



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 30, 2026 – 08:08 PM UTC

PDB ID : 4V8E / pdb_00004v8e
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 X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

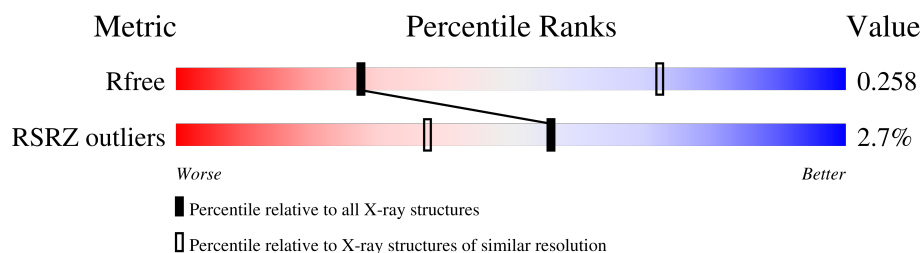
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	3144	-	-	-	X
55	MG	BA	1745	-	-	-	X
55	MG	BB	104	-	-	-	X
55	MG	BC	105	-	-	-	X
55	MG	CA	3045	-	-	-	X
55	MG	CA	3455	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 303952 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 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			

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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 (CCD ID: MG) (formula: Mg).

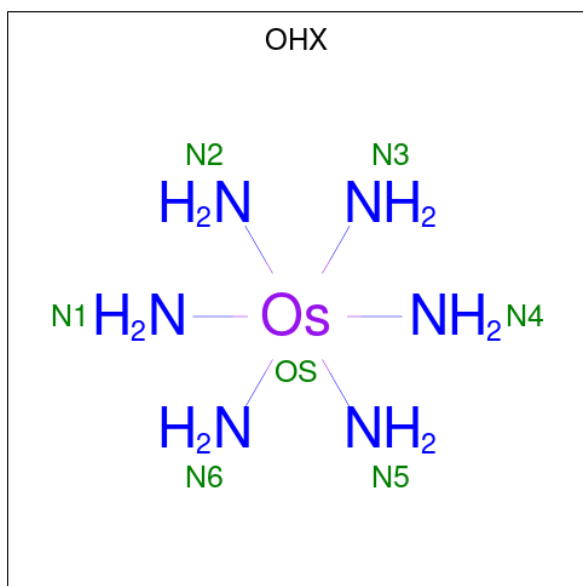
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	AA	331	Total Mg 331 331	0	0
55	AB	6	Total Mg 6 6	0	0
55	AE	3	Total Mg 3 3	0	0
55	AF	2	Total Mg 2 2	0	0
55	AO	3	Total Mg 3 3	0	0
55	A0	1	Total Mg 1 1	0	0
55	A1	1	Total Mg 1 1	0	0
55	A3	1	Total Mg 1 1	0	0
55	A5	1	Total Mg 1 1	0	0
55	BA	115	Total Mg 115 115	0	0
55	BN	1	Total Mg 1 1	0	0
55	BQ	1	Total Mg 1 1	0	0
55	BS	1	Total Mg 1 1	0	0
55	BB	5	Total Mg 5 5	0	0
55	BC	5	Total Mg 5 5	0	0
55	BD	1	Total Mg 1 1	0	0
55	B1	1	Total Mg 1 1	0	0
55	CA	274	Total Mg 274 274	0	0
55	CB	7	Total Mg 7 7	0	0
55	CE	1	Total Mg 1 1	0	0
55	C0	1	Total Mg 1 1	0	0
55	C5	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	C7	1	Total 1	Mg 1	0	0
55	DA	119	Total 119	Mg 119	0	0
55	DL	1	Total 1	Mg 1	0	0
55	DN	1	Total 1	Mg 1	0	0
55	DB	2	Total 2	Mg 2	0	0
55	DC	6	Total 6	Mg 6	0	0
55	D1	1	Total 1	Mg 1	0	0

- Molecule 56 is osmium (III) hexammine (CCD ID: 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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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
			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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	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	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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	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	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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	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	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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	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	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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	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	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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	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	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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	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	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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	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	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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	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	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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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 (CCD ID: ZN) (formula: Zn).

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

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

3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.25Å 450.87Å 622.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	256.19 – 3.30 256.19 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (256.19-3.30) 94.2 (256.19-3.30)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.19Å)	Xtriage
Refinement program	PHENIX dev_810	Depositor
R, R_{free}	0.206 , 0.259 0.206 , 0.258	Depositor DCC
R_{free} test set	2000 reflections (0.21%)	wwPDB-VP
Wilson B-factor (Å ²)	90.6	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 72.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	303952	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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	BD	38	52	28,31,32	1.90	3 (10%)	38,44,47	2.80	12 (31%)
52	MIA	DB	38	52	28,31,32	2.02	2 (7%)	38,44,47	2.70	13 (34%)
52	MIA	BB	38	52	28,31,32	1.95	3 (10%)	38,44,47	2.53	13 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	MIA	DD	38	52	28,31,32	1.94	3 (10%)	38,44,47	2.58	12 (31%)

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	BD	38	52	-	8/15/33/34	0/3/3/3
52	MIA	DB	38	52	-	4/15/33/34	0/3/3/3
52	MIA	BB	38	52	-	3/15/33/34	0/3/3/3
52	MIA	DD	38	52	-	8/15/33/34	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	DB	38	MIA	C6-N6	7.70	1.46	1.34
52	BB	38	MIA	C6-N6	7.41	1.46	1.34
52	DD	38	MIA	C6-N6	7.37	1.45	1.34
52	BD	38	MIA	C6-N6	7.22	1.45	1.34
52	DB	38	MIA	C13-C14	6.06	1.50	1.32

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	BD	38	MIA	C11-S10-C2	9.55	109.41	102.25
52	DB	38	MIA	C11-S10-C2	9.07	109.06	102.25
52	BB	38	MIA	C5-C4-N3	-7.68	119.09	127.18
52	BD	38	MIA	C5-C4-N3	-7.57	119.20	127.18
52	DB	38	MIA	C5-C4-N3	-7.45	119.33	127.18

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	BB	38	MIA	N1-C2-S10-C11
52	BB	38	MIA	N3-C2-S10-C11
52	BB	38	MIA	C12-C13-C14-C16
52	BD	38	MIA	N1-C2-S10-C11
52	BD	38	MIA	N3-C2-S10-C11

