)	0	1
26	C4	61/71 (86%)	23 (38%)	20 (33%)	18 (30%)	0	0
27	A5	57/60 (95%)	42 (74%)	9 (16%)	6 (10%)	1	6
27	C5	57/60 (95%)	47 (82%)	8 (14%)	2 (4%)	6	41
28	A6	43/54 (80%)	23 (54%)	13 (30%)	7 (16%)	0	1
28	C6	43/54 (80%)	23 (54%)	11 (26%)	9 (21%)	0	1
29	A7	43/49 (88%)	41 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	C7	43/49 (88%)	40 (93%)	3 (7%)	0	100	100
30	A8	58/65 (89%)	47 (81%)	8 (14%)	3 (5%)	3	27
30	C8	58/65 (89%)	41 (71%)	6 (10%)	11 (19%)	0	1
32	BE	235/256 (92%)	181 (77%)	38 (16%)	16 (7%)	2	18
32	DE	235/256 (92%)	177 (75%)	40 (17%)	18 (8%)	1	14
33	BF	203/239 (85%)	161 (79%)	36 (18%)	6 (3%)	7	46
33	DF	204/239 (85%)	163 (80%)	35 (17%)	6 (3%)	7	47
34	BG	206/208 (99%)	179 (87%)	19 (9%)	8 (4%)	5	37
34	DG	206/208 (99%)	159 (77%)	35 (17%)	12 (6%)	3	23
35	BH	149/162 (92%)	127 (85%)	16 (11%)	6 (4%)	5	36
35	DH	149/162 (92%)	132 (89%)	15 (10%)	2 (1%)	18	69
36	BI	99/101 (98%)	89 (90%)	7 (7%)	3 (3%)	7	46
36	DI	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	11	58
37	BJ	153/156 (98%)	128 (84%)	21 (14%)	4 (3%)	8	50
37	DJ	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	18	69
38	BK	136/138 (99%)	116 (85%)	16 (12%)	4 (3%)	7	47
38	DK	136/138 (99%)	116 (85%)	15 (11%)	5 (4%)	5	39
39	BL	125/128 (98%)	95 (76%)	25 (20%)	5 (4%)	5	36
39	DL	125/128 (98%)	97 (78%)	21 (17%)	7 (6%)	3	25
40	BM	97/105 (92%)	83 (86%)	13 (13%)	1 (1%)	22	74
40	DM	97/105 (92%)	82 (84%)	14 (14%)	1 (1%)	22	74
41	BN	117/129 (91%)	99 (85%)	12 (10%)	6 (5%)	3	28
41	DN	117/129 (91%)	103 (88%)	8 (7%)	6 (5%)	3	28
42	BO	123/132 (93%)	100 (81%)	17 (14%)	6 (5%)	3	29
42	DO	123/132 (93%)	94 (76%)	17 (14%)	12 (10%)	1	8
43	BP	114/126 (90%)	82 (72%)	22 (19%)	10 (9%)	1	11
43	DP	115/126 (91%)	85 (74%)	18 (16%)	12 (10%)	1	7
44	BQ	56/61 (92%)	40 (71%)	10 (18%)	6 (11%)	1	6
44	DQ	56/61 (92%)	41 (73%)	8 (14%)	7 (12%)	1	4
45	BR	86/89 (97%)	76 (88%)	8 (9%)	2 (2%)	10	54
45	DR	86/89 (97%)	77 (90%)	8 (9%)	1 (1%)	19	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	BS	82/88 (93%)	60 (73%)	20 (24%)	2 (2%)	9	53
46	DS	82/88 (93%)	70 (85%)	11 (13%)	1 (1%)	19	71
47	BT	98/105 (93%)	82 (84%)	13 (13%)	3 (3%)	7	45
47	DT	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	11	58
48	BU	70/88 (80%)	59 (84%)	10 (14%)	1 (1%)	16	67
48	DU	70/88 (80%)	57 (81%)	12 (17%)	1 (1%)	16	67
49	BV	76/93 (82%)	59 (78%)	14 (18%)	3 (4%)	5	37
49	DV	76/93 (82%)	55 (72%)	17 (22%)	4 (5%)	3	26
50	BW	97/106 (92%)	78 (80%)	16 (16%)	3 (3%)	7	45
50	DW	97/106 (92%)	82 (84%)	9 (9%)	6 (6%)	2	21
51	BX	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	4	34
51	DX	23/27 (85%)	21 (91%)	0	2 (9%)	1	11
All	All	11319/12052 (94%)	8877 (78%)	1684 (15%)	758 (7%)	2	18

5 of 758 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AD	28	GLU
3	AD	32	SER
3	AD	122	ASP
3	AD	123	ALA
3	AD	238	GLY

### 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%)	172 (80%)	42 (20%)	2	9
3	CD	214/218 (98%)	187 (87%)	27 (13%)	7	31
4	AE	165/166 (99%)	137 (83%)	28 (17%)	3	15
4	CE	165/166 (99%)	125 (76%)	40 (24%)	1	4
5	AF	161/166 (97%)	137 (85%)	24 (15%)	4	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	CF	165/166 (99%)	137 (83%)	28 (17%)	3	15
6	AG	155/156 (99%)	136 (88%)	19 (12%)	7	32
6	CG	155/156 (99%)	139 (90%)	16 (10%)	10	41
7	AH	142/148 (96%)	112 (79%)	30 (21%)	1	7
7	CH	142/148 (96%)	123 (87%)	19 (13%)	6	27
8	AK	122/124 (98%)	98 (80%)	24 (20%)	2	9
8	CK	122/124 (98%)	104 (85%)	18 (15%)	4	21
9	AM	117/119 (98%)	98 (84%)	19 (16%)	3	17
9	CM	117/119 (98%)	95 (81%)	22 (19%)	2	11
10	AN	100/100 (100%)	92 (92%)	8 (8%)	17	58
10	CN	100/100 (100%)	88 (88%)	12 (12%)	7	33
11	AO	116/116 (100%)	84 (72%)	32 (28%)	0	2
11	CO	116/116 (100%)	84 (72%)	32 (28%)	0	2
12	AP	111/111 (100%)	91 (82%)	20 (18%)	2	13
12	CP	111/111 (100%)	88 (79%)	23 (21%)	2	8
13	A0	101/101 (100%)	83 (82%)	18 (18%)	2	13
13	C0	100/101 (99%)	84 (84%)	16 (16%)	3	18
14	AQ	87/88 (99%)	70 (80%)	17 (20%)	2	9
14	CQ	87/88 (99%)	72 (83%)	15 (17%)	3	15
15	AR	120/127 (94%)	103 (86%)	17 (14%)	5	24
15	CR	120/127 (94%)	105 (88%)	15 (12%)	7	31
16	A1	93/94 (99%)	79 (85%)	14 (15%)	4	21
16	C1	93/94 (99%)	80 (86%)	13 (14%)	5	25
17	A2	82/82 (100%)	69 (84%)	13 (16%)	4	18
17	C2	82/82 (100%)	62 (76%)	20 (24%)	1	3
18	AS	92/92 (100%)	73 (79%)	19 (21%)	2	8
18	CS	92/92 (100%)	80 (87%)	12 (13%)	6	29
19	AT	74/78 (95%)	65 (88%)	9 (12%)	7	32
19	CT	74/78 (95%)	64 (86%)	10 (14%)	6	27
20	AU	85/91 (93%)	72 (85%)	13 (15%)	4	20
20	CU	85/91 (93%)	65 (76%)	20 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	AV	154/179 (86%)	130 (84%)	24 (16%)	4	19
21	CV	158/179 (88%)	137 (87%)	21 (13%)	6	27
22	A3	61/67 (91%)	55 (90%)	6 (10%)	12	45
22	C3	62/67 (92%)	58 (94%)	4 (6%)	24	69
23	AZ	82/83 (99%)	70 (85%)	12 (15%)	5	23
23	CZ	82/83 (99%)	73 (89%)	9 (11%)	9	38
24	AW	62/67 (92%)	49 (79%)	13 (21%)	1	8
24	CW	62/67 (92%)	52 (84%)	10 (16%)	3	17
25	AX	51/52 (98%)	43 (84%)	8 (16%)	4	19
25	CX	51/52 (98%)	46 (90%)	5 (10%)	12	45
26	A4	59/63 (94%)	52 (88%)	7 (12%)	8	34
26	C4	57/63 (90%)	45 (79%)	12 (21%)	1	7
27	A5	51/52 (98%)	41 (80%)	10 (20%)	2	9
27	C5	51/52 (98%)	44 (86%)	7 (14%)	5	26
28	A6	44/52 (85%)	30 (68%)	14 (32%)	0	1
28	C6	44/52 (85%)	38 (86%)	6 (14%)	5	26
29	A7	38/42 (90%)	33 (87%)	5 (13%)	6	28
29	C7	38/42 (90%)	31 (82%)	7 (18%)	2	12
30	A8	50/55 (91%)	39 (78%)	11 (22%)	1	6
30	C8	50/55 (91%)	37 (74%)	13 (26%)	1	2
32	BE	205/220 (93%)	172 (84%)	33 (16%)	3	17
32	DE	205/220 (93%)	177 (86%)	28 (14%)	5	26
33	BF	159/188 (85%)	134 (84%)	25 (16%)	4	19
33	DF	160/188 (85%)	141 (88%)	19 (12%)	8	34
34	BG	180/180 (100%)	158 (88%)	22 (12%)	7	32
34	DG	180/180 (100%)	156 (87%)	24 (13%)	6	27
35	BH	116/123 (94%)	100 (86%)	16 (14%)	5	25
35	DH	116/123 (94%)	95 (82%)	21 (18%)	2	12
36	BI	90/90 (100%)	82 (91%)	8 (9%)	14	51
36	DI	90/90 (100%)	80 (89%)	10 (11%)	9	37
37	BJ	126/127 (99%)	106 (84%)	20 (16%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DJ	126/127 (99%)	109 (86%)	17 (14%)	6	27
38	BK	119/119 (100%)	99 (83%)	20 (17%)	3	16
38	DK	119/119 (100%)	105 (88%)	14 (12%)	8	34
39	BL	98/99 (99%)	85 (87%)	13 (13%)	6	27
39	DL	98/99 (99%)	82 (84%)	16 (16%)	3	17
40	BM	89/92 (97%)	76 (85%)	13 (15%)	5	23
40	DM	89/92 (97%)	80 (90%)	9 (10%)	11	42
41	BN	90/99 (91%)	78 (87%)	12 (13%)	6	27
41	DN	90/99 (91%)	83 (92%)	7 (8%)	18	60
42	BO	104/109 (95%)	92 (88%)	12 (12%)	8	35
42	DO	104/109 (95%)	85 (82%)	19 (18%)	2	12
43	BP	94/101 (93%)	80 (85%)	14 (15%)	4	21
43	DP	94/101 (93%)	82 (87%)	12 (13%)	6	29
44	BQ	48/50 (96%)	42 (88%)	6 (12%)	7	31
44	DQ	48/50 (96%)	44 (92%)	4 (8%)	16	56
45	BR	79/80 (99%)	74 (94%)	5 (6%)	25	70
45	DR	79/80 (99%)	72 (91%)	7 (9%)	14	51
46	BS	72/74 (97%)	60 (83%)	12 (17%)	3	16
46	DS	72/74 (97%)	66 (92%)	6 (8%)	16	56
47	BT	95/97 (98%)	84 (88%)	11 (12%)	8	35
47	DT	95/97 (98%)	88 (93%)	7 (7%)	20	63
48	BU	63/77 (82%)	61 (97%)	2 (3%)	51	88
48	DU	63/77 (82%)	54 (86%)	9 (14%)	5	23
49	BV	67/80 (84%)	55 (82%)	12 (18%)	2	13
49	DV	67/80 (84%)	55 (82%)	12 (18%)	2	13
50	BW	76/82 (93%)	68 (90%)	8 (10%)	10	40
50	DW	76/82 (93%)	68 (90%)	8 (10%)	10	40
51	BX	20/22 (91%)	19 (95%)	1 (5%)	34	78
51	DX	20/22 (91%)	19 (95%)	1 (5%)	34	78
All	All	9565/9996 (96%)	8122 (85%)	1443 (15%)	4	21

5 of 1443 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	BN	93	GLN
4	CE	203	LYS
39	DL	79	LEU
43	BP	32	GLU
50	BW	10	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 281 such sidechains are listed below:

Mol	Chain	Res	Type
42	BO	6	GLN
5	CF	169	ASN
41	DN	93	GLN
43	BP	101	GLN
50	BW	42	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2911/2912 (99%)	616 (21%)	54 (1%)
1	CA	2905/2912 (99%)	632 (21%)	51 (1%)
2	AB	121/122 (99%)	16 (13%)	0
2	CB	121/122 (99%)	29 (23%)	2 (1%)
31	BA	1501/1506 (99%)	318 (21%)	42 (2%)
31	DA	1501/1506 (99%)	325 (21%)	46 (3%)
52	BB	83/85 (97%)	47 (56%)	10 (12%)
52	BD	83/85 (97%)	32 (38%)	5 (6%)
52	DB	83/85 (97%)	49 (59%)	9 (10%)
52	DD	83/85 (97%)	31 (37%)	5 (6%)
53	BC	76/77 (98%)	16 (21%)	2 (2%)
53	DC	76/77 (98%)	15 (19%)	2 (2%)
54	B1	15/16 (93%)	5 (33%)	3 (20%)
54	D1	15/16 (93%)	5 (33%)	3 (20%)
All	All	9574/9606 (99%)	2136 (22%)	234 (2%)

5 of 2136 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	U
1	AA	12	U
1	AA	17	G
1	AA	18	C

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Mol	Chain	Res	Type
1	AA	27	G

5 of 234 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	BB	78	C
1	CA	936	C
52	DB	6	G
52	BD	17	G
1	CA	126	C

## 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	1.67	3 (10%)	41,44,47	2.01	10 (24%)
52	MIA	BD	38	52	29,31,32	1.65	3 (10%)	41,44,47	2.36	9 (21%)
52	MIA	DB	38	52	29,31,32	1.74	3 (10%)	41,44,47	2.25	10 (24%)
52	MIA	DD	38	52	29,31,32	1.68	3 (10%)	41,44,47	2.11	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	-	1/16/33/34	0/3/3/3
52	MIA	DB	38	52	-	0/16/33/34	0/3/3/3
52	MIA	DD	38	52	-	1/16/33/34	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	DB	38	MIA	C6-N6	6.64	1.46	1.34
52	BB	38	MIA	C6-N6	6.39	1.46	1.34
52	DD	38	MIA	C6-N6	6.35	1.45	1.34
52	BD	38	MIA	C6-N6	6.23	1.45	1.34
52	DB	38	MIA	P-OP1	4.62	1.52	1.46

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	BD	38	MIA	C11-S10-C2	9.89	109.41	102.23
52	DB	38	MIA	C11-S10-C2	9.39	109.06	102.23
52	DD	38	MIA	C11-S10-C2	7.66	107.80	102.23
52	BB	38	MIA	C11-S10-C2	6.46	106.93	102.23
52	BB	38	MIA	C5-C4-N3	-6.06	119.09	126.07

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	DD	38	MIA	OP2-P-O5'-C5'
52	BD	38	MIA	OP2-P-O5'-C5'

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 1610 ligands modelled in this entry, 898 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	202	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	A1	203	-	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	3138	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3147	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3154	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3160	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3263	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3287	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3288	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3289	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3290	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3291	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3292	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3293	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3294	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3295	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3296	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3297	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3298	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3299	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3300	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3301	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3302	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3303	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3304	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3305	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3306	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3307	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3308	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3309	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3310	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3311	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3312	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3313	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3314	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3315	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3316	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3317	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3318	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3319	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3320	-	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	3321	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3322	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3323	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3324	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3325	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AA	3326	-	0,6,6	0.00	-	0,15,15	0.00	-
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	3334	-	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	3337	-	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	3339	-	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	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	3372	-	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	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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	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	-
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	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-
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	204	-	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	AO	205	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	AW	101	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1656	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1657	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1659	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1661	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1662	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1663	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1664	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1665	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1666	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1667	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1668	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1669	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1670	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1671	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1672	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1673	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1674	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1675	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1676	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1677	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1678	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1679	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1680	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1681	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1682	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1683	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1684	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1685	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1686	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1687	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1688	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1689	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1690	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1691	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1692	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1693	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1694	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1695	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1696	-	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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-
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	BA	1815	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BA	1816	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BB	106	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	BB	107	-	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	BR	101	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	C1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	C3	101	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	C5	102	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	C6	101	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3232	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3233	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3234	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3235	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3236	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3237	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3238	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3239	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3240	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3241	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3242	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3243	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3244	-	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	3245	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3246	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3247	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3248	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3249	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3250	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3251	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3252	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3253	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3254	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3255	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3256	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3269	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3270	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3271	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3272	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3273	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3274	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3275	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3276	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3277	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3278	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3279	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3280	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3281	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3282	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3283	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3284	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3285	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3286	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3287	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3288	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3289	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3290	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3291	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3292	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3293	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3294	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3295	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3296	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3297	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3298	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3299	-	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	3300	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3301	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3302	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3303	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3304	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3305	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3306	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3307	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3308	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3309	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3310	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3311	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3312	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3313	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3314	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3315	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3316	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3317	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3318	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3319	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3320	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3321	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3322	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3323	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3324	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3325	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3326	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3327	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3328	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3329	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3330	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3331	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3332	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3333	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3334	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3335	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3336	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3337	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3338	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3339	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3340	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3341	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3342	-	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	3343	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3344	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3345	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3346	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3347	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3348	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3349	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3350	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3351	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3352	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3353	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3354	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3355	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3356	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3357	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3358	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3359	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3360	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3361	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3362	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3363	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3364	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3365	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3366	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3367	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3368	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3369	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3370	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3371	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3372	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3373	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3374	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3375	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3376	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3377	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3378	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3379	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3380	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3381	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3382	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3383	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3384	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3385	-	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	3386	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3387	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3388	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3389	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3390	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3391	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3392	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3393	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3394	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3395	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3396	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3397	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3398	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3399	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3400	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3401	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3402	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3403	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3404	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3405	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3406	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3407	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3408	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3409	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3410	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3411	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3412	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3413	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3414	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3415	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3416	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3417	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3418	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3419	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3420	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3421	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3422	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3423	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3424	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3426	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3427	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3428	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	CA	3429	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3430	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3431	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3432	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3433	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3434	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3435	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3437	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3438	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3450	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3461	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3462	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3463	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3464	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3465	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3466	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3467	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3468	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3469	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3470	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3481	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3482	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3483	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3485	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3486	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3487	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3488	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3489	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3491	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CA	3492	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	208	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	209	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	210	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	211	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	212	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	213	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	214	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	215	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	216	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	217	-	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	CB	218	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	219	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CB	220	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CF	301	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	CO	201	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1718	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1719	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1721	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1722	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1723	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1724	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1726	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1727	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1728	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1729	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1730	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1731	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1732	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1733	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1734	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1735	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1736	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1737	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1738	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1739	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1740	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1741	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1742	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1743	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1744	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1745	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1746	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1747	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1748	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1749	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1750	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1751	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1752	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1753	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1754	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1755	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1756	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1757	-	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	1758	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1759	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1760	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1761	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1762	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1763	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1764	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1765	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1766	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1767	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1768	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1769	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1770	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1771	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1772	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1773	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1774	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1775	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1776	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1777	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1778	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1779	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1780	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1781	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1782	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1783	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1784	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1785	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1786	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1787	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1788	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1789	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1790	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1791	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1792	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1793	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1794	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1795	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1796	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1797	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1798	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1799	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1800	-	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	1801	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1802	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1803	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1804	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1805	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1806	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1807	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1808	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1809	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1810	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1811	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DA	1812	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DB	103	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DB	104	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DB	105	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DC	107	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DC	108	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DC	109	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DC	110	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DD	101	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DG	302	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DK	201	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DR	101	-	0,6,6	0.00	-	0,15,15	0.00	-