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 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	DA	1721	-	0,6,6	-	-	-		
56	OHX	DA	1803	-	0,6,6	-	-	-		
56	OHX	BA	1816	-	0,6,6	-	-	-		
56	OHX	AO	204	-	0,6,6	-	-	-		
56	OHX	AA	3553	-	0,6,6	-	-	-		
56	OHX	CO	201	-	0,6,6	-	-	-		
56	OHX	CA	3287	-	0,6,6	-	-	-		
56	OHX	AB	217	-	0,6,6	-	-	-		
56	OHX	DA	1734	-	0,6,6	-	-	-		
56	OHX	CA	3320	-	0,6,6	-	-	-		
56	OHX	AA	3518	-	0,6,6	-	-	-		
56	OHX	DA	1808	-	0,6,6	-	-	-		
56	OHX	AA	3567	-	0,6,6	-	-	-		
56	OHX	DV	101	-	0,6,6	-	-	-		
56	OHX	BA	1668	-	0,6,6	-	-	-		
56	OHX	CA	3332	-	0,6,6	-	-	-		
56	OHX	CA	3298	-	0,6,6	-	-	-		
56	OHX	BA	1797	-	0,6,6	-	-	-		
56	OHX	AA	3472	-	0,6,6	-	-	-		
56	OHX	AA	3322	-	0,6,6	-	-	-		
56	OHX	AA	3543	-	0,6,6	-	-	-		
56	OHX	DA	1774	-	0,6,6	-	-	-		
56	OHX	CA	3280	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	AA	3530	-	0,6,6	-	-	-		
56	OHX	AE	304	-	0,6,6	-	-	-		
56	OHX	AA	3506	-	0,6,6	-	-	-		
56	OHX	AA	3502	-	0,6,6	-	-	-		
56	OHX	BA	1802	-	0,6,6	-	-	-		
56	OHX	AA	3445	-	0,6,6	-	-	-		
56	OHX	AA	3500	-	0,6,6	-	-	-		
56	OHX	BA	1791	-	0,6,6	-	-	-		
56	OHX	CA	3436	-	0,6,6	-	-	-		
56	OHX	AA	3318	-	0,6,6	-	-	-		
56	OHX	AA	3463	-	0,6,6	-	-	-		
56	OHX	A1	203	-	0,6,6	-	-	-		
56	OHX	CA	3390	-	0,6,6	-	-	-		
56	OHX	DA	1752	-	0,6,6	-	-	-		
56	OHX	DA	1800	-	0,6,6	-	-	-		
56	OHX	AA	3432	-	0,6,6	-	-	-		
56	OHX	AO	205	-	0,6,6	-	-	-		
56	OHX	DA	1736	-	0,6,6	-	-	-		
56	OHX	AA	3402	-	0,6,6	-	-	-		
56	OHX	AA	3455	-	0,6,6	-	-	-		
56	OHX	CA	3376	-	0,6,6	-	-	-		
56	OHX	DA	1761	-	0,6,6	-	-	-		
56	OHX	AA	3509	-	0,6,6	-	-	-		
56	OHX	AA	3316	-	0,6,6	-	-	-		
56	OHX	AA	3474	-	0,6,6	-	-	-		
56	OHX	BA	1682	-	0,6,6	-	-	-		
56	OHX	CA	3400	-	0,6,6	-	-	-		
56	OHX	CA	3304	-	0,6,6	-	-	-		
56	OHX	CA	3300	-	0,6,6	-	-	-		
56	OHX	AA	3369	-	0,6,6	-	-	-		
56	OHX	BA	1691	-	0,6,6	-	-	-		
56	OHX	AA	3511	-	0,6,6	-	-	-		
56	OHX	CA	3434	-	0,6,6	-	-	-		
56	OHX	AA	3454	-	0,6,6	-	-	-		
56	OHX	DA	1745	-	0,6,6	-	-	-		
56	OHX	AA	3477	-	0,6,6	-	-	-		
56	OHX	AA	3325	-	0,6,6	-	-	-		
56	OHX	AA	3305	-	0,6,6	-	-	-		
56	OHX	AA	3337	-	0,6,6	-	-	-		
56	OHX	DA	1788	-	0,6,6	-	-	-		
56	OHX	AA	3528	-	0,6,6	-	-	-		
56	OHX	AA	3287	-	0,6,6	-	-	-		
56	OHX	AA	3536	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	CA	3370	-	0,6,6	-	-	-		
56	OHX	CA	3416	-	0,6,6	-	-	-		
56	OHX	DA	1782	-	0,6,6	-	-	-		
56	OHX	CA	3323	-	0,6,6	-	-	-		
56	OHX	CA	3421	-	0,6,6	-	-	-		
56	OHX	CA	3336	-	0,6,6	-	-	-		
56	OHX	AA	3488	-	0,6,6	-	-	-		
56	OHX	AA	3494	-	0,6,6	-	-	-		
56	OHX	CA	3239	-	0,6,6	-	-	-		
56	OHX	AA	3566	-	0,6,6	-	-	-		
56	OHX	CA	3329	-	0,6,6	-	-	-		
56	OHX	CB	212	-	0,6,6	-	-	-		
56	OHX	DA	1741	-	0,6,6	-	-	-		
56	OHX	CA	3425	-	0,6,6	-	-	-		
56	OHX	DA	1792	-	0,6,6	-	-	-		
56	OHX	BA	1787	-	0,6,6	-	-	-		
56	OHX	AA	3565	-	0,6,6	-	-	-		
56	OHX	AA	3406	-	0,6,6	-	-	-		
56	OHX	CA	3464	-	0,6,6	-	-	-		
56	OHX	AA	3469	-	0,6,6	-	-	-		
56	OHX	AA	3524	-	0,6,6	-	-	-		
56	OHX	CA	3302	-	0,6,6	-	-	-		
56	OHX	DA	1805	-	0,6,6	-	-	-		
56	OHX	AA	3486	-	0,6,6	-	-	-		
56	OHX	BA	1772	-	0,6,6	-	-	-		
56	OHX	DA	1732	-	0,6,6	-	-	-		
56	OHX	BA	1756	-	0,6,6	-	-	-		
56	OHX	AA	3485	-	0,6,6	-	-	-		
56	OHX	BA	1766	-	0,6,6	-	-	-		
56	OHX	AA	3510	-	0,6,6	-	-	-		
56	OHX	DA	1786	-	0,6,6	-	-	-		
56	OHX	AA	3332	-	0,6,6	-	-	-		
56	OHX	CA	3379	-	0,6,6	-	-	-		
56	OHX	CA	3423	-	0,6,6	-	-	-		
56	OHX	AA	3495	-	0,6,6	-	-	-		
56	OHX	BA	1780	-	0,6,6	-	-	-		
56	OHX	DA	1749	-	0,6,6	-	-	-		
56	OHX	AF	303	-	0,6,6	-	-	-		
56	OHX	CA	3236	-	0,6,6	-	-	-		
56	OHX	AA	3562	-	0,6,6	-	-	-		
56	OHX	AA	3522	-	0,6,6	-	-	-		
56	OHX	AA	3460	-	0,6,6	-	-	-		
56	OHX	BA	1662	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	AA	3296	-	0,6,6	-	-	-		
56	OHX	DA	1738	-	0,6,6	-	-	-		
56	OHX	CA	3333	-	0,6,6	-	-	-		
56	OHX	DA	1809	-	0,6,6	-	-	-		
56	OHX	CA	3385	-	0,6,6	-	-	-		
56	OHX	DA	1796	-	0,6,6	-	-	-		
56	OHX	CA	3362	-	0,6,6	-	-	-		
56	OHX	BA	1810	-	0,6,6	-	-	-		
56	OHX	AA	3473	-	0,6,6	-	-	-		
56	OHX	AB	218	-	0,6,6	-	-	-		
56	OHX	CA	3334	-	0,6,6	-	-	-		
56	OHX	CA	3238	-	0,6,6	-	-	-		
56	OHX	BA	1782	-	0,6,6	-	-	-		
56	OHX	AA	3537	-	0,6,6	-	-	-		
56	OHX	CB	211	-	0,6,6	-	-	-		
56	OHX	AA	3160	-	0,6,6	-	-	-		
56	OHX	DA	1810	-	0,6,6	-	-	-		
56	OHX	C1	201	-	0,6,6	-	-	-		
56	OHX	AB	215	-	0,6,6	-	-	-		
56	OHX	CA	3433	-	0,6,6	-	-	-		
56	OHX	AA	3539	-	0,6,6	-	-	-		
56	OHX	AA	3520	-	0,6,6	-	-	-		
56	OHX	CA	3417	-	0,6,6	-	-	-		
56	OHX	AA	3360	-	0,6,6	-	-	-		
56	OHX	BA	1779	-	0,6,6	-	-	-		
56	OHX	BG	302	-	0,6,6	-	-	-		
56	OHX	CA	3326	-	0,6,6	-	-	-		
56	OHX	BA	1759	-	0,6,6	-	-	-		
56	OHX	AA	3310	-	0,6,6	-	-	-		
56	OHX	CA	3419	-	0,6,6	-	-	-		
56	OHX	DA	1763	-	0,6,6	-	-	-		
56	OHX	DA	1798	-	0,6,6	-	-	-		
56	OHX	AA	3329	-	0,6,6	-	-	-		
56	OHX	CA	3357	-	0,6,6	-	-	-		
56	OHX	AA	3295	-	0,6,6	-	-	-		
56	OHX	CB	218	-	0,6,6	-	-	-		
56	OHX	BA	1769	-	0,6,6	-	-	-		
56	OHX	AA	3302	-	0,6,6	-	-	-		
56	OHX	AA	3359	-	0,6,6	-	-	-		
56	OHX	DC	110	-	0,6,6	-	-	-		
56	OHX	CA	3372	-	0,6,6	-	-	-		
56	OHX	CA	3310	-	0,6,6	-	-	-		
56	OHX	CA	3315	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	AA	3288	-	0,6,6	-	-	-		
56	OHX	AA	3436	-	0,6,6	-	-	-		
56	OHX	AA	3512	-	0,6,6	-	-	-		
56	OHX	AA	3326	-	0,6,6	-	-	-		
56	OHX	CA	3252	-	0,6,6	-	-	-		
56	OHX	CA	3237	-	0,6,6	-	-	-		
56	OHX	CA	3414	-	0,6,6	-	-	-		
56	OHX	CA	3299	-	0,6,6	-	-	-		
56	OHX	AA	3403	-	0,6,6	-	-	-		
56	OHX	AA	3516	-	0,6,6	-	-	-		
56	OHX	BA	1667	-	0,6,6	-	-	-		
56	OHX	CA	3308	-	0,6,6	-	-	-		
56	OHX	AA	3323	-	0,6,6	-	-	-		
56	OHX	AA	3421	-	0,6,6	-	-	-		
56	OHX	AA	3303	-	0,6,6	-	-	-		
56	OHX	CA	3241	-	0,6,6	-	-	-		
56	OHX	CA	3277	-	0,6,6	-	-	-		
56	OHX	BA	1788	-	0,6,6	-	-	-		
56	OHX	BA	1656	-	0,6,6	-	-	-		
56	OHX	AA	3449	-	0,6,6	-	-	-		
56	OHX	CA	3342	-	0,6,6	-	-	-		
56	OHX	DA	1733	-	0,6,6	-	-	-		
56	OHX	AA	3423	-	0,6,6	-	-	-		
56	OHX	AA	3540	-	0,6,6	-	-	-		
56	OHX	AA	3304	-	0,6,6	-	-	-		
56	OHX	DA	1757	-	0,6,6	-	-	-		
56	OHX	DA	1766	-	0,6,6	-	-	-		
56	OHX	AA	3479	-	0,6,6	-	-	-		
56	OHX	CA	3292	-	0,6,6	-	-	-		
56	OHX	CA	3314	-	0,6,6	-	-	-		
56	OHX	BA	1664	-	0,6,6	-	-	-		
56	OHX	BA	1669	-	0,6,6	-	-	-		
56	OHX	BA	1776	-	0,6,6	-	-	-		
56	OHX	CA	3276	-	0,6,6	-	-	-		
56	OHX	AA	3542	-	0,6,6	-	-	-		
56	OHX	CA	3272	-	0,6,6	-	-	-		
56	OHX	DA	1760	-	0,6,6	-	-	-		
56	OHX	CA	3350	-	0,6,6	-	-	-		
56	OHX	AA	3560	-	0,6,6	-	-	-		
56	OHX	CA	3352	-	0,6,6	-	-	-		
56	OHX	AA	3471	-	0,6,6	-	-	-		
56	OHX	AA	3482	-	0,6,6	-	-	-		
56	OHX	CA	3406	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	AA	3330	-	0,6,6	-	-	-		
56	OHX	BA	1689	-	0,6,6	-	-	-		
56	OHX	BC	107	-	0,6,6	-	-	-		
56	OHX	AA	3531	-	0,6,6	-	-	-		
56	OHX	AA	3468	-	0,6,6	-	-	-		
56	OHX	BR	101	-	0,6,6	-	-	-		
56	OHX	A3	102	-	0,6,6	-	-	-		
56	OHX	CA	3426	-	0,6,6	-	-	-		
56	OHX	BA	1789	-	0,6,6	-	-	-		
56	OHX	AA	3419	-	0,6,6	-	-	-		
56	OHX	C6	101	-	0,6,6	-	-	-		
56	OHX	CA	3431	-	0,6,6	-	-	-		
56	OHX	DB	104	-	0,6,6	-	-	-		
56	OHX	CA	3487	-	0,6,6	-	-	-		
56	OHX	BA	1771	-	0,6,6	-	-	-		
56	OHX	BB	107	-	0,6,6	-	-	-		
56	OHX	CA	3321	-	0,6,6	-	-	-		
56	OHX	CA	3285	-	0,6,6	-	-	-		
56	OHX	BA	1777	-	0,6,6	-	-	-		
56	OHX	AA	3450	-	0,6,6	-	-	-		
56	OHX	AA	3365	-	0,6,6	-	-	-		
56	OHX	BA	1804	-	0,6,6	-	-	-		
56	OHX	CA	3392	-	0,6,6	-	-	-		
56	OHX	CA	3364	-	0,6,6	-	-	-		
56	OHX	BA	1686	-	0,6,6	-	-	-		
56	OHX	CA	3275	-	0,6,6	-	-	-		
56	OHX	CA	3401	-	0,6,6	-	-	-		
56	OHX	CA	3402	-	0,6,6	-	-	-		
56	OHX	DA	1740	-	0,6,6	-	-	-		
56	OHX	DA	1765	-	0,6,6	-	-	-		
56	OHX	AA	3526	-	0,6,6	-	-	-		
56	OHX	AA	3407	-	0,6,6	-	-	-		
56	OHX	AA	3544	-	0,6,6	-	-	-		
56	OHX	AA	3299	-	0,6,6	-	-	-		
56	OHX	AA	3341	-	0,6,6	-	-	-		
56	OHX	CA	3363	-	0,6,6	-	-	-		
56	OHX	CA	3306	-	0,6,6	-	-	-		
56	OHX	CA	3373	-	0,6,6	-	-	-		
56	OHX	CA	3450	-	0,6,6	-	-	-		
56	OHX	CA	3375	-	0,6,6	-	-	-		
56	OHX	CA	3413	-	0,6,6	-	-	-		
56	OHX	AA	3519	-	0,6,6	-	-	-		
56	OHX	CA	3293	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	BA	1695	-	0,6,6	-	-	-		
56	OHX	DG	302	-	0,6,6	-	-	-		
56	OHX	CA	3341	-	0,6,6	-	-	-		
56	OHX	BA	1770	-	0,6,6	-	-	-		
56	OHX	CA	3307	-	0,6,6	-	-	-		
56	OHX	AA	3368	-	0,6,6	-	-	-		
56	OHX	DA	1722	-	0,6,6	-	-	-		
56	OHX	AA	3458	-	0,6,6	-	-	-		
56	OHX	AA	3499	-	0,6,6	-	-	-		
56	OHX	CA	3430	-	0,6,6	-	-	-		
56	OHX	C5	102	-	0,6,6	-	-	-		
56	OHX	AA	3466	-	0,6,6	-	-	-		
56	OHX	BA	1665	-	0,6,6	-	-	-		
56	OHX	BA	1767	-	0,6,6	-	-	-		
56	OHX	CA	3349	-	0,6,6	-	-	-		
56	OHX	AA	3363	-	0,6,6	-	-	-		
56	OHX	AA	3331	-	0,6,6	-	-	-		
56	OHX	CA	3365	-	0,6,6	-	-	-		
56	OHX	CA	3469	-	0,6,6	-	-	-		
56	OHX	DA	1719	-	0,6,6	-	-	-		
56	OHX	CA	3490	-	0,6,6	-	-	-		
56	OHX	AA	3324	-	0,6,6	-	-	-		
56	OHX	AA	3442	-	0,6,6	-	-	-		
56	OHX	CA	3398	-	0,6,6	-	-	-		
56	OHX	DC	109	-	0,6,6	-	-	-		
56	OHX	AA	3557	-	0,6,6	-	-	-		
56	OHX	CA	3391	-	0,6,6	-	-	-		
56	OHX	AA	3430	-	0,6,6	-	-	-		
56	OHX	BB	106	-	0,6,6	-	-	-		
56	OHX	AA	3308	-	0,6,6	-	-	-		
56	OHX	CA	3279	-	0,6,6	-	-	-		
56	OHX	CA	3330	-	0,6,6	-	-	-		
56	OHX	BA	1685	-	0,6,6	-	-	-		
56	OHX	CA	3311	-	0,6,6	-	-	-		
56	OHX	CB	216	-	0,6,6	-	-	-		
56	OHX	DA	1744	-	0,6,6	-	-	-		
56	OHX	CA	3269	-	0,6,6	-	-	-		
56	OHX	CA	3393	-	0,6,6	-	-	-		
56	OHX	DA	1802	-	0,6,6	-	-	-		
56	OHX	AA	3300	-	0,6,6	-	-	-		
56	OHX	AA	3480	-	0,6,6	-	-	-		
56	OHX	AA	3465	-	0,6,6	-	-	-		
56	OHX	DA	1787	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	AA	3507	-	0,6,6	-	-	-		
56	OHX	AA	3428	-	0,6,6	-	-	-		
56	OHX	AA	3461	-	0,6,6	-	-	-		
56	OHX	BA	1786	-	0,6,6	-	-	-		
56	OHX	CA	3286	-	0,6,6	-	-	-		
56	OHX	BA	1807	-	0,6,6	-	-	-		
56	OHX	AA	3314	-	0,6,6	-	-	-		
56	OHX	AA	3336	-	0,6,6	-	-	-		
56	OHX	AA	3311	-	0,6,6	-	-	-		
56	OHX	BA	1666	-	0,6,6	-	-	-		
56	OHX	AA	3339	-	0,6,6	-	-	-		
56	OHX	AA	3504	-	0,6,6	-	-	-		
56	OHX	AA	3447	-	0,6,6	-	-	-		
56	OHX	BA	1799	-	0,6,6	-	-	-		
56	OHX	AA	3546	-	0,6,6	-	-	-		
56	OHX	A1	202	-	0,6,6	-	-	-		
56	OHX	AA	3498	-	0,6,6	-	-	-		
56	OHX	AA	3425	-	0,6,6	-	-	-		
56	OHX	CA	3242	-	0,6,6	-	-	-		
56	OHX	BA	1672	-	0,6,6	-	-	-		
56	OHX	AA	3487	-	0,6,6	-	-	-		
56	OHX	AB	207	-	0,6,6	-	-	-		
56	OHX	BA	1785	-	0,6,6	-	-	-		
56	OHX	DA	1767	-	0,6,6	-	-	-		
56	OHX	DA	1730	-	0,6,6	-	-	-		
56	OHX	BA	1793	-	0,6,6	-	-	-		
56	OHX	DA	1780	-	0,6,6	-	-	-		
56	OHX	AA	3561	-	0,6,6	-	-	-		
56	OHX	CA	3378	-	0,6,6	-	-	-		
56	OHX	CA	3317	-	0,6,6	-	-	-		
56	OHX	AA	3293	-	0,6,6	-	-	-		
56	OHX	AB	210	-	0,6,6	-	-	-		
56	OHX	CA	3251	-	0,6,6	-	-	-		
56	OHX	CA	3288	-	0,6,6	-	-	-		
56	OHX	BA	1801	-	0,6,6	-	-	-		
56	OHX	AA	3514	-	0,6,6	-	-	-		
56	OHX	AA	3320	-	0,6,6	-	-	-		
56	OHX	CA	3335	-	0,6,6	-	-	-		
56	OHX	CA	3396	-	0,6,6	-	-	-		
56	OHX	AA	3475	-	0,6,6	-	-	-		
56	OHX	CA	3387	-	0,6,6	-	-	-		
56	OHX	DA	1750	-	0,6,6	-	-	-		
56	OHX	DA	1731	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	CA	3399	-	0,6,6	-	-	-		
56	OHX	DA	1768	-	0,6,6	-	-	-		
56	OHX	BA	1764	-	0,6,6	-	-	-		
56	OHX	CA	3410	-	0,6,6	-	-	-		
56	OHX	CA	3355	-	0,6,6	-	-	-		
56	OHX	DA	1718	-	0,6,6	-	-	-		
56	OHX	BA	1688	-	0,6,6	-	-	-		
56	OHX	BA	1805	-	0,6,6	-	-	-		
56	OHX	AA	3535	-	0,6,6	-	-	-		
56	OHX	CA	3437	-	0,6,6	-	-	-		
56	OHX	AA	3489	-	0,6,6	-	-	-		
56	OHX	AB	208	-	0,6,6	-	-	-		
56	OHX	DA	1794	-	0,6,6	-	-	-		
56	OHX	BA	1760	-	0,6,6	-	-	-		
56	OHX	AA	3568	-	0,6,6	-	-	-		
56	OHX	CA	3348	-	0,6,6	-	-	-		
56	OHX	BA	1811	-	0,6,6	-	-	-		
56	OHX	DA	1806	-	0,6,6	-	-	-		
56	OHX	AA	3298	-	0,6,6	-	-	-		
56	OHX	AA	3306	-	0,6,6	-	-	-		
56	OHX	AA	3373	-	0,6,6	-	-	-		
56	OHX	CA	3382	-	0,6,6	-	-	-		
56	OHX	DA	1747	-	0,6,6	-	-	-		
56	OHX	CA	3435	-	0,6,6	-	-	-		
56	OHX	CA	3319	-	0,6,6	-	-	-		
56	OHX	DA	1799	-	0,6,6	-	-	-		
56	OHX	CA	3483	-	0,6,6	-	-	-		
56	OHX	DA	1775	-	0,6,6	-	-	-		
56	OHX	CA	3245	-	0,6,6	-	-	-		
56	OHX	CA	3438	-	0,6,6	-	-	-		
56	OHX	BA	1671	-	0,6,6	-	-	-		
56	OHX	AB	219	-	0,6,6	-	-	-		
56	OHX	CA	3404	-	0,6,6	-	-	-		
56	OHX	CA	3389	-	0,6,6	-	-	-		
56	OHX	CA	3405	-	0,6,6	-	-	-		
56	OHX	CB	214	-	0,6,6	-	-	-		
56	OHX	BA	1783	-	0,6,6	-	-	-		
56	OHX	CA	3482	-	0,6,6	-	-	-		
56	OHX	DA	1751	-	0,6,6	-	-	-		
56	OHX	CA	3408	-	0,6,6	-	-	-		
56	OHX	CA	3491	-	0,6,6	-	-	-		
56	OHX	CA	3331	-	0,6,6	-	-	-		
56	OHX	CA	3340	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	AA	3444	-	0,6,6	-	-	-		
56	OHX	DA	1777	-	0,6,6	-	-	-		
56	OHX	BA	1803	-	0,6,6	-	-	-		
56	OHX	CA	3345	-	0,6,6	-	-	-		
56	OHX	CA	3369	-	0,6,6	-	-	-		
56	OHX	CA	3253	-	0,6,6	-	-	-		
56	OHX	BA	1775	-	0,6,6	-	-	-		
56	OHX	CA	3359	-	0,6,6	-	-	-		
56	OHX	CA	3468	-	0,6,6	-	-	-		
56	OHX	DA	1776	-	0,6,6	-	-	-		
56	OHX	AA	3529	-	0,6,6	-	-	-		
56	OHX	AA	3426	-	0,6,6	-	-	-		
56	OHX	CA	3427	-	0,6,6	-	-	-		
56	OHX	AA	3370	-	0,6,6	-	-	-		
56	OHX	AA	3448	-	0,6,6	-	-	-		
56	OHX	AA	3484	-	0,6,6	-	-	-		
56	OHX	CA	3395	-	0,6,6	-	-	-		
56	OHX	BA	1794	-	0,6,6	-	-	-		
56	OHX	AA	3505	-	0,6,6	-	-	-		
56	OHX	CA	3381	-	0,6,6	-	-	-		
56	OHX	DA	1742	-	0,6,6	-	-	-		
56	OHX	AA	3476	-	0,6,6	-	-	-		
56	OHX	CA	3327	-	0,6,6	-	-	-		
56	OHX	CA	3338	-	0,6,6	-	-	-		
56	OHX	AA	3420	-	0,6,6	-	-	-		
56	OHX	AA	3467	-	0,6,6	-	-	-		
56	OHX	AA	3470	-	0,6,6	-	-	-		
56	OHX	CA	3322	-	0,6,6	-	-	-		
56	OHX	CB	210	-	0,6,6	-	-	-		
56	OHX	BA	1670	-	0,6,6	-	-	-		
56	OHX	CA	3291	-	0,6,6	-	-	-		
56	OHX	CA	3343	-	0,6,6	-	-	-		
56	OHX	CA	3481	-	0,6,6	-	-	-		
56	OHX	AA	3459	-	0,6,6	-	-	-		
56	OHX	DA	1789	-	0,6,6	-	-	-		
56	OHX	AA	3313	-	0,6,6	-	-	-		
56	OHX	BA	1692	-	0,6,6	-	-	-		
56	OHX	CB	215	-	0,6,6	-	-	-		
56	OHX	DA	1781	-	0,6,6	-	-	-		
56	OHX	AA	3552	-	0,6,6	-	-	-		
56	OHX	CA	3380	-	0,6,6	-	-	-		
56	OHX	BA	1687	-	0,6,6	-	-	-		
56	OHX	BA	1806	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	DA	1770	-	0,6,6	-	-	-		
56	OHX	CA	3489	-	0,6,6	-	-	-		
56	OHX	DA	1801	-	0,6,6	-	-	-		
56	OHX	BA	1693	-	0,6,6	-	-	-		
56	OHX	DA	1729	-	0,6,6	-	-	-		
56	OHX	CA	3274	-	0,6,6	-	-	-		
56	OHX	BA	1762	-	0,6,6	-	-	-		
56	OHX	AA	3328	-	0,6,6	-	-	-		
56	OHX	AA	3400	-	0,6,6	-	-	-		
56	OHX	CA	3313	-	0,6,6	-	-	-		
56	OHX	AA	3333	-	0,6,6	-	-	-		
56	OHX	DK	201	-	0,6,6	-	-	-		
56	OHX	BA	1808	-	0,6,6	-	-	-		
56	OHX	AA	3517	-	0,6,6	-	-	-		
56	OHX	AB	209	-	0,6,6	-	-	-		
56	OHX	AA	3451	-	0,6,6	-	-	-		
56	OHX	CA	3358	-	0,6,6	-	-	-		
56	OHX	DA	1773	-	0,6,6	-	-	-		
56	OHX	CA	3244	-	0,6,6	-	-	-		
56	OHX	AA	3548	-	0,6,6	-	-	-		
56	OHX	CA	3361	-	0,6,6	-	-	-		
56	OHX	DA	1804	-	0,6,6	-	-	-		
56	OHX	AA	3334	-	0,6,6	-	-	-		
56	OHX	CB	219	-	0,6,6	-	-	-		
56	OHX	BA	1675	-	0,6,6	-	-	-		
56	OHX	AA	3431	-	0,6,6	-	-	-		
56	OHX	CA	3397	-	0,6,6	-	-	-		
56	OHX	AA	3362	-	0,6,6	-	-	-		
56	OHX	AA	3550	-	0,6,6	-	-	-		
56	OHX	CA	3282	-	0,6,6	-	-	-		
56	OHX	CA	3356	-	0,6,6	-	-	-		
56	OHX	CA	3367	-	0,6,6	-	-	-		
56	OHX	AA	3290	-	0,6,6	-	-	-		
56	OHX	BA	1798	-	0,6,6	-	-	-		
56	OHX	CA	3488	-	0,6,6	-	-	-		
56	OHX	AA	3515	-	0,6,6	-	-	-		
56	OHX	BA	1676	-	0,6,6	-	-	-		
56	OHX	CA	3465	-	0,6,6	-	-	-		
56	OHX	CA	3486	-	0,6,6	-	-	-		
56	OHX	CA	3273	-	0,6,6	-	-	-		
56	OHX	AA	3427	-	0,6,6	-	-	-		
56	OHX	BA	1681	-	0,6,6	-	-	-		
56	OHX	CA	3377	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	DA	1772	-	0,6,6	-	-	-		
56	OHX	DA	1743	-	0,6,6	-	-	-		
56	OHX	AA	3534	-	0,6,6	-	-	-		
56	OHX	DA	1769	-	0,6,6	-	-	-		
56	OHX	AA	3545	-	0,6,6	-	-	-		
56	OHX	DA	1785	-	0,6,6	-	-	-		
56	OHX	AA	3549	-	0,6,6	-	-	-		
56	OHX	BD	104	-	0,6,6	-	-	-		
56	OHX	AA	3154	-	0,6,6	-	-	-		
56	OHX	CA	3246	-	0,6,6	-	-	-		
56	OHX	AA	3371	-	0,6,6	-	-	-		
56	OHX	DA	1812	-	0,6,6	-	-	-		
56	OHX	AA	3424	-	0,6,6	-	-	-		
56	OHX	BA	1680	-	0,6,6	-	-	-		
56	OHX	CA	3467	-	0,6,6	-	-	-		
56	OHX	AA	3372	-	0,6,6	-	-	-		
56	OHX	CA	3346	-	0,6,6	-	-	-		
56	OHX	AA	3315	-	0,6,6	-	-	-		
56	OHX	AA	3493	-	0,6,6	-	-	-		
56	OHX	DC	107	-	0,6,6	-	-	-		
56	OHX	CA	3270	-	0,6,6	-	-	-		
56	OHX	BA	1757	-	0,6,6	-	-	-		
56	OHX	CA	3418	-	0,6,6	-	-	-		
56	OHX	BA	1768	-	0,6,6	-	-	-		
56	OHX	AA	3532	-	0,6,6	-	-	-		
56	OHX	BA	1815	-	0,6,6	-	-	-		
56	OHX	DA	1779	-	0,6,6	-	-	-		
56	OHX	AA	3508	-	0,6,6	-	-	-		
56	OHX	CA	3305	-	0,6,6	-	-	-		
56	OHX	DA	1807	-	0,6,6	-	-	-		
56	OHX	DA	1759	-	0,6,6	-	-	-		
56	OHX	CA	3316	-	0,6,6	-	-	-		
56	OHX	CA	3353	-	0,6,6	-	-	-		
56	OHX	CA	3328	-	0,6,6	-	-	-		
56	OHX	DA	1756	-	0,6,6	-	-	-		
56	OHX	AA	3292	-	0,6,6	-	-	-		
56	OHX	AA	3297	-	0,6,6	-	-	-		
56	OHX	CB	220	-	0,6,6	-	-	-		
56	OHX	CA	3249	-	0,6,6	-	-	-		
56	OHX	AA	3361	-	0,6,6	-	-	-		
56	OHX	BA	1758	-	0,6,6	-	-	-		
56	OHX	CB	209	-	0,6,6	-	-	-		
56	OHX	DA	1726	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	CA	3354	-	0,6,6	-	-	-		
56	OHX	BA	1814	-	0,6,6	-	-	-		
56	OHX	DA	1727	-	0,6,6	-	-	-		
56	OHX	AA	3541	-	0,6,6	-	-	-		
56	OHX	BA	1792	-	0,6,6	-	-	-		
56	OHX	DR	101	-	0,6,6	-	-	-		
56	OHX	BA	1813	-	0,6,6	-	-	-		
56	OHX	AA	3452	-	0,6,6	-	-	-		
56	OHX	CA	3297	-	0,6,6	-	-	-		
56	OHX	CA	3271	-	0,6,6	-	-	-		
56	OHX	CA	3295	-	0,6,6	-	-	-		
56	OHX	CA	3309	-	0,6,6	-	-	-		
56	OHX	CA	3243	-	0,6,6	-	-	-		
56	OHX	AA	3554	-	0,6,6	-	-	-		
56	OHX	AB	213	-	0,6,6	-	-	-		
56	OHX	DA	1762	-	0,6,6	-	-	-		
56	OHX	AA	3422	-	0,6,6	-	-	-		
56	OHX	BA	1674	-	0,6,6	-	-	-		
56	OHX	AA	3481	-	0,6,6	-	-	-		
56	OHX	BA	1774	-	0,6,6	-	-	-		
56	OHX	CA	3384	-	0,6,6	-	-	-		
56	OHX	AA	3446	-	0,6,6	-	-	-		
56	OHX	AA	3263	-	0,6,6	-	-	-		
56	OHX	CA	3383	-	0,6,6	-	-	-		
56	OHX	AA	3401	-	0,6,6	-	-	-		
56	OHX	CA	3432	-	0,6,6	-	-	-		
56	OHX	AA	3555	-	0,6,6	-	-	-		
56	OHX	AA	3321	-	0,6,6	-	-	-		
56	OHX	AB	211	-	0,6,6	-	-	-		
56	OHX	AA	3418	-	0,6,6	-	-	-		
56	OHX	AA	3438	-	0,6,6	-	-	-		
56	OHX	DA	1758	-	0,6,6	-	-	-		
56	OHX	AA	3335	-	0,6,6	-	-	-		
56	OHX	AA	3342	-	0,6,6	-	-	-		
56	OHX	BA	1755	-	0,6,6	-	-	-		
56	OHX	CA	3289	-	0,6,6	-	-	-		
56	OHX	BA	1812	-	0,6,6	-	-	-		
56	OHX	CB	213	-	0,6,6	-	-	-		
56	OHX	DA	1783	-	0,6,6	-	-	-		
56	OHX	AA	3558	-	0,6,6	-	-	-		
56	OHX	BA	1795	-	0,6,6	-	-	-		
56	OHX	BA	1659	-	0,6,6	-	-	-		
56	OHX	CA	3360	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	BA	1678	-	0,6,6	-	-	-		
56	OHX	AW	101	-	0,6,6	-	-	-		
56	OHX	CA	3420	-	0,6,6	-	-	-		
56	OHX	DA	1746	-	0,6,6	-	-	-		
56	OHX	DA	1797	-	0,6,6	-	-	-		
56	OHX	CA	3374	-	0,6,6	-	-	-		
56	OHX	AA	3547	-	0,6,6	-	-	-		
56	OHX	AA	3307	-	0,6,6	-	-	-		
56	OHX	A6	101	-	0,6,6	-	-	-		
56	OHX	BA	1683	-	0,6,6	-	-	-		
56	OHX	AA	3439	-	0,6,6	-	-	-		
56	OHX	AA	3559	-	0,6,6	-	-	-		
56	OHX	DA	1771	-	0,6,6	-	-	-		
56	OHX	CA	3278	-	0,6,6	-	-	-		
56	OHX	CA	3388	-	0,6,6	-	-	-		
56	OHX	CB	217	-	0,6,6	-	-	-		
56	OHX	CA	3233	-	0,6,6	-	-	-		
56	OHX	CA	3484	-	0,6,6	-	-	-		
56	OHX	CA	3344	-	0,6,6	-	-	-		
56	OHX	AA	3440	-	0,6,6	-	-	-		
56	OHX	BA	1673	-	0,6,6	-	-	-		
56	OHX	DA	1737	-	0,6,6	-	-	-		
56	OHX	BA	1773	-	0,6,6	-	-	-		
56	OHX	CA	3429	-	0,6,6	-	-	-		
56	OHX	BA	1694	-	0,6,6	-	-	-		
56	OHX	BD	103	-	0,6,6	-	-	-		
56	OHX	AA	3538	-	0,6,6	-	-	-		
56	OHX	AA	3569	-	0,6,6	-	-	-		
56	OHX	CA	3312	-	0,6,6	-	-	-		
56	OHX	AA	3503	-	0,6,6	-	-	-		
56	OHX	BD	102	-	0,6,6	-	-	-		
56	OHX	AA	3405	-	0,6,6	-	-	-		
56	OHX	AA	3435	-	0,6,6	-	-	-		
56	OHX	DA	1791	-	0,6,6	-	-	-		
56	OHX	BA	1690	-	0,6,6	-	-	-		
56	OHX	BA	1763	-	0,6,6	-	-	-		
56	OHX	BC	106	-	0,6,6	-	-	-		
56	OHX	AA	3533	-	0,6,6	-	-	-		
56	OHX	BA	1784	-	0,6,6	-	-	-		
56	OHX	DB	105	-	0,6,6	-	-	-		
56	OHX	CA	3351	-	0,6,6	-	-	-		
56	OHX	DA	1754	-	0,6,6	-	-	-		
56	OHX	CA	3255	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	CA	3290	-	0,6,6	-	-	-		
56	OHX	CA	3240	-	0,6,6	-	-	-		
56	OHX	AA	3364	-	0,6,6	-	-	-		
56	OHX	AA	3138	-	0,6,6	-	-	-		
56	OHX	AA	3462	-	0,6,6	-	-	-		
56	OHX	DA	1790	-	0,6,6	-	-	-		
56	OHX	DA	1753	-	0,6,6	-	-	-		
56	OHX	AA	3513	-	0,6,6	-	-	-		
56	OHX	CA	3281	-	0,6,6	-	-	-		
56	OHX	CA	3412	-	0,6,6	-	-	-		
56	OHX	AA	3147	-	0,6,6	-	-	-		
56	OHX	CA	3411	-	0,6,6	-	-	-		
56	OHX	DA	1755	-	0,6,6	-	-	-		
56	OHX	AA	3367	-	0,6,6	-	-	-		
56	OHX	AA	3289	-	0,6,6	-	-	-		
56	OHX	BA	1657	-	0,6,6	-	-	-		
56	OHX	CA	3294	-	0,6,6	-	-	-		
56	OHX	AA	3291	-	0,6,6	-	-	-		
56	OHX	CA	3284	-	0,6,6	-	-	-		
56	OHX	CA	3366	-	0,6,6	-	-	-		
56	OHX	CA	3394	-	0,6,6	-	-	-		
56	OHX	CA	3325	-	0,6,6	-	-	-		
56	OHX	CA	3337	-	0,6,6	-	-	-		
56	OHX	CA	3386	-	0,6,6	-	-	-		
56	OHX	DB	103	-	0,6,6	-	-	-		
56	OHX	AA	3490	-	0,6,6	-	-	-		
56	OHX	CA	3371	-	0,6,6	-	-	-		
56	OHX	BA	1696	-	0,6,6	-	-	-		
56	OHX	CA	3424	-	0,6,6	-	-	-		
56	OHX	CA	3296	-	0,6,6	-	-	-		
56	OHX	AA	3453	-	0,6,6	-	-	-		
56	OHX	CA	3422	-	0,6,6	-	-	-		
56	OHX	AA	3496	-	0,6,6	-	-	-		
56	OHX	AA	3309	-	0,6,6	-	-	-		
56	OHX	BA	1790	-	0,6,6	-	-	-		
56	OHX	AA	3433	-	0,6,6	-	-	-		
56	OHX	DA	1724	-	0,6,6	-	-	-		
56	OHX	CA	3415	-	0,6,6	-	-	-		
56	OHX	AA	3457	-	0,6,6	-	-	-		
56	OHX	AA	3437	-	0,6,6	-	-	-		
56	OHX	CA	3470	-	0,6,6	-	-	-		
56	OHX	CA	3232	-	0,6,6	-	-	-		
56	OHX	CA	3256	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	AB	214	-	0,6,6	-	-	-		
56	OHX	CA	3407	-	0,6,6	-	-	-		
56	OHX	CA	3235	-	0,6,6	-	-	-		
56	OHX	CA	3485	-	0,6,6	-	-	-		
56	OHX	BA	1677	-	0,6,6	-	-	-		
56	OHX	AA	3312	-	0,6,6	-	-	-		
56	OHX	DA	1793	-	0,6,6	-	-	-		
56	OHX	AA	3456	-	0,6,6	-	-	-		
56	OHX	BA	1809	-	0,6,6	-	-	-		
56	OHX	BA	1663	-	0,6,6	-	-	-		
56	OHX	AA	3521	-	0,6,6	-	-	-		
56	OHX	DA	1795	-	0,6,6	-	-	-		
56	OHX	AA	3441	-	0,6,6	-	-	-		
56	OHX	AA	3478	-	0,6,6	-	-	-		
56	OHX	CA	3368	-	0,6,6	-	-	-		
56	OHX	AA	3443	-	0,6,6	-	-	-		
56	OHX	CA	3303	-	0,6,6	-	-	-		
56	OHX	CA	3466	-	0,6,6	-	-	-		
56	OHX	CA	3318	-	0,6,6	-	-	-		
56	OHX	CA	3463	-	0,6,6	-	-	-		
56	OHX	DC	108	-	0,6,6	-	-	-		
56	OHX	BA	1781	-	0,6,6	-	-	-		
56	OHX	C3	101	-	0,6,6	-	-	-		
56	OHX	AA	3404	-	0,6,6	-	-	-		
56	OHX	AA	3497	-	0,6,6	-	-	-		
56	OHX	AA	3399	-	0,6,6	-	-	-		
56	OHX	AA	3319	-	0,6,6	-	-	-		
56	OHX	CA	3347	-	0,6,6	-	-	-		
56	OHX	AA	3527	-	0,6,6	-	-	-		
56	OHX	AA	3434	-	0,6,6	-	-	-		
56	OHX	DA	1723	-	0,6,6	-	-	-		
56	OHX	DA	1811	-	0,6,6	-	-	-		
56	OHX	DA	1764	-	0,6,6	-	-	-		
56	OHX	CA	3462	-	0,6,6	-	-	-		
56	OHX	BA	1684	-	0,6,6	-	-	-		
56	OHX	AA	3464	-	0,6,6	-	-	-		
56	OHX	AA	3564	-	0,6,6	-	-	-		
56	OHX	AA	3501	-	0,6,6	-	-	-		
56	OHX	CA	3324	-	0,6,6	-	-	-		
56	OHX	DA	1784	-	0,6,6	-	-	-		
56	OHX	BA	1778	-	0,6,6	-	-	-		
56	OHX	AA	3417	-	0,6,6	-	-	-		
56	OHX	AA	3429	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	OHX	AA	3491	-	0,6,6	-	-	-		
56	OHX	AA	3294	-	0,6,6	-	-	-		
56	OHX	CA	3283	-	0,6,6	-	-	-		
56	OHX	AA	3317	-	0,6,6	-	-	-		
56	OHX	AA	3366	-	0,6,6	-	-	-		
56	OHX	AA	3523	-	0,6,6	-	-	-		
56	OHX	AA	3563	-	0,6,6	-	-	-		
56	OHX	AA	3340	-	0,6,6	-	-	-		
56	OHX	BA	1796	-	0,6,6	-	-	-		
56	OHX	CA	3234	-	0,6,6	-	-	-		
56	OHX	BA	1679	-	0,6,6	-	-	-		
56	OHX	CF	301	-	0,6,6	-	-	-		
56	OHX	CA	3428	-	0,6,6	-	-	-		
56	OHX	CA	3461	-	0,6,6	-	-	-		
56	OHX	DA	1728	-	0,6,6	-	-	-		
56	OHX	CB	208	-	0,6,6	-	-	-		
56	OHX	DA	1735	-	0,6,6	-	-	-		
56	OHX	DA	1739	-	0,6,6	-	-	-		
56	OHX	AA	3492	-	0,6,6	-	-	-		
56	OHX	BA	1800	-	0,6,6	-	-	-		
56	OHX	CA	3247	-	0,6,6	-	-	-		
56	OHX	CA	3492	-	0,6,6	-	-	-		
56	OHX	AA	3551	-	0,6,6	-	-	-		
56	OHX	DD	101	-	0,6,6	-	-	-		
56	OHX	DA	1748	-	0,6,6	-	-	-		
56	OHX	BA	1761	-	0,6,6	-	-	-		
56	OHX	BA	1661	-	0,6,6	-	-	-		
56	OHX	AA	3327	-	0,6,6	-	-	-		
56	OHX	AA	3338	-	0,6,6	-	-	-		
56	OHX	CA	3248	-	0,6,6	-	-	-		
56	OHX	CA	3250	-	0,6,6	-	-	-		
56	OHX	CA	3339	-	0,6,6	-	-	-		
56	OHX	CA	3403	-	0,6,6	-	-	-		
56	OHX	AA	3556	-	0,6,6	-	-	-		
56	OHX	BA	1765	-	0,6,6	-	-	-		
56	OHX	CA	3254	-	0,6,6	-	-	-		
56	OHX	DA	1778	-	0,6,6	-	-	-		
56	OHX	AA	3483	-	0,6,6	-	-	-		
56	OHX	AB	212	-	0,6,6	-	-	-		
56	OHX	CA	3409	-	0,6,6	-	-	-		
56	OHX	AA	3301	-	0,6,6	-	-	-		
56	OHX	CA	3301	-	0,6,6	-	-	-		
56	OHX	AB	216	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	OHX	AA	3525	-	0,6,6	-	-	-		

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.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	2912/2912 (100%)	-0.73	7 (0%) 91 86	45, 76, 209, 243	0
1	CA	2907/2912 (99%)	-0.49	10 (0%) 90 82	58, 92, 230, 245	0
2	AB	122/122 (100%)	-0.68	0 100 100	73, 95, 116, 177	0
2	CB	122/122 (100%)	-0.42	1 (0%) 82 68	92, 126, 146, 198	0
3	AD	272/276 (98%)	0.10	7 (2%) 57 38	39, 66, 84, 105	0
3	CD	272/276 (98%)	0.39	15 (5%) 30 21	55, 78, 96, 128	0
4	AE	205/206 (99%)	0.40	17 (8%) 17 13	51, 86, 130, 142	0
4	CE	205/206 (99%)	0.30	9 (4%) 39 25	64, 100, 148, 165	0
5	AF	202/210 (96%)	-0.22	3 (1%) 72 53	47, 81, 118, 130	0
5	CF	208/210 (99%)	0.26	6 (2%) 53 35	62, 106, 160, 184	0
6	AG	181/182 (99%)	0.15	6 (3%) 49 33	84, 107, 138, 149	0
6	CG	181/182 (99%)	0.70	14 (7%) 19 14	120, 141, 164, 171	0
7	AH	170/180 (94%)	0.43	10 (5%) 28 19	86, 112, 130, 157	0
7	CH	170/180 (94%)	0.76	20 (11%) 9 8	155, 198, 220, 229	0
8	AK	146/148 (98%)	0.30	10 (6%) 23 16	79, 131, 147, 150	0
8	CK	146/148 (98%)	0.25	2 (1%) 73 55	84, 130, 152, 158	0
9	AM	138/140 (98%)	0.40	8 (5%) 29 19	66, 87, 124, 136	0
9	CM	138/140 (98%)	0.53	4 (2%) 53 35	83, 114, 140, 156	0
10	AN	122/122 (100%)	0.06	1 (0%) 82 68	57, 78, 93, 101	0
10	CN	122/122 (100%)	0.31	1 (0%) 82 68	75, 95, 111, 124	0
11	AO	150/150 (100%)	-0.07	1 (0%) 84 70	48, 88, 117, 160	0
11	CO	150/150 (100%)	0.36	9 (6%) 27 19	45, 108, 146, 178	0
12	AP	141/141 (100%)	0.88	20 (14%) 6 5	58, 83, 105, 127	0
12	CP	141/141 (100%)	1.21	29 (20%) 2 2	58, 109, 140, 159	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	A0	118/118 (100%)	-0.22	0 100 100	61, 81, 103, 113	0
13	C0	117/118 (99%)	-0.32	0 100 100	69, 87, 106, 121	0
14	AQ	111/112 (99%)	-0.06	2 (1%) 67 49	70, 92, 117, 131	0
14	CQ	111/112 (99%)	0.13	5 (4%) 38 25	86, 123, 147, 162	0
15	AR	137/146 (93%)	0.10	4 (2%) 53 35	73, 93, 143, 170	0
15	CR	137/146 (93%)	0.12	6 (4%) 39 25	84, 104, 163, 183	0
16	A1	117/118 (99%)	-0.07	0 100 100	52, 75, 108, 139	0
16	C1	117/118 (99%)	0.22	1 (0%) 81 65	67, 106, 143, 162	0
17	A2	101/101 (100%)	0.51	7 (6%) 23 16	53, 98, 122, 141	0
17	C2	101/101 (100%)	0.97	9 (8%) 15 12	67, 129, 142, 151	0
18	AS	113/113 (100%)	-0.08	1 (0%) 81 65	54, 73, 104, 156	0
18	CS	113/113 (100%)	0.03	1 (0%) 81 65	64, 80, 114, 158	0
19	AT	92/96 (95%)	-0.02	2 (2%) 62 43	57, 71, 95, 107	0
19	CT	92/96 (95%)	0.46	6 (6%) 25 17	74, 88, 113, 127	0
20	AU	102/110 (92%)	0.38	6 (5%) 28 19	74, 101, 152, 162	0
20	CU	102/110 (92%)	0.85	15 (14%) 6 5	95, 118, 166, 181	0
21	AV	175/206 (84%)	0.75	15 (8%) 16 12	87, 126, 188, 191	0
21	CV	179/206 (86%)	0.73	9 (5%) 34 23	122, 160, 208, 216	0
22	A3	76/85 (89%)	-0.16	1 (1%) 75 56	59, 77, 91, 132	0
22	C3	77/85 (90%)	0.12	3 (3%) 43 29	83, 95, 117, 147	0
23	AZ	97/98 (98%)	0.01	5 (5%) 33 22	58, 78, 126, 156	0
23	CZ	97/98 (98%)	0.51	5 (5%) 33 22	68, 86, 132, 155	0
24	AW	66/72 (91%)	0.05	2 (3%) 52 35	63, 84, 98, 125	0
24	CW	66/72 (91%)	0.28	3 (4%) 38 25	84, 107, 130, 139	0
25	AX	59/60 (98%)	-0.02	1 (1%) 69 50	63, 83, 112, 130	0
25	CX	59/60 (98%)	0.34	2 (3%) 48 32	80, 110, 141, 162	0
26	A4	66/71 (92%)	0.48	2 (3%) 52 35	120, 156, 173, 179	0
26	C4	63/71 (88%)	1.11	9 (14%) 6 5	146, 185, 194, 199	0
27	A5	59/60 (98%)	0.67	9 (15%) 5 5	49, 88, 168, 171	0
27	C5	59/60 (98%)	0.33	2 (3%) 48 32	65, 92, 173, 187	0
28	A6	45/54 (83%)	1.00	8 (17%) 4 3	124, 151, 168, 177	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	C6	45/54 (83%)	1.36	11 (24%) 2 1	141, 169, 183, 186	0
29	A7	45/49 (91%)	-0.22	3 (6%) 24 16	47, 55, 69, 78	0
29	C7	45/49 (91%)	0.02	1 (2%) 62 43	56, 66, 77, 100	0
30	A8	60/65 (92%)	-0.04	0 100 100	55, 73, 90, 114	0
30	C8	60/65 (92%)	0.61	8 (13%) 7 6	78, 90, 112, 137	0
31	BA	1502/1506 (99%)	-0.57	10 (0%) 84 70	58, 107, 187, 244	0
31	DA	1502/1506 (99%)	-0.65	2 (0%) 92 90	71, 119, 189, 244	0
32	BE	237/256 (92%)	0.46	8 (3%) 48 32	111, 144, 182, 193	0
32	DE	237/256 (92%)	0.20	1 (0%) 88 79	126, 161, 196, 211	0
33	BF	205/239 (85%)	0.36	5 (2%) 59 40	96, 119, 152, 160	0
33	DF	206/239 (86%)	0.29	5 (2%) 59 40	127, 147, 175, 180	0
34	BG	208/208 (100%)	0.55	10 (4%) 35 24	92, 116, 136, 147	0
34	DG	208/208 (100%)	0.25	5 (2%) 59 40	93, 111, 132, 145	0
35	BH	151/162 (93%)	0.31	2 (1%) 75 56	81, 105, 127, 161	0
35	DH	151/162 (93%)	0.18	3 (1%) 65 46	104, 121, 142, 165	0
36	BI	101/101 (100%)	0.12	0 100 100	81, 108, 122, 145	0
36	DI	101/101 (100%)	0.39	0 100 100	81, 106, 124, 149	0
37	BJ	155/156 (99%)	0.20	5 (3%) 50 34	106, 121, 149, 158	0
37	DJ	155/156 (99%)	0.10	2 (1%) 75 56	113, 131, 153, 164	0
38	BK	138/138 (100%)	-0.05	1 (0%) 84 70	89, 110, 123, 129	0
38	DK	138/138 (100%)	-0.24	0 100 100	104, 125, 136, 146	0
39	BL	127/128 (99%)	-0.12	0 100 100	87, 142, 160, 169	0
39	DL	127/128 (99%)	-0.16	1 (0%) 82 68	117, 155, 168, 174	0
40	BM	99/105 (94%)	0.10	2 (2%) 65 46	91, 142, 170, 174	0
40	DM	99/105 (94%)	0.17	1 (1%) 79 63	124, 159, 175, 179	0
41	BN	119/129 (92%)	0.27	5 (4%) 40 26	72, 104, 133, 161	0
41	DN	119/129 (92%)	0.46	6 (5%) 34 23	91, 112, 139, 167	0
42	BO	125/132 (94%)	0.45	7 (5%) 30 20	69, 83, 112, 158	0
42	DO	125/132 (94%)	0.57	9 (7%) 21 15	93, 110, 134, 166	0
43	BP	116/126 (92%)	0.13	3 (2%) 57 38	92, 128, 145, 153	0
43	DP	117/126 (92%)	0.38	7 (5%) 27 19	106, 156, 169, 171	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	58/61 (95%)	0.06	1 (1%) 69 50	91, 108, 122, 129	0
44	DQ	58/61 (95%)	-0.14	0 100 100	126, 140, 157, 160	0
45	BR	88/89 (98%)	-0.18	0 100 100	80, 100, 121, 125	0
45	DR	88/89 (98%)	0.01	0 100 100	85, 112, 133, 140	0
46	BS	84/88 (95%)	0.09	0 100 100	100, 118, 139, 175	0
46	DS	84/88 (95%)	-0.04	0 100 100	96, 107, 127, 158	0
47	BT	100/105 (95%)	0.01	4 (4%) 42 28	93, 112, 125, 133	0
47	DT	100/105 (95%)	0.05	3 (3%) 52 35	94, 114, 135, 143	0
48	BU	72/88 (81%)	0.29	1 (1%) 73 55	88, 106, 139, 164	0
48	DU	72/88 (81%)	0.43	4 (5%) 30 20	97, 114, 155, 169	0
49	BV	78/93 (83%)	0.38	4 (5%) 33 22	109, 130, 147, 152	0
49	DV	78/93 (83%)	0.36	2 (2%) 57 38	145, 163, 182, 185	0
50	BW	99/106 (93%)	-0.07	0 100 100	105, 124, 155, 160	0
50	DW	99/106 (93%)	-0.25	0 100 100	95, 117, 153, 163	0
51	BX	25/27 (92%)	-0.34	0 100 100	102, 117, 137, 154	0
51	DX	25/27 (92%)	-0.05	1 (4%) 42 28	122, 143, 158, 168	0
52	BB	84/85 (98%)	1.23	25 (29%) 1 1	82, 123, 154, 169	0
52	BD	84/85 (98%)	0.20	7 (8%) 17 13	75, 137, 217, 227	0
52	DB	84/85 (98%)	1.23	17 (20%) 3 2	93, 128, 156, 171	0
52	DD	84/85 (98%)	0.53	9 (10%) 11 9	84, 137, 217, 225	0
53	BC	77/77 (100%)	0.23	5 (6%) 25 17	77, 114, 139, 153	0
53	DC	77/77 (100%)	0.17	2 (2%) 57 38	88, 122, 150, 157	0
54	B1	16/16 (100%)	0.82	3 (18%) 3 3	76, 104, 156, 163	0
54	D1	16/16 (100%)	0.36	2 (12%) 8 6	85, 109, 157, 165	0
All	All	21100/21658 (97%)	-0.10	564 (2%) 56 37	39, 105, 182, 245	0

The worst 5 of 564 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	CW	41	ILE	7.6
27	A5	2	ALA	7.3
11	CO	61	ARG	7.2
12	AP	86	GLY	7.1
27	C5	2	ALA	6.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
52	MIA	DB	38	29/30	0.79	0.12	84,93,111,126	0
52	MIA	BD	38	29/30	0.87	0.15	116,135,182,198	0
52	MIA	DD	38	29/30	0.88	0.12	120,140,186,205	0
52	MIA	BB	38	29/30	0.93	0.12	68,83,97,106	0