56	OHX	DV	101	-	0,6,6	0.00	-	0,15,15	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	A1	202	-	-	0/0/0/0	0/0/0/0
56	OHX	A1	203	-	-	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	3138	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3147	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3154	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3160	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3263	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3287	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3288	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3289	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	AA	3290	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3291	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3292	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3293	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3294	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3295	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3296	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3297	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3298	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3299	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3300	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3301	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3302	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3303	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3304	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3305	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3306	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3307	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3308	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3309	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3310	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3311	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3312	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3313	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3314	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3315	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3316	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3317	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3318	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3319	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3320	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3321	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3322	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3323	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3324	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3325	-	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	3334	-	-	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	3337	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3338	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3339	-	-	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
56	OHX	AA	3342	-	-	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	3372	-	-	0/0/0/0	0/0/0/0
56	OHX	AA	3373	-	-	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	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	204	-	-	0/0/0/0	0/0/0/0
56	OHX	AO	205	-	-	0/0/0/0	0/0/0/0
56	OHX	AW	101	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1656	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1657	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1659	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1661	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	BA	1662	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1663	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1664	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1665	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1666	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1667	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1668	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1669	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1670	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1671	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1672	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1673	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1674	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1675	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1676	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1677	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1678	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1679	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1680	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1681	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1682	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1683	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1684	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1685	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1686	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1687	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1688	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1689	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1690	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1691	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1692	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1693	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1694	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1695	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1696	-	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	BA	1815	-	-	0/0/0/0	0/0/0/0
56	OHX	BA	1816	-	-	0/0/0/0	0/0/0/0
56	OHX	BB	106	-	-	0/0/0/0	0/0/0/0
56	OHX	BB	107	-	-	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	BR	101	-	-	0/0/0/0	0/0/0/0
56	OHX	C1	201	-	-	0/0/0/0	0/0/0/0
56	OHX	C3	101	-	-	0/0/0/0	0/0/0/0
56	OHX	C5	102	-	-	0/0/0/0	0/0/0/0
56	OHX	C6	101	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3232	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3233	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3234	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3235	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3236	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3237	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3238	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3239	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3240	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3241	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3242	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3243	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3244	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3245	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3246	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3247	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	CA	3248	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3249	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3250	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3251	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3252	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3253	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3254	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3255	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3256	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3269	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3270	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3271	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3272	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3273	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3274	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3275	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3276	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3277	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3278	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3279	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3280	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3281	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3282	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3283	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3284	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3285	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3286	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3287	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3288	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3289	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3290	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3291	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3292	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3293	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3294	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3295	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3296	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3297	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3298	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3299	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3300	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3301	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	CA	3302	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3303	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3304	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3305	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3306	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3307	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3308	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3309	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3310	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3311	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3312	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3313	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3314	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3315	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3316	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3317	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3318	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3319	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3320	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3321	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3322	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3323	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3324	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3325	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3326	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3327	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3328	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3329	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3330	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3331	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3332	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3333	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3334	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3335	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3336	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3337	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3338	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3339	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3340	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3341	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3342	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3343	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	CA	3344	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3345	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3346	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3347	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3348	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3349	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3350	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3351	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3352	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3353	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3354	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3355	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3356	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3357	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3358	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3359	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3360	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3361	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3362	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3363	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3364	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3365	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3366	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3367	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3368	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3369	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3370	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3371	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3372	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3373	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3374	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3375	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3376	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3377	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3378	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3379	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3380	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3381	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3382	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3383	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3384	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3385	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	CA	3386	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3387	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3388	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3389	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3390	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3391	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3392	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3393	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3394	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3395	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3396	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3397	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3398	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3399	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3400	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3401	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3402	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3403	