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	CA	3213	1/1	0.26	0.15	121,121,121,121	0
55	MG	AA	3095	1/1	0.40	0.24	89,89,89,89	0
55	MG	AA	3086	1/1	0.43	0.31	95,95,95,95	0
55	MG	DA	1631	1/1	0.43	0.28	111,111,111,111	0
55	MG	DA	1619	1/1	0.48	0.31	98,98,98,98	0
55	MG	CA	3455	1/1	0.52	0.61	97,97,97,97	0
55	MG	BA	1699	1/1	0.54	0.37	79,79,79,79	0
55	MG	DA	1681	1/1	0.54	0.18	100,100,100,100	0
55	MG	DA	1622	1/1	0.57	0.21	122,122,122,122	0
55	MG	BA	1648	1/1	0.58	0.25	99,99,99,99	0
55	MG	AA	3100	1/1	0.58	0.23	108,108,108,108	0
55	MG	BB	104	1/1	0.58	0.44	87,87,87,87	0
55	MG	BA	1632	1/1	0.59	0.21	108,108,108,108	0
55	MG	AA	3247	1/1	0.60	0.26	81,81,81,81	0
55	MG	DA	1714	1/1	0.60	0.20	97,97,97,97	0
55	MG	DA	1618	1/1	0.61	0.25	105,105,105,105	0
55	MG	AA	3137	1/1	0.62	0.38	51,51,51,51	0
55	MG	AA	3067	1/1	0.62	0.19	97,97,97,97	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	1673	1/1	0.62	0.20	80,80,80,80	0
55	MG	CA	3034	1/1	0.62	0.25	91,91,91,91	0
55	MG	CA	3209	1/1	0.62	0.33	85,85,85,85	0
56	OHX	AA	3526	7/7	0.62	0.12	120,129,136,176	1
55	MG	BA	1629	1/1	0.63	0.18	112,112,112,112	0
55	MG	BC	102	1/1	0.63	0.18	68,68,68,68	0
55	MG	CA	3220	1/1	0.63	0.35	85,85,85,85	0
55	MG	AA	3245	1/1	0.63	0.26	68,68,68,68	0
56	OHX	DB	104	7/7	0.63	0.09	129,133,143,205	2
55	MG	BA	1634	1/1	0.64	0.34	74,74,74,74	0
55	MG	AA	3087	1/1	0.64	0.29	83,83,83,83	0
55	MG	DA	1642	1/1	0.64	0.21	112,112,112,112	0
56	OHX	DA	1794	7/7	0.64	0.09	124,130,139,205	1
55	MG	CA	3198	1/1	0.64	0.23	118,118,118,118	0
55	MG	DA	1659	1/1	0.65	0.22	89,89,89,89	0
55	MG	DA	1641	1/1	0.65	0.27	130,130,130,130	0
55	MG	DA	1643	1/1	0.65	0.24	136,136,136,136	0
55	MG	DA	1682	1/1	0.65	0.35	87,87,87,87	0
55	MG	AA	3248	1/1	0.66	0.25	86,86,86,86	0
55	MG	CA	3085	1/1	0.66	0.28	102,102,102,102	0
55	MG	CA	3107	1/1	0.66	0.25	82,82,82,82	0
55	MG	DB	102	1/1	0.66	0.21	102,102,102,102	0
55	MG	CA	3197	1/1	0.66	0.32	79,79,79,79	0
55	MG	BA	1749	1/1	0.66	0.27	88,88,88,88	0
55	MG	BC	105	1/1	0.66	0.40	87,87,87,87	0
55	MG	CA	3264	1/1	0.67	0.40	49,49,49,49	0
56	OHX	CB	218	7/7	0.67	0.10	141,159,166,235	1
55	MG	DA	1720	1/1	0.67	0.25	105,105,105,105	0
55	MG	DA	1688	1/1	0.67	0.30	101,101,101,101	0
55	MG	AA	3009	1/1	0.68	0.16	89,89,89,89	0
55	MG	DA	1717	1/1	0.68	0.20	100,100,100,100	0
55	MG	BA	1746	1/1	0.68	0.28	82,82,82,82	0
55	MG	AA	3108	1/1	0.68	0.19	82,82,82,82	0
55	MG	AA	3347	1/1	0.68	0.32	70,70,70,70	0
55	MG	CA	3141	1/1	0.68	0.32	77,77,77,77	0
55	MG	BA	1622	1/1	0.68	0.16	123,123,123,123	0
55	MG	DA	1705	1/1	0.68	0.24	108,108,108,108	0
55	MG	DA	1649	1/1	0.69	0.27	87,87,87,87	0
55	MG	CA	3458	1/1	0.69	0.20	82,82,82,82	0
55	MG	DA	1668	1/1	0.69	0.22	86,86,86,86	0
55	MG	BA	1607	1/1	0.69	0.24	93,93,93,93	0
55	MG	DA	1623	1/1	0.70	0.24	124,124,124,124	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3280	1/1	0.70	0.24	77,77,77,77	0
55	MG	CE	301	1/1	0.70	0.39	56,56,56,56	0
55	MG	DA	1617	1/1	0.70	0.20	115,115,115,115	0
56	OHX	BD	104	7/7	0.70	0.12	82,85,90,147	2
55	MG	CA	3146	1/1	0.70	0.29	77,77,77,77	0
55	MG	CA	3062	1/1	0.70	0.14	78,78,78,78	0
55	MG	CA	3457	1/1	0.70	0.20	66,66,66,66	0
56	OHX	DB	105	7/7	0.70	0.14	88,91,103,175	5
55	MG	BA	1611	1/1	0.71	0.34	84,84,84,84	0
55	MG	DC	103	1/1	0.71	0.34	96,96,96,96	0
55	MG	AA	3131	1/1	0.71	0.20	94,94,94,94	0
55	MG	CA	3448	1/1	0.71	0.25	63,63,63,63	0
55	MG	AA	3144	1/1	0.72	0.45	71,71,71,71	0
55	MG	CA	3079	1/1	0.72	0.28	73,73,73,73	0
55	MG	BA	1602	1/1	0.72	0.29	75,75,75,75	0
55	MG	AA	3232	1/1	0.72	0.23	75,75,75,75	0
55	MG	CA	3215	1/1	0.72	0.15	137,137,137,137	0
55	MG	CA	3023	1/1	0.72	0.30	85,85,85,85	0
55	MG	AA	3065	1/1	0.72	0.40	49,49,49,49	0
55	MG	CA	3172	1/1	0.72	0.22	86,86,86,86	0
55	MG	BA	1615	1/1	0.73	0.21	113,113,113,113	0
56	OHX	AA	3536	7/7	0.73	0.10	116,124,157,192	1
55	MG	CA	3196	1/1	0.73	0.36	92,92,92,92	0
56	OHX	CA	3429	7/7	0.73	0.10	127,129,142,209	1
55	MG	DA	1678	1/1	0.73	0.13	118,118,118,118	0
55	MG	AA	3141	1/1	0.73	0.32	44,44,44,44	0
55	MG	AA	3098	1/1	0.73	0.23	77,77,77,77	0
55	MG	AA	3218	1/1	0.73	0.27	82,82,82,82	0
55	MG	BA	1712	1/1	0.74	0.29	95,95,95,95	0
56	OHX	AA	3555	7/7	0.74	0.10	112,114,124,192	1
56	OHX	BA	1669	7/7	0.74	0.14	124,127,142,200	1
55	MG	BA	1745	1/1	0.74	0.44	83,83,83,83	0
55	MG	AA	3282	1/1	0.74	0.18	69,69,69,69	0
55	MG	AA	3037	1/1	0.74	0.30	63,63,63,63	0
55	MG	DA	1630	1/1	0.74	0.20	95,95,95,95	0
55	MG	AA	3045	1/1	0.74	0.28	65,65,65,65	0
56	OHX	AA	3534	7/7	0.74	0.10	136,141,145,222	1
55	MG	CA	3086	1/1	0.75	0.29	68,68,68,68	0
55	MG	BA	1722	1/1	0.75	0.34	91,91,91,91	0
55	MG	CA	3136	1/1	0.75	0.19	91,91,91,91	0
55	MG	BA	1704	1/1	0.75	0.13	88,88,88,88	0
55	MG	AA	3268	1/1	0.75	0.30	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	1720	1/1	0.75	0.30	58,58,58,58	0
55	MG	DA	1634	1/1	0.75	0.09	118,118,118,118	0
55	MG	DA	1637	1/1	0.75	0.23	106,106,106,106	0
55	MG	CA	3193	1/1	0.75	0.25	80,80,80,80	0
55	MG	AA	3273	1/1	0.76	0.31	66,66,66,66	0
55	MG	BA	1601	1/1	0.76	0.11	81,81,81,81	0
55	MG	CA	3183	1/1	0.76	0.29	93,93,93,93	0
55	MG	CA	3187	1/1	0.76	0.36	86,86,86,86	0
56	OHX	AA	3562	7/7	0.76	0.10	98,105,127,189	1
55	MG	BA	1747	1/1	0.76	0.28	74,74,74,74	0
55	MG	AA	3125	1/1	0.76	0.20	92,92,92,92	0
56	OHX	CA	3421	7/7	0.76	0.10	113,126,135,198	1
55	MG	BA	1605	1/1	0.76	0.16	104,104,104,104	0
55	MG	AA	3209	1/1	0.76	0.26	57,57,57,57	0
55	MG	CA	3117	1/1	0.76	0.17	69,69,69,69	0
55	MG	BA	1609	1/1	0.76	0.22	73,73,73,73	0
55	MG	BA	1744	1/1	0.76	0.16	90,90,90,90	0
55	MG	AA	3058	1/1	0.77	0.20	73,73,73,73	0
55	MG	AA	3150	1/1	0.77	0.27	68,68,68,68	0
55	MG	AA	3397	1/1	0.77	0.14	80,80,80,80	0
55	MG	DC	104	1/1	0.77	0.28	77,77,77,77	0
56	OHX	AA	3523	7/7	0.77	0.12	109,114,123,180	1
55	MG	CA	3460	1/1	0.77	0.36	72,72,72,72	0
55	MG	BA	1718	1/1	0.77	0.20	78,78,78,78	0
55	MG	BA	1633	1/1	0.77	0.18	59,59,59,59	0
55	MG	CA	3201	1/1	0.77	0.29	79,79,79,79	0
55	MG	CA	3129	1/1	0.77	0.39	81,81,81,81	0
55	MG	AA	3190	1/1	0.77	0.32	69,69,69,69	0
55	MG	BA	1729	1/1	0.77	0.33	73,73,73,73	0
55	MG	BA	1640	1/1	0.77	0.26	73,73,73,73	0
55	MG	DA	1694	1/1	0.77	0.20	104,104,104,104	0
55	MG	CA	3045	1/1	0.77	0.41	91,91,91,91	0
55	MG	CA	3266	1/1	0.77	0.30	64,64,64,64	0
55	MG	DA	1715	1/1	0.77	0.22	89,89,89,89	0
55	MG	AA	3076	1/1	0.77	0.37	72,72,72,72	0
55	MG	CA	3046	1/1	0.78	0.18	76,76,76,76	0
55	MG	DA	1675	1/1	0.78	0.19	92,92,92,92	0
55	MG	DA	1676	1/1	0.78	0.29	83,83,83,83	0
55	MG	BA	1706	1/1	0.78	0.32	79,79,79,79	0
56	OHX	AA	3535	7/7	0.78	0.10	104,112,123,191	1
55	MG	DA	1627	1/1	0.78	0.32	77,77,77,77	0
56	OHX	AA	3545	7/7	0.78	0.14	90,96,105,167	2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	1631	1/1	0.78	0.15	78,78,78,78	0
55	MG	CA	3200	1/1	0.78	0.24	56,56,56,56	0
56	OHX	BA	1657	7/7	0.78	0.15	116,125,141,215	1
56	OHX	BA	1667	7/7	0.78	0.12	118,130,146,200	1
55	MG	AA	3159	1/1	0.78	0.19	65,65,65,65	0
56	OHX	BA	1686	7/7	0.78	0.09	141,143,153,230	1
56	OHX	BA	1692	7/7	0.78	0.10	126,131,140,209	1
55	MG	CA	3202	1/1	0.78	0.33	79,79,79,79	0
56	OHX	CA	3396	7/7	0.78	0.08	135,136,150,198	1
55	MG	AA	3164	1/1	0.78	0.17	70,70,70,70	0
55	MG	CA	3095	1/1	0.78	0.16	54,54,54,54	0
55	MG	DA	1609	1/1	0.78	0.25	91,91,91,91	0
55	MG	AA	3074	1/1	0.78	0.24	73,73,73,73	0
55	MG	CA	3216	1/1	0.78	0.28	91,91,91,91	0
55	MG	BA	1728	1/1	0.78	0.28	90,90,90,90	0
55	MG	AA	3391	1/1	0.79	0.27	59,59,59,59	0
55	MG	CA	3170	1/1	0.79	0.12	65,65,65,65	0
55	MG	CA	3217	1/1	0.79	0.28	58,58,58,58	0
55	MG	BA	1612	1/1	0.79	0.28	81,81,81,81	0
55	MG	CA	3053	1/1	0.79	0.12	99,99,99,99	0
55	MG	AA	3187	1/1	0.79	0.32	86,86,86,86	0
55	MG	AO	201	1/1	0.79	0.23	80,80,80,80	0
55	MG	DA	1635	1/1	0.79	0.36	96,96,96,96	0
56	OHX	BA	1677	7/7	0.79	0.10	141,145,154,220	1
55	MG	AA	3035	1/1	0.79	0.31	64,64,64,64	0
55	MG	BA	1751	1/1	0.79	0.35	95,95,95,95	0
55	MG	AA	3258	1/1	0.79	0.25	65,65,65,65	0
55	MG	AA	3176	1/1	0.79	0.17	60,60,60,60	0
56	OHX	CA	3420	7/7	0.79	0.09	131,141,152,216	1
55	MG	DA	1647	1/1	0.79	0.30	90,90,90,90	0
55	MG	BA	1606	1/1	0.79	0.24	92,92,92,92	0
56	OHX	CA	3470	7/7	0.79	0.10	113,126,137,181	1
55	MG	AA	3350	1/1	0.79	0.32	80,80,80,80	0
55	MG	DA	1660	1/1	0.79	0.33	88,88,88,88	0
55	MG	AA	3378	1/1	0.79	0.25	47,47,47,47	0
55	MG	CA	3035	1/1	0.79	0.18	92,92,92,92	0
55	MG	DA	1662	1/1	0.80	0.29	73,73,73,73	0
55	MG	BA	1610	1/1	0.80	0.19	92,92,92,92	0
55	MG	CA	3207	1/1	0.80	0.23	68,68,68,68	0
55	MG	CA	3042	1/1	0.80	0.24	67,67,67,67	0
56	OHX	AA	3552	7/7	0.80	0.13	105,122,135,199	1
55	MG	CA	3044	1/1	0.80	0.20	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3231	1/1	0.80	0.30	66,66,66,66	0
55	MG	AA	3169	1/1	0.80	0.30	76,76,76,76	0
55	MG	DA	1629	1/1	0.80	0.15	93,93,93,93	0
55	MG	CA	3164	1/1	0.80	0.26	97,97,97,97	0
55	MG	AA	3062	1/1	0.80	0.34	73,73,73,73	0
55	MG	DA	1696	1/1	0.80	0.16	112,112,112,112	0
55	MG	CA	3223	1/1	0.80	0.29	88,88,88,88	0
55	MG	DA	1708	1/1	0.80	0.27	87,87,87,87	0
55	MG	BA	1724	1/1	0.80	0.24	59,59,59,59	0
55	MG	CA	3072	1/1	0.80	0.36	43,43,43,43	0
55	MG	CA	3076	1/1	0.80	0.37	64,64,64,64	0
55	MG	AA	3217	1/1	0.80	0.23	60,60,60,60	0
55	MG	BA	1625	1/1	0.80	0.32	65,65,65,65	0
55	MG	AA	3132	1/1	0.80	0.34	81,81,81,81	0
56	OHX	DA	1753	7/7	0.80	0.13	120,124,134,196	1
55	MG	CA	3088	1/1	0.80	0.30	86,86,86,86	0
55	MG	CA	3028	1/1	0.80	0.19	73,73,73,73	0
55	MG	AA	3285	1/1	0.80	0.32	80,80,80,80	0
55	MG	DA	1657	1/1	0.81	0.33	70,70,70,70	0
55	MG	AA	3235	1/1	0.81	0.21	50,50,50,50	0
55	MG	CA	3225	1/1	0.81	0.18	48,48,48,48	0
55	MG	BA	1725	1/1	0.81	0.35	69,69,69,69	0
55	MG	AB	201	1/1	0.81	0.27	73,73,73,73	0
55	MG	CA	3267	1/1	0.81	0.22	65,65,65,65	0
55	MG	CA	3440	1/1	0.81	0.31	54,54,54,54	0
55	MG	CA	3060	1/1	0.81	0.16	75,75,75,75	0
55	MG	CA	3206	1/1	0.81	0.30	90,90,90,90	0
55	MG	AB	206	1/1	0.81	0.37	83,83,83,83	0
55	MG	BQ	101	1/1	0.81	0.41	96,96,96,96	0
55	MG	CA	3191	1/1	0.81	0.28	72,72,72,72	0
55	MG	CA	3192	1/1	0.81	0.23	87,87,87,87	0
55	MG	BA	1703	1/1	0.81	0.27	108,108,108,108	0
55	MG	BA	1635	1/1	0.81	0.23	96,96,96,96	0
55	MG	CA	3081	1/1	0.81	0.34	63,63,63,63	0
56	OHX	AA	3565	7/7	0.81	0.09	117,122,134,195	1
56	OHX	DC	108	7/7	0.81	0.10	120,132,142,180	1
55	MG	CA	3221	1/1	0.82	0.29	69,69,69,69	0
55	MG	CA	3171	1/1	0.82	0.20	82,82,82,82	0
55	MG	AA	3019	1/1	0.82	0.31	72,72,72,72	0
56	OHX	AA	3522	7/7	0.82	0.10	118,131,145,201	1
55	MG	CA	3262	1/1	0.82	0.41	74,74,74,74	0
55	MG	CA	3178	1/1	0.82	0.19	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	3064	1/1	0.82	0.12	89,89,89,89	0
55	MG	AA	3130	1/1	0.82	0.17	75,75,75,75	0
55	MG	AA	3354	1/1	0.82	0.33	57,57,57,57	0
55	MG	CA	3441	1/1	0.82	0.33	99,99,99,99	0
55	MG	AA	3165	1/1	0.82	0.24	84,84,84,84	0
55	MG	CA	3449	1/1	0.82	0.32	54,54,54,54	0
55	MG	AA	3066	1/1	0.82	0.26	83,83,83,83	0
55	MG	BA	1709	1/1	0.82	0.24	100,100,100,100	0
55	MG	DA	1672	1/1	0.82	0.26	83,83,83,83	0
55	MG	AA	3096	1/1	0.82	0.27	71,71,71,71	0
55	MG	DA	1674	1/1	0.82	0.22	99,99,99,99	0
55	MG	AA	3080	1/1	0.82	0.31	55,55,55,55	0
55	MG	AB	203	1/1	0.82	0.29	71,71,71,71	0
55	MG	AA	3083	1/1	0.82	0.15	88,88,88,88	0
55	MG	AA	3014	1/1	0.82	0.34	44,44,44,44	0
55	MG	AA	3276	1/1	0.82	0.21	69,69,69,69	0
56	OHX	CA	3419	7/7	0.82	0.08	153,156,164,238	1
55	MG	AA	3145	1/1	0.82	0.32	56,56,56,56	0
55	MG	BA	1604	1/1	0.82	0.22	72,72,72,72	0
56	OHX	CA	3427	7/7	0.82	0.08	114,126,136,203	1
55	MG	CA	3144	1/1	0.82	0.30	54,54,54,54	0
55	MG	DA	1626	1/1	0.82	0.33	84,84,84,84	0
55	MG	CA	3145	1/1	0.82	0.42	74,74,74,74	0
55	MG	DA	1710	1/1	0.82	0.15	103,103,103,103	0
56	OHX	DA	1765	7/7	0.82	0.15	117,133,141,227	1
55	MG	AA	3119	1/1	0.82	0.28	64,64,64,64	0
55	MG	AA	3156	1/1	0.82	0.27	45,45,45,45	0
55	MG	BA	1646	1/1	0.82	0.24	95,95,95,95	0
55	MG	DA	1633	1/1	0.82	0.32	74,74,74,74	0
55	MG	CA	3477	1/1	0.83	0.27	60,60,60,60	0
55	MG	CB	206	1/1	0.83	0.23	83,83,83,83	0
55	MG	AA	3021	1/1	0.83	0.30	80,80,80,80	0
55	MG	AA	3129	1/1	0.83	0.20	83,83,83,83	0
55	MG	CA	3163	1/1	0.83	0.28	80,80,80,80	0
55	MG	BA	1710	1/1	0.83	0.25	97,97,97,97	0
55	MG	CA	3065	1/1	0.83	0.29	55,55,55,55	0
55	MG	AA	3091	1/1	0.83	0.20	77,77,77,77	0
55	MG	AA	3072	1/1	0.83	0.22	65,65,65,65	0
55	MG	AA	3166	1/1	0.83	0.25	66,66,66,66	0
55	MG	AA	3351	1/1	0.83	0.30	53,53,53,53	0
55	MG	CA	3227	1/1	0.83	0.32	79,79,79,79	0
55	MG	CA	3230	1/1	0.83	0.27	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	BB	107	7/7	0.83	0.12	71,92,103,147	3
55	MG	DA	1703	1/1	0.83	0.30	73,73,73,73	0
55	MG	AA	3052	1/1	0.83	0.24	85,85,85,85	0
55	MG	AA	3024	1/1	0.83	0.27	63,63,63,63	0
55	MG	BA	1644	1/1	0.83	0.49	94,94,94,94	0
55	MG	CA	3091	1/1	0.83	0.29	74,74,74,74	0
55	MG	CA	3268	1/1	0.83	0.16	52,52,52,52	0
55	MG	CA	3040	1/1	0.83	0.31	70,70,70,70	0
56	OHX	CA	3432	7/7	0.83	0.08	119,135,143,173	1
56	OHX	CA	3435	7/7	0.83	0.13	105,108,131,192	1
55	MG	AA	3252	1/1	0.83	0.32	47,47,47,47	0
55	MG	AA	3034	1/1	0.83	0.27	56,56,56,56	0
56	OHX	C3	101	7/7	0.83	0.10	119,129,151,179	2
55	MG	DA	1644	1/1	0.83	0.10	149,149,149,149	0
55	MG	AA	3017	1/1	0.83	0.23	100,100,100,100	0
56	OHX	DA	1774	7/7	0.83	0.12	131,135,155,208	1
56	OHX	DA	1782	7/7	0.83	0.08	117,128,138,207	1
55	MG	AA	3110	1/1	0.83	0.38	48,48,48,48	0
55	MG	AA	3005	1/1	0.83	0.29	43,43,43,43	0
55	MG	CA	3142	1/1	0.83	0.27	71,71,71,71	0
55	MG	CA	3054	1/1	0.83	0.19	54,54,54,54	0
55	MG	BA	1723	1/1	0.84	0.20	82,82,82,82	0
55	MG	DA	1624	1/1	0.84	0.07	73,73,73,73	0
56	OHX	AA	3564	7/7	0.84	0.07	102,105,128,167	1
55	MG	AB	205	1/1	0.84	0.17	50,50,50,50	0
55	MG	AA	3026	1/1	0.84	0.26	92,92,92,92	0
55	MG	CA	3039	1/1	0.84	0.28	65,65,65,65	0
55	MG	BA	1647	1/1	0.84	0.18	112,112,112,112	0
55	MG	AE	301	1/1	0.84	0.32	52,52,52,52	0
55	MG	DA	1698	1/1	0.84	0.31	95,95,95,95	0
55	MG	DA	1701	1/1	0.84	0.36	90,90,90,90	0
55	MG	AA	3220	1/1	0.84	0.26	64,64,64,64	0
55	MG	AA	3139	1/1	0.84	0.30	48,48,48,48	0
56	OHX	CA	3250	7/7	0.84	0.13	106,109,126,164	1
55	MG	DA	1706	1/1	0.84	0.09	100,100,100,100	0
56	OHX	CA	3399	7/7	0.84	0.13	97,104,115,165	2
55	MG	CA	3134	1/1	0.84	0.25	65,65,65,65	0
55	MG	AA	3015	1/1	0.84	0.26	76,76,76,76	0
55	MG	AA	3038	1/1	0.84	0.15	46,46,46,46	0
55	MG	AA	3208	1/1	0.84	0.23	65,65,65,65	0
55	MG	AA	3281	1/1	0.84	0.38	70,70,70,70	0
55	MG	BA	1753	1/1	0.84	0.24	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3059	1/1	0.84	0.26	85,85,85,85	0
55	MG	DC	101	1/1	0.84	0.34	85,85,85,85	0
56	OHX	CA	3486	7/7	0.84	0.13	87,109,129,181	2
56	OHX	CB	216	7/7	0.84	0.10	117,132,146,206	1
55	MG	CA	3214	1/1	0.84	0.22	65,65,65,65	0
55	MG	CB	204	1/1	0.84	0.24	73,73,73,73	0
55	MG	BA	1715	1/1	0.84	0.26	74,74,74,74	0
55	MG	AB	202	1/1	0.84	0.13	72,72,72,72	0
55	MG	BA	1639	1/1	0.84	0.10	102,102,102,102	0
55	MG	DA	1613	1/1	0.84	0.20	87,87,87,87	0
55	MG	CA	3078	1/1	0.84	0.37	76,76,76,76	0
55	MG	AA	3148	1/1	0.84	0.23	65,65,65,65	0
55	MG	CA	3175	1/1	0.84	0.43	64,64,64,64	0
55	MG	CA	3027	1/1	0.84	0.26	81,81,81,81	0
55	MG	DA	1712	1/1	0.85	0.33	98,98,98,98	0
55	MG	DA	1670	1/1	0.85	0.24	64,64,64,64	0
55	MG	CA	3037	1/1	0.85	0.23	89,89,89,89	0
56	OHX	BA	1695	7/7	0.85	0.07	129,147,158,217	1
56	OHX	BA	1806	7/7	0.85	0.14	97,127,142,180	2
55	MG	DA	1632	1/1	0.85	0.20	83,83,83,83	0
55	MG	CA	3057	1/1	0.85	0.26	95,95,95,95	0
55	MG	DA	1601	1/1	0.85	0.25	87,87,87,87	0
55	MG	DA	1603	1/1	0.85	0.39	71,71,71,71	0
55	MG	CA	3189	1/1	0.85	0.31	67,67,67,67	0
56	OHX	CA	3413	7/7	0.85	0.10	121,130,144,215	1
56	OHX	CA	3414	7/7	0.85	0.09	155,156,163,215	1
55	MG	BA	1608	1/1	0.85	0.23	55,55,55,55	0
56	OHX	AA	3333	7/7	0.85	0.12	91,114,128,179	2
56	OHX	AA	3369	7/7	0.85	0.14	80,102,119,165	1
56	OHX	CA	3422	7/7	0.85	0.09	126,137,143,193	1
56	OHX	AA	3513	7/7	0.85	0.09	80,88,116,153	1
55	MG	AA	3216	1/1	0.85	0.28	71,71,71,71	0
55	MG	DA	1686	1/1	0.85	0.14	73,73,73,73	0
55	MG	BA	1660	1/1	0.85	0.20	97,97,97,97	0
56	OHX	AA	3530	7/7	0.85	0.12	101,121,143,206	1
55	MG	CA	3195	1/1	0.85	0.17	68,68,68,68	0
56	OHX	CA	3491	7/7	0.85	0.11	92,108,117,175	1
55	MG	AA	3107	1/1	0.85	0.11	79,79,79,79	0
55	MG	DA	1697	1/1	0.85	0.25	72,72,72,72	0
56	OHX	CB	219	7/7	0.85	0.08	145,151,161,232	1
55	MG	CA	3071	1/1	0.85	0.26	51,51,51,51	0
55	MG	DA	1656	1/1	0.85	0.28	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	1702	1/1	0.85	0.11	122,122,122,122	0
55	MG	CA	3114	1/1	0.85	0.32	57,57,57,57	0
55	MG	AA	3126	1/1	0.85	0.21	85,85,85,85	0
56	OHX	DA	1783	7/7	0.85	0.09	123,123,145,185	1
55	MG	AA	3105	1/1	0.85	0.23	124,124,124,124	0
56	OHX	DA	1805	7/7	0.85	0.07	155,158,165,245	1
56	OHX	DA	1809	7/7	0.85	0.07	124,126,139,221	1
56	OHX	DR	101	7/7	0.85	0.07	135,141,146,189	1
55	MG	DA	1707	1/1	0.85	0.26	85,85,85,85	0
55	MG	CA	3051	1/1	0.85	0.31	69,69,69,69	0
55	MG	AA	3379	1/1	0.85	0.35	55,55,55,55	0
55	MG	AA	3079	1/1	0.86	0.26	88,88,88,88	0
56	OHX	BA	1674	7/7	0.86	0.09	117,122,137,199	1
56	OHX	BA	1675	7/7	0.86	0.09	120,128,140,197	1
55	MG	BA	1714	1/1	0.86	0.18	56,56,56,56	0
55	MG	CA	3109	1/1	0.86	0.23	56,56,56,56	0
55	MG	AA	3046	1/1	0.86	0.24	68,68,68,68	0
55	MG	BB	102	1/1	0.86	0.19	85,85,85,85	0
56	OHX	BA	1790	7/7	0.86	0.11	96,123,133,185	1
55	MG	DA	1640	1/1	0.86	0.20	83,83,83,83	0
55	MG	CA	3118	1/1	0.86	0.26	69,69,69,69	0
55	MG	DA	1709	1/1	0.86	0.36	80,80,80,80	0
55	MG	CA	3124	1/1	0.86	0.29	44,44,44,44	0
56	OHX	CA	3252	7/7	0.86	0.13	108,118,136,203	1
56	OHX	CA	3371	7/7	0.86	0.14	67,90,123,162	1
55	MG	AO	203	1/1	0.86	0.19	56,56,56,56	0
55	MG	DA	1713	1/1	0.86	0.30	79,79,79,79	0
56	OHX	CA	3409	7/7	0.86	0.11	97,100,119,183	1
55	MG	BA	1641	1/1	0.86	0.16	85,85,85,85	0
55	MG	BA	1721	1/1	0.86	0.25	70,70,70,70	0
56	OHX	CA	3415	7/7	0.86	0.10	134,135,143,187	1
55	MG	DA	1716	1/1	0.86	0.26	85,85,85,85	0
55	MG	CA	3014	1/1	0.86	0.22	76,76,76,76	0
55	MG	CA	3479	1/1	0.86	0.33	64,64,64,64	0
55	MG	DA	1725	1/1	0.86	0.32	87,87,87,87	0
55	MG	AA	3382	1/1	0.86	0.27	36,36,36,36	0
55	MG	BA	1617	1/1	0.86	0.25	71,71,71,71	0
55	MG	BA	1618	1/1	0.86	0.27	63,63,63,63	0
55	MG	AA	3157	1/1	0.86	0.35	49,49,49,49	0
55	MG	CA	3151	1/1	0.86	0.22	76,76,76,76	0
55	MG	DA	1607	1/1	0.86	0.23	82,82,82,82	0
56	OHX	CA	3487	7/7	0.86	0.08	135,139,147,210	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	3156	1/1	0.86	0.38	84,84,84,84	0
55	MG	AA	3256	1/1	0.86	0.33	53,53,53,53	0
55	MG	DA	1614	1/1	0.86	0.17	91,91,91,91	0
55	MG	BA	1628	1/1	0.86	0.28	80,80,80,80	0
55	MG	CA	3218	1/1	0.86	0.26	83,83,83,83	0
55	MG	AA	3211	1/1	0.86	0.36	62,62,62,62	0
55	MG	CA	3082	1/1	0.86	0.34	62,62,62,62	0
55	MG	CA	3084	1/1	0.86	0.39	60,60,60,60	0
55	MG	DA	1684	1/1	0.86	0.29	79,79,79,79	0
55	MG	AA	3048	1/1	0.86	0.34	94,94,94,94	0
55	MG	DA	1687	1/1	0.86	0.15	63,63,63,63	0
55	MG	CA	3177	1/1	0.86	0.21	57,57,57,57	0
55	MG	AA	3270	1/1	0.86	0.09	94,94,94,94	0
55	MG	AA	3084	1/1	0.86	0.23	58,58,58,58	0
55	MG	AA	3275	1/1	0.86	0.28	64,64,64,64	0
56	OHX	BA	1666	7/7	0.86	0.09	117,122,134,158	2
55	MG	CA	3188	1/1	0.86	0.33	60,60,60,60	0
55	MG	BA	1649	1/1	0.87	0.14	74,74,74,74	0
55	MG	AA	3392	1/1	0.87	0.35	64,64,64,64	0
55	MG	CA	3056	1/1	0.87	0.28	79,79,79,79	0
55	MG	BA	1698	1/1	0.87	0.30	62,62,62,62	0
55	MG	AA	3040	1/1	0.87	0.27	47,47,47,47	0
55	MG	CA	3125	1/1	0.87	0.16	52,52,52,52	0
55	MG	CA	3446	1/1	0.87	0.33	47,47,47,47	0
55	MG	A1	201	1/1	0.87	0.30	71,71,71,71	0
55	MG	A3	101	1/1	0.87	0.31	60,60,60,60	0
55	MG	AA	3171	1/1	0.87	0.20	48,48,48,48	0
55	MG	CA	3456	1/1	0.87	0.23	66,66,66,66	0
55	MG	CA	3066	1/1	0.87	0.38	56,56,56,56	0
55	MG	BA	1734	1/1	0.87	0.32	70,70,70,70	0
55	MG	CA	3029	1/1	0.87	0.19	76,76,76,76	0
56	OHX	CA	3348	7/7	0.87	0.15	104,111,132,178	1
55	MG	CA	3471	1/1	0.87	0.30	57,57,57,57	0
56	OHX	CA	3379	7/7	0.87	0.07	134,137,155,207	1
55	MG	DA	1655	1/1	0.87	0.24	78,78,78,78	0
56	OHX	CA	3397	7/7	0.87	0.07	128,138,154,219	1
55	MG	BA	1741	1/1	0.87	0.38	73,73,73,73	0
55	MG	CA	3478	1/1	0.87	0.29	82,82,82,82	0
55	MG	BA	1708	1/1	0.87	0.28	77,77,77,77	0
55	MG	CA	3036	1/1	0.87	0.22	87,87,87,87	0
55	MG	AA	3106	1/1	0.87	0.24	70,70,70,70	0
55	MG	DA	1665	1/1	0.87	0.27	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	AA	3331	7/7	0.87	0.14	72,87,130,163	3
55	MG	AA	3267	1/1	0.87	0.30	80,80,80,80	0
55	MG	AA	3068	1/1	0.87	0.20	61,61,61,61	0
56	OHX	AA	3403	7/7	0.87	0.10	109,110,128,178	1
56	OHX	AA	3488	7/7	0.87	0.10	86,101,105,150	1
56	OHX	AA	3510	7/7	0.87	0.12	92,103,113,152	2
56	OHX	CA	3434	7/7	0.87	0.10	96,110,126,177	1
56	OHX	AA	3512	7/7	0.87	0.11	99,114,126,166	2
56	OHX	CA	3436	7/7	0.87	0.08	115,121,137,192	1
55	MG	CA	3041	1/1	0.87	0.14	73,73,73,73	0
55	MG	AA	3053	1/1	0.87	0.26	60,60,60,60	0
55	MG	DA	1608	1/1	0.87	0.19	78,78,78,78	0
55	MG	BA	1626	1/1	0.87	0.14	81,81,81,81	0
55	MG	CA	3219	1/1	0.87	0.44	79,79,79,79	0
56	OHX	CB	217	7/7	0.87	0.08	128,135,146,182	1
56	OHX	AA	3532	7/7	0.87	0.08	89,105,116,172	1
55	MG	AA	3061	1/1	0.87	0.22	49,49,49,49	0
55	MG	CA	3176	1/1	0.87	0.40	67,67,67,67	0
55	MG	CA	3222	1/1	0.87	0.20	81,81,81,81	0
55	MG	DA	1683	1/1	0.87	0.37	71,71,71,71	0
55	MG	AF	302	1/1	0.87	0.23	81,81,81,81	0
55	MG	DA	1620	1/1	0.87	0.32	79,79,79,79	0
55	MG	CA	3101	1/1	0.87	0.31	59,59,59,59	0
55	MG	CA	3102	1/1	0.87	0.31	67,67,67,67	0
56	OHX	DA	1801	7/7	0.87	0.08	141,143,154,216	1
55	MG	CA	3184	1/1	0.87	0.35	60,60,60,60	0
56	OHX	DA	1808	7/7	0.87	0.10	119,124,131,178	1
56	OHX	AA	3566	7/7	0.87	0.09	92,97,126,175	2
56	OHX	DK	201	7/7	0.87	0.08	137,138,149,200	1
56	OHX	AB	216	7/7	0.87	0.12	88,124,141,184	1
55	MG	CA	3231	1/1	0.87	0.27	89,89,89,89	0
56	OHX	BA	1661	7/7	0.87	0.09	108,124,128,170	1
55	MG	BS	101	1/1	0.87	0.20	93,93,93,93	0
55	MG	AA	3381	1/1	0.88	0.27	59,59,59,59	0
55	MG	CA	3258	1/1	0.88	0.33	56,56,56,56	0
55	MG	CA	3050	1/1	0.88	0.24	65,65,65,65	0
55	MG	AA	3226	1/1	0.88	0.28	42,42,42,42	0
55	MG	CA	3052	1/1	0.88	0.28	66,66,66,66	0
55	MG	BA	1603	1/1	0.88	0.20	63,63,63,63	0
55	MG	BA	1711	1/1	0.88	0.29	94,94,94,94	0
56	OHX	AA	3524	7/7	0.88	0.07	111,120,128,172	1
55	MG	AA	3013	1/1	0.88	0.22	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3143	1/1	0.88	0.30	46,46,46,46	0
56	OHX	CA	3417	7/7	0.88	0.07	151,167,187,222	1
55	MG	AA	3396	1/1	0.88	0.40	71,71,71,71	0
55	MG	AA	3279	1/1	0.88	0.25	81,81,81,81	0
55	MG	CA	3140	1/1	0.88	0.27	59,59,59,59	0
55	MG	CA	3003	1/1	0.88	0.22	51,51,51,51	0
56	OHX	CA	3426	7/7	0.88	0.06	142,146,155,215	1
55	MG	CA	3008	1/1	0.88	0.23	52,52,52,52	0
55	MG	CA	3204	1/1	0.88	0.29	73,73,73,73	0
56	OHX	CA	3431	7/7	0.88	0.08	105,117,132,179	1
56	OHX	AA	3554	7/7	0.88	0.07	116,128,150,205	1
55	MG	AA	3193	1/1	0.88	0.08	58,58,58,58	0
55	MG	AA	3206	1/1	0.88	0.34	64,64,64,64	0
55	MG	CA	3208	1/1	0.88	0.29	70,70,70,70	0
55	MG	BA	1643	1/1	0.88	0.10	78,78,78,78	0
55	MG	AA	3163	1/1	0.88	0.20	61,61,61,61	0
56	OHX	AA	3567	7/7	0.88	0.08	103,106,118,172	1
55	MG	AA	3115	1/1	0.88	0.20	51,51,51,51	0
56	OHX	A1	203	7/7	0.88	0.11	100,107,140,182	3
55	MG	CA	3480	1/1	0.88	0.17	72,72,72,72	0
55	MG	DA	1650	1/1	0.88	0.23	67,67,67,67	0
55	MG	CB	201	1/1	0.88	0.12	77,77,77,77	0
55	MG	CA	3033	1/1	0.88	0.15	71,71,71,71	0
55	MG	AA	3057	1/1	0.88	0.29	72,72,72,72	0
55	MG	AA	3123	1/1	0.88	0.18	72,72,72,72	0
55	MG	AE	302	1/1	0.88	0.22	71,71,71,71	0
55	MG	BA	1652	1/1	0.88	0.20	63,63,63,63	0
55	MG	DA	1663	1/1	0.88	0.19	66,66,66,66	0
55	MG	AA	3049	1/1	0.88	0.25	64,64,64,64	0
55	MG	AA	3353	1/1	0.88	0.21	39,39,39,39	0
55	MG	AA	3151	1/1	0.88	0.21	62,62,62,62	0
55	MG	AA	3044	1/1	0.88	0.33	72,72,72,72	0
56	OHX	BA	1816	7/7	0.88	0.09	127,130,142,194	1
56	OHX	DA	1810	7/7	0.88	0.05	134,135,143,197	1
56	OHX	DG	302	7/7	0.88	0.07	133,142,147,197	1
55	MG	D1	101	1/1	0.88	0.28	78,78,78,78	0
55	MG	CA	3179	1/1	0.88	0.09	73,73,73,73	0
55	MG	BA	1627	1/1	0.88	0.29	80,80,80,80	0
55	MG	AA	3224	1/1	0.88	0.22	68,68,68,68	0
56	OHX	CA	3284	7/7	0.88	0.09	136,147,155,216	1
55	MG	BA	1650	1/1	0.89	0.36	72,72,72,72	0
55	MG	CA	3018	1/1	0.89	0.34	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	1651	1/1	0.89	0.10	90,90,90,90	0
55	MG	CA	3211	1/1	0.89	0.12	116,116,116,116	0
55	MG	CA	3026	1/1	0.89	0.10	58,58,58,58	0
55	MG	CA	3157	1/1	0.89	0.31	76,76,76,76	0
55	MG	AA	3234	1/1	0.89	0.13	56,56,56,56	0
55	MG	BA	1727	1/1	0.89	0.28	70,70,70,70	0
55	MG	CB	202	1/1	0.89	0.14	99,99,99,99	0
56	OHX	CA	3269	7/7	0.89	0.14	98,100,123,153	2
55	MG	AA	3063	1/1	0.89	0.20	76,76,76,76	0
55	MG	DC	106	1/1	0.89	0.41	91,91,91,91	0
56	OHX	CA	3358	7/7	0.89	0.07	128,130,147,230	1
55	MG	CB	205	1/1	0.89	0.33	74,74,74,74	0
56	OHX	CA	3378	7/7	0.89	0.09	128,141,148,178	1
56	OHX	AA	3138	7/7	0.89	0.12	88,92,127,173	1
56	OHX	AA	3302	7/7	0.89	0.10	88,114,124,193	1
56	OHX	AA	3306	7/7	0.89	0.08	134,139,151,214	1
55	MG	CA	3030	1/1	0.89	0.22	89,89,89,89	0
56	OHX	CA	3407	7/7	0.89	0.08	142,149,155,227	1
55	MG	AA	3244	1/1	0.89	0.21	49,49,49,49	0
56	OHX	AA	3366	7/7	0.89	0.13	85,90,106,173	1
55	MG	BA	1730	1/1	0.89	0.30	73,73,73,73	0
56	OHX	AA	3370	7/7	0.89	0.10	115,126,140,200	1
55	MG	DA	1667	1/1	0.89	0.32	68,68,68,68	0
55	MG	AA	3102	1/1	0.89	0.25	79,79,79,79	0
56	OHX	AA	3490	7/7	0.89	0.07	94,113,129,158	1
55	MG	DA	1669	1/1	0.89	0.31	64,64,64,64	0
55	MG	BA	1702	1/1	0.89	0.17	62,62,62,62	0
55	MG	AA	3167	1/1	0.89	0.32	53,53,53,53	0
55	MG	AA	3155	1/1	0.89	0.10	85,85,85,85	0
55	MG	AA	3212	1/1	0.89	0.24	35,35,35,35	0
55	MG	AA	3128	1/1	0.89	0.23	54,54,54,54	0
55	MG	DA	1615	1/1	0.89	0.15	98,98,98,98	0
55	MG	DA	1677	1/1	0.89	0.23	76,76,76,76	0
55	MG	DA	1616	1/1	0.89	0.24	88,88,88,88	0
55	MG	AA	3175	1/1	0.89	0.25	39,39,39,39	0
55	MG	CA	3257	1/1	0.89	0.21	60,60,60,60	0
55	MG	AA	3023	1/1	0.89	0.24	52,52,52,52	0
56	OHX	AA	3539	7/7	0.89	0.07	116,125,136,193	1
56	OHX	AA	3540	7/7	0.89	0.08	109,134,164,188	2
56	OHX	CB	214	7/7	0.89	0.09	129,139,146,186	1
55	MG	CA	3260	1/1	0.89	0.22	71,71,71,71	0
55	MG	AA	3117	1/1	0.89	0.19	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	1613	1/1	0.89	0.17	65,65,65,65	0
55	MG	BA	1713	1/1	0.89	0.15	59,59,59,59	0
55	MG	DA	1625	1/1	0.89	0.12	97,97,97,97	0
55	MG	DA	1695	1/1	0.89	0.30	76,76,76,76	0
55	MG	BB	101	1/1	0.89	0.34	70,70,70,70	0
55	MG	BA	1614	1/1	0.89	0.25	73,73,73,73	0
56	OHX	DA	1775	7/7	0.89	0.08	133,145,148,215	1
55	MG	DA	1628	1/1	0.89	0.31	78,78,78,78	0
55	MG	CA	3439	1/1	0.89	0.32	63,63,63,63	0
56	OHX	DA	1786	7/7	0.89	0.08	143,151,161,223	1
56	OHX	DA	1787	7/7	0.89	0.09	95,113,121,162	2
56	OHX	AB	218	7/7	0.89	0.07	128,132,146,199	1
56	OHX	DA	1796	7/7	0.89	0.07	134,139,149,195	1
55	MG	AA	3070	1/1	0.89	0.13	52,52,52,52	0
56	OHX	DA	1803	7/7	0.89	0.07	135,141,144,207	1
55	MG	AA	3041	1/1	0.89	0.15	49,49,49,49	0
55	MG	CA	3443	1/1	0.89	0.36	49,49,49,49	0
55	MG	AA	3199	1/1	0.89	0.33	76,76,76,76	0
55	MG	BD	101	1/1	0.89	0.24	93,93,93,93	0
56	OHX	DA	1812	7/7	0.89	0.08	149,158,168,252	1
55	MG	CA	3059	1/1	0.89	0.32	63,63,63,63	0
55	MG	DA	1636	1/1	0.89	0.21	75,75,75,75	0
55	MG	AA	3390	1/1	0.89	0.28	46,46,46,46	0
55	MG	CA	3005	1/1	0.89	0.15	48,48,48,48	0
55	MG	AA	3201	1/1	0.89	0.22	45,45,45,45	0
56	OHX	BA	1690	7/7	0.89	0.08	118,127,134,188	1
55	MG	CA	3476	1/1	0.90	0.26	52,52,52,52	0
55	MG	BA	1623	1/1	0.90	0.20	67,67,67,67	0
55	MG	AA	3221	1/1	0.90	0.13	68,68,68,68	0
55	MG	DA	1658	1/1	0.90	0.31	64,64,64,64	0
55	MG	AA	3127	1/1	0.90	0.27	57,57,57,57	0
55	MG	CA	3119	1/1	0.90	0.19	61,61,61,61	0
56	OHX	CA	3306	7/7	0.90	0.09	98,106,119,148	1
55	MG	AA	3261	1/1	0.90	0.36	64,64,64,64	0
56	OHX	AA	3365	7/7	0.90	0.14	90,106,114,161	2
55	MG	AA	3109	1/1	0.90	0.34	47,47,47,47	0
55	MG	CB	203	1/1	0.90	0.11	111,111,111,111	0
55	MG	AA	3229	1/1	0.90	0.28	59,59,59,59	0
56	OHX	CA	3380	7/7	0.90	0.07	106,119,130,170	1
55	MG	CA	3131	1/1	0.90	0.27	65,65,65,65	0
56	OHX	AA	3407	7/7	0.90	0.10	108,117,126,165	1
56	OHX	AA	3484	7/7	0.90	0.11	76,100,111,147	2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3380	1/1	0.90	0.21	66,66,66,66	0
55	MG	CA	3212	1/1	0.90	0.29	75,75,75,75	0
56	OHX	CA	3411	7/7	0.90	0.07	117,123,138,184	1
56	OHX	AA	3505	7/7	0.90	0.12	86,108,110,156	1
55	MG	AA	3060	1/1	0.90	0.13	70,70,70,70	0
55	MG	AA	3114	1/1	0.90	0.22	47,47,47,47	0
55	MG	DA	1604	1/1	0.90	0.28	82,82,82,82	0
56	OHX	AA	3519	7/7	0.90	0.08	140,146,150,214	1
55	MG	BB	103	1/1	0.90	0.27	91,91,91,91	0
55	MG	CA	3055	1/1	0.90	0.17	66,66,66,66	0
55	MG	AA	3386	1/1	0.90	0.14	42,42,42,42	0
55	MG	DA	1611	1/1	0.90	0.18	92,92,92,92	0
55	MG	DA	1679	1/1	0.90	0.17	69,69,69,69	0
55	MG	BB	105	1/1	0.90	0.39	63,63,63,63	0
55	MG	AA	3274	1/1	0.90	0.28	89,89,89,89	0
55	MG	AA	3078	1/1	0.90	0.24	59,59,59,59	0
56	OHX	CA	3433	7/7	0.90	0.07	121,129,144,183	1
55	MG	CA	3153	1/1	0.90	0.23	56,56,56,56	0
56	OHX	AA	3537	7/7	0.90	0.07	171,189,202,242	1
55	MG	AA	3103	1/1	0.90	0.08	97,97,97,97	0
56	OHX	CA	3437	7/7	0.90	0.10	98,105,117,166	2
56	OHX	CA	3466	7/7	0.90	0.12	96,98,116,157	1
56	OHX	CA	3467	7/7	0.90	0.11	131,146,152,199	1
55	MG	CA	3002	1/1	0.90	0.29	50,50,50,50	0
55	MG	BA	1716	1/1	0.90	0.21	55,55,55,55	0
55	MG	AA	3243	1/1	0.90	0.30	51,51,51,51	0
55	MG	CA	3229	1/1	0.90	0.27	80,80,80,80	0
56	OHX	CB	213	7/7	0.90	0.08	131,144,166,188	1
55	MG	CA	3165	1/1	0.90	0.25	57,57,57,57	0
56	OHX	CB	215	7/7	0.90	0.08	108,133,144,220	1
56	OHX	AA	3560	7/7	0.90	0.07	102,104,127,184	1
55	MG	CA	3166	1/1	0.90	0.35	58,58,58,58	0
55	MG	CA	3067	1/1	0.90	0.26	49,49,49,49	0
55	MG	BA	1642	1/1	0.90	0.10	102,102,102,102	0
55	MG	AA	3071	1/1	0.90	0.33	68,68,68,68	0
55	MG	AA	3409	1/1	0.90	0.30	56,56,56,56	0
56	OHX	AA	3568	7/7	0.90	0.09	78,93,100,118	1
56	OHX	AB	210	7/7	0.90	0.10	83,107,129,146	3
55	MG	CA	3021	1/1	0.90	0.12	60,60,60,60	0
55	MG	BA	1645	1/1	0.90	0.33	51,51,51,51	0
55	MG	AA	3020	1/1	0.90	0.39	44,44,44,44	0
56	OHX	DA	1785	7/7	0.90	0.09	110,114,129,164	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3158	1/1	0.90	0.26	50,50,50,50	0