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3404	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3405	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3406	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3407	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3408	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3409	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3410	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3411	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3412	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3413	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3414	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3415	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3416	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3417	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3418	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3419	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3420	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3421	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3422	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3423	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3424	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3425	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3426	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3427	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	CA	3428	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3429	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3430	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3431	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3432	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3433	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3434	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3435	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3436	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3437	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3438	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3450	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3461	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3462	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3463	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3464	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3465	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3466	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3467	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3468	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3469	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3470	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3481	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3482	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3483	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3484	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3485	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3486	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3487	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3488	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3489	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3490	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3491	-	-	0/0/0/0	0/0/0/0
56	OHX	CA	3492	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	208	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	209	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	210	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	211	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	212	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	213	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	214	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	215	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	CB	216	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	217	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	218	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	219	-	-	0/0/0/0	0/0/0/0
56	OHX	CB	220	-	-	0/0/0/0	0/0/0/0
56	OHX	CF	301	-	-	0/0/0/0	0/0/0/0
56	OHX	CO	201	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1718	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1719	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1721	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1722	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1723	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1724	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1726	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1727	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1728	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1729	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1730	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1731	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1732	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1733	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1734	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1735	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1736	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1737	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1738	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1739	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1740	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1741	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1742	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1743	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1744	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1745	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1746	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1747	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1748	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1749	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1750	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1751	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1752	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1753	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1754	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	DA	1755	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1756	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1757	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1758	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1759	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1760	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1761	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1762	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1763	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1764	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1765	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1766	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1767	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1768	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1769	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1770	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1771	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1772	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1773	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1774	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1775	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1776	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1777	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1778	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1779	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1780	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1781	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1782	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1783	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1784	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1785	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1786	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1787	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1788	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1789	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1790	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1791	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1792	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1793	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1794	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1795	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1796	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	OHX	DA	1797	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1798	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1799	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1800	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1801	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1802	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1803	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1804	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1805	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1806	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1807	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1808	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1809	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1810	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1811	-	-	0/0/0/0	0/0/0/0
56	OHX	DA	1812	-	-	0/0/0/0	0/0/0/0
56	OHX	DB	103	-	-	0/0/0/0	0/0/0/0
56	OHX	DB	104	-	-	0/0/0/0	0/0/0/0
56	OHX	DB	105	-	-	0/0/0/0	0/0/0/0
56	OHX	DC	107	-	-	0/0/0/0	0/0/0/0
56	OHX	DC	108	-	-	0/0/0/0	0/0/0/0
56	OHX	DC	109	-	-	0/0/0/0	0/0/0/0
56	OHX	DC	110	-	-	0/0/0/0	0/0/0/0
56	OHX	DD	101	-	-	0/0/0/0	0/0/0/0
56	OHX	DG	302	-	-	0/0/0/0	0/0/0/0
56	OHX	DK	201	-	-	0/0/0/0	0/0/0/0
56	OHX	DR	101	-	-	0/0/0/0	0/0/0/0
56	OHX	DV	101	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	2912/2912 (100%)	-0.29	45 (1%) 70 24	45, 76, 209, 243	0
1	CA	2907/2912 (99%)	-0.43	39 (1%) 74 27	58, 92, 230, 245	0
2	AB	122/122 (100%)	-0.40	3 (2%) 54 14	73, 95, 116, 177	0
2	CB	122/122 (100%)	-0.61	1 (0%) 83 39	92, 127, 146, 198	0
3	AD	272/276 (98%)	-0.00	1 (0%) 90 57	39, 66, 84, 105	0
3	CD	272/276 (98%)	0.26	2 (0%) 84 42	55, 78, 96, 128	0
4	AE	205/206 (99%)	0.45	12 (5%) 22 5	51, 86, 130, 142	0
4	CE	205/206 (99%)	0.28	6 (2%) 49 12	64, 100, 148, 165	0
5	AF	202/210 (96%)	-0.10	0 100 100	47, 81, 118, 130	0
5	CF	208/210 (99%)	0.35	9 (4%) 34 8	62, 106, 160, 184	0
6	AG	181/182 (99%)	0.42	7 (3%) 37 8	84, 107, 138, 149	0
6	CG	181/182 (99%)	0.50	8 (4%) 33 7	120, 141, 164, 171	0
7	AH	170/180 (94%)	0.16	3 (1%) 65 20	86, 112, 130, 157	0
7	CH	170/180 (94%)	1.97	69 (40%) 1 0	155, 198, 220, 229	0
8	AK	146/148 (98%)	0.37	4 (2%) 52 13	79, 131, 147, 150	0
8	CK	146/148 (98%)	0.42	1 (0%) 84 42	84, 130, 152, 158	0
9	AM	138/140 (98%)	0.31	2 (1%) 72 25	66, 87, 124, 136	0
9	CM	138/140 (98%)	0.74	11 (7%) 12 4	83, 114, 140, 156	0
10	AN	122/122 (100%)	0.17	0 100 100	57, 78, 93, 101	0
10	CN	122/122 (100%)	0.20	0 100 100	75, 95, 111, 124	0
11	AO	150/150 (100%)	-0.05	1 (0%) 84 42	48, 88, 117, 160	0
11	CO	150/150 (100%)	0.69	13 (8%) 10 3	45, 108, 146, 178	0
12	AP	141/141 (100%)	0.32	1 (0%) 84 42	58, 83, 105, 127	0
12	CP	141/141 (100%)	0.49	8 (5%) 23 5	58, 109, 140, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	A0	118/118 (100%)	0.28	1 (0%) 83 39	61, 81, 103, 113	0
13	C0	117/118 (99%)	-0.11	0 100 100	69, 87, 106, 121	0
14	AQ	111/112 (99%)	0.20	1 (0%) 81 37	70, 92, 117, 131	0
14	CQ	111/112 (99%)	-0.15	1 (0%) 81 37	86, 123, 147, 162	0
15	AR	137/146 (93%)	0.50	5 (3%) 41 9	73, 93, 143, 170	0
15	CR	137/146 (93%)	0.12	3 (2%) 59 16	84, 104, 163, 183	0
16	A1	117/118 (99%)	-0.01	0 100 100	52, 75, 108, 139	0
16	C1	117/118 (99%)	0.52	5 (4%) 34 8	67, 106, 143, 162	0
17	A2	101/101 (100%)	0.62	8 (7%) 13 4	53, 98, 122, 141	0
17	C2	101/101 (100%)	1.10	19 (18%) 2 1	67, 129, 142, 151	0
18	AS	113/113 (100%)	0.31	3 (2%) 52 13	54, 73, 104, 156	0
18	CS	113/113 (100%)	0.13	2 (1%) 65 20	64, 80, 114, 158	0
19	AT	92/96 (95%)	0.06	1 (1%) 77 30	57, 71, 95, 107	0
19	CT	92/96 (95%)	0.22	1 (1%) 77 30	74, 88, 113, 127	0
20	AU	102/110 (92%)	0.54	6 (5%) 22 5	74, 101, 152, 162	0
20	CU	102/110 (92%)	0.44	8 (7%) 13 4	95, 118, 166, 181	0
21	AV	175/206 (84%)	1.10	27 (15%) 3 1	87, 126, 188, 191	0
21	CV	179/206 (86%)	1.16	29 (16%) 2 1	122, 160, 208, 216	0
22	A3	76/85 (89%)	0.07	1 (1%) 74 27	59, 77, 91, 132	0
22	C3	77/85 (90%)	-0.05	0 100 100	83, 95, 117, 147	0
23	AZ	97/98 (98%)	0.03	1 (1%) 79 33	58, 78, 126, 156	0
23	CZ	97/98 (98%)	0.28	2 (2%) 60 17	68, 86, 132, 155	0
24	AW	66/72 (91%)	0.22	1 (1%) 70 24	63, 84, 98, 125	0
24	CW	66/72 (91%)	0.22	2 (3%) 48 11	84, 107, 130, 139	0
25	AX	59/60 (98%)	0.11	1 (1%) 67 21	63, 83, 112, 130	0
25	CX	59/60 (98%)	0.48	0 100 100	80, 110, 141, 162	0
26	A4	66/71 (92%)	1.33	17 (25%) 1 1	120, 156, 173, 179	0
26	C4	63/71 (88%)	2.02	26 (41%) 1 0	146, 185, 194, 199	0
27	A5	59/60 (98%)	0.85	10 (16%) 2 1	49, 88, 168, 171	0
27	C5	59/60 (98%)	0.39	6 (10%) 7 2	65, 92, 173, 187	0
28	A6	45/54 (83%)	2.85	31 (68%) 0 0	124, 151, 168, 177	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	C6	45/54 (83%)	1.88	15 (33%) 1 0	141, 169, 183, 186	0
29	A7	45/49 (91%)	-0.21	0 100 100	47, 55, 69, 78	0
29	C7	45/49 (91%)	-0.16	0 100 100	56, 66, 77, 100	0
30	A8	60/65 (92%)	0.06	0 100 100	55, 73, 90, 114	0
30	C8	60/65 (92%)	0.36	0 100 100	78, 90, 112, 137	0
31	BA	1502/1506 (99%)	-0.50	8 (0%) 88 51	58, 107, 187, 244	0
31	DA	1502/1506 (99%)	-0.62	10 (0%) 84 42	71, 119, 189, 244	0
32	BE	237/256 (92%)	0.35	5 (2%) 60 17	111, 144, 182, 193	0
32	DE	237/256 (92%)	0.23	8 (3%) 43 10	126, 161, 196, 211	0
33	BF	205/239 (85%)	0.41	3 (1%) 70 24	96, 119, 152, 160	0
33	DF	206/239 (86%)	0.85	23 (11%) 6 2	127, 147, 175, 180	0
34	BG	208/208 (100%)	-0.02	0 100 100	92, 116, 136, 147	0
34	DG	208/208 (100%)	-0.07	0 100 100	93, 111, 132, 145	0
35	BH	151/162 (93%)	0.16	1 (0%) 84 42	81, 105, 127, 161	0
35	DH	151/162 (93%)	-0.05	1 (0%) 84 42	104, 121, 142, 165	0
36	BI	101/101 (100%)	-0.04	1 (0%) 79 33	81, 108, 122, 145	0
36	DI	101/101 (100%)	0.36	0 100 100	81, 106, 124, 149	0
37	BJ	155/156 (99%)	0.59	14 (9%) 10 3	106, 121, 149, 158	0
37	DJ	155/156 (99%)	0.14	0 100 100	113, 131, 153, 164	0
38	BK	138/138 (100%)	-0.09	0 100 100	89, 110, 123, 129	0
38	DK	138/138 (100%)	-0.16	0 100 100	104, 125, 136, 146	0
39	BL	127/128 (99%)	0.10	1 (0%) 83 39	87, 142, 160, 169	0
39	DL	127/128 (99%)	-0.03	0 100 100	117, 155, 168, 174	0
40	BM	99/105 (94%)	0.15	1 (1%) 79 33	91, 142, 170, 174	0
40	DM	99/105 (94%)	0.20	4 (4%) 36 8	124, 159, 175, 179	0
41	BN	119/129 (92%)	0.61	7 (5%) 22 5	72, 104, 133, 161	0
41	DN	119/129 (92%)	0.48	5 (4%) 35 8	91, 112, 139, 167	0
42	BO	125/132 (94%)	0.34	4 (3%) 45 11	69, 83, 112, 158	0
42	DO	125/132 (94%)	0.47	6 (4%) 29 7	93, 110, 134, 166	0
43	BP	116/126 (92%)	0.09	1 (0%) 81 37	92, 128, 145, 153	0
43	DP	117/126 (92%)	0.03	3 (2%) 53 13	106, 156, 169, 171	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BQ	58/61 (95%)	-0.12	0 100 100	91, 108, 122, 129	0
44	DQ	58/61 (95%)	0.40	2 (3%) 43 10	126, 140, 157, 160	0
45	BR	88/89 (98%)	-0.26	0 100 100	80, 100, 121, 125	0
45	DR	88/89 (98%)	-0.06	0 100 100	85, 112, 133, 140	0
46	BS	84/88 (95%)	-0.11	1 (1%) 75 29	100, 118, 139, 175	0
46	DS	84/88 (95%)	-0.15	0 100 100	96, 107, 127, 158	0
47	BT	100/105 (95%)	-0.17	0 100 100	93, 112, 125, 133	0
47	DT	100/105 (95%)	-0.06	0 100 100	94, 114, 135, 143	0
48	BU	72/88 (81%)	0.14	3 (4%) 35 8	88, 106, 139, 164	0
48	DU	72/88 (81%)	0.32	2 (2%) 50 12	97, 114, 155, 169	0
49	BV	78/93 (83%)	0.17	2 (2%) 53 13	109, 130, 147, 152	0
49	DV	78/93 (83%)	0.03	1 (1%) 74 27	145, 163, 182, 185	0
50	BW	99/106 (93%)	0.05	1 (1%) 79 33	105, 124, 155, 160	0
50	DW	99/106 (93%)	-0.02	1 (1%) 79 33	95, 117, 153, 163	0
51	BX	25/27 (92%)	-0.46	0 100 100	102, 117, 137, 154	0
51	DX	25/27 (92%)	-0.46	0 100 100	122, 143, 158, 168	0
52	BB	84/85 (98%)	0.76	15 (17%) 2 1	82, 123, 154, 169	0
52	BD	84/85 (98%)	-0.23	5 (5%) 21 5	75, 137, 217, 227	0
52	DB	84/85 (98%)	0.84	14 (16%) 2 1	93, 128, 156, 171	0
52	DD	84/85 (98%)	-0.46	2 (2%) 56 15	84, 137, 217, 225	0
53	BC	77/77 (100%)	-0.33	0 100 100	77, 114, 139, 153	0
53	DC	77/77 (100%)	-0.63	1 (1%) 74 27	88, 122, 150, 157	0
54	B1	16/16 (100%)	0.14	1 (6%) 19 5	76, 104, 156, 163	0
54	D1	16/16 (100%)	-0.38	0 100 100	85, 109, 157, 165	0
All	All	21100/21658 (97%)	-0.01	636 (3%) 48 11	39, 105, 182, 245	0

The worst 5 of 636 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CA	691	C	11.4
1	CA	2911	C	11.4
1	CA	690	A	11.3
1	CA	689	C	10.4
1	AA	654(K)	C	9.2

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
52	MIA	DB	38	29/30	0.23	-	84,93,111,126	0
52	MIA	BB	38	29/30	0.20	-	68,83,97,106	0
52	MIA	BD	38	29/30	0.24	-	116,135,182,198	0