55	MG	CA	3083	1/1	0.90	0.27	44,44,44,44	0
55	MG	AA	3284	1/1	0.90	0.11	66,66,66,66	0
55	MG	CA	3185	1/1	0.90	0.39	75,75,75,75	0
55	MG	AA	3073	1/1	0.90	0.18	69,69,69,69	0
55	MG	AA	3250	1/1	0.90	0.35	56,56,56,56	0
55	MG	AA	3348	1/1	0.90	0.36	46,46,46,46	0
56	OHX	DA	1807	7/7	0.90	0.07	117,126,135,195	1
55	MG	AA	3069	1/1	0.90	0.26	62,62,62,62	0
55	MG	BA	1735	1/1	0.90	0.15	48,48,48,48	0
55	MG	CA	3096	1/1	0.90	0.18	64,64,64,64	0
55	MG	BA	1739	1/1	0.90	0.32	70,70,70,70	0
55	MG	DA	1645	1/1	0.90	0.26	91,91,91,91	0
56	OHX	BA	1783	7/7	0.90	0.14	77,87,125,141	2
55	MG	BA	1658	1/1	0.90	0.25	71,71,71,71	0
56	OHX	BA	1805	7/7	0.90	0.11	90,105,122,143	3
55	MG	BA	1621	1/1	0.90	0.27	55,55,55,55	0
55	MG	AF	301	1/1	0.90	0.23	83,83,83,83	0
55	MG	AA	3077	1/1	0.91	0.22	73,73,73,73	0
56	OHX	AA	3487	7/7	0.91	0.07	95,110,116,167	1
55	MG	AA	3124	1/1	0.91	0.24	70,70,70,70	0
56	OHX	CA	3375	7/7	0.91	0.10	103,118,131,145	1
55	MG	CA	3143	1/1	0.91	0.24	60,60,60,60	0
55	MG	DA	1605	1/1	0.91	0.23	63,63,63,63	0
55	MG	AA	3101	1/1	0.91	0.22	63,63,63,63	0
56	OHX	CA	3390	7/7	0.91	0.07	117,128,152,209	1
56	OHX	CA	3393	7/7	0.91	0.12	93,114,121,181	1
55	MG	CA	3025	1/1	0.91	0.12	83,83,83,83	0
55	MG	AA	3249	1/1	0.91	0.31	58,58,58,58	0
56	OHX	AA	3515	7/7	0.91	0.08	100,121,139,211	1
56	OHX	CA	3404	7/7	0.91	0.09	149,155,166,217	1
55	MG	CA	3148	1/1	0.91	0.21	57,57,57,57	0
55	MG	BA	1742	1/1	0.91	0.37	86,86,86,86	0
55	MG	AA	3036	1/1	0.91	0.26	36,36,36,36	0
55	MG	CA	3154	1/1	0.91	0.26	46,46,46,46	0
55	MG	CA	3155	1/1	0.91	0.20	58,58,58,58	0
55	MG	AA	3162	1/1	0.91	0.33	38,38,38,38	0
55	MG	AA	3398	1/1	0.91	0.23	51,51,51,51	0
55	MG	CA	3224	1/1	0.91	0.25	77,77,77,77	0
55	MG	CA	3159	1/1	0.91	0.28	75,75,75,75	0
55	MG	CA	3031	1/1	0.91	0.08	53,53,53,53	0
55	MG	CA	3032	1/1	0.91	0.33	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3012	1/1	0.91	0.20	46,46,46,46	0
55	MG	AA	3414	1/1	0.91	0.24	57,57,57,57	0
56	OHX	AA	3542	7/7	0.91	0.08	118,127,135,189	1
55	MG	CA	3167	1/1	0.91	0.29	75,75,75,75	0
55	MG	BA	1750	1/1	0.91	0.24	72,72,72,72	0
55	MG	AA	3416	1/1	0.91	0.25	74,74,74,74	0
55	MG	AA	3227	1/1	0.91	0.26	63,63,63,63	0
55	MG	DA	1704	1/1	0.91	0.31	73,73,73,73	0
55	MG	CA	3087	1/1	0.91	0.06	70,70,70,70	0
55	MG	CA	3038	1/1	0.91	0.15	74,74,74,74	0
55	MG	AA	3349	1/1	0.91	0.32	61,61,61,61	0
55	MG	AA	3033	1/1	0.91	0.18	48,48,48,48	0
55	MG	AA	3266	1/1	0.91	0.12	78,78,78,78	0
55	MG	CA	3099	1/1	0.91	0.24	51,51,51,51	0
56	OHX	AA	3569	7/7	0.91	0.07	116,117,125,191	1
55	MG	CA	3100	1/1	0.91	0.36	63,63,63,63	0
55	MG	BA	1717	1/1	0.91	0.26	51,51,51,51	0
55	MG	CA	3186	1/1	0.91	0.17	75,75,75,75	0
55	MG	AA	3064	1/1	0.91	0.11	66,66,66,66	0
55	MG	CA	3103	1/1	0.91	0.23	70,70,70,70	0
55	MG	AA	3149	1/1	0.91	0.15	74,74,74,74	0
56	OHX	BA	1662	7/7	0.91	0.08	105,117,141,193	1
56	OHX	BA	1664	7/7	0.91	0.07	108,126,142,197	1
55	MG	AA	3356	1/1	0.91	0.34	58,58,58,58	0
55	MG	AA	3118	1/1	0.91	0.20	53,53,53,53	0
55	MG	DB	101	1/1	0.91	0.33	78,78,78,78	0
56	OHX	BA	1673	7/7	0.91	0.08	117,123,127,191	1
55	MG	CA	3116	1/1	0.91	0.24	69,69,69,69	0
55	MG	AA	3056	1/1	0.91	0.16	36,36,36,36	0
55	MG	DC	102	1/1	0.91	0.41	69,69,69,69	0
56	OHX	DA	1784	7/7	0.91	0.07	150,153,166,225	1
56	OHX	BA	1680	7/7	0.91	0.07	120,125,145,238	1
55	MG	AA	3241	1/1	0.91	0.22	60,60,60,60	0
55	MG	DA	1654	1/1	0.91	0.26	61,61,61,61	0
55	MG	BA	1624	1/1	0.91	0.20	70,70,70,70	0
55	MG	CA	3121	1/1	0.91	0.28	55,55,55,55	0
56	OHX	DA	1798	7/7	0.91	0.07	128,133,140,212	1
55	MG	BA	1653	1/1	0.91	0.17	63,63,63,63	0
55	MG	AA	3122	1/1	0.91	0.22	62,62,62,62	0
55	MG	AA	3174	1/1	0.91	0.29	76,76,76,76	0
55	MG	CA	3203	1/1	0.91	0.21	47,47,47,47	0
55	MG	DA	1661	1/1	0.91	0.39	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	3009	1/1	0.91	0.24	39,39,39,39	0
55	MG	CA	3013	1/1	0.91	0.15	47,47,47,47	0
56	OHX	CA	3245	7/7	0.91	0.09	99,120,129,189	1
55	MG	AA	3383	1/1	0.91	0.22	46,46,46,46	0
55	MG	CA	3138	1/1	0.91	0.43	53,53,53,53	0
55	MG	CA	3061	1/1	0.91	0.30	64,64,64,64	0
56	OHX	AA	3406	7/7	0.91	0.13	84,92,109,162	1
56	OHX	CA	3304	7/7	0.91	0.09	113,122,141,181	2
55	MG	CA	3210	1/1	0.91	0.34	74,74,74,74	0
56	OHX	CA	3340	7/7	0.92	0.09	115,122,140,168	1
55	MG	CA	3068	1/1	0.92	0.29	44,44,44,44	0
55	MG	CA	3069	1/1	0.92	0.36	69,69,69,69	0
56	OHX	CA	3359	7/7	0.92	0.07	115,123,136,171	2
55	MG	AA	3152	1/1	0.92	0.23	56,56,56,56	0
56	OHX	CA	3373	7/7	0.92	0.09	113,122,129,160	1
56	OHX	AA	3525	7/7	0.92	0.09	100,109,122,187	1
55	MG	CA	3139	1/1	0.92	0.21	56,56,56,56	0
56	OHX	AA	3527	7/7	0.92	0.06	130,134,147,188	1
55	MG	AA	3255	1/1	0.92	0.16	64,64,64,64	0
56	OHX	CA	3383	7/7	0.92	0.07	111,116,132,194	1
56	OHX	CA	3386	7/7	0.92	0.08	110,116,134,181	1
55	MG	CA	3452	1/1	0.92	0.13	51,51,51,51	0
56	OHX	CA	3392	7/7	0.92	0.08	126,132,142,192	1
56	OHX	AA	3533	7/7	0.92	0.10	98,103,114,150	2
56	OHX	CA	3395	7/7	0.92	0.09	106,111,125,156	1
55	MG	CA	3454	1/1	0.92	0.30	51,51,51,51	0
55	MG	CA	3074	1/1	0.92	0.35	64,64,64,64	0
55	MG	BA	1754	1/1	0.92	0.29	61,61,61,61	0
56	OHX	CA	3400	7/7	0.92	0.08	116,133,145,220	1
56	OHX	CA	3402	7/7	0.92	0.07	159,162,170,218	1
55	MG	CA	3077	1/1	0.92	0.16	57,57,57,57	0
55	MG	AA	3153	1/1	0.92	0.36	64,64,64,64	0
56	OHX	CA	3408	7/7	0.92	0.05	136,139,143,209	1
55	MG	CA	3459	1/1	0.92	0.17	56,56,56,56	0
56	OHX	AA	3541	7/7	0.92	0.09	102,114,134,158	2
55	MG	AA	3135	1/1	0.92	0.20	67,67,67,67	0
55	MG	AA	3177	1/1	0.92	0.23	37,37,37,37	0
56	OHX	AA	3546	7/7	0.92	0.09	98,103,119,179	1
56	OHX	AA	3551	7/7	0.92	0.06	141,143,149,194	1
56	OHX	CA	3418	7/7	0.92	0.08	115,119,129,166	1
55	MG	CA	3473	1/1	0.92	0.22	50,50,50,50	0
55	MG	CA	3475	1/1	0.92	0.18	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3136	1/1	0.92	0.15	57,57,57,57	0
56	OHX	AA	3559	7/7	0.92	0.05	124,133,143,186	1
56	OHX	CA	3424	7/7	0.92	0.06	141,145,151,214	1
56	OHX	CA	3425	7/7	0.92	0.06	101,110,125,187	1
55	MG	AA	3055	1/1	0.92	0.26	65,65,65,65	0
55	MG	AA	3081	1/1	0.92	0.39	56,56,56,56	0
56	OHX	CA	3428	7/7	0.92	0.07	123,134,138,182	1
55	MG	AA	3357	1/1	0.92	0.36	73,73,73,73	0
55	MG	BC	101	1/1	0.92	0.37	69,69,69,69	0
55	MG	AA	3097	1/1	0.92	0.11	59,59,59,59	0
55	MG	AA	3271	1/1	0.92	0.12	39,39,39,39	0
55	MG	AA	3272	1/1	0.92	0.27	50,50,50,50	0
55	MG	CA	3093	1/1	0.92	0.32	81,81,81,81	0
55	MG	CA	3001	1/1	0.92	0.18	46,46,46,46	0
55	MG	AO	202	1/1	0.92	0.24	55,55,55,55	0
55	MG	AA	3161	1/1	0.92	0.19	50,50,50,50	0
56	OHX	AO	205	7/7	0.92	0.08	83,89,107,180	1
56	OHX	CA	3468	7/7	0.92	0.08	115,126,133,180	1
55	MG	C0	201	1/1	0.92	0.16	61,61,61,61	0
55	MG	DC	105	1/1	0.92	0.36	54,54,54,54	0
55	MG	AA	3142	1/1	0.92	0.40	45,45,45,45	0
55	MG	CA	3007	1/1	0.92	0.16	45,45,45,45	0
55	MG	AA	3028	1/1	0.92	0.24	66,66,66,66	0
55	MG	AA	3384	1/1	0.92	0.31	59,59,59,59	0
55	MG	CA	3106	1/1	0.92	0.24	61,61,61,61	0
55	MG	CA	3011	1/1	0.92	0.24	46,46,46,46	0
55	MG	BA	1630	1/1	0.92	0.11	90,90,90,90	0
55	MG	CA	3228	1/1	0.92	0.10	65,65,65,65	0
55	MG	CA	3110	1/1	0.92	0.37	85,85,85,85	0
56	OHX	BA	1676	7/7	0.92	0.07	143,151,156,210	1
56	OHX	C5	102	7/7	0.92	0.07	114,118,133,165	1
55	MG	AA	3006	1/1	0.92	0.36	45,45,45,45	0
56	OHX	DA	1755	7/7	0.92	0.10	103,120,143,191	1
56	OHX	DA	1757	7/7	0.92	0.10	123,127,134,157	1
56	OHX	BA	1678	7/7	0.92	0.07	115,118,134,165	1
55	MG	CA	3182	1/1	0.92	0.34	59,59,59,59	0
56	OHX	AA	3371	7/7	0.92	0.10	93,107,117,177	1
56	OHX	DA	1781	7/7	0.92	0.08	107,126,135,195	1
55	MG	CA	3115	1/1	0.92	0.23	63,63,63,63	0
56	OHX	AA	3404	7/7	0.92	0.10	74,98,116,164	1
55	MG	CA	3015	1/1	0.92	0.21	54,54,54,54	0
55	MG	AA	3051	1/1	0.92	0.17	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	BA	1784	7/7	0.92	0.09	122,129,148,203	0
56	OHX	BA	1787	7/7	0.92	0.09	107,117,138,149	2
55	MG	AA	3027	1/1	0.92	0.21	42,42,42,42	0
56	OHX	BA	1803	7/7	0.92	0.09	101,126,136,190	1
56	OHX	BA	1804	7/7	0.92	0.09	134,142,150,227	1
56	OHX	DA	1799	7/7	0.92	0.06	122,127,139,209	1
56	OHX	AA	3485	7/7	0.92	0.07	104,114,127,171	1
55	MG	CA	3022	1/1	0.92	0.20	55,55,55,55	0
55	MG	AA	3215	1/1	0.92	0.36	50,50,50,50	0
55	MG	AA	3090	1/1	0.92	0.14	85,85,85,85	0
56	OHX	AA	3493	7/7	0.92	0.07	109,111,123,166	1
55	MG	AA	3283	1/1	0.92	0.25	55,55,55,55	0
56	OHX	CA	3247	7/7	0.92	0.11	95,104,117,152	1
56	OHX	AA	3509	7/7	0.92	0.07	92,96,122,175	1
55	MG	AA	3047	1/1	0.92	0.26	54,54,54,54	0
55	MG	AA	3092	1/1	0.92	0.04	73,73,73,73	0
55	MG	DA	1689	1/1	0.92	0.17	87,87,87,87	0
56	OHX	DB	103	7/7	0.92	0.09	166,171,179,191	1
56	OHX	CA	3302	7/7	0.92	0.10	79,86,104,139	1
55	MG	DA	1690	1/1	0.92	0.27	63,63,63,63	0
55	MG	DA	1692	1/1	0.92	0.30	70,70,70,70	0
55	MG	DA	1711	1/1	0.93	0.15	107,107,107,107	0
55	MG	CA	3147	1/1	0.93	0.27	51,51,51,51	0
56	OHX	CA	3382	7/7	0.93	0.07	129,131,148,199	1
55	MG	AA	3387	1/1	0.93	0.22	42,42,42,42	0
56	OHX	CA	3384	7/7	0.93	0.07	118,124,135,184	1
55	MG	CA	3090	1/1	0.93	0.19	55,55,55,55	0
56	OHX	CA	3387	7/7	0.93	0.07	111,127,150,170	2
56	OHX	CA	3388	7/7	0.93	0.11	112,116,127,180	1
56	OHX	AA	3544	7/7	0.93	0.06	103,105,124,176	1
55	MG	DA	1648	1/1	0.93	0.07	91,91,91,91	0
55	MG	CA	3152	1/1	0.93	0.35	54,54,54,54	0
56	OHX	AA	3547	7/7	0.93	0.07	69,84,101,157	2
55	MG	CA	3048	1/1	0.93	0.29	44,44,44,44	0
55	MG	DA	1653	1/1	0.93	0.37	73,73,73,73	0
56	OHX	AA	3553	7/7	0.93	0.06	113,118,133,183	1
55	MG	AA	3259	1/1	0.93	0.20	35,35,35,35	0
55	MG	DL	201	1/1	0.93	0.28	92,92,92,92	0
55	MG	BA	1736	1/1	0.93	0.41	64,64,64,64	0
55	MG	CA	3010	1/1	0.93	0.13	47,47,47,47	0
56	OHX	AA	3561	7/7	0.93	0.07	152,158,173,226	1
55	MG	CA	3097	1/1	0.93	0.25	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	AA	3563	7/7	0.93	0.06	124,125,134,183	1
56	OHX	CA	3412	7/7	0.93	0.11	99,116,129,164	2
55	MG	AA	3260	1/1	0.93	0.37	58,58,58,58	0
55	MG	CA	3162	1/1	0.93	0.32	65,65,65,65	0
55	MG	BA	1740	1/1	0.93	0.34	61,61,61,61	0
56	OHX	CA	3416	7/7	0.93	0.07	114,117,128,182	1
55	MG	CB	207	1/1	0.93	0.33	76,76,76,76	0
55	MG	AA	3286	1/1	0.93	0.33	68,68,68,68	0
55	MG	AA	3395	1/1	0.93	0.13	40,40,40,40	0
55	MG	CA	3016	1/1	0.93	0.20	55,55,55,55	0
56	OHX	AB	215	7/7	0.93	0.10	105,114,120,153	1
55	MG	DA	1602	1/1	0.93	0.23	68,68,68,68	0
56	OHX	AB	217	7/7	0.93	0.09	85,105,116,146	1
55	MG	CA	3104	1/1	0.93	0.32	41,41,41,41	0
56	OHX	AB	219	7/7	0.93	0.08	104,111,125,162	1
55	MG	CA	3169	1/1	0.93	0.18	71,71,71,71	0
55	MG	BA	1707	1/1	0.93	0.21	70,70,70,70	0
55	MG	DA	1671	1/1	0.93	0.12	64,64,64,64	0
56	OHX	CA	3430	7/7	0.93	0.08	96,106,114,197	1
55	MG	AA	3344	1/1	0.93	0.24	48,48,48,48	0
55	MG	AA	3032	1/1	0.93	0.23	41,41,41,41	0
55	MG	AA	3264	1/1	0.93	0.27	76,76,76,76	0
55	MG	CA	3112	1/1	0.93	0.28	41,41,41,41	0
55	MG	AA	3408	1/1	0.93	0.30	47,47,47,47	0
55	MG	AA	3184	1/1	0.93	0.16	38,38,38,38	0
56	OHX	BA	1672	7/7	0.93	0.07	156,159,170,224	1
56	OHX	CA	3464	7/7	0.93	0.12	78,109,122,137	3
55	MG	AA	3413	1/1	0.93	0.20	57,57,57,57	0
55	MG	CA	3259	1/1	0.93	0.28	65,65,65,65	0
56	OHX	AA	3476	7/7	0.93	0.10	102,122,137,175	1
56	OHX	AA	3482	7/7	0.93	0.07	105,118,127,177	1
56	OHX	AA	3483	7/7	0.93	0.07	124,141,146,196	1
55	MG	AA	3113	1/1	0.93	0.20	32,32,32,32	0
55	MG	AA	3188	1/1	0.93	0.16	40,40,40,40	0
56	OHX	CB	211	7/7	0.93	0.07	122,128,152,168	1
55	MG	AA	3189	1/1	0.93	0.27	42,42,42,42	0
55	MG	AA	3134	1/1	0.93	0.15	82,82,82,82	0
55	MG	DA	1685	1/1	0.93	0.10	59,59,59,59	0
56	OHX	BA	1694	7/7	0.93	0.06	159,161,173,226	1
56	OHX	AA	3491	7/7	0.93	0.08	162,182,190,220	1
56	OHX	AA	3492	7/7	0.93	0.09	79,89,95,107	3
55	MG	DA	1621	1/1	0.93	0.17	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	AA	3495	7/7	0.93	0.09	86,93,120,158	1
55	MG	CA	3123	1/1	0.93	0.14	36,36,36,36	0
56	OHX	BA	1797	7/7	0.93	0.13	71,104,132,136	3
56	OHX	AA	3506	7/7	0.93	0.06	97,110,123,157	1
56	OHX	DA	1756	7/7	0.93	0.06	145,145,160,212	1
56	OHX	AA	3507	7/7	0.93	0.07	101,111,128,158	1
55	MG	AA	3120	1/1	0.93	0.15	71,71,71,71	0
56	OHX	DA	1769	7/7	0.93	0.07	133,140,147,188	1
56	OHX	DA	1772	7/7	0.93	0.07	131,135,143,214	1
55	MG	BA	1719	1/1	0.93	0.31	51,51,51,51	0
55	MG	CA	3075	1/1	0.93	0.21	45,45,45,45	0
56	OHX	DA	1777	7/7	0.93	0.06	150,152,155,232	1
56	OHX	BR	101	7/7	0.93	0.06	117,129,143,169	1
55	MG	AB	204	1/1	0.93	0.33	68,68,68,68	0
56	OHX	AA	3514	7/7	0.93	0.08	84,93,104,149	1
55	MG	CA	3133	1/1	0.93	0.23	48,48,48,48	0
55	MG	AA	3197	1/1	0.93	0.27	50,50,50,50	0
56	OHX	CA	3248	7/7	0.93	0.06	116,128,134,203	1
55	MG	AA	3198	1/1	0.93	0.22	54,54,54,54	0
55	MG	CA	3137	1/1	0.93	0.33	74,74,74,74	0
55	MG	CA	3451	1/1	0.93	0.22	46,46,46,46	0
55	MG	AA	3004	1/1	0.93	0.23	37,37,37,37	0
55	MG	CA	3080	1/1	0.93	0.10	57,57,57,57	0
55	MG	AA	3008	1/1	0.93	0.27	42,42,42,42	0
56	OHX	AA	3529	7/7	0.93	0.08	90,106,115,167	1
56	OHX	DA	1804	7/7	0.93	0.07	107,115,128,173	1
55	MG	AA	3203	1/1	0.93	0.18	50,50,50,50	0
56	OHX	DA	1806	7/7	0.93	0.05	142,150,160,228	1
56	OHX	CA	3342	7/7	0.93	0.07	116,123,130,201	1
56	OHX	CA	3343	7/7	0.93	0.09	109,118,132,184	1
56	OHX	CA	3344	7/7	0.93	0.10	96,110,117,162	1
56	OHX	AA	3531	7/7	0.93	0.06	119,124,135,185	1
56	OHX	CA	3350	7/7	0.93	0.08	112,134,144,175	1
55	MG	AA	3204	1/1	0.93	0.12	61,61,61,61	0
55	MG	AA	3228	1/1	0.93	0.18	67,67,67,67	0
55	MG	AA	3089	1/1	0.93	0.47	84,84,84,84	0
55	MG	CA	3205	1/1	0.93	0.15	63,63,63,63	0
55	MG	AA	3230	1/1	0.93	0.19	66,66,66,66	0
56	OHX	CA	3376	7/7	0.93	0.07	113,130,136,172	1
56	OHX	DC	107	7/7	0.93	0.09	131,132,141,177	1
55	MG	BA	1731	1/1	0.93	0.33	57,57,57,57	0
57	ZN	DG	301	1/1	0.93	0.20	122,122,122,122	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	3093	1/1	0.94	0.26	91,91,91,91	0
55	MG	AA	3003	1/1	0.94	0.17	39,39,39,39	0
56	OHX	AA	3452	7/7	0.94	0.11	61,75,91,137	2
55	MG	AA	3233	1/1	0.94	0.16	59,59,59,59	0
56	OHX	AA	3477	7/7	0.94	0.06	108,119,125,208	1
56	OHX	A1	202	7/7	0.94	0.08	85,95,114,146	1
56	OHX	CA	3403	7/7	0.94	0.08	88,108,114,167	1
55	MG	AA	3210	1/1	0.94	0.33	41,41,41,41	0
56	OHX	CA	3405	7/7	0.94	0.06	112,116,119,187	1
56	OHX	BA	1656	7/7	0.94	0.07	160,162,176,267	0
55	MG	AA	3082	1/1	0.94	0.12	50,50,50,50	0
55	MG	CA	3181	1/1	0.94	0.21	62,62,62,62	0
55	MG	CA	3017	1/1	0.94	0.15	92,92,92,92	0
56	OHX	AA	3486	7/7	0.94	0.07	127,135,138,199	1
55	MG	AA	3236	1/1	0.94	0.26	40,40,40,40	0
55	MG	CA	3122	1/1	0.94	0.19	40,40,40,40	0
55	MG	CA	3020	1/1	0.94	0.21	70,70,70,70	0
55	MG	AA	3237	1/1	0.94	0.23	45,45,45,45	0
55	MG	BA	1737	1/1	0.94	0.18	46,46,46,46	0
55	MG	CA	3126	1/1	0.94	0.20	54,54,54,54	0
56	OHX	AA	3494	7/7	0.94	0.08	59,86,128,185	1
55	MG	AA	3238	1/1	0.94	0.29	50,50,50,50	0
56	OHX	AA	3504	7/7	0.94	0.06	112,118,129,179	1
55	MG	CA	3445	1/1	0.94	0.19	38,38,38,38	0
55	MG	AA	3191	1/1	0.94	0.19	45,45,45,45	0
56	OHX	BA	1681	7/7	0.94	0.06	153,163,173,229	1
55	MG	AA	3278	1/1	0.94	0.24	35,35,35,35	0
56	OHX	BA	1688	7/7	0.94	0.09	107,112,123,154	1
56	OHX	BA	1689	7/7	0.94	0.07	113,130,139,190	1
56	OHX	AA	3508	7/7	0.94	0.07	122,129,136,204	1
56	OHX	BA	1691	7/7	0.94	0.06	148,150,156,215	1
55	MG	AA	3214	1/1	0.94	0.21	46,46,46,46	0
56	OHX	BA	1693	7/7	0.94	0.08	112,112,134,152	1
55	MG	DA	1699	1/1	0.94	0.21	78,78,78,78	0
55	MG	AA	3192	1/1	0.94	0.27	48,48,48,48	0
56	OHX	BA	1771	7/7	0.94	0.11	77,100,122,150	1
55	MG	AA	3104	1/1	0.94	0.31	68,68,68,68	0
55	MG	BA	1616	1/1	0.94	0.15	61,61,61,61	0
56	OHX	BA	1785	7/7	0.94	0.08	109,122,129,170	1
55	MG	AA	3246	1/1	0.94	0.21	36,36,36,36	0
55	MG	CA	3199	1/1	0.94	0.23	62,62,62,62	0
56	OHX	BA	1791	7/7	0.94	0.10	82,106,122,150	2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	BA	1793	7/7	0.94	0.07	95,105,117,163	1
56	OHX	CA	3482	7/7	0.94	0.07	84,120,131,181	0
55	MG	AA	3195	1/1	0.94	0.25	43,43,43,43	0
55	MG	DA	1639	1/1	0.94	0.24	70,70,70,70	0
56	OHX	CA	3489	7/7	0.94	0.09	91,101,112,140	1
55	MG	AA	3030	1/1	0.94	0.18	44,44,44,44	0
56	OHX	CB	209	7/7	0.94	0.09	117,133,147,190	1
56	OHX	CB	210	7/7	0.94	0.08	104,124,140,171	1
55	MG	BA	1705	1/1	0.94	0.18	63,63,63,63	0
55	MG	AA	3011	1/1	0.94	0.21	49,49,49,49	0
56	OHX	BA	1811	7/7	0.94	0.09	88,104,115,154	1
55	MG	AA	3180	1/1	0.94	0.19	65,65,65,65	0
55	MG	CA	3472	1/1	0.94	0.10	59,59,59,59	0
56	OHX	BB	106	7/7	0.94	0.12	164,167,173,198	1
55	MG	AA	3251	1/1	0.94	0.28	49,49,49,49	0
56	OHX	BD	102	7/7	0.94	0.07	153,174,197,228	0
55	MG	AA	3345	1/1	0.94	0.48	47,47,47,47	0
56	OHX	CA	3244	7/7	0.94	0.07	94,113,121,172	1
56	OHX	DA	1747	7/7	0.94	0.09	109,122,155,200	1
56	OHX	DA	1749	7/7	0.94	0.10	91,120,126,173	1
56	OHX	DA	1752	7/7	0.94	0.06	107,121,128,186	1
55	MG	AA	3222	1/1	0.94	0.28	64,64,64,64	0
55	MG	CA	3089	1/1	0.94	0.15	60,60,60,60	0
55	MG	AA	3254	1/1	0.94	0.20	42,42,42,42	0
55	MG	AA	3223	1/1	0.94	0.21	56,56,56,56	0
56	OHX	DA	1760	7/7	0.94	0.07	142,145,152,204	1
55	MG	CA	3092	1/1	0.94	0.35	52,52,52,52	0
55	MG	AA	3182	1/1	0.94	0.29	45,45,45,45	0
55	MG	AA	3257	1/1	0.94	0.22	57,57,57,57	0
56	OHX	DA	1773	7/7	0.94	0.06	122,126,137,197	1
55	MG	AA	3225	1/1	0.94	0.16	63,63,63,63	0
55	MG	AA	3183	1/1	0.94	0.24	88,88,88,88	0
56	OHX	DA	1776	7/7	0.94	0.07	114,116,125,160	1
55	MG	AA	3039	1/1	0.94	0.21	40,40,40,40	0
56	OHX	DA	1778	7/7	0.94	0.07	142,148,154,267	0
56	OHX	CA	3318	7/7	0.94	0.11	34,112,130,183	1
55	MG	CA	3161	1/1	0.94	0.20	71,71,71,71	0
55	MG	CA	3049	1/1	0.94	0.19	62,62,62,62	0
55	MG	AA	3205	1/1	0.94	0.18	40,40,40,40	0
55	MG	AA	3358	1/1	0.94	0.24	51,51,51,51	0
56	OHX	CA	3346	7/7	0.94	0.09	99,104,119,151	1
56	OHX	AA	3548	7/7	0.94	0.06	113,118,133,172	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	DA	1790	7/7	0.94	0.06	135,136,148,199	1
56	OHX	CA	3349	7/7	0.94	0.07	115,117,131,178	1
56	OHX	AA	3550	7/7	0.94	0.07	111,121,131,187	1
56	OHX	CA	3355	7/7	0.94	0.09	108,110,119,149	1
55	MG	BA	1636	1/1	0.94	0.14	61,61,61,61	0
55	MG	DA	1666	1/1	0.94	0.30	62,62,62,62	0
56	OHX	CA	3365	7/7	0.94	0.07	164,171,176,213	1
56	OHX	AA	3147	7/7	0.94	0.09	89,98,103,163	1
56	OHX	AA	3160	7/7	0.94	0.06	116,121,130,182	1
55	MG	BA	1638	1/1	0.94	0.20	57,57,57,57	0
55	MG	AA	3374	1/1	0.94	0.22	29,29,29,29	0
56	OHX	CA	3377	7/7	0.94	0.10	90,95,111,135	2
56	OHX	AA	3312	7/7	0.94	0.08	64,87,123,173	1
56	OHX	AA	3324	7/7	0.94	0.09	92,110,118,165	1
55	MG	CA	3168	1/1	0.94	0.24	72,72,72,72	0
55	MG	AA	3377	1/1	0.94	0.23	51,51,51,51	0
55	MG	DA	1606	1/1	0.94	0.13	84,84,84,84	0
55	MG	CA	3226	1/1	0.94	0.41	65,65,65,65	0
56	OHX	DV	101	7/7	0.94	0.07	162,169,185,231	1
55	MG	AA	3168	1/1	0.94	0.26	89,89,89,89	0
55	MG	AA	3265	1/1	0.94	0.30	85,85,85,85	0
55	MG	AA	3207	1/1	0.94	0.31	57,57,57,57	0
56	OHX	AA	3402	7/7	0.94	0.14	87,110,129,141	3
55	MG	DA	1612	1/1	0.94	0.21	86,86,86,86	0
56	OHX	DD	101	7/7	0.94	0.08	155,165,187,227	0
57	ZN	BQ	102	1/1	0.94	0.12	130,130,130,130	0
55	MG	CA	3173	1/1	0.94	0.16	53,53,53,53	0
55	MG	AA	3240	1/1	0.95	0.17	43,43,43,43	0
55	MG	CA	3174	1/1	0.95	0.32	52,52,52,52	0
55	MG	BA	1619	1/1	0.95	0.18	50,50,50,50	0
55	MG	AA	3173	1/1	0.95	0.19	52,52,52,52	0
55	MG	AA	3242	1/1	0.95	0.21	37,37,37,37	0
55	MG	BA	1726	1/1	0.95	0.27	61,61,61,61	0
56	OHX	AA	3528	7/7	0.95	0.07	112,118,137,160	2
56	OHX	BA	1778	7/7	0.95	0.08	99,120,131,182	0
55	MG	AA	3262	1/1	0.95	0.28	52,52,52,52	0
55	MG	CA	3130	1/1	0.95	0.41	58,58,58,58	0
55	MG	BA	1654	1/1	0.95	0.24	47,47,47,47	0
55	MG	AA	3002	1/1	0.95	0.28	41,41,41,41	0
55	MG	AA	3010	1/1	0.95	0.17	40,40,40,40	0
55	MG	DA	1610	1/1	0.95	0.14	96,96,96,96	0
55	MG	CA	3135	1/1	0.95	0.29	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	BA	1794	7/7	0.95	0.06	118,138,149,184	1
55	MG	CA	3043	1/1	0.95	0.11	82,82,82,82	0
56	OHX	BA	1798	7/7	0.95	0.06	140,143,151,221	1
56	OHX	BA	1800	7/7	0.95	0.08	106,107,118,143	1
56	OHX	BA	1801	7/7	0.95	0.06	118,138,142,207	1
55	MG	CA	3263	1/1	0.95	0.25	69,69,69,69	0
56	OHX	AA	3304	7/7	0.95	0.06	109,115,135,200	1
55	MG	CA	3004	1/1	0.95	0.13	49,49,49,49	0
55	MG	BA	1697	1/1	0.95	0.26	37,37,37,37	0
56	OHX	BA	1807	7/7	0.95	0.06	135,141,150,224	0
56	OHX	AA	3313	7/7	0.95	0.08	96,112,122,174	0
56	OHX	BA	1813	7/7	0.95	0.07	128,130,137,174	1
56	OHX	BA	1814	7/7	0.95	0.06	101,109,125,174	1
56	OHX	BA	1815	7/7	0.95	0.07	110,125,133,172	1
56	OHX	AA	3543	7/7	0.95	0.05	113,117,131,189	1
56	OHX	AA	3319	7/7	0.95	0.08	87,95,122,151	1
55	MG	CA	3006	1/1	0.95	0.19	47,47,47,47	0
56	OHX	AA	3330	7/7	0.95	0.07	102,112,122,166	1
55	MG	CA	3190	1/1	0.95	0.11	60,60,60,60	0
56	OHX	CA	3488	7/7	0.95	0.06	113,123,127,179	1
55	MG	AA	3343	1/1	0.95	0.28	34,34,34,34	0
55	MG	AA	3099	1/1	0.95	0.18	65,65,65,65	0
55	MG	AA	3389	1/1	0.95	0.29	44,44,44,44	0
55	MG	CA	3442	1/1	0.95	0.18	61,61,61,61	0
55	MG	CA	3194	1/1	0.95	0.26	63,63,63,63	0
56	OHX	CB	212	7/7	0.95	0.07	101,120,135,155	1
55	MG	AA	3029	1/1	0.95	0.24	38,38,38,38	0
56	OHX	AA	3373	7/7	0.95	0.08	75,103,110,155	1
56	OHX	AA	3557	7/7	0.95	0.09	75,87,101,114	1
55	MG	CA	3094	1/1	0.95	0.35	79,79,79,79	0
56	OHX	CA	3285	7/7	0.95	0.12	94,107,126,147	1
55	MG	A5	101	1/1	0.95	0.19	41,41,41,41	0
55	MG	AA	3178	1/1	0.95	0.31	39,39,39,39	0
56	OHX	CB	220	7/7	0.95	0.07	133,142,154,201	0
56	OHX	C1	201	7/7	0.95	0.08	102,111,123,165	1
55	MG	AA	3269	1/1	0.95	0.23	72,72,72,72	0
55	MG	AA	3179	1/1	0.95	0.32	60,60,60,60	0
56	OHX	DA	1730	7/7	0.95	0.09	102,111,123,157	0
56	OHX	DA	1731	7/7	0.95	0.07	129,139,145,172	1
56	OHX	DA	1741	7/7	0.95	0.08	97,116,128,170	1
56	OHX	DA	1745	7/7	0.95	0.07	115,123,143,223	0
56	OHX	CA	3325	7/7	0.95	0.13	108,122,148,156	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	CA	3334	7/7	0.95	0.07	110,115,136,183	0
56	OHX	DA	1751	7/7	0.95	0.13	66,109,137,183	2
55	MG	CA	3149	1/1	0.95	0.27	55,55,55,55	0
56	OHX	AA	3474	7/7	0.95	0.09	51,85,127,151	2
56	OHX	DA	1754	7/7	0.95	0.07	98,102,118,156	1
56	OHX	AA	3475	7/7	0.95	0.07	67,93,111,167	1
55	MG	CA	3150	1/1	0.95	0.23	55,55,55,55	0
55	MG	DA	1691	1/1	0.95	0.22	54,54,54,54	0
56	OHX	AA	3479	7/7	0.95	0.07	106,122,142,174	1
56	OHX	DA	1762	7/7	0.95	0.08	107,112,122,180	1
56	OHX	AB	209	7/7	0.95	0.08	63,88,125,152	2
55	MG	BA	1743	1/1	0.95	0.26	69,69,69,69	0
56	OHX	DA	1771	7/7	0.95	0.10	97,105,129,152	1
55	MG	AA	3025	1/1	0.95	0.20	59,59,59,59	0
55	MG	AA	3146	1/1	0.95	0.20	41,41,41,41	0
55	MG	CA	3019	1/1	0.95	0.13	46,46,46,46	0
56	OHX	CA	3362	7/7	0.95	0.05	129,136,141,186	1
56	OHX	CA	3364	7/7	0.95	0.07	117,120,133,182	1
55	MG	AA	3352	1/1	0.95	0.13	41,41,41,41	0
56	OHX	CA	3368	7/7	0.95	0.07	108,126,135,177	1
56	OHX	DA	1780	7/7	0.95	0.07	127,131,138,167	1
56	OHX	CA	3370	7/7	0.95	0.07	116,120,142,180	1
55	MG	AA	3088	1/1	0.95	0.09	60,60,60,60	0
55	MG	AA	3202	1/1	0.95	0.27	45,45,45,45	0
56	OHX	CA	3374	7/7	0.95	0.08	106,124,128,169	1
55	MG	CA	3158	1/1	0.95	0.21	56,56,56,56	0
55	MG	CA	3474	1/1	0.95	0.16	70,70,70,70	0
56	OHX	AW	101	7/7	0.95	0.09	103,112,128,156	1
56	OHX	DA	1788	7/7	0.95	0.08	96,113,128,168	1
55	MG	CA	3108	1/1	0.95	0.22	52,52,52,52	0
56	OHX	DA	1791	7/7	0.95	0.09	103,104,121,153	1
56	OHX	DA	1792	7/7	0.95	0.07	110,118,129,172	1
55	MG	AA	3412	1/1	0.95	0.23	39,39,39,39	0
56	OHX	DA	1795	7/7	0.95	0.06	112,118,132,167	1
56	OHX	BA	1659	7/7	0.95	0.07	114,130,135,179	1
56	OHX	DA	1797	7/7	0.95	0.05	149,152,159,218	1
56	OHX	CA	3381	7/7	0.95	0.07	102,112,121,159	1
55	MG	AA	3018	1/1	0.95	0.20	43,43,43,43	0
55	MG	BA	1752	1/1	0.95	0.31	53,53,53,53	0
56	OHX	AA	3497	7/7	0.95	0.08	94,106,111,138	2
56	OHX	AA	3500	7/7	0.95	0.07	94,114,122,159	1
55	MG	CA	3113	1/1	0.95	0.21	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	BA	1668	7/7	0.95	0.07	116,121,137,182	1
55	MG	DA	1646	1/1	0.95	0.16	64,64,64,64	0
56	OHX	CA	3391	7/7	0.95	0.06	140,144,157,182	1
56	OHX	BA	1670	7/7	0.95	0.06	135,143,147,201	1
55	MG	AA	3186	1/1	0.95	0.21	49,49,49,49	0
55	MG	AA	3277	1/1	0.95	0.27	46,46,46,46	0
55	MG	AA	3170	1/1	0.95	0.14	50,50,50,50	0
55	MG	AA	3375	1/1	0.95	0.25	31,31,31,31	0
56	OHX	CA	3398	7/7	0.95	0.06	129,132,142,192	1
55	MG	DA	1651	1/1	0.95	0.38	62,62,62,62	0
55	MG	DA	1652	1/1	0.95	0.33	52,52,52,52	0
55	MG	AA	3376	1/1	0.95	0.25	33,33,33,33	0
55	MG	AA	3121	1/1	0.95	0.30	53,53,53,53	0
55	MG	CA	3120	1/1	0.95	0.25	48,48,48,48	0
56	OHX	BA	1683	7/7	0.95	0.06	124,130,146,183	1
56	OHX	AA	3516	7/7	0.95	0.06	101,109,121,183	1
56	OHX	AA	3517	7/7	0.95	0.10	88,111,115,145	1
55	MG	AA	3239	1/1	0.95	0.15	44,44,44,44	0
55	MG	AA	3043	1/1	0.96	0.23	46,46,46,46	0
55	MG	AA	3050	1/1	0.96	0.20	60,60,60,60	0
56	OHX	AA	3558	7/7	0.96	0.06	95,121,125,156	1
55	MG	CA	3012	1/1	0.96	0.18	53,53,53,53	0
55	MG	CA	3047	1/1	0.96	0.33	41,41,41,41	0
56	OHX	CA	3423	7/7	0.96	0.04	123,126,136,189	1
56	OHX	BA	1810	7/7	0.96	0.07	106,108,121,152	1
55	MG	BA	1748	1/1	0.96	0.20	66,66,66,66	0
56	OHX	BA	1812	7/7	0.96	0.06	151,164,170,231	1
55	MG	AA	3415	1/1	0.96	0.12	52,52,52,52	0
55	MG	AA	3007	1/1	0.96	0.11	31,31,31,31	0
55	MG	BA	1655	1/1	0.96	0.19	60,60,60,60	0
55	MG	AA	3133	1/1	0.96	0.15	54,54,54,54	0
55	MG	AA	3385	1/1	0.96	0.29	34,34,34,34	0
55	MG	AA	3111	1/1	0.96	0.22	35,35,35,35	0
55	MG	BN	201	1/1	0.96	0.11	80,80,80,80	0
55	MG	AA	3112	1/1	0.96	0.13	47,47,47,47	0
56	OHX	BD	103	7/7	0.96	0.06	86,95,103,174	1
56	OHX	AB	207	7/7	0.96	0.07	89,99,126,152	1
56	OHX	AB	208	7/7	0.96	0.07	113,119,131,170	1
56	OHX	CA	3463	7/7	0.96	0.10	107,129,139,156	1
55	MG	CA	3180	1/1	0.96	0.17	75,75,75,75	0
56	OHX	CA	3465	7/7	0.96	0.07	131,136,147,181	1
55	MG	AA	3022	1/1	0.96	0.12	15,15,15,15	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	AB	212	7/7	0.96	0.08	81,99,131,153	1
56	OHX	AB	213	7/7	0.96	0.10	85,93,130,132	3
56	OHX	CA	3469	7/7	0.96	0.07	89,110,121,162	1
56	OHX	AB	214	7/7	0.96	0.07	110,118,132,162	1
56	OHX	CA	3253	7/7	0.96	0.08	107,120,133,155	1
55	MG	BA	1701	1/1	0.96	0.20	57,57,57,57	0
56	OHX	AA	3496	7/7	0.96	0.06	117,124,142,215	0
55	MG	CA	3024	1/1	0.96	0.11	48,48,48,48	0
55	MG	AA	3181	1/1	0.96	0.25	61,61,61,61	0
56	OHX	CA	3490	7/7	0.96	0.07	102,105,118,156	1
56	OHX	AA	3501	7/7	0.96	0.08	101,109,129,149	1
56	OHX	AA	3503	7/7	0.96	0.06	99,121,138,179	1
56	OHX	CA	3314	7/7	0.96	0.10	84,93,97,114	1
55	MG	DA	1680	1/1	0.96	0.18	72,72,72,72	0
55	MG	BA	1637	1/1	0.96	0.06	83,83,83,83	0
56	OHX	CA	3328	7/7	0.96	0.07	50,117,131,206	0
56	OHX	CA	3331	7/7	0.96	0.09	101,112,120,147	1
56	OHX	CA	3333	7/7	0.96	0.07	104,127,133,184	1
56	OHX	A3	102	7/7	0.96	0.10	90,98,113,134	2
56	OHX	CA	3335	7/7	0.96	0.07	96,110,125,200	0
56	OHX	CA	3337	7/7	0.96	0.08	109,124,136,185	0
56	OHX	CA	3339	7/7	0.96	0.08	100,105,127,171	1
55	MG	CA	3063	1/1	0.96	0.15	70,70,70,70	0
56	OHX	A6	101	7/7	0.96	0.07	113,122,137,155	1
55	MG	AA	3016	1/1	0.96	0.20	39,39,39,39	0
55	MG	AA	3200	1/1	0.96	0.27	45,45,45,45	0
56	OHX	C6	101	7/7	0.96	0.07	132,145,157,184	1
55	MG	CA	3105	1/1	0.96	0.41	68,68,68,68	0
55	MG	BA	1732	1/1	0.96	0.27	52,52,52,52	0
56	OHX	DA	1732	7/7	0.96	0.07	134,143,157,195	0
56	OHX	DA	1733	7/7	0.96	0.07	146,151,163,202	0
56	OHX	DA	1735	7/7	0.96	0.07	110,115,118,170	1
56	OHX	DA	1736	7/7	0.96	0.07	130,135,157,193	0
56	OHX	DA	1737	7/7	0.96	0.08	87,110,131,158	1
56	OHX	AA	3305	7/7	0.96	0.10	83,97,103,135	1
55	MG	AE	303	1/1	0.96	0.15	32,32,32,32	0
56	OHX	CA	3351	7/7	0.96	0.07	102,107,134,173	1
56	OHX	CA	3352	7/7	0.96	0.05	133,145,147,191	1
56	OHX	DA	1750	7/7	0.96	0.07	127,137,146,202	1
56	OHX	CA	3353	7/7	0.96	0.07	81,96,110,140	1
56	OHX	BA	1665	7/7	0.96	0.08	82,92,111,128	1
56	OHX	CA	3356	7/7	0.96	0.06	96,109,118,157	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BC	103	1/1	0.96	0.31	62,62,62,62	0
55	MG	BC	104	1/1	0.96	0.34	57,57,57,57	0
56	OHX	CA	3360	7/7	0.96	0.06	116,124,135,193	1
56	OHX	CA	3361	7/7	0.96	0.06	113,119,132,166	1
56	OHX	AA	3317	7/7	0.96	0.07	79,88,118,156	1
56	OHX	CA	3363	7/7	0.96	0.08	94,99,114,167	1
56	OHX	DA	1763	7/7	0.96	0.05	154,159,173,250	0
55	MG	CA	3070	1/1	0.96	0.14	44,44,44,44	0
56	OHX	DA	1768	7/7	0.96	0.06	121,132,163,218	0
55	MG	CA	3261	1/1	0.96	0.36	48,48,48,48	0
56	OHX	DA	1770	7/7	0.96	0.05	136,142,156,217	1
56	OHX	CA	3366	7/7	0.96	0.07	140,148,168,207	0
56	OHX	CA	3367	7/7	0.96	0.05	129,137,147,194	1
56	OHX	AA	3327	7/7	0.96	0.06	107,115,135,188	1
56	OHX	CA	3369	7/7	0.96	0.08	97,113,121,158	1
56	OHX	AA	3328	7/7	0.96	0.09	89,97,114,142	1
55	MG	AA	3393	1/1	0.96	0.13	56,56,56,56	0
55	MG	DA	1693	1/1	0.96	0.32	54,54,54,54	0
55	MG	C5	101	1/1	0.96	0.24	50,50,50,50	0
56	OHX	AA	3334	7/7	0.96	0.09	66,79,94,105	1
56	OHX	AA	3336	7/7	0.96	0.07	146,153,168,218	0
56	OHX	BA	1679	7/7	0.96	0.05	116,125,129,189	1
55	MG	AA	3394	1/1	0.96	0.23	43,43,43,43	0
55	MG	CA	3073	1/1	0.96	0.18	54,54,54,54	0
56	OHX	BA	1682	7/7	0.96	0.06	119,124,130,186	1
56	OHX	AA	3368	7/7	0.96	0.10	76,83,98,126	1
55	MG	AA	3054	1/1	0.96	0.13	49,49,49,49	0
56	OHX	BA	1687	7/7	0.96	0.08	94,99,108,140	1
55	MG	BA	1738	1/1	0.96	0.09	41,41,41,41	0
56	OHX	CA	3385	7/7	0.96	0.06	115,124,135,193	1
55	MG	AA	3140	1/1	0.96	0.09	41,41,41,41	0
56	OHX	AA	3372	7/7	0.96	0.07	93,103,121,167	1
55	MG	CA	3160	1/1	0.96	0.28	49,49,49,49	0
55	MG	AA	3185	1/1	0.96	0.26	36,36,36,36	0
56	OHX	AA	3538	7/7	0.96	0.09	88,94,114,159	1
55	MG	AA	3116	1/1	0.96	0.17	45,45,45,45	0
55	MG	AA	3001	1/1	0.96	0.25	28,28,28,28	0
56	OHX	DA	1800	7/7	0.96	0.05	137,140,150,220	1
56	OHX	AA	3405	7/7	0.96	0.06	103,111,138,161	1
56	OHX	BA	1772	7/7	0.96	0.07	106,118,144,175	0
56	OHX	BA	1777	7/7	0.96	0.07	114,118,140,171	1
55	MG	AA	3346	1/1	0.96	0.16	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	3444	1/1	0.96	0.21	52,52,52,52	0
56	OHX	AA	3447	7/7	0.96	0.07	91,102,120,163	1
56	OHX	CA	3401	7/7	0.96	0.06	136,149,158,185	1
55	MG	AA	3410	1/1	0.96	0.23	61,61,61,61	0
56	OHX	AA	3458	7/7	0.96	0.10	34,48,113,148	3
56	OHX	BA	1788	7/7	0.96	0.07	118,118,132,157	1
56	OHX	BA	1789	7/7	0.96	0.07	108,112,133,182	1
56	OHX	AA	3464	7/7	0.96	0.07	117,125,139,188	0
56	OHX	AA	3465	7/7	0.96	0.08	85,99,124,159	1
56	OHX	AA	3549	7/7	0.96	0.08	97,102,111,165	1