52	MIA	DD	38	29/30	0.19	-	120,140,186,205	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	OHX	AA	3556	7/7	0.09	-	212,217,223,266	1
56	OHX	AB	214	7/7	0.15	-	110,118,132,162	1
56	OHX	CA	3382	7/7	0.09	-	129,131,148,199	1
55	MG	CA	3023	1/1	0.28	-	85,85,85,85	0
56	OHX	AA	3503	7/7	0.12	-	99,121,138,179	1
56	OHX	CB	214	7/7	0.12	-	129,139,146,186	1
56	OHX	DA	1794	7/7	0.14	-	124,130,139,205	1
55	MG	AA	3221	1/1	0.27	-	68,68,68,68	0
56	OHX	CA	3429	7/7	0.14	-	127,129,142,209	1
55	MG	CA	3197	1/1	0.40	-	79,79,79,79	0
56	OHX	CA	3306	7/7	0.13	-	98,106,119,148	1
55	MG	AA	3223	1/1	0.38	-	56,56,56,56	0
56	OHX	AA	3361	7/7	0.19	-	51,71,83,107	0
55	MG	CA	3074	1/1	0.31	-	64,64,64,64	0
55	MG	AA	3037	1/1	0.48	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	CA	3383	7/7	0.14	-	111,116,132,194	1
55	MG	BA	1620	1/1	0.46	-	70,70,70,70	0
56	OHX	CA	3338	7/7	0.17	-	95,103,117,121	1
56	OHX	DA	1786	7/7	0.15	-	143,151,161,223	1
55	MG	AA	3098	1/1	0.32	-	77,77,77,77	0
55	MG	BA	1613	1/1	0.32	-	65,65,65,65	0
56	OHX	BA	1795	7/7	0.12	-	109,127,134,173	1
56	OHX	DA	1737	7/7	0.13	-	87,110,131,158	1
56	OHX	CA	3430	7/7	0.11	-	96,106,114,197	1
55	MG	BA	1712	1/1	0.57	-	95,95,95,95	0
55	MG	CA	3205	1/1	0.31	-	63,63,63,63	0
56	OHX	DA	1739	7/7	0.12	-	98,110,124,155	1
55	MG	BA	1649	1/1	0.30	-	74,74,74,74	0
55	MG	CA	3025	1/1	0.18	-	83,83,83,83	0
55	MG	AA	3008	1/1	0.40	-	42,42,42,42	0
56	OHX	CA	3403	7/7	0.14	-	88,108,114,167	1
56	OHX	CB	211	7/7	0.10	-	122,128,152,168	1
55	MG	DA	1693	1/1	0.53	-	54,54,54,54	0
56	OHX	AA	3457	7/7	0.15	-	73,83,101,131	1
55	MG	AA	3275	1/1	0.43	-	64,64,64,64	0
55	MG	CA	3457	1/1	0.32	-	66,66,66,66	0
56	OHX	BA	1765	7/7	0.12	-	111,119,130,164	0
55	MG	DA	1631	1/1	0.52	-	111,111,111,111	0
56	OHX	CA	3363	7/7	0.11	-	94,99,114,167	1
55	MG	DA	1662	1/1	0.35	-	73,73,73,73	0
56	OHX	CA	3417	7/7	0.09	-	151,167,187,222	1
55	MG	AA	3028	1/1	0.40	-	66,66,66,66	0
55	MG	CA	3028	1/1	0.17	-	73,73,73,73	0
56	OHX	AB	208	7/7	0.16	-	113,119,131,170	1
55	MG	BA	1735	1/1	0.20	-	48,48,48,48	0
55	MG	AA	3114	1/1	0.39	-	47,47,47,47	0
55	MG	CA	3447	1/1	0.46	-	58,58,58,58	0
56	OHX	BA	1762	7/7	0.15	-	72,94,107,136	0
56	OHX	AA	3502	7/7	0.11	-	97,102,112,146	1
56	OHX	AA	3329	7/7	0.12	-	85,90,103,133	1
55	MG	CA	3072	1/1	0.32	-	43,43,43,43	0
55	MG	BA	1718	1/1	0.28	-	78,78,78,78	0
55	MG	BA	1746	1/1	0.41	-	82,82,82,82	0
55	MG	BA	1626	1/1	0.16	-	81,81,81,81	0
55	MG	AA	3237	1/1	0.35	-	45,45,45,45	0
56	OHX	AA	3548	7/7	0.12	-	113,118,133,172	1
55	MG	AA	3103	1/1	0.11	-	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	1730	1/1	0.56	-	73,73,73,73	0
55	MG	BA	1748	1/1	0.27	-	66,66,66,66	0
55	MG	CA	3229	1/1	0.41	-	80,80,80,80	0
56	OHX	DA	1773	7/7	0.10	-	122,126,137,197	1
55	MG	BA	1738	1/1	0.16	-	41,41,41,41	0
55	MG	AA	3187	1/1	0.57	-	86,86,86,86	0
56	OHX	AO	204	7/7	0.15	-	83,94,106,121	1
55	MG	AA	3171	1/1	0.25	-	48,48,48,48	0
55	MG	BA	1725	1/1	0.47	-	69,69,69,69	0
55	MG	AA	3002	1/1	0.44	-	41,41,41,41	0
55	MG	CA	3170	1/1	0.21	-	65,65,65,65	0
56	OHX	DA	1788	7/7	0.12	-	96,113,128,168	1
56	OHX	AA	3314	7/7	0.14	-	81,93,123,149	1
56	OHX	AA	3263	7/7	0.15	-	76,102,114,143	1
55	MG	DA	1687	1/1	0.18	-	63,63,63,63	0
55	MG	CA	3207	1/1	0.32	-	68,68,68,68	0
55	MG	DA	1637	1/1	0.56	-	106,106,106,106	0
55	MG	DA	1710	1/1	0.25	-	103,103,103,103	0
55	MG	CA	3259	1/1	0.25	-	65,65,65,65	0
56	OHX	CA	3436	7/7	0.14	-	115,121,137,192	1
55	MG	CA	3182	1/1	0.45	-	59,59,59,59	0
56	OHX	CA	3289	7/7	0.14	-	69,83,106,125	0
55	MG	AA	3067	1/1	0.20	-	97,97,97,97	0
56	OHX	DA	1722	7/7	0.15	-	84,90,106,116	0
56	OHX	AA	3444	7/7	0.15	-	80,103,116,131	1
55	MG	AA	3075	1/1	0.50	-	44,44,44,44	0
56	OHX	CA	3333	7/7	0.10	-	104,127,133,184	1
55	MG	BA	1641	1/1	0.39	-	85,85,85,85	0
55	MG	AA	3173	1/1	0.33	-	52,52,52,52	0
56	OHX	DA	1733	7/7	0.15	-	146,151,163,202	0
55	MG	BA	1605	1/1	0.22	-	104,104,104,104	0
56	OHX	AA	3470	7/7	0.15	-	107,109,130,160	1
55	MG	CA	3440	1/1	0.34	-	54,54,54,54	0
56	OHX	AA	3458	7/7	0.22	-	34,48,113,148	3
55	MG	AA	3269	1/1	0.42	-	72,72,72,72	0
55	MG	CA	3053	1/1	0.18	-	99,99,99,99	0
56	OHX	AA	3407	7/7	0.15	-	108,117,126,165	1
55	MG	AA	3162	1/1	0.55	-	38,38,38,38	0
55	MG	AA	3273	1/1	0.58	-	66,66,66,66	0
56	OHX	AA	3522	7/7	0.17	-	118,131,145,201	1
56	OHX	DA	1730	7/7	0.14	-	102,111,123,157	0
56	OHX	AA	3449	7/7	0.17	-	64,74,89,112	2

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	OHX	CA	3402	7/7	0.10	-	159,162,170,218	1
56	OHX	BA	1657	7/7	0.19	-	116,125,141,215	1
55	MG	CA	3225	1/1	0.28	-	48,48,48,48	0
55	MG	DA	1613	1/1	0.27	-	87,87,87,87	0
56	OHX	CA	3374	7/7	0.11	-	106,124,128,169	1
55	MG	DA	1629	1/1	0.25	-	93,93,93,93	0
55	MG	CA	3168	1/1	0.43	-	72,72,72,72	0
55	MG	AA	3057	1/1	0.47	-	72,72,72,72	0
56	OHX	BA	1798	7/7	0.12	-	140,143,151,221	1
56	OHX	CA	3364	7/7	0.10	-	117,120,133,182	1
55	MG	AA	3270	1/1	0.13	-	94,94,94,94	0
55	MG	AB	206	1/1	0.57	-	83,83,83,83	0
56	OHX	BA	1680	7/7	0.12	-	120,125,145,238	1
55	MG	AA	3074	1/1	0.38	-	73,73,73,73	0
55	MG	CA	3004	1/1	0.26	-	49,49,49,49	0
55	MG	CA	3054	1/1	0.34	-	54,54,54,54	0
56	OHX	BA	1789	7/7	0.18	-	108,112,133,182	1
55	MG	BA	1709	1/1	0.35	-	100,100,100,100	0
55	MG	CA	3150	1/1	0.36	-	55,55,55,55	0
55	MG	DA	1630	1/1	0.39	-	95,95,95,95	0
56	OHX	AA	3339	7/7	0.11	-	151,155,164,211	1
55	MG	BA	1717	1/1	0.47	-	51,51,51,51	0
56	OHX	BA	1810	7/7	0.13	-	106,108,121,152	1
55	MG	CA	3179	1/1	0.13	-	73,73,73,73	0
56	OHX	AA	3424	7/7	0.17	-	92,97,108,112	0
56	OHX	BA	1792	7/7	0.09	-	150,163,168,209	1
56	OHX	BA	1667	7/7	0.18	-	118,130,146,200	1
56	OHX	AA	3290	7/7	0.17	-	10,72,91,128	0
56	OHX	BA	1671	7/7	0.08	-	127,131,133,210	1
55	MG	CA	3260	1/1	0.26	-	71,71,71,71	0
55	MG	AA	3261	1/1	0.41	-	64,64,64,64	0
55	MG	BB	101	1/1	0.49	-	70,70,70,70	0
56	OHX	CA	3411	7/7	0.10	-	117,123,138,184	1
55	MG	CA	3044	1/1	0.18	-	74,74,74,74	0
55	MG	DA	1639	1/1	0.49	-	70,70,70,70	0
56	OHX	CA	3358	7/7	0.11	-	128,130,147,230	1
55	MG	CA	3202	1/1	0.49	-	79,79,79,79	0
55	MG	BA	1753	1/1	0.48	-	67,67,67,67	0
55	MG	CA	3126	1/1	0.30	-	54,54,54,54	0
55	MG	CA	3118	1/1	0.39	-	69,69,69,69	0
57	ZN	BG	301	1/1	0.30	-	79,79,79,79	0
55	MG	BC	104	1/1	0.51	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3410	1/1	0.47	-	61,61,61,61	0
55	MG	CA	3132	1/1	0.24	-	80,80,80,80	0
56	OHX	CA	3485	7/7	0.15	-	88,102,109,144	1
56	OHX	DB	103	7/7	0.12	-	166,171,179,191	1
56	OHX	CA	3351	7/7	0.12	-	102,107,134,173	1
55	MG	BA	1719	1/1	0.43	-	51,51,51,51	0
56	OHX	DA	1748	7/7	0.11	-	95,111,122,149	1
56	OHX	CA	3396	7/7	0.13	-	135,136,150,198	1
56	OHX	BA	1661	7/7	0.13	-	108,124,128,170	1
55	MG	BA	1634	1/1	0.19	-	74,74,74,74	0
55	MG	BA	1601	1/1	0.23	-	81,81,81,81	0
55	MG	AA	3076	1/1	0.39	-	72,72,72,72	0
55	MG	DA	1716	1/1	0.34	-	85,85,85,85	0
56	OHX	CA	3438	7/7	0.11	-	97,104,116,167	1
55	MG	CA	3177	1/1	0.29	-	57,57,57,57	0
56	OHX	BA	1670	7/7	0.10	-	135,143,147,201	1
55	MG	BA	1706	1/1	0.42	-	79,79,79,79	0
56	OHX	CA	3283	7/7	0.16	-	81,83,86,120	1
56	OHX	BA	1800	7/7	0.13	-	106,107,118,143	1
56	OHX	BA	1756	7/7	0.20	-	59,79,107,108	0
55	MG	CB	205	1/1	0.43	-	74,74,74,74	0
56	OHX	DA	1811	7/7	0.07	-	137,141,149,222	1
55	MG	DA	1601	1/1	0.24	-	87,87,87,87	0
55	MG	BC	103	1/1	0.44	-	62,62,62,62	0
55	MG	AA	3105	1/1	0.48	-	124,124,124,124	0
56	OHX	AA	3292	7/7	0.17	-	50,75,88,112	0
56	OHX	CA	3302	7/7	0.18	-	79,86,104,139	1
56	OHX	CA	3277	7/7	0.17	-	73,81,99,107	1
55	MG	BA	1622	1/1	0.16	-	123,123,123,123	0
56	OHX	DA	1771	7/7	0.11	-	97,105,129,152	1
55	MG	CA	3010	1/1	0.22	-	47,47,47,47	0
55	MG	CA	3022	1/1	0.17	-	55,55,55,55	0
56	OHX	AA	3287	7/7	0.14	-	75,88,103,129	2
56	OHX	AA	3307	7/7	0.15	-	85,90,103,127	1
56	OHX	CF	301	7/7	0.17	-	54,58,79,92	0
55	MG	CA	3039	1/1	0.39	-	65,65,65,65	0
56	OHX	CB	218	7/7	0.12	-	141,159,166,235	1
56	OHX	CA	3343	7/7	0.16	-	109,118,132,184	1
55	MG	DA	1611	1/1	0.29	-	92,92,92,92	0
55	MG	AA	3241	1/1	0.36	-	60,60,60,60	0
55	MG	AA	3101	1/1	0.46	-	63,63,63,63	0
56	OHX	CA	3482	7/7	0.12	-	84,120,131,181	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	AA	3328	7/7	0.11	-	89,97,114,142	1
56	OHX	CA	3323	7/7	0.13	-	107,111,118,169	0
55	MG	AA	3158	1/1	0.43	-	50,50,50,50	0
55	MG	CA	3454	1/1	0.30	-	51,51,51,51	0
55	MG	CA	3125	1/1	0.21	-	52,52,52,52	0
56	OHX	CA	3340	7/7	0.12	-	115,122,140,168	1
55	MG	AA	3106	1/1	0.45	-	70,70,70,70	0
55	MG	AA	3180	1/1	0.32	-	65,65,65,65	0
55	MG	AA	3017	1/1	0.54	-	100,100,100,100	0
55	MG	DA	1713	1/1	0.45	-	79,79,79,79	0
55	MG	DA	1654	1/1	0.36	-	61,61,61,61	0
56	OHX	AA	3367	7/7	0.14	-	121,129,147,173	1
56	OHX	CA	3274	7/7	0.15	-	67,83,114,118	0
55	MG	AA	3023	1/1	0.53	-	52,52,52,52	0
56	OHX	BA	1755	7/7	0.18	-	72,74,97,109	0
56	OHX	BA	1785	7/7	0.14	-	109,122,129,170	1
56	OHX	CA	3251	7/7	0.12	-	88,107,125,141	1
55	MG	AA	3344	1/1	0.38	-	48,48,48,48	0
55	MG	CA	3478	1/1	0.50	-	82,82,82,82	0
55	MG	CA	3144	1/1	0.34	-	54,54,54,54	0
56	OHX	AA	3514	7/7	0.19	-	84,93,104,149	1
56	OHX	AA	3456	7/7	0.20	-	59,75,90,132	2
55	MG	CA	3017	1/1	0.24	-	92,92,92,92	0
55	MG	DA	1636	1/1	0.37	-	75,75,75,75	0
56	OHX	AA	3400	7/7	0.18	-	69,80,83,116	1
56	OHX	A6	101	7/7	0.13	-	113,122,137,155	1
55	MG	AO	203	1/1	0.28	-	56,56,56,56	0
56	OHX	AA	3431	7/7	0.16	-	74,81,100,115	0
56	OHX	DB	105	7/7	0.20	-	88,91,103,175	5
55	MG	AO	201	1/1	0.41	-	80,80,80,80	0
56	OHX	AA	3473	7/7	0.16	-	66,95,102,124	1
56	OHX	DA	1760	7/7	0.11	-	142,145,152,204	1
56	OHX	BA	1683	7/7	0.10	-	124,130,146,183	1
55	MG	AA	3240	1/1	0.33	-	43,43,43,43	0
55	MG	AA	3148	1/1	0.38	-	65,65,65,65	0
55	MG	DA	1652	1/1	0.44	-	52,52,52,52	0
56	OHX	AA	3537	7/7	0.10	-	171,189,202,242	1
55	MG	AA	3051	1/1	0.35	-	49,49,49,49	0
56	OHX	CA	3342	7/7	0.14	-	116,123,130,201	1
55	MG	AE	301	1/1	0.32	-	52,52,52,52	0
56	OHX	BA	1781	7/7	0.13	-	91,111,121,156	1
56	OHX	CA	3316	7/7	0.09	-	119,122,129,158	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	1725	1/1	0.40	-	87,87,87,87	0
55	MG	AA	3392	1/1	0.61	-	64,64,64,64	0
55	MG	AA	3049	1/1	0.42	-	64,64,64,64	0
56	OHX	AA	3369	7/7	0.18	-	80,102,119,165	1
56	OHX	AA	3334	7/7	0.17	-	66,79,94,105	1
56	OHX	CA	3294	7/7	0.14	-	91,93,107,125	1
55	MG	CA	3011	1/1	0.36	-	46,46,46,46	0
55	MG	BA	1699	1/1	0.42	-	79,79,79,79	0
56	OHX	CA	3321	7/7	0.13	-	111,119,144,156	0
55	MG	CA	3016	1/1	0.24	-	55,55,55,55	0
55	MG	CA	3473	1/1	0.30	-	50,50,50,50	0
56	OHX	BA	1688	7/7	0.13	-	107,112,123,154	1
56	OHX	DR	101	7/7	0.15	-	135,141,146,189	1
56	OHX	BA	1774	7/7	0.15	-	80,98,111,147	1
55	MG	AA	3226	1/1	0.49	-	42,42,42,42	0
55	MG	CA	3085	1/1	0.38	-	102,102,102,102	0
56	OHX	CA	3293	7/7	0.16	-	100,117,128,163	0
55	MG	BB	102	1/1	0.28	-	85,85,85,85	0
56	OHX	AA	3402	7/7	0.20	-	87,110,129,141	3
56	OHX	AA	3399	7/7	0.20	-	42,51,73,98	0
56	OHX	CA	3240	7/7	0.12	-	96,99,103,148	1
55	MG	CA	3041	1/1	0.25	-	73,73,73,73	0
55	MG	AA	3388	1/1	0.42	-	41,41,41,41	0
55	MG	BA	1737	1/1	0.25	-	46,46,46,46	0
55	MG	AA	3010	1/1	0.27	-	40,40,40,40	0
56	OHX	DA	1772	7/7	0.09	-	131,135,143,214	1
55	MG	CA	3140	1/1	0.39	-	59,59,59,59	0
55	MG	AA	3065	1/1	0.39	-	49,49,49,49	0
55	MG	AA	3207	1/1	0.47	-	57,57,57,57	0
56	OHX	AA	3430	7/7	0.17	-	63,78,92,111	1
56	OHX	AA	3509	7/7	0.13	-	92,96,122,175	1
56	OHX	AA	3494	7/7	0.16	-	59,86,128,185	1
55	MG	CA	3073	1/1	0.17	-	54,54,54,54	0
55	MG	CA	3068	1/1	0.33	-	44,44,44,44	0
55	MG	AA	3212	1/1	0.39	-	35,35,35,35	0
56	OHX	AA	3529	7/7	0.16	-	90,106,115,167	1
55	MG	AA	3355	1/1	0.47	-	36,36,36,36	0
55	MG	AA	3015	1/1	0.45	-	76,76,76,76	0
55	MG	CA	3163	1/1	0.39	-	80,80,80,80	0
55	MG	DA	1689	1/1	0.41	-	87,87,87,87	0
56	OHX	AA	3439	7/7	0.15	-	69,82,92,115	1
55	MG	AA	3395	1/1	0.20	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3139	1/1	0.31	-	56,56,56,56	0
56	OHX	AA	3366	7/7	0.20	-	85,90,106,173	1
55	MG	CA	3086	1/1	0.38	-	68,68,68,68	0
56	OHX	AA	3498	7/7	0.16	-	92,94,127,136	1
56	OHX	DA	1804	7/7	0.16	-	107,115,128,173	1
56	OHX	AA	3552	7/7	0.18	-	105,122,135,199	1
56	OHX	DA	1734	7/7	0.10	-	102,105,122,149	1
56	OHX	CA	3248	7/7	0.10	-	116,128,134,203	1
56	OHX	AA	3521	7/7	0.13	-	87,94,107,160	1
55	MG	A5	101	1/1	0.24	-	41,41,41,41	0
56	OHX	AA	3508	7/7	0.11	-	122,129,136,204	1
55	MG	BA	1655	1/1	0.23	-	60,60,60,60	0
55	MG	BA	1651	1/1	0.11	-	90,90,90,90	0
55	MG	AA	3032	1/1	0.30	-	41,41,41,41	0
56	OHX	CA	3372	7/7	0.12	-	112,137,145,182	0
55	MG	AA	3046	1/1	0.53	-	68,68,68,68	0
55	MG	DA	1605	1/1	0.26	-	63,63,63,63	0
55	MG	DA	1676	1/1	0.43	-	83,83,83,83	0
56	OHX	CA	3276	7/7	0.16	-	81,100,117,133	0
56	OHX	DB	104	7/7	0.15	-	129,133,143,205	2
55	MG	BA	1726	1/1	0.34	-	61,61,61,61	0
55	MG	DA	1686	1/1	0.26	-	73,73,73,73	0
56	OHX	CA	3419	7/7	0.13	-	153,156,164,238	1
56	OHX	CA	3386	7/7	0.14	-	110,116,134,181	1
56	OHX	CA	3330	7/7	0.10	-	102,106,115,169	0
55	MG	BA	1714	1/1	0.27	-	56,56,56,56	0
55	MG	DA	1706	1/1	0.19	-	100,100,100,100	0
55	MG	AA	3384	1/1	0.44	-	59,59,59,59	0
55	MG	DA	1664	1/1	0.48	-	31,31,31,31	0
56	OHX	AW	101	7/7	0.14	-	103,112,128,156	1
55	MG	DA	1608	1/1	0.25	-	78,78,78,78	0
55	MG	CB	203	1/1	0.13	-	111,111,111,111	0
55	MG	AA	3193	1/1	0.21	-	58,58,58,58	0
56	OHX	CB	212	7/7	0.15	-	101,120,135,155	1
55	MG	AA	3050	1/1	0.37	-	60,60,60,60	0
55	MG	BA	1731	1/1	0.40	-	57,57,57,57	0
56	OHX	CA	3483	7/7	0.14	-	84,93,103,136	1
56	OHX	BA	1809	7/7	0.10	-	141,153,160,232	0
55	MG	AA	3196	1/1	0.40	-	36,36,36,36	0
56	OHX	BA	1695	7/7	0.09	-	129,147,158,217	1
56	OHX	BR	101	7/7	0.10	-	117,129,143,169	1
56	OHX	CA	3487	7/7	0.08	-	135,139,147,210	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	OHX	CA	3489	7/7	0.14	-	91,101,112,140	1
55	MG	AA	3089	1/1	0.53	-	84,84,84,84	0
56	OHX	CA	3300	7/7	0.15	-	66,75,91,101	1
55	MG	CA	3064	1/1	0.21	-	89,89,89,89	0
56	OHX	CA	3301	7/7	0.14	-	55,85,123,136	3
56	OHX	AA	3568	7/7	0.14	-	78,93,100,118	1
56	OHX	CA	3407	7/7	0.12	-	142,149,155,227	1
55	MG	AA	3272	1/1	0.50	-	50,50,50,50	0
56	OHX	CA	3313	7/7	0.12	-	103,112,124,157	0
55	MG	CA	3208	1/1	0.35	-	70,70,70,70	0
55	MG	AA	3206	1/1	0.51	-	64,64,64,64	0
56	OHX	AA	3304	7/7	0.13	-	109,115,135,200	1
56	OHX	BA	1675	7/7	0.08	-	120,128,140,197	1
56	OHX	BA	1778	7/7	0.13	-	99,120,131,182	0
55	MG	DA	1681	1/1	0.34	-	100,100,100,100	0
55	MG	CA	3142	1/1	0.35	-	71,71,71,71	0
56	OHX	AA	3333	7/7	0.20	-	91,114,128,179	2
56	OHX	DA	1778	7/7	0.15	-	142,148,154,267	0
56	OHX	CA	3367	7/7	0.09	-	129,137,147,194	1
56	OHX	AA	3520	7/7	0.11	-	127,132,145,185	1
56	OHX	AB	218	7/7	0.17	-	128,132,146,199	1
56	OHX	BA	1786	7/7	0.10	-	93,97,101,149	1
55	MG	AA	3178	1/1	0.45	-	39,39,39,39	0
55	MG	CA	3265	1/1	0.22	-	55,55,55,55	0
55	MG	AA	3210	1/1	0.49	-	41,41,41,41	0
55	MG	AA	3198	1/1	0.30	-	54,54,54,54	0
55	MG	CA	3099	1/1	0.34	-	51,51,51,51	0
55	MG	AA	3230	1/1	0.26	-	66,66,66,66	0
55	MG	AA	3346	1/1	0.26	-	42,42,42,42	0
55	MG	CA	3217	1/1	0.37	-	58,58,58,58	0
55	MG	DA	1617	1/1	0.30	-	115,115,115,115	0
56	OHX	AA	3427	7/7	0.18	-	29,70,88,108	0
56	OHX	CA	3334	7/7	0.11	-	110,115,136,183	0
55	MG	AE	302	1/1	0.21	-	71,71,71,71	0
56	OHX	CA	3236	7/7	0.20	-	81,104,120,146	0
55	MG	DA	1671	1/1	0.25	-	64,64,64,64	0
56	OHX	AA	3372	7/7	0.12	-	93,103,121,167	1
55	MG	CA	3100	1/1	0.44	-	63,63,63,63	0
56	OHX	AA	3551	7/7	0.10	-	141,143,149,194	1
56	OHX	CA	3281	7/7	0.19	-	101,105,126,132	0
56	OHX	AA	3481	7/7	0.16	-	95,108,126,156	2
55	MG	AA	3104	1/1	0.53	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	AB	210	7/7	0.21	-	83,107,129,146	3
55	MG	CA	3220	1/1	0.34	-	85,85,85,85	0
55	MG	CA	3033	1/1	0.27	-	71,71,71,71	0
56	OHX	CA	3410	7/7	0.12	-	114,125,132,190	1
55	MG	AA	3172	1/1	0.44	-	38,38,38,38	0
56	OHX	CA	3405	7/7	0.10	-	112,116,119,187	1
56	OHX	CA	3433	7/7	0.19	-	121,129,144,183	1
55	MG	AA	3169	1/1	0.52	-	76,76,76,76	0
55	MG	AA	3279	1/1	0.42	-	81,81,81,81	0
55	MG	DA	1646	1/1	0.26	-	64,64,64,64	0
55	MG	AA	3152	1/1	0.35	-	56,56,56,56	0
56	OHX	BA	1790	7/7	0.22	-	96,123,133,185	1
55	MG	DA	1673	1/1	0.36	-	80,80,80,80	0
56	OHX	AA	3468	7/7	0.14	-	99,111,119,167	1
55	MG	DL	201	1/1	0.49	-	92,92,92,92	0
55	MG	BA	1732	1/1	0.46	-	52,52,52,52	0
55	MG	BD	101	1/1	0.30	-	93,93,93,93	0
56	OHX	DA	1782	7/7	0.14	-	117,128,138,207	1
56	OHX	AA	3567	7/7	0.15	-	103,106,118,172	1
56	OHX	BA	1676	7/7	0.10	-	143,151,156,210	1
55	MG	CA	3459	1/1	0.29	-	56,56,56,56	0
55	MG	DA	1622	1/1	0.27	-	122,122,122,122	0
56	OHX	CA	3359	7/7	0.14	-	115,123,136,171	2
55	MG	CA	3203	1/1	0.40	-	47,47,47,47	0
55	MG	AA	3004	1/1	0.45	-	37,37,37,37	0
55	MG	DA	1642	1/1	0.48	-	112,112,112,112	0
56	OHX	CA	3308	7/7	0.16	-	88,90,121,161	0
56	OHX	AA	3526	7/7	0.18	-	120,129,136,176	1
56	OHX	AB	212	7/7	0.17	-	81,99,131,153	1
55	MG	CA	3257	1/1	0.31	-	60,60,60,60	0
56	OHX	AA	3517	7/7	0.17	-	88,111,115,145	1
56	OHX	AA	3491	7/7	0.15	-	162,182,190,220	1
55	MG	CA	3175	1/1	0.37	-	64,64,64,64	0
55	MG	A0	201	1/1	0.20	-	48,48,48,48	0
55	MG	AA	3134	1/1	0.21	-	82,82,82,82	0
55	MG	BA	1606	1/1	0.45	-	92,92,92,92	0
55	MG	BA	1621	1/1	0.43	-	55,55,55,55	0
55	MG	AA	3174	1/1	0.47	-	76,76,76,76	0
56	OHX	AA	3302	7/7	0.13	-	88,114,124,193	1
55	MG	CA	3071	1/1	0.26	-	51,51,51,51	0
56	OHX	CA	3385	7/7	0.10	-	115,124,135,193	1
55	MG	BA	1705	1/1	0.31	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	CA	3282	7/7	0.15	-	79,83,97,109	0
55	MG	CA	3095	1/1	0.28	-	54,54,54,54	0
56	OHX	DA	1783	7/7	0.12	-	123,123,145,185	1
55	MG	AA	3119	1/1	0.36	-	64,64,64,64	0
56	OHX	AA	3298	7/7	0.20	-	71,88,99,110	1
55	MG	DA	1659	1/1	0.27	-	89,89,89,89	0
56	OHX	AA	3368	7/7	0.18	-	76,83,98,126	1
56	OHX	AA	3306	7/7	0.12	-	134,139,151,214	1
55	MG	AA	3204	1/1	0.18	-	61,61,61,61	0
55	MG	BA	1729	1/1	0.54	-	73,73,73,73	0
55	MG	CA	3472	1/1	0.19	-	59,59,59,59	0
56	OHX	CA	3397	7/7	0.11	-	128,138,154,219	1
56	OHX	CA	3271	7/7	0.22	-	67,82,101,115	0
56	OHX	DA	1758	7/7	0.08	-	132,137,143,204	0
55	MG	AA	3142	1/1	0.56	-	45,45,45,45	0
56	OHX	DA	1809	7/7	0.08	-	124,126,139,221	1
55	MG	CA	3264	1/1	0.35	-	49,49,49,49	0
55	MG	AA	3047	1/1	0.39	-	54,54,54,54	0
56	OHX	AA	3497	7/7	0.14	-	94,106,111,138	2
56	OHX	CA	3466	7/7	0.14	-	96,98,116,157	1
56	OHX	CA	3388	7/7	0.12	-	112,116,127,180	1
55	MG	DA	1632	1/1	0.30	-	83,83,83,83	0
55	MG	BA	1609	1/1	0.34	-	73,73,73,73	0
55	MG	CA	3445	1/1	0.22	-	38,38,38,38	0
55	MG	AA	3398	1/1	0.41	-	51,51,51,51	0
55	MG	CA	3167	1/1	0.48	-	75,75,75,75	0
55	MG	CA	3442	1/1	0.21	-	61,61,61,61	0
56	OHX	DA	1791	7/7	0.15	-	103,104,121,153	1
55	MG	DA	1690	1/1	0.44	-	63,63,63,63	0
55	MG	AA	3170	1/1	0.22	-	50,50,50,50	0
56	OHX	CA	3368	7/7	0.14	-	108,126,135,177	1
55	MG	BA	1604	1/1	0.44	-	72,72,72,72	0
55	MG	AA	3250	1/1	0.37	-	56,56,56,56	0
55	MG	CA	3005	1/1	0.21	-	48,48,48,48	0
56	OHX	AA	3446	7/7	0.15	-	68,90,101,115	2
55	MG	AA	3084	1/1	0.35	-	58,58,58,58	0
55	MG	AA	3132	1/1	0.51	-	81,81,81,81	0
55	MG	AA	3157	1/1	0.48	-	49,49,49,49	0
55	MG	AA	3149	1/1	0.31	-	74,74,74,74	0
56	OHX	DA	1768	7/7	0.10	-	121,132,163,218	0
56	OHX	DA	1746	7/7	0.08	-	126,134,146,189	1
55	MG	AA	3112	1/1	0.26	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3161	1/1	0.33	-	50,50,50,50	0
55	MG	CA	3084	1/1	0.38	-	60,60,60,60	0
56	OHX	CA	3399	7/7	0.19	-	97,104,115,165	2
56	OHX	DA	1781	7/7	0.13	-	107,126,135,195	1
55	MG	DA	1615	1/1	0.28	-	98,98,98,98	0
55	MG	AA	3041	1/1	0.25	-	49,49,49,49	0
55	MG	DA	1625	1/1	0.10	-	97,97,97,97	0
56	OHX	AA	3320	7/7	0.18	-	69,81,96,121	1
56	OHX	DA	1726	7/7	0.17	-	87,101,123,159	0
56	OHX	DA	1780	7/7	0.10	-	127,131,138,167	1
55	MG	CA	3149	1/1	0.35	-	55,55,55,55	0
55	MG	CA	3015	1/1	0.28	-	54,54,54,54	0
55	MG	AA	3409	1/1	0.47	-	56,56,56,56	0
55	MG	BA	1603	1/1	0.35	-	63,63,63,63	0
56	OHX	CA	3365	7/7	0.08	-	164,171,176,213	1
55	MG	AA	3096	1/1	0.34	-	71,71,71,71	0
56	OHX	CA	3373	7/7	0.16	-	113,122,129,160	1
56	OHX	DA	1796	7/7	0.11	-	134,139,149,195	1
56	OHX	AA	3480	7/7	0.18	-	90,100,124,135	1
55	MG	CA	3120	1/1	0.35	-	48,48,48,48	0
56	OHX	AA	3558	7/7	0.12	-	95,121,125,156	1
55	MG	DA	1626	1/1	0.54	-	84,84,84,84	0
55	MG	AA	3093	1/1	0.47	-	91,91,91,91	0
56	OHX	AB	219	7/7	0.15	-	104,111,125,162	1
56	OHX	AA	3342	7/7	0.17	-	78,85,104,123	1
55	MG	BA	1751	1/1	0.50	-	95,95,95,95	0
55	MG	AA	3228	1/1	0.26	-	67,67,67,67	0
55	MG	CA	3092	1/1	0.56	-	52,52,52,52	0
55	MG	BA	1715	1/1	0.35	-	74,74,74,74	0
55	MG	CA	3267	1/1	0.16	-	65,65,65,65	0
56	OHX	DA	1736	7/7	0.12	-	130,135,157,193	0
55	MG	AA	3252	1/1	0.39	-	47,47,47,47	0
56	OHX	BA	1669	7/7	0.18	-	124,127,142,200	1
55	MG	AA	3267	1/1	0.45	-	80,80,80,80	0
56	OHX	DA	1806	7/7	0.07	-	142,150,160,228	1
55	MG	AA	3116	1/1	0.31	-	45,45,45,45	0
56	OHX	DA	1751	7/7	0.18	-	66,109,137,183	2
55	MG	BB	104	1/1	0.50	-	87,87,87,87	0
56	OHX	AA	3452	7/7	0.21	-	61,75,91,137	2
55	MG	CA	3065	1/1	0.35	-	55,55,55,55	0
55	MG	CA	3449	1/1	0.46	-	54,54,54,54	0
55	MG	CA	3046	1/1	0.29	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3102	1/1	0.45	-	67,67,67,67	0
56	OHX	DA	1767	7/7	0.09	-	120,124,135,184	1
55	MG	CA	3134	1/1	0.36	-	65,65,65,65	0
55	MG	AA	3249	1/1	0.43	-	58,58,58,58	0
55	MG	CA	3212	1/1	0.47	-	75,75,75,75	0
55	MG	AA	3094	1/1	0.56	-	39,39,39,39	0
56	OHX	CA	3253	7/7	0.16	-	107,120,133,155	1
55	MG	BA	1648	1/1	0.51	-	99,99,99,99	0
56	OHX	CA	3422	7/7	0.11	-	126,137,143,193	1
55	MG	CA	3195	1/1	0.29	-	68,68,68,68	0
55	MG	DA	1620	1/1	0.52	-	79,79,79,79	0
56	OHX	CA	3418	7/7	0.12	-	115,119,129,166	1
56	OHX	CA	3348	7/7	0.23	-	104,111,132,178	1
56	OHX	DA	1784	7/7	0.09	-	150,153,166,225	1
55	MG	AO	202	1/1	0.29	-	55,55,55,55	0
55	MG	DA	1696	1/1	0.26	-	112,112,112,112	0
55	MG	D1	101	1/1	0.36	-	78,78,78,78	0
55	MG	BA	1615	1/1	0.26	-	113,113,113,113	0
56	OHX	CA	3329	7/7	0.11	-	102,103,123,146	1
55	MG	AE	303	1/1	0.29	-	32,32,32,32	0
55	MG	AA	3102	1/1	0.42	-	79,79,79,79	0
55	MG	AA	3227	1/1	0.41	-	63,63,63,63	0
55	MG	AA	3277	1/1	0.50	-	46,46,46,46	0
55	MG	CA	3098	1/1	0.17	-	63,63,63,63	0
55	MG	DA	1705	1/1	0.49	-	108,108,108,108	0
55	MG	CA	3047	1/1	0.38	-	41,41,41,41	0
56	OHX	CA	3304	7/7	0.14	-	113,122,141,181	2
56	OHX	CA	3424	7/7	0.08	-	141,145,151,214	1
55	MG	BA	1654	1/1	0.35	-	47,47,47,47	0
55	MG	CA	3109	1/1	0.29	-	56,56,56,56	0
55	MG	AA	3259	1/1	0.35	-	35,35,35,35	0
55	MG	CA	3081	1/1	0.31	-	63,63,63,63	0
55	MG	AA	3058	1/1	0.35	-	73,73,73,73	0
56	OHX	AA	3518	7/7	0.16	-	67,73,103,130	1
56	OHX	CA	3426	7/7	0.10	-	142,146,155,215	1
56	OHX	CA	3243	7/7	0.12	-	121,128,140,172	0
56	OHX	CA	3346	7/7	0.13	-	99,104,119,151	1
56	OHX	DA	1724	7/7	0.13	-	84,106,133,148	1
56	OHX	DA	1740	7/7	0.12	-	139,153,162,184	0
55	MG	CA	3115	1/1	0.35	-	63,63,63,63	0
56	OHX	BA	1799	7/7	0.11	-	158,163,176,213	1
55	MG	BA	1637	1/1	0.08	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	1643	1/1	0.39	-	136,136,136,136	0
56	OHX	C5	102	7/7	0.15	-	114,118,133,165	1
56	OHX	AA	3448	7/7	0.14	-	87,90,112,131	1
55	MG	CA	3201	1/1	0.51	-	79,79,79,79	0
55	MG	DA	1672	1/1	0.32	-	83,83,83,83	0
55	MG	AA	3257	1/1	0.42	-	57,57,57,57	0
55	MG	CA	3121	1/1	0.34	-	55,55,55,55	0
56	OHX	AA	3557	7/7	0.15	-	75,87,101,114	1
56	OHX	AA	3475	7/7	0.17	-	67,93,111,167	1
56	OHX	AA	3547	7/7	0.16	-	69,84,101,157	2
56	OHX	AA	3305	7/7	0.17	-	83,97,103,135	1
56	OHX	DC	110	7/7	0.13	-	78,91,106,144	4
56	OHX	CA	3317	7/7	0.10	-	116,126,142,180	1
55	MG	AA	3229	1/1	0.52	-	59,59,59,59	0
56	OHX	CB	210	7/7	0.14	-	104,124,140,171	1
55	MG	AA	3068	1/1	0.29	-	61,61,61,61	0
55	MG	BA	1630	1/1	0.19	-	90,90,90,90	0
56	OHX	CA	3249	7/7	0.15	-	86,90,104,128	1
56	OHX	BD	104	7/7	0.26	-	82,85,90,147	2
55	MG	DC	105	1/1	0.50	-	54,54,54,54	0
55	MG	AA	3244	1/1	0.22	-	49,49,49,49	0
55	MG	BA	1727	1/1	0.43	-	70,70,70,70	0
56	OHX	DA	1800	7/7	0.08	-	137,140,150,220	1
56	OHX	AB	207	7/7	0.15	-	89,99,126,152	1
55	MG	CA	3045	1/1	0.60	-	91,91,91,91	0
56	OHX	AA	3490	7/7	0.16	-	94,113,129,158	1
56	OHX	AA	3501	7/7	0.16	-	101,109,129,149	1
56	OHX	AA	3469	7/7	0.12	-	79,91,98,161	1
55	MG	CA	3158	1/1	0.41	-	56,56,56,56	0
55	MG	CA	3206	1/1	0.47	-	90,90,90,90	0
55	MG	CA	3059	1/1	0.41	-	63,63,63,63	0
56	OHX	BA	1757	7/7	0.18	-	57,66,87,98	2
55	MG	CA	3194	1/1	0.25	-	63,63,63,63	0
56	OHX	CA	3326	7/7	0.11	-	97,110,130,136	2
55	MG	AA	3016	1/1	0.36	-	39,39,39,39	0
56	OHX	CA	3465	7/7	0.10	-	131,136,147,181	1
56	OHX	CA	3337	7/7	0.13	-	109,124,136,185	0
56	OHX	AA	3478	7/7	0.17	-	77,90,100,131	1
55	MG	AA	3014	1/1	0.46	-	44,44,44,44	0
55	MG	AA	3260	1/1	0.53	-	58,58,58,58	0
56	OHX	C1	201	7/7	0.14	-	102,111,123,165	1
55	MG	BA	1708	1/1	0.42	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	OHX	DA	1802	7/7	0.12	-	120,122,140,196	1
55	MG	BA	1747	1/1	0.41	-	74,74,74,74	0
56	OHX	AA	3160	7/7	0.11	-	116,121,130,182	1
55	MG	AA	3195	1/1	0.38	-	43,43,43,43	0
55	MG	AA	3118	1/1	0.31	-	53,53,53,53	0
56	OHX	CA	3356	7/7	0.13	-	96,109,118,157	1
56	OHX	BA	1775	7/7	0.09	-	111,114,129,169	1
56	OHX	AA	3417	7/7	0.21	-	68,72,82,103	0
55	MG	BA	1645	1/1	0.38	-	51,51,51,51	0
55	MG	C7	101	1/1	0.38	-	54,54,54,54	0
55	MG	AA	3218	1/1	0.40	-	82,82,82,82	0
55	MG	AA	3211	1/1	0.51	-	62,62,62,62	0
56	OHX	BA	1773	7/7	0.10	-	101,102,110,142	1
55	MG	BA	1643	1/1	0.11	-	78,78,78,78	0
56	OHX	AA	3486	7/7	0.16	-	127,135,138,199	1
56	OHX	CA	3255	7/7	0.12	-	103,107,122,145	1
56	OHX	AA	3426	7/7	0.20	-	70,84,89,118	0
56	OHX	CA	3318	7/7	0.18	-	34,112,130,183	1
55	MG	CA	3185	1/1	0.46	-	75,75,75,75	0
56	OHX	CA	3427	7/7	0.10	-	114,126,136,203	1
56	OHX	CA	3404	7/7	0.10	-	149,155,166,217	1
55	MG	AA	3003	1/1	0.35	-	39,39,39,39	0
55	MG	AA	3107	1/1	0.43	-	79,79,79,79	0
55	MG	AA	3081	1/1	0.43	-	56,56,56,56	0
55	MG	DC	106	1/1	0.55	-	91,91,91,91	0
55	MG	AA	3351	1/1	0.40	-	53,53,53,53	0
55	MG	DA	1715	1/1	0.30	-	89,89,89,89	0
55	MG	BA	1635	1/1	0.25	-	96,96,96,96	0
56	OHX	AA	3360	7/7	0.17	-	58,67,70,97	1
55	MG	CA	3133	1/1	0.36	-	48,48,48,48	0
56	OHX	C6	101	7/7	0.11	-	132,145,157,184	1
56	OHX	AA	3550	7/7	0.17	-	111,121,131,187	1
56	OHX	AA	3338	7/7	0.13	-	82,93,108,126	1
55	MG	CA	3221	1/1	0.47	-	69,69,69,69	0
56	OHX	DA	1810	7/7	0.11	-	134,135,143,197	1
55	MG	AA	3214	1/1	0.34	-	46,46,46,46	0
56	OHX	AA	3442	7/7	0.17	-	70,87,119,140	0
55	MG	CA	3031	1/1	0.10	-	53,53,53,53	0
55	MG	BA	1653	1/1	0.34	-	63,63,63,63	0
55	MG	AA	3070	1/1	0.20	-	52,52,52,52	0
55	MG	CA	3119	1/1	0.28	-	61,61,61,61	0
55	MG	AA	3150	1/1	0.45	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	OHX	AA	3528	7/7	0.14	-	112,118,137,160	2
55	MG	CA	3110	1/1	0.38	-	85,85,85,85	0
55	MG	CA	3228	1/1	0.12	-	65,65,65,65	0
56	OHX	AA	3322	7/7	0.12	-	89,98,107,146	1
56	OHX	CA	3490	7/7	0.12	-	102,105,118,156	1
56	OHX	CA	3470	7/7	0.14	-	113,126,137,181	1
55	MG	BA	1744	1/1	0.14	-	90,90,90,90	0
56	OHX	AA	3560	7/7	0.15	-	102,104,127,184	1
55	MG	DA	1624	1/1	0.10	-	73,73,73,73	0
55	MG	DA	1700	1/1	0.48	-	70,70,70,70	0
56	OHX	DA	1803	7/7	0.09	-	135,141,144,207	1
55	MG	DA	1704	1/1	0.42	-	73,73,73,73	0
55	MG	AA	3159	1/1	0.29	-	65,65,65,65	0
56	OHX	CA	3233	7/7	0.15	-	74,85,95,121	0
56	OHX	DA	1769	7/7	0.11	-	133,140,147,188	1
56	OHX	BA	1766	7/7	0.16	-	89,96,106,129	1
55	MG	A1	201	1/1	0.30	-	71,71,71,71	0
55	MG	CA	3027	1/1	0.40	-	81,81,81,81	0
56	OHX	AA	3471	7/7	0.16	-	98,107,114,163	1
55	MG	AA	3113	1/1	0.39	-	32,32,32,32	0
55	MG	DA	1661	1/1	0.42	-	76,76,76,76	0
55	MG	AA	3111	1/1	0.36	-	35,35,35,35	0
56	OHX	DA	1745	7/7	0.13	-	115,123,143,223	0
55	MG	AA	3413	1/1	0.31	-	57,57,57,57	0
56	OHX	AA	3516	7/7	0.13	-	101,109,121,183	1
56	OHX	AA	3450	7/7	0.18	-	65,94,112,113	3
56	OHX	AA	3312	7/7	0.17	-	64,87,123,173	1
55	MG	AB	201	1/1	0.41	-	73,73,73,73	0
56	OHX	AA	3461	7/7	0.17	-	60,78,98,143	1
56	OHX	CA	3278	7/7	0.15	-	81,96,114,120	0
56	OHX	AA	3496	7/7	0.15	-	117,124,142,215	0
56	OHX	DC	108	7/7	0.10	-	120,132,142,180	1
56	OHX	CA	3390	7/7	0.10	-	117,128,152,209	1
55	MG	AA	3353	1/1	0.24	-	39,39,39,39	0
56	OHX	CB	216	7/7	0.13	-	117,132,146,206	1
55	MG	CA	3069	1/1	0.26	-	69,69,69,69	0
56	OHX	CA	3375	7/7	0.14	-	103,118,131,145	1
55	MG	AA	3080	1/1	0.42	-	55,55,55,55	0
55	MG	AA	3286	1/1	0.54	-	68,68,68,68	0
55	MG	CA	3161	1/1	0.27	-	71,71,71,71	0
55	MG	BB	105	1/1	0.51	-	63,63,63,63	0
56	OHX	DA	1744	7/7	0.13	-	103,108,120,148	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	AA	3534	7/7	0.13	-	136,141,145,222	1
55	MG	DA	1607	1/1	0.36	-	82,82,82,82	0
56	OHX	AA	3294	7/7	0.12	-	94,100,117,120	0
55	MG	AA	3045	1/1	0.43	-	65,65,65,65	0
55	MG	CA	3173	1/1	0.31	-	53,53,53,53	0
56	OHX	A1	202	7/7	0.16	-	85,95,114,146	1
55	MG	AA	3083	1/1	0.34	-	88,88,88,88	0
55	MG	AA	3143	1/1	0.42	-	46,46,46,46	0
56	OHX	BA	1681	7/7	0.11	-	153,163,173,229	1
56	OHX	AA	3331	7/7	0.27	-	72,87,130,163	3
55	MG	CA	3171	1/1	0.34	-	82,82,82,82	0
56	OHX	CA	3398	7/7	0.10	-	129,132,142,192	1
56	OHX	CA	3246	7/7	0.16	-	113,116,120,151	1
55	MG	AA	3066	1/1	0.39	-	83,83,83,83	0
56	OHX	DA	1749	7/7	0.15	-	91,120,126,173	1
56	OHX	DA	1801	7/7	0.12	-	141,143,154,216	1
56	OHX	AA	3325	7/7	0.11	-	91,103,115,154	1
56	OHX	AA	3405	7/7	0.11	-	103,111,138,161	1
55	MG	CA	3475	1/1	0.21	-	55,55,55,55	0
56	OHX	AA	3336	7/7	0.11	-	146,153,168,218	0
56	OHX	AA	3311	7/7	0.15	-	97,106,117,155	1
55	MG	CA	3444	1/1	0.26	-	52,52,52,52	0
56	OHX	AA	3432	7/7	0.15	-	72,98,103,107	0
56	OHX	CA	3285	7/7	0.12	-	94,107,126,147	1
56	OHX	CA	3254	7/7	0.08	-	167,174,181,211	0
55	MG	AA	3348	1/1	0.43	-	46,46,46,46	0
55	MG	AA	3100	1/1	0.38	-	108,108,108,108	0
56	OHX	BA	1764	7/7	0.17	-	88,94,120,157	0
56	OHX	CA	3250	7/7	0.18	-	106,109,126,164	1
55	MG	CA	3200	1/1	0.37	-	56,56,56,56	0
55	MG	CA	3067	1/1	0.29	-	49,49,49,49	0
56	OHX	AA	3319	7/7	0.15	-	87,95,122,151	1
55	MG	AA	3040	1/1	0.48	-	47,47,47,47	0
55	MG	AA	3085	1/1	0.12	-	58,58,58,58	0
55	MG	BA	1652	1/1	0.34	-	63,63,63,63	0
55	MG	BA	1740	1/1	0.45	-	61,61,61,61	0
55	MG	CA	3030	1/1	0.37	-	89,89,89,89	0
56	OHX	CA	3413	7/7	0.14	-	121,130,144,215	1
56	OHX	CA	3486	7/7	0.16	-	87,109,129,181	2
55	MG	CA	3230	1/1	0.50	-	79,79,79,79	0
55	MG	CA	3147	1/1	0.35	-	51,51,51,51	0
55	MG	CA	3263	1/1	0.29	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	DA	1812	7/7	0.14	-	149,158,168,252	1
55	MG	DA	1616	1/1	0.40	-	88,88,88,88	0
56	OHX	DA	1787	7/7	0.13	-	95,113,121,162	2
55	MG	AA	3224	1/1	0.55	-	68,68,68,68	0
56	OHX	CA	3311	7/7	0.16	-	79,95,105,127	1
56	OHX	AA	3443	7/7	0.15	-	69,76,84,127	1
56	OHX	DA	1732	7/7	0.17	-	134,143,157,195	0
56	OHX	CA	3401	7/7	0.09	-	136,149,158,185	1
56	OHX	DA	1775	7/7	0.11	-	133,145,148,215	1
56	OHX	CA	3270	7/7	0.15	-	73,87,105,117	0
55	MG	BQ	101	1/1	0.58	-	96,96,96,96	0
56	OHX	DG	302	7/7	0.10	-	133,142,147,197	1
55	MG	CA	3188	1/1	0.46	-	60,60,60,60	0
56	OHX	CA	3290	7/7	0.13	-	94,101,123,130	0
56	OHX	DA	1763	7/7	0.11	-	154,159,173,250	0
55	MG	AA	3145	1/1	0.45	-	56,56,56,56	0
56	OHX	CA	3360	7/7	0.10	-	116,124,135,193	1
56	OHX	CA	3273	7/7	0.20	-	58,69,86,110	0
55	MG	CA	3080	1/1	0.09	-	57,57,57,57	0
55	MG	CA	3009	1/1	0.33	-	39,39,39,39	0
55	MG	AA	3378	1/1	0.34	-	47,47,47,47	0
55	MG	BA	1646	1/1	0.43	-	95,95,95,95	0
55	MG	AA	3166	1/1	0.48	-	66,66,66,66	0
55	MG	CA	3181	1/1	0.37	-	62,62,62,62	0
55	MG	AA	3059	1/1	0.59	-	85,85,85,85	0
55	MG	AA	3376	1/1	0.34	-	33,33,33,33	0
56	OHX	CA	3288	7/7	0.15	-	87,95,104,133	0
55	MG	CB	204	1/1	0.40	-	73,73,73,73	0
55	MG	CA	3024	1/1	0.18	-	48,48,48,48	0
55	MG	BC	102	1/1	0.21	-	68,68,68,68	0
55	MG	AA	3219	1/1	0.35	-	48,48,48,48	0
56	OHX	CA	3319	7/7	0.15	-	87,97,106,138	1
55	MG	AA	3038	1/1	0.25	-	46,46,46,46	0
55	MG	AA	3146	1/1	0.34	-	41,41,41,41	0
56	OHX	CA	3392	7/7	0.11	-	126,132,142,192	1
56	OHX	DA	1747	7/7	0.14	-	109,122,155,200	1
56	OHX	AA	3460	7/7	0.14	-	87,98,107,140	0
56	OHX	CA	3395	7/7	0.16	-	106,111,125,156	1
55	MG	DA	1656	1/1	0.35	-	68,68,68,68	0
55	MG	CA	3441	1/1	0.36	-	99,99,99,99	0
55	MG	CA	3196	1/1	0.54	-	92,92,92,92	0
55	MG	CA	3455	1/1	0.41	-	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	DC	109	7/7	0.14	-	88,92,104,159	3
55	MG	AA	3087	1/1	0.54	-	83,83,83,83	0
56	OHX	AA	3531	7/7	0.12	-	119,124,135,185	1
55	MG	CA	3152	1/1	0.37	-	54,54,54,54	0
55	MG	AA	3126	1/1	0.35	-	85,85,85,85	0
56	OHX	DA	1793	7/7	0.09	-	146,150,161,207	1
56	OHX	AA	3441	7/7	0.17	-	84,93,115,140	0
55	MG	BA	1629	1/1	0.28	-	112,112,112,112	0
55	MG	AA	3375	1/1	0.38	-	31,31,31,31	0
55	MG	AA	3201	1/1	0.33	-	45,45,45,45	0
56	OHX	BA	1802	7/7	0.14	-	107,121,133,185	1
55	MG	AA	3177	1/1	0.43	-	37,37,37,37	0
55	MG	BA	1616	1/1	0.28	-	61,61,61,61	0
55	MG	CA	3021	1/1	0.18	-	60,60,60,60	0
55	MG	BA	1754	1/1	0.40	-	61,61,61,61	0
55	MG	DA	1647	1/1	0.44	-	90,90,90,90	0
55	MG	BA	1745	1/1	0.55	-	83,83,83,83	0
55	MG	CA	3211	1/1	0.17	-	116,116,116,116	0
55	MG	DA	1614	1/1	0.22	-	91,91,91,91	0
56	OHX	DA	1723	7/7	0.15	-	107,111,116,151	0
56	OHX	AA	3313	7/7	0.16	-	96,112,122,174	0
55	MG	CA	3032	1/1	0.30	-	70,70,70,70	0
55	MG	AA	3258	1/1	0.46	-	65,65,65,65	0
55	MG	CA	3002	1/1	0.33	-	50,50,50,50	0
55	MG	AA	3412	1/1	0.42	-	39,39,39,39	0
55	MG	BA	1700	1/1	0.41	-	61,61,61,61	0
55	MG	CA	3012	1/1	0.26	-	53,53,53,53	0
55	MG	BA	1633	1/1	0.15	-	59,59,59,59	0
55	MG	AA	3035	1/1	0.57	-	64,64,64,64	0
56	OHX	BA	1682	7/7	0.11	-	119,124,130,186	1
56	OHX	AA	3453	7/7	0.12	-	95,106,114,148	0
56	OHX	AA	3326	7/7	0.15	-	83,94,100,118	1
56	OHX	CB	213	7/7	0.11	-	131,144,166,188	1
55	MG	AA	3283	1/1	0.33	-	55,55,55,55	0
56	OHX	CA	3435	7/7	0.17	-	105,108,131,192	1
55	MG	DA	1612	1/1	0.43	-	86,86,86,86	0
55	MG	DA	1627	1/1	0.53	-	77,77,77,77	0
55	MG	AA	3054	1/1	0.34	-	49,49,49,49	0
55	MG	BA	1711	1/1	0.51	-	94,94,94,94	0
55	MG	AA	3121	1/1	0.46	-	53,53,53,53	0
55	MG	DA	1691	1/1	0.39	-	54,54,54,54	0
56	OHX	CA	3280	7/7	0.18	-	82,87,100,129	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3018	1/1	0.40	-	43,43,43,43	0
56	OHX	BA	1772	7/7	0.14	-	106,118,144,175	0
56	OHX	BA	1664	7/7	0.14	-	108,126,142,197	1
55	MG	AA	3061	1/1	0.41	-	49,49,49,49	0
56	OHX	BA	1813	7/7	0.13	-	128,130,137,174	1
56	OHX	CA	3377	7/7	0.14	-	90,95,111,135	2
55	MG	AA	3095	1/1	0.43	-	89,89,89,89	0
56	OHX	CA	3416	7/7	0.17	-	114,117,128,182	1
55	MG	CA	3131	1/1	0.33	-	65,65,65,65	0
56	OHX	AA	3492	7/7	0.17	-	79,89,95,107	3
55	MG	BA	1647	1/1	0.21	-	112,112,112,112	0
56	OHX	CA	3354	7/7	0.13	-	78,88,98,105	1
55	MG	AA	3053	1/1	0.51	-	60,60,60,60	0
55	MG	BA	1703	1/1	0.51	-	108,108,108,108	0
55	MG	AA	3231	1/1	0.50	-	66,66,66,66	0
55	MG	AA	3216	1/1	0.44	-	71,71,71,71	0
56	OHX	AF	303	7/7	0.20	-	45,52,58,77	0
56	OHX	CA	3241	7/7	0.13	-	90,96,101,122	1
55	MG	AA	3151	1/1	0.36	-	62,62,62,62	0
55	MG	AA	3256	1/1	0.55	-	53,53,53,53	0
55	MG	CA	3066	1/1	0.38	-	56,56,56,56	0
56	OHX	AA	3546	7/7	0.17	-	98,103,119,179	1
55	MG	DA	1609	1/1	0.38	-	91,91,91,91	0
55	MG	AA	3239	1/1	0.27	-	44,44,44,44	0
56	OHX	CA	3425	7/7	0.12	-	101,110,125,187	1
55	MG	DA	1602	1/1	0.41	-	68,68,68,68	0
56	OHX	CA	3415	7/7	0.13	-	134,135,143,187	1
56	OHX	AA	3359	7/7	0.17	-	61,75,93,113	0
56	OHX	CA	3370	7/7	0.13	-	116,120,142,180	1
55	MG	DC	101	1/1	0.27	-	85,85,85,85	0
55	MG	AA	3060	1/1	0.27	-	70,70,70,70	0
56	OHX	BB	107	7/7	0.23	-	71,92,103,147	3
56	OHX	DA	1759	7/7	0.11	-	120,137,147,190	0
56	OHX	BA	1687	7/7	0.16	-	94,99,108,140	1
55	MG	AA	3029	1/1	0.28	-	38,38,38,38	0
56	OHX	DA	1797	7/7	0.06	-	149,152,159,218	1
56	OHX	BA	1770	7/7	0.15	-	102,113,126,149	1
55	MG	AA	3243	1/1	0.40	-	51,51,51,51	0
56	OHX	AA	3459	7/7	0.14	-	71,92,105,129	1
56	OHX	CA	3468	7/7	0.11	-	115,126,133,180	1
55	MG	AA	3217	1/1	0.44	-	60,60,60,60	0
55	MG	CA	3137	1/1	0.47	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	CA	3353	7/7	0.15	-	81,96,110,140	1
55	MG	AA	3042	1/1	0.28	-	43,43,43,43	0
55	MG	BA	1623	1/1	0.31	-	67,67,67,67	0
57	ZN	BQ	102	1/1	0.10	-	130,130,130,130	0
55	MG	AA	3389	1/1	0.39	-	44,44,44,44	0
56	OHX	CA	3287	7/7	0.17	-	69,74,104,109	3
56	OHX	BA	1812	7/7	0.13	-	151,164,170,231	1
56	OHX	AA	3438	7/7	0.17	-	51,64,72,96	2
56	OHX	AA	3484	7/7	0.19	-	76,100,111,147	2
55	MG	DA	1660	1/1	0.51	-	88,88,88,88	0
56	OHX	DA	1719	7/7	0.15	-	79,99,112,124	0
56	OHX	CA	3467	7/7	0.12	-	131,146,152,199	1
56	OHX	CA	3357	7/7	0.15	-	86,98,106,151	1
56	OHX	CA	3297	7/7	0.13	-	84,94,129,142	1
56	OHX	DA	1731	7/7	0.10	-	129,139,145,172	1
55	MG	CA	3103	1/1	0.27	-	70,70,70,70	0
55	MG	DA	1674	1/1	0.32	-	99,99,99,99	0
55	MG	DA	1712	1/1	0.32	-	98,98,98,98	0
56	OHX	BA	1797	7/7	0.21	-	71,104,132,136	3
55	MG	CA	3176	1/1	0.33	-	67,67,67,67	0
55	MG	AA	3246	1/1	0.39	-	36,36,36,36	0
55	MG	AA	3236	1/1	0.41	-	40,40,40,40	0
55	MG	CA	3231	1/1	0.34	-	89,89,89,89	0
56	OHX	CA	3272	7/7	0.18	-	54,70,84,85	1
56	OHX	AA	3303	7/7	0.12	-	93,102,117,145	1
55	MG	DA	1603	1/1	0.42	-	71,71,71,71	0
56	OHX	BA	1691	7/7	0.10	-	148,150,156,215	1
55	MG	DA	1641	1/1	0.45	-	130,130,130,130	0
55	MG	BA	1722	1/1	0.52	-	91,91,91,91	0
55	MG	AA	3163	1/1	0.39	-	61,61,61,61	0
56	OHX	BA	1674	7/7	0.17	-	117,122,137,199	1
56	OHX	BA	1807	7/7	0.09	-	135,141,150,224	0
55	MG	CA	3204	1/1	0.41	-	73,73,73,73	0
56	OHX	AA	3364	7/7	0.15	-	92,103,108,119	1
56	OHX	AA	3406	7/7	0.23	-	84,92,109,162	1
55	MG	AF	302	1/1	0.37	-	81,81,81,81	0
55	MG	CA	3130	1/1	0.44	-	58,58,58,58	0
56	OHX	BA	1787	7/7	0.14	-	107,117,138,149	2
56	OHX	AA	3337	7/7	0.14	-	97,106,127,177	1
56	OHX	C3	101	7/7	0.16	-	119,129,151,179	2
55	MG	CA	3261	1/1	0.40	-	48,48,48,48	0
55	MG	DA	1682	1/1	0.58	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	BA	1689	7/7	0.13	-	113,130,139,190	1
56	OHX	BA	1692	7/7	0.13	-	126,131,140,209	1
56	OHX	CA	3295	7/7	0.14	-	102,105,117,137	1
56	OHX	AA	3500	7/7	0.14	-	94,114,122,159	1
56	OHX	CA	3275	7/7	0.14	-	56,80,112,114	1
55	MG	BA	1639	1/1	0.14	-	102,102,102,102	0
55	MG	AA	3176	1/1	0.22	-	60,60,60,60	0
55	MG	AA	3062	1/1	0.39	-	73,73,73,73	0
55	MG	AA	3127	1/1	0.40	-	57,57,57,57	0
55	MG	BA	1631	1/1	0.33	-	78,78,78,78	0
56	OHX	CA	3387	7/7	0.16	-	111,127,150,170	2
56	OHX	CO	201	7/7	0.13	-	104,109,121,141	1
55	MG	AA	3188	1/1	0.29	-	40,40,40,40	0
55	MG	AB	203	1/1	0.48	-	71,71,71,71	0
56	OHX	AA	3310	7/7	0.12	-	94,104,125,156	0
55	MG	AA	3078	1/1	0.33	-	59,59,59,59	0
55	MG	CA	3160	1/1	0.42	-	49,49,49,49	0
55	MG	DA	1679	1/1	0.30	-	69,69,69,69	0
55	MG	BA	1650	1/1	0.56	-	72,72,72,72	0
55	MG	CA	3079	1/1	0.28	-	73,73,73,73	0
56	OHX	CA	3239	7/7	0.15	-	66,92,107,113	1
55	MG	DA	1606	1/1	0.20	-	84,84,84,84	0
56	OHX	CA	3325	7/7	0.14	-	108,122,148,156	1
55	MG	AA	3194	1/1	0.11	-	26,26,26,26	0
56	OHX	AA	3566	7/7	0.18	-	92,97,126,175	2
55	MG	DA	1635	1/1	0.43	-	96,96,96,96	0
56	OHX	AA	3447	7/7	0.15	-	91,102,120,163	1
55	MG	AA	3073	1/1	0.36	-	69,69,69,69	0
56	OHX	AA	3317	7/7	0.17	-	79,88,118,156	1
55	MG	AA	3182	1/1	0.56	-	45,45,45,45	0
56	OHX	BA	1805	7/7	0.17	-	90,105,122,143	3
56	OHX	AA	3371	7/7	0.15	-	93,107,117,177	1
55	MG	CA	3218	1/1	0.29	-	83,83,83,83	0
56	OHX	DA	1798	7/7	0.09	-	128,133,140,212	1
56	OHX	AA	3511	7/7	0.12	-	133,145,154,207	0
55	MG	AA	3030	1/1	0.34	-	44,44,44,44	0
55	MG	DA	1694	1/1	0.40	-	104,104,104,104	0
55	MG	DA	1669	1/1	0.38	-	64,64,64,64	0
56	OHX	CA	3238	7/7	0.15	-	80,102,103,125	1
55	MG	AA	3009	1/1	0.46	-	89,89,89,89	0
56	OHX	DA	1729	7/7	0.14	-	104,108,118,152	1
55	MG	AA	3086	1/1	0.41	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3278	1/1	0.43	-	35,35,35,35	0
56	OHX	BA	1771	7/7	0.19	-	77,100,122,150	1
55	MG	DA	1670	1/1	0.43	-	64,64,64,64	0
55	MG	CE	301	1/1	0.36	-	56,56,56,56	0
55	MG	DA	1685	1/1	0.18	-	59,59,59,59	0
56	OHX	BA	1814	7/7	0.10	-	101,109,125,174	1
56	OHX	CA	3406	7/7	0.08	-	151,161,169,211	1
55	MG	CA	3003	1/1	0.36	-	51,51,51,51	0
56	OHX	DA	1721	7/7	0.14	-	94,108,116,135	0
55	MG	AA	3264	1/1	0.42	-	76,76,76,76	0
55	MG	CA	3474	1/1	0.14	-	70,70,70,70	0
55	MG	CA	3063	1/1	0.26	-	70,70,70,70	0
55	MG	CA	3458	1/1	0.24	-	82,82,82,82	0
55	MG	CA	3154	1/1	0.32	-	46,46,46,46	0
56	OHX	CA	3245	7/7	0.12	-	99,120,129,189	1
56	OHX	DA	1741	7/7	0.14	-	97,116,128,170	1
56	OHX	BA	1808	7/7	0.16	-	84,90,96,110	2
56	OHX	AA	3418	7/7	0.20	-	39,61,82,95	0
56	OHX	AA	3545	7/7	0.21	-	90,96,105,167	2
55	MG	CA	3056	1/1	0.49	-	79,79,79,79	0
55	MG	AA	3167	1/1	0.54	-	53,53,53,53	0
55	MG	AA	3092	1/1	0.15	-	73,73,73,73	0
56	OHX	BA	1666	7/7	0.17	-	117,122,134,158	2
55	MG	AA	3117	1/1	0.34	-	48,48,48,48	0
55	MG	CA	3070	1/1	0.24	-	44,44,44,44	0
55	MG	BB	103	1/1	0.36	-	91,91,91,91	0
55	MG	CA	3453	1/1	0.30	-	58,58,58,58	0
55	MG	AA	3386	1/1	0.25	-	42,42,42,42	0
56	OHX	BA	1776	7/7	0.12	-	102,114,119,153	1
55	MG	AA	3192	1/1	0.38	-	48,48,48,48	0
55	MG	AA	3144	1/1	0.54	-	71,71,71,71	0
55	MG	AA	3128	1/1	0.40	-	54,54,54,54	0
55	MG	AA	3254	1/1	0.35	-	42,42,42,42	0
55	MG	AA	3136	1/1	0.28	-	57,57,57,57	0
56	OHX	AA	3373	7/7	0.16	-	75,103,110,155	1
56	OHX	AA	3324	7/7	0.15	-	92,110,118,165	1
55	MG	AA	3357	1/1	0.39	-	73,73,73,73	0
55	MG	CA	3145	1/1	0.44	-	74,74,74,74	0
55	MG	AA	3048	1/1	0.61	-	94,94,94,94	0
56	OHX	AA	3535	7/7	0.14	-	104,112,123,191	1
55	MG	AA	3281	1/1	0.54	-	70,70,70,70	0
55	MG	AA	3024	1/1	0.39	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	DA	1738	7/7	0.09	-	115,122,137,171	1
56	OHX	CA	3462	7/7	0.16	-	71,82,94,110	1
55	MG	DC	103	1/1	0.31	-	96,96,96,96	0
55	MG	CA	3097	1/1	0.37	-	67,67,67,67	0
55	MG	DA	1618	1/1	0.28	-	105,105,105,105	0
56	OHX	AA	3401	7/7	0.12	-	93,112,116,173	1
56	OHX	AA	3318	7/7	0.15	-	92,102,113,133	1
55	MG	CA	3122	1/1	0.32	-	40,40,40,40	0
56	OHX	DA	1792	7/7	0.10	-	110,118,129,172	1
55	MG	AA	3039	1/1	0.34	-	40,40,40,40	0
56	OHX	AA	3138	7/7	0.14	-	88,92,127,173	1
55	MG	AA	3191	1/1	0.31	-	45,45,45,45	0
55	MG	BA	1607	1/1	0.38	-	93,93,93,93	0
55	MG	CA	3199	1/1	0.37	-	62,62,62,62	0
55	MG	B1	101	1/1	0.49	-	26,26,26,26	0
55	MG	CA	3157	1/1	0.30	-	76,76,76,76	0
55	MG	AA	3377	1/1	0.32	-	51,51,51,51	0
55	MG	AA	3069	1/1	0.44	-	62,62,62,62	0
55	MG	BA	1702	1/1	0.30	-	62,62,62,62	0
56	OHX	CB	217	7/7	0.22	-	128,135,146,182	1
55	MG	CA	3219	1/1	0.53	-	79,79,79,79	0
57	ZN	DQ	101	1/1	0.14	-	123,123,123,123	0
56	OHX	BA	1793	7/7	0.09	-	95,105,117,163	1
55	MG	AA	3242	1/1	0.38	-	37,37,37,37	0
56	OHX	CA	3298	7/7	0.14	-	90,98,134,148	0
55	MG	AA	3345	1/1	0.42	-	47,47,47,47	0
56	OHX	DA	1808	7/7	0.14	-	119,124,131,178	1
56	OHX	CA	3347	7/7	0.13	-	86,102,110,148	1
56	OHX	AA	3440	7/7	0.17	-	59,88,102,124	0
56	OHX	AA	3297	7/7	0.15	-	87,98,102,106	1
55	MG	AA	3397	1/1	0.21	-	80,80,80,80	0
55	MG	CA	3018	1/1	0.33	-	55,55,55,55	0
56	OHX	BA	1806	7/7	0.19	-	97,127,142,180	2
56	OHX	AA	3420	7/7	0.21	-	63,69,102,115	0
55	MG	AA	3253	1/1	0.40	-	53,53,53,53	0
55	MG	CA	3112	1/1	0.37	-	41,41,41,41	0
55	MG	AA	3248	1/1	0.39	-	86,86,86,86	0
55	MG	AA	3181	1/1	0.46	-	61,61,61,61	0
55	MG	AA	3131	1/1	0.34	-	94,94,94,94	0
56	OHX	AA	3428	7/7	0.19	-	67,79,86,113	0
56	OHX	DD	101	7/7	0.14	-	155,165,187,227	0
55	MG	CA	3104	1/1	0.42	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	CA	3428	7/7	0.13	-	123,134,138,182	1
56	OHX	AA	3154	7/7	0.17	-	76,89,110,133	1
56	OHX	BA	1782	7/7	0.14	-	133,144,159,198	0
56	OHX	CA	3408	7/7	0.09	-	136,139,143,209	1
55	MG	CA	3189	1/1	0.42	-	67,67,67,67	0
56	OHX	CA	3320	7/7	0.13	-	140,142,153,174	0
56	OHX	AB	213	7/7	0.18	-	85,93,130,132	3
55	MG	BA	1612	1/1	0.42	-	81,81,81,81	0
56	OHX	CA	3237	7/7	0.15	-	109,109,122,166	0
55	MG	CA	3187	1/1	0.42	-	86,86,86,86	0
56	OHX	BD	103	7/7	0.13	-	86,95,103,174	1
56	OHX	CA	3284	7/7	0.13	-	136,147,155,216	1
55	MG	CA	3180	1/1	0.34	-	75,75,75,75	0
56	OHX	AA	3536	7/7	0.24	-	116,124,157,192	1
56	OHX	CA	3269	7/7	0.17	-	98,100,123,153	2
55	MG	DC	102	1/1	0.38	-	69,69,69,69	0
55	MG	AA	3408	1/1	0.45	-	47,47,47,47	0
55	MG	CA	3460	1/1	0.26	-	72,72,72,72	0
55	MG	AA	3391	1/1	0.30	-	59,59,59,59	0
56	OHX	BA	1693	7/7	0.14	-	112,112,134,152	1
56	OHX	BA	1804	7/7	0.17	-	134,142,150,227	1
55	MG	BN	201	1/1	0.13	-	80,80,80,80	0
56	OHX	BA	1663	7/7	0.09	-	132,137,143,190	1
56	OHX	BA	1672	7/7	0.11	-	156,159,170,224	1
55	MG	CA	3226	1/1	0.45	-	65,65,65,65	0
55	MG	BC	105	1/1	0.48	-	87,87,87,87	0
56	OHX	BA	1668	7/7	0.10	-	116,121,137,182	1
55	MG	CA	3216	1/1	0.44	-	91,91,91,91	0
55	MG	CA	3036	1/1	0.26	-	87,87,87,87	0
56	OHX	DA	1757	7/7	0.12	-	123,127,134,157	1
56	OHX	CA	3256	7/7	0.15	-	88,101,112,126	1
55	MG	CA	3127	1/1	0.29	-	53,53,53,53	0
55	MG	CA	3043	1/1	0.13	-	82,82,82,82	0
56	OHX	AA	3462	7/7	0.14	-	75,85,103,106	1
55	MG	CA	3129	1/1	0.60	-	81,81,81,81	0
56	OHX	CA	3412	7/7	0.14	-	99,116,129,164	2
55	MG	AA	3383	1/1	0.32	-	46,46,46,46	0
56	OHX	AA	3504	7/7	0.12	-	112,118,129,179	1
55	MG	BA	1734	1/1	0.42	-	70,70,70,70	0
55	MG	AA	3139	1/1	0.40	-	48,48,48,48	0
56	OHX	BA	1791	7/7	0.15	-	82,106,122,150	2
55	MG	DA	1633	1/1	0.53	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	CA	3247	7/7	0.17	-	95,104,117,152	1
56	OHX	DA	1805	7/7	0.09	-	155,158,165,245	1
56	OHX	CA	3391	7/7	0.10	-	140,144,157,182	1
56	OHX	CB	215	7/7	0.13	-	108,133,144,220	1
55	MG	AA	3411	1/1	0.33	-	63,63,63,63	0
56	OHX	AE	304	7/7	0.15	-	74,87,107,110	1
56	OHX	DA	1742	7/7	0.10	-	117,127,141,176	1
56	OHX	CA	3461	7/7	0.19	-	38,55,94,109	0
56	OHX	DA	1777	7/7	0.09	-	150,152,155,232	1
55	MG	AA	3156	1/1	0.47	-	45,45,45,45	0
55	MG	CA	3156	1/1	0.36	-	84,84,84,84	0
56	OHX	BA	1768	7/7	0.12	-	128,139,147,175	0
56	OHX	AA	3488	7/7	0.18	-	86,101,105,150	1
55	MG	DA	1668	1/1	0.25	-	86,86,86,86	0
55	MG	CA	3088	1/1	0.40	-	86,86,86,86	0
55	MG	CB	206	1/1	0.34	-	83,83,83,83	0
55	MG	BA	1741	1/1	0.50	-	73,73,73,73	0
56	OHX	CA	3307	7/7	0.12	-	92,104,131,164	0
55	MG	CA	3184	1/1	0.41	-	60,60,60,60	0
55	MG	CA	3448	1/1	0.15	-	63,63,63,63	0
55	MG	DN	201	1/1	0.13	-	80,80,80,80	0
55	MG	CA	3038	1/1	0.19	-	74,74,74,74	0
56	OHX	BA	1783	7/7	0.19	-	77,87,125,141	2
55	MG	DA	1665	1/1	0.49	-	70,70,70,70	0
55	MG	AA	3122	1/1	0.46	-	62,62,62,62	0
56	OHX	DA	1770	7/7	0.11	-	136,142,156,217	1
55	MG	DA	1663	1/1	0.28	-	66,66,66,66	0
55	MG	DB	101	1/1	0.43	-	78,78,78,78	0
55	MG	BA	1710	1/1	0.55	-	97,97,97,97	0
55	MG	AA	3019	1/1	0.50	-	72,72,72,72	0
55	MG	BA	1624	1/1	0.27	-	70,70,70,70	0
55	MG	BA	1752	1/1	0.47	-	53,53,53,53	0
55	MG	AA	3123	1/1	0.26	-	72,72,72,72	0
56	OHX	DA	1765	7/7	0.21	-	117,133,141,227	1
55	MG	DA	1648	1/1	0.11	-	91,91,91,91	0
56	OHX	BA	1796	7/7	0.12	-	143,156,164,225	0
55	MG	BA	1750	1/1	0.43	-	72,72,72,72	0
55	MG	CA	3076	1/1	0.40	-	64,64,64,64	0
55	MG	DC	104	1/1	0.41	-	77,77,77,77	0
56	OHX	BA	1763	7/7	0.15	-	94,115,123,136	0
56	OHX	AA	3445	7/7	0.14	-	75,87,109,120	1
55	MG	DA	1610	1/1	0.25	-	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	CA	3314	7/7	0.14	-	84,93,97,114	1
56	OHX	CA	3484	7/7	0.12	-	104,113,129,146	1
56	OHX	CA	3292	7/7	0.19	-	69,105,113,146	0
55	MG	AA	3390	1/1	0.23	-	46,46,46,46	0
56	OHX	AA	3483	7/7	0.14	-	124,141,146,196	1
55	MG	AA	3021	1/1	0.52	-	80,80,80,80	0
55	MG	AA	3280	1/1	0.40	-	77,77,77,77	0
56	OHX	AA	3301	7/7	0.14	-	88,89,93,110	1
56	OHX	BC	106	7/7	0.14	-	110,133,144,147	1
55	MG	CA	3006	1/1	0.19	-	47,47,47,47	0
55	MG	CA	3159	1/1	0.38	-	75,75,75,75	0
56	OHX	DA	1743	7/7	0.14	-	109,113,118,148	1
55	MG	BA	1716	1/1	0.35	-	55,55,55,55	0
56	OHX	AA	3562	7/7	0.16	-	98,105,127,189	1
56	OHX	AA	3466	7/7	0.15	-	89,94,108,128	1
55	MG	AA	3120	1/1	0.28	-	71,71,71,71	0
55	MG	AA	3012	1/1	0.33	-	46,46,46,46	0
56	OHX	CA	3362	7/7	0.08	-	129,136,141,186	1
55	MG	AA	3155	1/1	0.14	-	85,85,85,85	0
56	OHX	CA	3344	7/7	0.16	-	96,110,117,162	1
55	MG	AA	3097	1/1	0.23	-	59,59,59,59	0
55	MG	CA	3008	1/1	0.21	-	52,52,52,52	0
55	MG	CA	3477	1/1	0.44	-	60,60,60,60	0
56	OHX	AA	3533	7/7	0.15	-	98,103,114,150	2
55	MG	BA	1743	1/1	0.40	-	69,69,69,69	0
56	OHX	AA	3464	7/7	0.14	-	117,125,139,188	0
56	OHX	DA	1756	7/7	0.11	-	145,145,160,212	1
56	OHX	AA	3429	7/7	0.14	-	69,73,84,102	1
56	OHX	AA	3472	7/7	0.12	-	120,126,137,153	1
55	MG	AA	3285	1/1	0.50	-	80,80,80,80	0
55	MG	BA	1632	1/1	0.31	-	108,108,108,108	0
56	OHX	CB	219	7/7	0.10	-	145,151,161,232	1
55	MG	AA	3005	1/1	0.41	-	43,43,43,43	0
55	MG	AA	3247	1/1	0.34	-	81,81,81,81	0
56	OHX	AA	3288	7/7	0.18	-	76,85,101,127	1
56	OHX	AA	3482	7/7	0.12	-	105,118,127,177	1
56	OHX	AA	3467	7/7	0.13	-	100,105,117,133	1
56	OHX	AA	3335	7/7	0.12	-	94,101,113,136	1
55	MG	AA	3007	1/1	0.26	-	31,31,31,31	0
55	MG	BA	1720	1/1	0.52	-	58,58,58,58	0
56	OHX	AA	3515	7/7	0.13	-	100,121,139,211	1
56	OHX	AA	3479	7/7	0.16	-	106,122,142,174	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	AA	3330	7/7	0.13	-	102,112,122,166	1
55	MG	DA	1619	1/1	0.40	-	98,98,98,98	0
55	MG	CB	201	1/1	0.24	-	77,77,77,77	0
56	OHX	AO	205	7/7	0.18	-	83,89,107,180	1
56	OHX	CA	3339	7/7	0.12	-	100,105,127,171	1
56	OHX	CA	3437	7/7	0.13	-	98,105,117,166	2
55	MG	DA	1650	1/1	0.23	-	67,67,67,67	0
55	MG	CA	3061	1/1	0.26	-	64,64,64,64	0
55	MG	AA	3115	1/1	0.38	-	51,51,51,51	0
55	MG	AA	3141	1/1	0.55	-	44,44,44,44	0
56	OHX	AA	3454	7/7	0.17	-	68,93,112,112	1
56	OHX	A3	102	7/7	0.13	-	90,98,113,134	2
55	MG	BA	1638	1/1	0.33	-	57,57,57,57	0
55	MG	CA	3266	1/1	0.33	-	64,64,64,64	0
56	OHX	AA	3340	7/7	0.10	-	159,167,171,209	0
55	MG	CA	3198	1/1	0.32	-	118,118,118,118	0
56	OHX	BA	1662	7/7	0.12	-	105,117,141,193	1
55	MG	BA	1713	1/1	0.29	-	59,59,59,59	0
55	MG	BA	1618	1/1	0.40	-	63,63,63,63	0
56	OHX	DA	1789	7/7	0.06	-	176,179,184,242	1
55	MG	DA	1651	1/1	0.45	-	62,62,62,62	0
56	OHX	CA	3434	7/7	0.13	-	96,110,126,177	1
56	OHX	BA	1686	7/7	0.17	-	141,143,153,230	1
55	MG	AA	3225	1/1	0.29	-	63,63,63,63	0
56	OHX	BA	1684	7/7	0.11	-	109,118,126,149	1
55	MG	CA	3116	1/1	0.39	-	69,69,69,69	0
56	OHX	CA	3450	7/7	0.12	-	112,125,137,206	0
56	OHX	DA	1754	7/7	0.12	-	98,102,118,156	1
55	MG	AA	3125	1/1	0.39	-	92,92,92,92	0
56	OHX	DK	201	7/7	0.09	-	137,138,149,200	1
56	OHX	AA	3465	7/7	0.13	-	85,99,124,159	1
56	OHX	CA	3394	7/7	0.12	-	97,100,116,155	1
56	OHX	AA	3315	7/7	0.12	-	89,99,111,137	1
56	OHX	DA	1776	7/7	0.10	-	114,116,125,160	1
56	OHX	CA	3244	7/7	0.16	-	94,113,121,172	1
55	MG	CA	3057	1/1	0.39	-	95,95,95,95	0
56	OHX	CA	3379	7/7	0.12	-	134,137,155,207	1
55	MG	AA	3033	1/1	0.37	-	48,48,48,48	0
56	OHX	AA	3544	7/7	0.17	-	103,105,124,176	1
56	OHX	AA	3289	7/7	0.18	-	53,58,81,93	0
56	OHX	AB	215	7/7	0.18	-	105,114,120,153	1
55	MG	C0	201	1/1	0.18	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3090	1/1	0.33	-	55,55,55,55	0
56	OHX	AA	3455	7/7	0.16	-	56,75,100,119	2
55	MG	BA	1658	1/1	0.44	-	71,71,71,71	0
55	MG	DA	1703	1/1	0.48	-	73,73,73,73	0
55	MG	AA	3071	1/1	0.61	-	68,68,68,68	0
55	MG	DA	1649	1/1	0.29	-	87,87,87,87	0
56	OHX	AA	3316	7/7	0.14	-	80,95,97,136	0
55	MG	BA	1721	1/1	0.39	-	70,70,70,70	0
55	MG	DA	1717	1/1	0.26	-	100,100,100,100	0
55	MG	DB	102	1/1	0.24	-	102,102,102,102	0
56	OHX	CA	3369	7/7	0.13	-	97,113,121,158	1
55	MG	AA	3129	1/1	0.34	-	83,83,83,83	0
55	MG	BA	1619	1/1	0.27	-	50,50,50,50	0
56	OHX	CA	3312	7/7	0.14	-	85,101,114,134	1
55	MG	DA	1644	1/1	0.18	-	149,149,149,149	0
56	OHX	BB	106	7/7	0.12	-	164,167,173,198	1
55	MG	DA	1666	1/1	0.44	-	62,62,62,62	0
56	OHX	CA	3400	7/7	0.12	-	116,133,145,220	1
55	MG	CB	202	1/1	0.18	-	99,99,99,99	0
56	OHX	BA	1803	7/7	0.15	-	101,126,136,190	1
55	MG	AA	3203	1/1	0.33	-	50,50,50,50	0
56	OHX	CA	3371	7/7	0.15	-	67,90,123,162	1
56	OHX	AB	216	7/7	0.19	-	88,124,141,184	1
56	OHX	BA	1659	7/7	0.15	-	114,130,135,179	1
55	MG	CA	3471	1/1	0.34	-	57,57,57,57	0
55	MG	AA	3215	1/1	0.53	-	50,50,50,50	0
56	OHX	BA	1777	7/7	0.13	-	114,118,140,171	1
55	MG	AA	3130	1/1	0.33	-	75,75,75,75	0
55	MG	DA	1634	1/1	0.15	-	118,118,118,118	0
56	OHX	DA	1807	7/7	0.09	-	117,126,135,195	1
55	MG	CA	3111	1/1	0.41	-	30,30,30,30	0
55	MG	AA	3374	1/1	0.34	-	29,29,29,29	0
56	OHX	AA	3507	7/7	0.12	-	101,111,128,158	1
55	MG	CA	3479	1/1	0.48	-	64,64,64,64	0
55	MG	CA	3013	1/1	0.20	-	47,47,47,47	0
55	MG	CA	3034	1/1	0.40	-	91,91,91,91	0
55	MG	BA	1617	1/1	0.51	-	71,71,71,71	0
55	MG	CA	3214	1/1	0.26	-	65,65,65,65	0
55	MG	CA	3083	1/1	0.35	-	44,44,44,44	0
55	MG	AA	3099	1/1	0.34	-	65,65,65,65	0
56	OHX	AA	3293	7/7	0.15	-	54,82,88,102	2
57	ZN	DG	301	1/1	0.27	-	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3106	1/1	0.26	-	61,61,61,61	0
55	MG	CA	3077	1/1	0.24	-	57,57,57,57	0
55	MG	BA	1707	1/1	0.31	-	70,70,70,70	0
55	MG	AB	205	1/1	0.33	-	50,50,50,50	0
56	OHX	CA	3305	7/7	0.15	-	70,83,99,129	1
56	OHX	CA	3310	7/7	0.14	-	74,88,107,129	1
56	OHX	AA	3512	7/7	0.18	-	99,114,126,166	2
55	MG	AA	3387	1/1	0.35	-	42,42,42,42	0
55	MG	BA	1614	1/1	0.36	-	73,73,73,73	0
55	MG	AB	202	1/1	0.23	-	72,72,72,72	0
55	MG	CA	3051	1/1	0.34	-	69,69,69,69	0
55	MG	AA	3238	1/1	0.53	-	50,50,50,50	0
56	OHX	CA	3423	7/7	0.08	-	123,126,136,189	1
55	MG	CA	3113	1/1	0.30	-	61,61,61,61	0
56	OHX	CB	209	7/7	0.16	-	117,133,147,190	1
56	OHX	DA	1766	7/7	0.10	-	118,124,133,175	1
56	OHX	AA	3327	7/7	0.13	-	107,115,135,188	1
55	MG	CA	3035	1/1	0.27	-	92,92,92,92	0
55	MG	DA	1711	1/1	0.27	-	107,107,107,107	0
55	MG	CA	3178	1/1	0.27	-	52,52,52,52	0
56	OHX	CA	3324	7/7	0.18	-	65,83,94,110	2
55	MG	CA	3166	1/1	0.54	-	58,58,58,58	0
55	MG	CA	3143	1/1	0.38	-	60,60,60,60	0
55	MG	CA	3055	1/1	0.29	-	66,66,66,66	0
55	MG	CA	3052	1/1	0.38	-	66,66,66,66	0
56	OHX	AA	3363	7/7	0.13	-	90,99,133,145	1
56	OHX	BD	102	7/7	0.10	-	153,174,197,228	0
55	MG	BA	1642	1/1	0.21	-	102,102,102,102	0
56	OHX	AA	3332	7/7	0.15	-	77,106,123,134	1
55	MG	AA	3140	1/1	0.24	-	41,41,41,41	0
55	MG	CA	3174	1/1	0.47	-	52,52,52,52	0
56	OHX	DC	107	7/7	0.12	-	131,132,141,177	1
56	OHX	CA	3242	7/7	0.12	-	95,107,117,129	1
56	OHX	CA	3299	7/7	0.14	-	99,105,124,141	1
55	MG	AA	3091	1/1	0.24	-	77,77,77,77	0
55	MG	CA	3014	1/1	0.31	-	76,76,76,76	0
55	MG	CA	3215	1/1	0.26	-	137,137,137,137	0
56	OHX	AA	3538	7/7	0.12	-	88,94,114,159	1
55	MG	AA	3013	1/1	0.44	-	41,41,41,41	0
56	OHX	CA	3352	7/7	0.08	-	133,145,147,191	1
56	OHX	CA	3420	7/7	0.13	-	131,141,152,216	1
56	OHX	BA	1677	7/7	0.13	-	141,145,154,220	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3148	1/1	0.27	-	57,57,57,57	0
55	MG	AA	3079	1/1	0.42	-	88,88,88,88	0
55	MG	CA	3258	1/1	0.34	-	56,56,56,56	0
56	OHX	CA	3235	7/7	0.15	-	43,79,99,118	0
55	MG	DA	1697	1/1	0.46	-	72,72,72,72	0
56	OHX	DA	1727	7/7	0.16	-	114,126,131,160	0
55	MG	DA	1640	1/1	0.38	-	83,83,83,83	0
55	MG	CA	3105	1/1	0.48	-	68,68,68,68	0
55	MG	AA	3056	1/1	0.22	-	36,36,36,36	0
55	MG	AA	3416	1/1	0.38	-	74,74,74,74	0
55	MG	AA	3251	1/1	0.38	-	49,49,49,49	0
56	OHX	BA	1760	7/7	0.15	-	71,106,126,148	0
56	OHX	AA	3403	7/7	0.18	-	109,110,128,178	1
56	OHX	AA	3563	7/7	0.09	-	124,125,134,183	1
55	MG	AA	3414	1/1	0.32	-	57,57,57,57	0
56	OHX	AA	3435	7/7	0.18	-	61,70,93,100	3
55	MG	CA	3087	1/1	0.12	-	70,70,70,70	0
55	MG	CA	3128	1/1	0.16	-	72,72,72,72	0
56	OHX	AA	3299	7/7	0.17	-	54,81,94,118	1
56	OHX	AA	3404	7/7	0.21	-	74,98,116,164	1
56	OHX	CA	3389	7/7	0.11	-	101,110,123,155	1
55	MG	CA	3451	1/1	0.32	-	46,46,46,46	0
56	OHX	CA	3349	7/7	0.12	-	115,117,131,178	1
56	OHX	CA	3409	7/7	0.16	-	97,100,119,183	1
55	MG	CA	3107	1/1	0.25	-	82,82,82,82	0
55	MG	CA	3060	1/1	0.25	-	75,75,75,75	0
56	OHX	DA	1785	7/7	0.13	-	110,114,129,164	1
56	OHX	AB	211	7/7	0.14	-	74,85,113,121	0
55	MG	DA	1707	1/1	0.47	-	85,85,85,85	0
55	MG	AA	3183	1/1	0.45	-	88,88,88,88	0
56	OHX	CA	3355	7/7	0.11	-	108,110,119,149	1
55	MG	BA	1704	1/1	0.24	-	88,88,88,88	0
55	MG	DA	1695	1/1	0.53	-	76,76,76,76	0
55	MG	AF	301	1/1	0.32	-	83,83,83,83	0
56	OHX	AA	3539	7/7	0.13	-	116,125,136,193	1
55	MG	DA	1621	1/1	0.35	-	98,98,98,98	0
56	OHX	AA	3527	7/7	0.10	-	130,134,147,188	1
56	OHX	AB	217	7/7	0.16	-	85,105,116,146	1
55	MG	CA	3193	1/1	0.36	-	80,80,80,80	0
55	MG	BA	1698	1/1	0.48	-	62,62,62,62	0
55	MG	CA	3183	1/1	0.39	-	93,93,93,93	0
55	MG	CA	3029	1/1	0.28	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3452	1/1	0.16	-	51,51,51,51	0
56	OHX	AA	3542	7/7	0.13	-	118,127,135,189	1
56	OHX	BA	1815	7/7	0.14	-	110,125,133,172	1
56	OHX	DA	1752	7/7	0.12	-	107,121,128,186	1
55	MG	CA	3151	1/1	0.36	-	76,76,76,76	0
55	MG	DA	1684	1/1	0.54	-	79,79,79,79	0
55	MG	CA	3040	1/1	0.44	-	70,70,70,70	0
56	OHX	BA	1673	7/7	0.12	-	117,123,127,191	1
56	OHX	BA	1784	7/7	0.13	-	122,129,148,203	0
55	MG	DA	1657	1/1	0.43	-	70,70,70,70	0
56	OHX	CA	3381	7/7	0.10	-	102,112,121,159	1
56	OHX	AA	3296	7/7	0.12	-	115,120,123,158	0
55	MG	CA	3049	1/1	0.34	-	62,62,62,62	0
55	MG	CA	3192	1/1	0.29	-	87,87,87,87	0
55	MG	CA	3062	1/1	0.17	-	78,78,78,78	0
56	OHX	CA	3327	7/7	0.14	-	76,83,103,129	1
56	OHX	CA	3328	7/7	0.15	-	50,117,131,206	0
55	MG	BA	1723	1/1	0.27	-	82,82,82,82	0
56	OHX	BA	1816	7/7	0.14	-	127,130,142,194	1
55	MG	AA	3245	1/1	0.27	-	68,68,68,68	0
56	OHX	AA	3362	7/7	0.20	-	40,81,119,136	1
56	OHX	CA	3361	7/7	0.10	-	113,119,132,166	1
55	MG	CA	3439	1/1	0.32	-	63,63,63,63	0
55	MG	CA	3082	1/1	0.42	-	62,62,62,62	0
56	OHX	CA	3345	7/7	0.13	-	91,108,114,146	1
55	MG	DA	1698	1/1	0.51	-	95,95,95,95	0
55	MG	CA	3213	1/1	0.26	-	121,121,121,121	0
55	MG	BA	1742	1/1	0.47	-	86,86,86,86	0
55	MG	DA	1667	1/1	0.45	-	68,68,68,68	0
55	MG	AA	3137	1/1	0.50	-	51,51,51,51	0
55	MG	CA	3186	1/1	0.22	-	75,75,75,75	0
56	OHX	BA	1759	7/7	0.19	-	78,93,120,156	0
55	MG	BA	1736	1/1	0.50	-	64,64,64,64	0
55	MG	BA	1627	1/1	0.41	-	80,80,80,80	0
55	MG	DA	1692	1/1	0.49	-	70,70,70,70	0
55	MG	DA	1702	1/1	0.24	-	122,122,122,122	0
55	MG	AA	3026	1/1	0.46	-	92,92,92,92	0
55	MG	AA	3006	1/1	0.47	-	45,45,45,45	0
56	OHX	BA	1665	7/7	0.14	-	82,92,111,128	1
56	OHX	CA	3309	7/7	0.17	-	92,108,125,150	1
56	OHX	CA	3252	7/7	0.17	-	108,118,136,203	1
56	OHX	AA	3451	7/7	0.18	-	75,85,92,125	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	CA	3463	7/7	0.14	-	107,129,139,156	1
55	MG	AA	3354	1/1	0.38	-	57,57,57,57	0
55	MG	AA	3043	1/1	0.41	-	46,46,46,46	0
56	OHX	AA	3433	7/7	0.17	-	63,65,104,122	1
55	MG	AA	3396	1/1	0.47	-	71,71,71,71	0
55	MG	CA	3224	1/1	0.28	-	77,77,77,77	0
56	OHX	CA	3481	7/7	0.14	-	35,87,114,138	2
56	OHX	CA	3492	7/7	0.14	-	97,102,115,126	1
55	MG	AA	3077	1/1	0.30	-	73,73,73,73	0
55	MG	BA	1640	1/1	0.36	-	73,73,73,73	0
56	OHX	AA	3309	7/7	0.16	-	64,84,90,112	1
56	OHX	A1	203	7/7	0.19	-	100,107,140,182	3
56	OHX	CA	3491	7/7	0.13	-	92,108,117,175	1
55	MG	CA	3172	1/1	0.31	-	86,86,86,86	0
56	OHX	BA	1761	7/7	0.15	-	102,104,115,161	0
55	MG	AA	3022	1/1	0.34	-	15,15,15,15	0
56	OHX	BA	1685	7/7	0.13	-	198,199,207,267	1
55	MG	BS	101	1/1	0.33	-	93,93,93,93	0
56	OHX	BA	1767	7/7	0.17	-	92,119,140,142	0
55	MG	BA	1739	1/1	0.44	-	70,70,70,70	0
56	OHX	AA	3300	7/7	0.14	-	67,91,120,167	1
55	MG	AA	3209	1/1	0.35	-	57,57,57,57	0
56	OHX	AA	3559	7/7	0.10	-	124,133,143,186	1
56	OHX	AA	3476	7/7	0.14	-	102,122,137,175	1
56	OHX	AA	3489	7/7	0.14	-	72,78,92,128	1
55	MG	AA	3185	1/1	0.46	-	36,36,36,36	0
55	MG	CA	3164	1/1	0.48	-	97,97,97,97	0
55	MG	AA	3356	1/1	0.57	-	58,58,58,58	0
56	OHX	CA	3488	7/7	0.07	-	113,123,127,179	1
56	OHX	CA	3421	7/7	0.14	-	113,126,135,198	1
55	MG	AA	3175	1/1	0.36	-	39,39,39,39	0
56	OHX	AA	3561	7/7	0.08	-	152,158,173,226	1
56	OHX	AA	3506	7/7	0.13	-	97,110,123,157	1
56	OHX	DA	1755	7/7	0.16	-	103,120,143,191	1
56	OHX	CA	3332	7/7	0.15	-	70,82,93,103	1
55	MG	CA	3124	1/1	0.31	-	44,44,44,44	0
55	MG	AA	3186	1/1	0.38	-	49,49,49,49	0
55	MG	AA	3381	1/1	0.31	-	59,59,59,59	0
55	MG	AA	3284	1/1	0.38	-	66,66,66,66	0
55	MG	AA	3063	1/1	0.32	-	76,76,76,76	0
55	MG	CA	3138	1/1	0.47	-	53,53,53,53	0
55	MG	AA	3110	1/1	0.51	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	CA	3366	7/7	0.10	-	140,148,168,207	0
56	OHX	CA	3341	7/7	0.13	-	74,100,107,145	2
55	MG	BA	1733	1/1	0.50	-	60,60,60,60	0
56	OHX	AA	3554	7/7	0.14	-	116,128,150,205	1
56	OHX	DA	1753	7/7	0.17	-	120,124,134,196	1
55	MG	CA	3093	1/1	0.36	-	81,81,81,81	0
55	MG	AA	3197	1/1	0.34	-	50,50,50,50	0
56	OHX	CA	3393	7/7	0.13	-	93,114,121,181	1
55	MG	AA	3164	1/1	0.29	-	70,70,70,70	0
55	MG	CA	3223	1/1	0.41	-	88,88,88,88	0
55	MG	AA	3232	1/1	0.45	-	75,75,75,75	0
56	OHX	CA	3414	7/7	0.10	-	155,156,163,215	1
56	OHX	DA	1795	7/7	0.11	-	112,118,132,167	1
55	MG	AA	3222	1/1	0.52	-	64,64,64,64	0
56	OHX	DA	1750	7/7	0.13	-	127,137,146,202	1
55	MG	BA	1728	1/1	0.47	-	90,90,90,90	0
55	MG	AA	3124	1/1	0.43	-	70,70,70,70	0
55	MG	AA	3168	1/1	0.34	-	89,89,89,89	0
56	OHX	DA	1799	7/7	0.15	-	122,127,139,209	1
55	MG	BA	1749	1/1	0.50	-	88,88,88,88	0
56	OHX	DA	1735	7/7	0.10	-	110,115,118,170	1
55	MG	AA	3271	1/1	0.16	-	39,39,39,39	0
56	OHX	AA	3365	7/7	0.22	-	90,106,114,161	2
55	MG	DA	1604	1/1	0.46	-	82,82,82,82	0
55	MG	AA	3208	1/1	0.38	-	65,65,65,65	0
56	OHX	BA	1801	7/7	0.09	-	118,138,142,207	1
55	MG	BA	1636	1/1	0.27	-	61,61,61,61	0
56	OHX	AA	3477	7/7	0.15	-	108,119,125,208	1
56	OHX	CA	3384	7/7	0.11	-	118,124,135,184	1
55	MG	AA	3034	1/1	0.46	-	56,56,56,56	0
56	OHX	AA	3422	7/7	0.17	-	74,81,107,116	0
55	MG	AA	3282	1/1	0.37	-	69,69,69,69	0
55	MG	AA	3213	1/1	0.21	-	49,49,49,49	0
56	OHX	AA	3499	7/7	0.13	-	101,113,131,183	1
55	MG	AA	3001	1/1	0.41	-	28,28,28,28	0
55	MG	AA	3179	1/1	0.52	-	60,60,60,60	0
56	OHX	BA	1696	7/7	0.15	-	47,75,99,113	0
56	OHX	CA	3331	7/7	0.14	-	101,112,120,147	1
56	OHX	AA	3423	7/7	0.21	-	44,66,84,86	1
55	MG	BA	1625	1/1	0.46	-	65,65,65,65	0
55	MG	AA	3189	1/1	0.39	-	42,42,42,42	0
55	MG	BA	1724	1/1	0.37	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	DA	1762	7/7	0.15	-	107,112,122,180	1
55	MG	AA	3235	1/1	0.34	-	50,50,50,50	0
55	MG	CA	3191	1/1	0.47	-	72,72,72,72	0
55	MG	CA	3091	1/1	0.46	-	74,74,74,74	0
55	MG	CA	3123	1/1	0.28	-	36,36,36,36	0
55	MG	CA	3007	1/1	0.25	-	45,45,45,45	0
55	MG	AA	3276	1/1	0.44	-	69,69,69,69	0
55	MG	AA	3394	1/1	0.47	-	43,43,43,43	0
55	MG	CA	3446	1/1	0.27	-	47,47,47,47	0
56	OHX	AA	3425	7/7	0.18	-	45,61,75,79	0
55	MG	AA	3274	1/1	0.58	-	89,89,89,89	0
55	MG	CB	207	1/1	0.47	-	76,76,76,76	0
55	MG	CA	3136	1/1	0.42	-	91,91,91,91	0
56	OHX	AA	3436	7/7	0.11	-	78,91,117,117	0
56	OHX	AA	3519	7/7	0.11	-	140,146,150,214	1
55	MG	AA	3031	1/1	0.23	-	35,35,35,35	0
55	MG	AA	3190	1/1	0.40	-	69,69,69,69	0
55	MG	AA	3108	1/1	0.36	-	82,82,82,82	0
56	OHX	BA	1690	7/7	0.13	-	118,127,134,188	1
56	OHX	AA	3540	7/7	0.13	-	109,134,164,188	2
56	OHX	CA	3279	7/7	0.13	-	80,89,109,118	0
55	MG	DA	1658	1/1	0.48	-	64,64,64,64	0
56	OHX	BA	1678	7/7	0.14	-	115,118,134,165	1
55	MG	CA	3050	1/1	0.28	-	65,65,65,65	0
56	OHX	BA	1656	7/7	0.10	-	160,162,176,267	0
55	MG	AA	3199	1/1	0.64	-	76,76,76,76	0
56	OHX	AA	3147	7/7	0.19	-	89,98,103,163	1
55	MG	DA	1701	1/1	0.43	-	90,90,90,90	0
56	OHX	CA	3315	7/7	0.15	-	90,101,110,160	1
55	MG	CA	3146	1/1	0.37	-	77,77,77,77	0
56	OHX	AA	3505	7/7	0.18	-	86,108,110,156	1
55	MG	AA	3379	1/1	0.45	-	55,55,55,55	0
55	MG	DA	1645	1/1	0.50	-	91,91,91,91	0
56	OHX	AA	3437	7/7	0.13	-	81,95,107,131	0
55	MG	AA	3265	1/1	0.29	-	85,85,85,85	0
56	OHX	DA	1779	7/7	0.09	-	144,146,155,215	1
55	MG	CA	3141	1/1	0.46	-	77,77,77,77	0
56	OHX	AA	3513	7/7	0.16	-	80,88,116,153	1
56	OHX	CA	3291	7/7	0.12	-	86,105,118,139	0
55	MG	BC	101	1/1	0.52	-	69,69,69,69	0
55	MG	AA	3233	1/1	0.19	-	59,59,59,59	0
55	MG	CA	3078	1/1	0.36	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	1697	1/1	0.40	-	37,37,37,37	0
56	OHX	BA	1788	7/7	0.14	-	118,118,132,157	1
55	MG	AA	3234	1/1	0.20	-	56,56,56,56	0
55	MG	AA	3220	1/1	0.50	-	64,64,64,64	0
55	MG	BA	1644	1/1	0.51	-	94,94,94,94	0
55	MG	CA	3153	1/1	0.22	-	56,56,56,56	0
56	OHX	CA	3232	7/7	0.20	-	72,77,83,137	0
55	MG	DA	1638	1/1	0.20	-	89,89,89,89	0
55	MG	AA	3165	1/1	0.58	-	84,84,84,84	0
55	MG	AA	3135	1/1	0.30	-	67,67,67,67	0
56	OHX	AA	3541	7/7	0.22	-	102,114,134,158	2
55	MG	AA	3109	1/1	0.48	-	47,47,47,47	0
56	OHX	CA	3380	7/7	0.09	-	106,119,130,170	1
56	OHX	AA	3474	7/7	0.18	-	51,85,127,151	2
55	MG	AA	3072	1/1	0.27	-	65,65,65,65	0
55	MG	AA	3350	1/1	0.45	-	80,80,80,80	0
56	OHX	CA	3350	7/7	0.15	-	112,134,144,175	1
56	OHX	AA	3553	7/7	0.12	-	113,118,133,183	1
55	MG	CA	3094	1/1	0.57	-	79,79,79,79	0
56	OHX	BA	1679	7/7	0.12	-	116,125,129,189	1
56	OHX	BC	107	7/7	0.14	-	105,124,134,145	1
55	MG	DA	1677	1/1	0.36	-	76,76,76,76	0
55	MG	AA	3343	1/1	0.42	-	34,34,34,34	0
55	MG	DA	1709	1/1	0.54	-	80,80,80,80	0
55	MG	AA	3415	1/1	0.26	-	52,52,52,52	0
55	MG	CA	3020	1/1	0.31	-	70,70,70,70	0
55	MG	DA	1675	1/1	0.42	-	92,92,92,92	0
56	OHX	AA	3555	7/7	0.16	-	112,114,124,192	1
56	OHX	AA	3323	7/7	0.15	-	72,87,96,117	1
55	MG	CA	3135	1/1	0.43	-	45,45,45,45	0
55	MG	AA	3349	1/1	0.45	-	61,61,61,61	0
56	OHX	DV	101	7/7	0.10	-	162,169,185,231	1
55	MG	DA	1683	1/1	0.48	-	71,71,71,71	0
55	MG	BA	1610	1/1	0.32	-	92,92,92,92	0
56	OHX	AA	3549	7/7	0.12	-	97,102,111,165	1
56	OHX	BA	1794	7/7	0.11	-	118,138,149,184	1
55	MG	AA	3347	1/1	0.47	-	70,70,70,70	0
55	MG	CA	3001	1/1	0.24	-	46,46,46,46	0
56	OHX	AA	3569	7/7	0.14	-	116,117,125,191	1
55	MG	DA	1720	1/1	0.50	-	105,105,105,105	0
55	MG	CA	3026	1/1	0.10	-	58,58,58,58	0
56	OHX	AA	3487	7/7	0.12	-	95,110,116,167	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3088	1/1	0.17	-	60,60,60,60	0
55	MG	DA	1708	1/1	0.48	-	87,87,87,87	0
55	MG	BA	1628	1/1	0.37	-	80,80,80,80	0
55	MG	CA	3268	1/1	0.14	-	52,52,52,52	0
56	OHX	AA	3524	7/7	0.12	-	111,120,128,172	1
55	MG	A3	101	1/1	0.46	-	60,60,60,60	0
55	MG	CA	3210	1/1	0.57	-	74,74,74,74	0
55	MG	CA	3075	1/1	0.19	-	45,45,45,45	0
55	MG	CA	3165	1/1	0.46	-	57,57,57,57	0
55	MG	BA	1608	1/1	0.25	-	55,55,55,55	0
56	OHX	CB	208	7/7	0.13	-	105,109,142,147	0
55	MG	DA	1655	1/1	0.12	-	78,78,78,78	0
55	MG	CA	3209	1/1	0.36	-	85,85,85,85	0
55	MG	CA	3162	1/1	0.47	-	65,65,65,65	0
56	OHX	AA	3523	7/7	0.16	-	109,114,123,180	1
56	OHX	AA	3295	7/7	0.14	-	84,98,116,152	0
55	MG	CA	3117	1/1	0.20	-	69,69,69,69	0
55	MG	AA	3352	1/1	0.21	-	41,41,41,41	0
56	OHX	AA	3525	7/7	0.13	-	100,109,122,187	1
55	MG	CA	3089	1/1	0.30	-	60,60,60,60	0
56	OHX	AA	3495	7/7	0.18	-	86,93,120,158	1
56	OHX	AA	3543	7/7	0.11	-	113,117,131,189	1
56	OHX	DA	1718	7/7	0.19	-	73,98,100,135	0
55	MG	AA	3184	1/1	0.34	-	38,38,38,38	0
55	MG	AA	3027	1/1	0.38	-	42,42,42,42	0
56	OHX	BA	1779	7/7	0.12	-	102,112,125,152	1
55	MG	BA	1602	1/1	0.47	-	75,75,75,75	0
56	OHX	CA	3286	7/7	0.14	-	87,94,108,115	0
55	MG	CA	3096	1/1	0.39	-	64,64,64,64	0
56	OHX	CA	3303	7/7	0.12	-	92,96,123,138	0
56	OHX	AA	3434	7/7	0.17	-	62,71,94,101	1
56	OHX	CA	3464	7/7	0.16	-	78,109,122,137	3
55	MG	CA	3058	1/1	0.40	-	50,50,50,50	0
55	MG	BA	1701	1/1	0.32	-	57,57,57,57	0
56	OHX	BA	1811	7/7	0.13	-	88,104,115,154	1
55	MG	CA	3476	1/1	0.34	-	52,52,52,52	0
56	OHX	DA	1764	7/7	0.09	-	115,121,127,171	1
56	OHX	AA	3341	7/7	0.13	-	75,103,114,126	1
55	MG	CA	3227	1/1	0.34	-	79,79,79,79	0
55	MG	AA	3090	1/1	0.21	-	85,85,85,85	0
55	MG	CA	3101	1/1	0.39	-	59,59,59,59	0
55	MG	AA	3385	1/1	0.46	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3153	1/1	0.68	-	64,64,64,64	0
55	MG	AA	3255	1/1	0.22	-	64,64,64,64	0
55	MG	C5	101	1/1	0.22	-	50,50,50,50	0
55	MG	CA	3114	1/1	0.45	-	57,57,57,57	0
55	MG	BA	1660	1/1	0.27	-	97,97,97,97	0
55	MG	AA	3052	1/1	0.49	-	85,85,85,85	0
55	MG	DA	1688	1/1	0.36	-	101,101,101,101	0
55	MG	CA	3480	1/1	0.20	-	72,72,72,72	0
56	OHX	AA	3565	7/7	0.20	-	117,122,134,195	1
56	OHX	CA	3335	7/7	0.16	-	96,110,125,200	0
56	OHX	BA	1694	7/7	0.08	-	159,161,173,226	1
55	MG	BA	1611	1/1	0.40	-	84,84,84,84	0
56	OHX	CA	3469	7/7	0.09	-	89,110,121,162	1
55	MG	DA	1678	1/1	0.15	-	118,118,118,118	0
56	OHX	AA	3485	7/7	0.14	-	104,114,127,171	1
56	OHX	CA	3296	7/7	0.14	-	65,90,108,135	2
55	MG	AA	3055	1/1	0.42	-	65,65,65,65	0
55	MG	AA	3205	1/1	0.17	-	40,40,40,40	0
55	MG	CA	3456	1/1	0.21	-	66,66,66,66	0
56	OHX	BA	1758	7/7	0.16	-	69,88,100,119	0
55	MG	AA	3025	1/1	0.30	-	59,59,59,59	0
55	MG	CA	3042	1/1	0.30	-	67,67,67,67	0
55	MG	DA	1714	1/1	0.33	-	97,97,97,97	0
55	MG	DA	1699	1/1	0.38	-	78,78,78,78	0
55	MG	CA	3169	1/1	0.26	-	71,71,71,71	0
56	OHX	AA	3530	7/7	0.17	-	101,121,143,206	1
55	MG	AA	3266	1/1	0.28	-	78,78,78,78	0
56	OHX	BA	1769	7/7	0.15	-	102,107,127,145	0
56	OHX	AA	3291	7/7	0.15	-	68,75,102,108	3
55	MG	CA	3190	1/1	0.17	-	60,60,60,60	0
55	MG	AA	3268	1/1	0.46	-	73,73,73,73	0
55	MG	AA	3064	1/1	0.25	-	66,66,66,66	0
55	MG	DA	1623	1/1	0.49	-	124,124,124,124	0
55	MG	DA	1628	1/1	0.48	-	78,78,78,78	0
55	MG	AA	3082	1/1	0.21	-	50,50,50,50	0
55	MG	CA	3048	1/1	0.33	-	44,44,44,44	0
55	MG	AA	3393	1/1	0.22	-	56,56,56,56	0
56	OHX	BA	1780	7/7	0.15	-	94,102,115,117	1
55	MG	CA	3019	1/1	0.20	-	46,46,46,46	0
55	MG	AB	204	1/1	0.61	-	68,68,68,68	0
55	MG	CA	3037	1/1	0.38	-	89,89,89,89	0
55	MG	CA	3108	1/1	0.31	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	CA	3378	7/7	0.12	-	128,141,148,178	1
55	MG	DA	1680	1/1	0.29	-	72,72,72,72	0
55	MG	AA	3382	1/1	0.43	-	36,36,36,36	0
56	OHX	CB	220	7/7	0.13	-	133,142,154,201	0
55	MG	AA	3358	1/1	0.32	-	51,51,51,51	0
56	OHX	AA	3463	7/7	0.14	-	77,89,96,134	1
56	OHX	CA	3322	7/7	0.12	-	104,117,127,154	1
56	OHX	AA	3321	7/7	0.11	-	97,109,121,173	1
56	OHX	AA	3419	7/7	0.17	-	67,75,91,95	0
56	OHX	AA	3308	7/7	0.17	-	66,73,104,120	2
56	OHX	CA	3431	7/7	0.13	-	105,117,132,179	1
55	MG	AA	3036	1/1	0.38	-	36,36,36,36	0
56	OHX	BG	302	7/7	0.07	-	128,137,145,186	1
56	OHX	CA	3336	7/7	0.14	-	114,127,138,191	0
56	OHX	AB	209	7/7	0.19	-	63,88,125,152	2
56	OHX	DA	1774	7/7	0.15	-	131,135,155,208	1
55	MG	AA	3044	1/1	0.53	-	72,72,72,72	0
55	MG	CA	3155	1/1	0.18	-	58,58,58,58	0
56	OHX	CA	3376	7/7	0.14	-	113,130,136,172	1
56	OHX	AA	3532	7/7	0.18	-	89,105,116,172	1
55	MG	AA	3202	1/1	0.39	-	45,45,45,45	0
56	OHX	DA	1761	7/7	0.11	-	130,132,145,205	0
56	OHX	CA	3432	7/7	0.12	-	119,135,143,173	1
55	MG	CA	3262	1/1	0.43	-	74,74,74,74	0
55	MG	DA	1653	1/1	0.50	-	73,73,73,73	0
55	MG	AA	3380	1/1	0.27	-	66,66,66,66	0
56	OHX	DA	1728	7/7	0.17	-	78,116,123,162	0
56	OHX	AA	3564	7/7	0.16	-	102,105,128,167	1
55	MG	CA	3443	1/1	0.39	-	49,49,49,49	0
56	OHX	AA	3510	7/7	0.18	-	92,103,113,152	2
55	MG	AA	3133	1/1	0.23	-	54,54,54,54	0
55	MG	AA	3011	1/1	0.38	-	49,49,49,49	0
56	OHX	AA	3370	7/7	0.20	-	115,126,140,200	1
55	MG	AA	3200	1/1	0.44	-	45,45,45,45	0
56	OHX	AA	3421	7/7	0.19	-	50,71,87,114	0
56	OHX	DA	1790	7/7	0.11	-	135,136,148,199	1
56	OHX	AA	3493	7/7	0.15	-	109,111,123,166	1
55	MG	AA	3262	1/1	0.41	-	52,52,52,52	0
55	MG	CA	3222	1/1	0.23	-	81,81,81,81	0
56	OHX	CA	3234	7/7	0.15	-	77,91,119,122	2
55	MG	AA	3020	1/1	0.38	-	44,44,44,44	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.