56	OHX	CA	3410	7/7	0.96	0.06	114,125,132,190	1
56	OHX	AA	3466	7/7	0.96	0.07	89,94,108,128	1
56	OHX	BA	1796	7/7	0.96	0.06	143,156,164,225	0
56	OHX	AA	3470	7/7	0.96	0.07	107,109,130,160	1
56	OHX	AA	3473	7/7	0.96	0.08	66,95,102,124	1
55	MG	AA	3042	1/1	0.96	0.17	43,43,43,43	0
55	MG	CA	3447	1/1	0.96	0.43	58,58,58,58	0
56	OHX	BA	1802	7/7	0.96	0.06	107,121,133,185	1
55	MG	CA	3127	1/1	0.97	0.18	53,53,53,53	0
56	OHX	AA	3480	7/7	0.97	0.07	90,100,124,135	1
56	OHX	AA	3481	7/7	0.97	0.06	95,108,126,156	2
56	OHX	CA	3372	7/7	0.97	0.07	112,137,145,182	0
56	OHX	AA	3332	7/7	0.97	0.08	77,106,123,134	1
55	MG	CA	3128	1/1	0.97	0.07	72,72,72,72	0
55	MG	AA	3075	1/1	0.97	0.34	44,44,44,44	0
56	OHX	BA	1663	7/7	0.97	0.05	132,137,143,190	1
56	OHX	BA	1808	7/7	0.97	0.11	84,90,96,110	2
56	OHX	BA	1809	7/7	0.97	0.05	141,153,160,232	0
56	OHX	AA	3335	7/7	0.97	0.06	94,101,113,136	1
56	OHX	CO	201	7/7	0.97	0.06	104,109,121,141	1
55	MG	AA	3085	1/1	0.97	0.12	58,58,58,58	0
56	OHX	AA	3337	7/7	0.97	0.06	97,106,127,177	1
56	OHX	AA	3339	7/7	0.97	0.06	151,155,164,211	1
56	OHX	AA	3489	7/7	0.97	0.07	72,78,92,128	1
56	OHX	DA	1728	7/7	0.97	0.07	78,116,123,162	0
56	OHX	AA	3363	7/7	0.97	0.09	90,99,133,145	1
55	MG	AA	3196	1/1	0.97	0.20	36,36,36,36	0
56	OHX	BG	302	7/7	0.97	0.06	128,137,145,186	1
56	OHX	BA	1671	7/7	0.97	0.04	127,131,133,210	1
55	MG	C7	101	1/1	0.97	0.28	54,54,54,54	0
56	OHX	CA	3389	7/7	0.97	0.06	101,110,123,155	1
56	OHX	AA	3367	7/7	0.97	0.06	121,129,147,173	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	3132	1/1	0.97	0.14	80,80,80,80	0
55	MG	AA	3253	1/1	0.97	0.20	53,53,53,53	0
56	OHX	AA	3263	7/7	0.97	0.06	76,102,114,143	1
56	OHX	DA	1748	7/7	0.97	0.06	95,111,122,149	1
56	OHX	CA	3394	7/7	0.97	0.07	97,100,116,155	1
56	OHX	AA	3288	7/7	0.97	0.08	76,85,101,127	1
56	OHX	AA	3498	7/7	0.97	0.07	92,94,127,136	1
56	OHX	CA	3246	7/7	0.97	0.10	113,116,120,151	1
56	OHX	AA	3298	7/7	0.97	0.11	71,88,99,110	1
56	OHX	AA	3299	7/7	0.97	0.07	54,81,94,118	1
56	OHX	AA	3556	7/7	0.97	0.05	212,217,223,266	1
56	OHX	AA	3502	7/7	0.97	0.07	97,102,112,146	1
56	OHX	AA	3401	7/7	0.97	0.05	93,112,116,173	1
56	OHX	CA	3254	7/7	0.97	0.06	167,174,181,211	0
56	OHX	DA	1761	7/7	0.97	0.05	130,132,145,205	0
56	OHX	BA	1685	7/7	0.97	0.05	198,199,207,267	1
55	MG	AA	3094	1/1	0.97	0.31	39,39,39,39	0
56	OHX	CA	3406	7/7	0.97	0.06	151,161,169,211	1
56	OHX	DA	1766	7/7	0.97	0.06	118,124,133,175	1
56	OHX	DA	1767	7/7	0.97	0.05	120,124,135,184	1
56	OHX	AA	3303	7/7	0.97	0.07	93,102,117,145	1
56	OHX	CA	3293	7/7	0.97	0.09	100,117,128,163	0
56	OHX	CA	3295	7/7	0.97	0.08	102,105,117,137	1
55	MG	DA	1638	1/1	0.97	0.11	89,89,89,89	0
55	MG	AA	3411	1/1	0.97	0.17	63,63,63,63	0
55	MG	CA	3453	1/1	0.97	0.24	58,58,58,58	0
56	OHX	CA	3308	7/7	0.97	0.07	88,90,121,161	0
56	OHX	CA	3309	7/7	0.97	0.07	92,108,125,150	1
56	OHX	AA	3307	7/7	0.97	0.07	85,90,103,127	1
56	OHX	CA	3317	7/7	0.97	0.07	116,126,142,180	1
55	MG	CA	3098	1/1	0.97	0.13	63,63,63,63	0
56	OHX	AA	3448	7/7	0.97	0.08	87,90,112,131	1
56	OHX	AA	3450	7/7	0.97	0.07	65,94,112,113	3
55	MG	CA	3058	1/1	0.97	0.29	50,50,50,50	0
56	OHX	BA	1764	7/7	0.97	0.08	88,94,120,157	0
56	OHX	BA	1768	7/7	0.97	0.07	128,139,147,175	0
56	OHX	BA	1770	7/7	0.97	0.07	102,113,126,149	1
56	OHX	CA	3336	7/7	0.97	0.06	114,127,138,191	0
55	MG	CA	3111	1/1	0.97	0.28	30,30,30,30	0
56	OHX	CA	3338	7/7	0.97	0.08	95,103,117,121	1
56	OHX	DA	1789	7/7	0.97	0.04	176,179,184,242	1
56	OHX	AA	3318	7/7	0.97	0.08	92,102,113,133	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	BA	1773	7/7	0.97	0.08	101,102,110,142	1
56	OHX	CA	3341	7/7	0.97	0.08	74,100,107,145	2
56	OHX	DA	1793	7/7	0.97	0.06	146,150,161,207	1
55	MG	DA	1700	1/1	0.97	0.35	70,70,70,70	0
56	OHX	AA	3322	7/7	0.97	0.06	89,98,107,146	1
56	OHX	BA	1780	7/7	0.97	0.09	94,102,115,117	1
56	OHX	BA	1781	7/7	0.97	0.06	91,111,121,156	1
56	OHX	BA	1782	7/7	0.97	0.07	133,144,159,198	0
56	OHX	AA	3520	7/7	0.97	0.05	127,132,145,185	1
56	OHX	AA	3521	7/7	0.97	0.06	87,94,107,160	1
56	OHX	AA	3467	7/7	0.97	0.06	100,105,117,133	1
56	OHX	DA	1802	7/7	0.97	0.07	120,122,140,196	1
56	OHX	CA	3438	7/7	0.97	0.05	97,104,116,167	1
56	OHX	CA	3450	7/7	0.97	0.06	112,125,137,206	0
56	OHX	CA	3462	7/7	0.97	0.09	71,82,94,110	1
56	OHX	BA	1786	7/7	0.97	0.07	93,97,101,149	1
56	OHX	AA	3468	7/7	0.97	0.06	99,111,119,167	1
56	OHX	AA	3469	7/7	0.97	0.08	79,91,98,161	1
55	MG	AA	3388	1/1	0.97	0.25	41,41,41,41	0
56	OHX	CA	3357	7/7	0.97	0.07	86,98,106,151	1
56	OHX	DA	1811	7/7	0.97	0.04	137,141,149,222	1
56	OHX	AA	3471	7/7	0.97	0.05	98,107,114,163	1
56	OHX	AA	3472	7/7	0.97	0.07	120,126,137,153	1
56	OHX	BA	1792	7/7	0.97	0.06	150,163,168,209	1
56	OHX	CA	3481	7/7	0.97	0.08	35,87,114,138	2
56	OHX	AA	3325	7/7	0.97	0.07	91,103,115,154	1
56	OHX	CA	3484	7/7	0.97	0.06	104,113,129,146	1
56	OHX	AA	3326	7/7	0.97	0.09	83,94,100,118	1
56	OHX	BA	1795	7/7	0.97	0.06	109,127,134,173	1
55	MG	BA	1700	1/1	0.97	0.34	61,61,61,61	0
55	MG	DA	1664	1/1	0.97	0.32	31,31,31,31	0
55	MG	AA	3219	1/1	0.97	0.15	48,48,48,48	0
56	OHX	BA	1799	7/7	0.97	0.06	158,163,176,213	1
56	OHX	AA	3478	7/7	0.97	0.06	77,90,100,131	1
55	MG	AA	3172	1/1	0.98	0.32	38,38,38,38	0
56	OHX	AA	3323	7/7	0.98	0.07	72,87,96,117	1
56	OHX	DA	1719	7/7	0.98	0.07	79,99,112,124	0
56	OHX	DA	1724	7/7	0.98	0.07	84,106,133,148	1
56	OHX	DA	1726	7/7	0.98	0.08	87,101,123,159	0
56	OHX	CA	3307	7/7	0.98	0.06	92,104,131,164	0
56	OHX	DA	1729	7/7	0.98	0.06	104,108,118,152	1
55	MG	BA	1620	1/1	0.98	0.37	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	AA	3518	7/7	0.98	0.06	67,73,103,130	1
56	OHX	CA	3310	7/7	0.98	0.06	74,88,107,129	1
56	OHX	CA	3311	7/7	0.98	0.07	79,95,105,127	1
56	OHX	CA	3312	7/7	0.98	0.07	85,101,114,134	1
56	OHX	CA	3313	7/7	0.98	0.05	103,112,124,157	0
56	OHX	AA	3300	7/7	0.98	0.06	67,91,120,167	1
56	OHX	DA	1738	7/7	0.98	0.05	115,122,137,171	1
56	OHX	DA	1739	7/7	0.98	0.04	98,110,124,155	1
56	OHX	CA	3315	7/7	0.98	0.07	90,101,110,160	1
56	OHX	DA	1742	7/7	0.98	0.05	117,127,141,176	1
56	OHX	DA	1743	7/7	0.98	0.06	109,113,118,148	1
56	OHX	DA	1744	7/7	0.98	0.06	103,108,120,148	1
55	MG	AA	3031	1/1	0.98	0.20	35,35,35,35	0
56	OHX	DA	1746	7/7	0.98	0.05	126,134,146,189	1
56	OHX	AA	3400	7/7	0.98	0.08	69,80,83,116	1
56	OHX	CA	3319	7/7	0.98	0.06	87,97,106,138	1
56	OHX	CA	3320	7/7	0.98	0.06	140,142,153,174	0
56	OHX	CA	3321	7/7	0.98	0.06	111,119,144,156	0
56	OHX	CA	3322	7/7	0.98	0.06	104,117,127,154	1
56	OHX	CA	3323	7/7	0.98	0.05	107,111,118,169	0
55	MG	DN	201	1/1	0.98	0.10	80,80,80,80	0
56	OHX	CA	3326	7/7	0.98	0.06	97,110,130,136	2
55	MG	BA	1733	1/1	0.98	0.35	60,60,60,60	0
56	OHX	CA	3329	7/7	0.98	0.06	102,103,123,146	1
56	OHX	AA	3329	7/7	0.98	0.06	85,90,103,133	1
56	OHX	DA	1758	7/7	0.98	0.04	132,137,143,204	0
56	OHX	DA	1759	7/7	0.98	0.05	120,137,147,190	0
56	OHX	CA	3332	7/7	0.98	0.07	70,82,93,103	1
55	MG	AA	3213	1/1	0.98	0.10	49,49,49,49	0
56	OHX	AA	3154	7/7	0.98	0.08	76,89,110,133	1
55	MG	CA	3265	1/1	0.98	0.14	55,55,55,55	0
56	OHX	DA	1764	7/7	0.98	0.05	115,121,127,171	1
56	OHX	AA	3308	7/7	0.98	0.06	66,73,104,120	2
56	OHX	AA	3440	7/7	0.98	0.07	59,88,102,124	0
56	OHX	BA	1684	7/7	0.98	0.05	109,118,126,149	1
56	OHX	AA	3441	7/7	0.98	0.07	84,93,115,140	0
56	OHX	AA	3443	7/7	0.98	0.06	69,76,84,127	1
56	OHX	AB	211	7/7	0.98	0.07	74,85,113,121	0
56	OHX	AA	3309	7/7	0.98	0.07	64,84,90,112	1
55	MG	A0	201	1/1	0.98	0.14	48,48,48,48	0
56	OHX	AA	3287	7/7	0.98	0.06	75,88,103,129	2
56	OHX	CA	3345	7/7	0.98	0.05	91,108,114,146	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	AA	3451	7/7	0.98	0.07	75,85,92,125	1
56	OHX	CA	3347	7/7	0.98	0.06	86,102,110,148	1
56	OHX	AA	3314	7/7	0.98	0.07	81,93,123,149	1
56	OHX	AA	3454	7/7	0.98	0.07	68,93,112,112	1
56	OHX	DA	1779	7/7	0.98	0.04	144,146,155,215	1
56	OHX	AA	3455	7/7	0.98	0.06	56,75,100,119	2
56	OHX	AA	3456	7/7	0.98	0.07	59,75,90,132	2
56	OHX	BA	1761	7/7	0.98	0.06	102,104,115,161	0
56	OHX	AA	3338	7/7	0.98	0.07	82,93,108,126	1
56	OHX	CA	3354	7/7	0.98	0.08	78,88,98,105	1
56	OHX	BA	1765	7/7	0.98	0.07	111,119,130,164	0
56	OHX	BA	1766	7/7	0.98	0.08	89,96,106,129	1
56	OHX	BA	1767	7/7	0.98	0.06	92,119,140,142	0
56	OHX	BC	106	7/7	0.98	0.07	110,133,144,147	1
56	OHX	BC	107	7/7	0.98	0.06	105,124,134,145	1
56	OHX	AA	3499	7/7	0.98	0.05	101,113,131,183	1
56	OHX	BA	1769	7/7	0.98	0.07	102,107,127,145	0
56	OHX	AA	3459	7/7	0.98	0.07	71,92,105,129	1
56	OHX	CA	3235	7/7	0.98	0.06	43,79,99,118	0
56	OHX	CA	3237	7/7	0.98	0.06	109,109,122,166	0
56	OHX	CA	3240	7/7	0.98	0.07	96,99,103,148	1
56	OHX	CA	3241	7/7	0.98	0.08	90,96,101,122	1
56	OHX	CA	3242	7/7	0.98	0.07	95,107,117,129	1
56	OHX	AA	3460	7/7	0.98	0.06	87,98,107,140	0
56	OHX	CA	3483	7/7	0.98	0.07	84,93,103,136	1
56	OHX	AA	3461	7/7	0.98	0.06	60,78,98,143	1
56	OHX	CA	3485	7/7	0.98	0.07	88,102,109,144	1
56	OHX	AA	3463	7/7	0.98	0.07	77,89,96,134	1
56	OHX	BA	1774	7/7	0.98	0.06	80,98,111,147	1
56	OHX	AA	3315	7/7	0.98	0.09	89,99,111,137	1
56	OHX	CA	3249	7/7	0.98	0.08	86,90,104,128	1
56	OHX	AA	3340	7/7	0.98	0.05	159,167,171,209	0
56	OHX	CA	3251	7/7	0.98	0.06	88,107,125,141	1
56	OHX	CA	3492	7/7	0.98	0.06	97,102,115,126	1
56	OHX	CB	208	7/7	0.98	0.06	105,109,142,147	0
56	OHX	AA	3341	7/7	0.98	0.06	75,103,114,126	1
56	OHX	AA	3342	7/7	0.98	0.06	78,85,104,123	1
55	MG	AA	3355	1/1	0.98	0.29	36,36,36,36	0
56	OHX	AA	3364	7/7	0.98	0.07	92,103,108,119	1
56	OHX	AA	3295	7/7	0.98	0.07	84,98,116,152	0
56	OHX	AA	3511	7/7	0.98	0.05	133,145,154,207	0
56	OHX	CA	3288	7/7	0.98	0.07	87,95,104,133	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	AA	3297	7/7	0.98	0.10	87,98,102,106	1
56	OHX	CA	3294	7/7	0.98	0.08	91,93,107,125	1
56	OHX	AA	3320	7/7	0.98	0.09	69,81,96,121	1
56	OHX	CA	3297	7/7	0.98	0.05	84,94,129,142	1
56	OHX	CA	3298	7/7	0.98	0.05	90,98,134,148	0
56	OHX	DC	109	7/7	0.98	0.05	88,92,104,159	3
56	OHX	DC	110	7/7	0.98	0.07	78,91,106,144	4
56	OHX	CA	3299	7/7	0.98	0.06	99,105,124,141	1
57	ZN	BG	301	1/1	0.98	0.18	79,79,79,79	0
56	OHX	CA	3301	7/7	0.98	0.07	55,85,123,136	3
56	OHX	AA	3321	7/7	0.98	0.04	97,109,121,173	1
56	OHX	AA	3433	7/7	0.99	0.04	63,65,104,122	1
56	OHX	AA	3434	7/7	0.99	0.06	62,71,94,101	1
56	OHX	CA	3303	7/7	0.99	0.04	92,96,123,138	0
56	OHX	AA	3435	7/7	0.99	0.07	61,70,93,100	3
56	OHX	CA	3305	7/7	0.99	0.06	70,83,99,129	1
56	OHX	AA	3436	7/7	0.99	0.05	78,91,117,117	0
56	OHX	AA	3437	7/7	0.99	0.05	81,95,107,131	0
56	OHX	AA	3438	7/7	0.99	0.06	51,64,72,96	2
56	OHX	AA	3439	7/7	0.99	0.04	69,82,92,115	1
56	OHX	AA	3310	7/7	0.99	0.04	94,104,125,156	0
56	OHX	DA	1740	7/7	0.99	0.05	139,153,162,184	0
56	OHX	AA	3311	7/7	0.99	0.06	97,106,117,155	1
56	OHX	AA	3442	7/7	0.99	0.05	70,87,119,140	0
56	OHX	AA	3301	7/7	0.99	0.06	88,89,93,110	1
56	OHX	AA	3444	7/7	0.99	0.05	80,103,116,131	1
56	OHX	AA	3445	7/7	0.99	0.05	75,87,109,120	1
56	OHX	CA	3316	7/7	0.99	0.05	119,122,129,158	0
56	OHX	AA	3446	7/7	0.99	0.07	68,90,101,115	2
56	OHX	AA	3293	7/7	0.99	0.07	54,82,88,102	2
56	OHX	AA	3294	7/7	0.99	0.05	94,100,117,120	0
56	OHX	AA	3449	7/7	0.99	0.04	64,74,89,112	2
55	MG	B1	101	1/1	0.99	0.33	26,26,26,26	0
56	OHX	BA	1696	7/7	0.99	0.04	47,75,99,113	0
56	OHX	BA	1755	7/7	0.99	0.06	72,74,97,109	0
56	OHX	CA	3324	7/7	0.99	0.07	65,83,94,110	2
56	OHX	BA	1756	7/7	0.99	0.08	59,79,107,108	0
56	OHX	BA	1757	7/7	0.99	0.07	57,66,87,98	2
56	OHX	CA	3327	7/7	0.99	0.05	76,83,103,129	1
56	OHX	BA	1758	7/7	0.99	0.07	69,88,100,119	0
56	OHX	BA	1759	7/7	0.99	0.07	78,93,120,156	0
56	OHX	CA	3330	7/7	0.99	0.04	102,106,115,169	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	BA	1760	7/7	0.99	0.06	71,106,126,148	0
56	OHX	AE	304	7/7	0.99	0.06	74,87,107,110	1
56	OHX	BA	1762	7/7	0.99	0.07	72,94,107,136	0
56	OHX	BA	1763	7/7	0.99	0.05	94,115,123,136	0
56	OHX	AO	204	7/7	0.99	0.05	83,94,106,121	1
56	OHX	AA	3316	7/7	0.99	0.05	80,95,97,136	0
56	OHX	AA	3296	7/7	0.99	0.05	115,120,123,158	0
56	OHX	AA	3453	7/7	0.99	0.06	95,106,114,148	0
56	OHX	CA	3232	7/7	0.99	0.10	72,77,83,137	0
56	OHX	CA	3233	7/7	0.99	0.08	74,85,95,121	0
56	OHX	CA	3234	7/7	0.99	0.06	77,91,119,122	2
56	OHX	AA	3399	7/7	0.99	0.10	42,51,73,98	0
56	OHX	CA	3236	7/7	0.99	0.06	81,104,120,146	0
56	OHX	AA	3289	7/7	0.99	0.07	53,58,81,93	0
56	OHX	CA	3238	7/7	0.99	0.08	80,102,103,125	1
56	OHX	CA	3239	7/7	0.99	0.06	66,92,107,113	1
56	OHX	AA	3359	7/7	0.99	0.05	61,75,93,113	0
56	OHX	AA	3457	7/7	0.99	0.04	73,83,101,131	1
56	OHX	CA	3461	7/7	0.99	0.08	38,55,94,109	0
56	OHX	AA	3360	7/7	0.99	0.07	58,67,70,97	1
56	OHX	CA	3243	7/7	0.99	0.05	121,128,140,172	0
56	OHX	AA	3361	7/7	0.99	0.06	51,71,83,107	0
56	OHX	AA	3362	7/7	0.99	0.08	40,81,119,136	1
56	OHX	BA	1775	7/7	0.99	0.04	111,114,129,169	1
56	OHX	BA	1776	7/7	0.99	0.05	102,114,119,153	1
56	OHX	AA	3290	7/7	0.99	0.06	10,72,91,128	0
56	OHX	AA	3462	7/7	0.99	0.06	75,85,103,106	1
56	OHX	BA	1779	7/7	0.99	0.05	102,112,125,152	1
56	OHX	AA	3291	7/7	0.99	0.07	68,75,102,108	3
56	OHX	AA	3292	7/7	0.99	0.06	50,75,88,112	0
56	OHX	AA	3420	7/7	0.99	0.08	63,69,102,115	0
56	OHX	AA	3421	7/7	0.99	0.07	50,71,87,114	0
56	OHX	CA	3255	7/7	0.99	0.05	103,107,122,145	1
56	OHX	CA	3256	7/7	0.99	0.06	88,101,112,126	1
56	OHX	AA	3422	7/7	0.99	0.07	74,81,107,116	0
56	OHX	CA	3270	7/7	0.99	0.05	73,87,105,117	0
56	OHX	CA	3272	7/7	0.99	0.08	54,70,84,85	1
56	OHX	CA	3273	7/7	0.99	0.06	58,69,86,110	0
56	OHX	CA	3274	7/7	0.99	0.07	67,83,114,118	0
56	OHX	CA	3276	7/7	0.99	0.06	81,100,117,133	0
56	OHX	CA	3277	7/7	0.99	0.06	73,81,99,107	1
56	OHX	CA	3278	7/7	0.99	0.05	81,96,114,120	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	OHX	CA	3279	7/7	0.99	0.07	80,89,109,118	0
56	OHX	CA	3280	7/7	0.99	0.07	82,87,100,129	0
56	OHX	CA	3283	7/7	0.99	0.07	81,83,86,120	1
56	OHX	AA	3423	7/7	0.99	0.08	44,66,84,86	1
56	OHX	AA	3424	7/7	0.99	0.06	92,97,108,112	0
56	OHX	CA	3286	7/7	0.99	0.04	87,94,108,115	0
56	OHX	CA	3287	7/7	0.99	0.08	69,74,104,109	3
56	OHX	AA	3426	7/7	0.99	0.08	70,84,89,118	0
56	OHX	CA	3289	7/7	0.99	0.04	69,83,106,125	0
56	OHX	CA	3290	7/7	0.99	0.05	94,101,123,130	0
56	OHX	CA	3291	7/7	0.99	0.07	86,105,118,139	0
56	OHX	CA	3292	7/7	0.99	0.08	69,105,113,146	0
56	OHX	AA	3427	7/7	0.99	0.05	29,70,88,108	0
56	OHX	AA	3428	7/7	0.99	0.07	67,79,86,113	0
56	OHX	AA	3429	7/7	0.99	0.06	69,73,84,102	1
56	OHX	CA	3296	7/7	0.99	0.06	65,90,108,135	2
56	OHX	DA	1718	7/7	0.99	0.08	73,98,100,135	0
56	OHX	AA	3430	7/7	0.99	0.06	63,78,92,111	1
56	OHX	DA	1721	7/7	0.99	0.04	94,108,116,135	0
56	OHX	DA	1722	7/7	0.99	0.06	84,90,106,116	0
56	OHX	DA	1723	7/7	0.99	0.06	107,111,116,151	0
56	OHX	AA	3431	7/7	0.99	0.05	74,81,100,115	0
56	OHX	AA	3432	7/7	0.99	0.05	72,98,103,107	0
56	OHX	DA	1727	7/7	0.99	0.05	114,126,131,160	0
56	OHX	CA	3300	7/7	0.99	0.07	66,75,91,101	1
57	ZN	DQ	101	1/1	0.99	0.04	123,123,123,123	0
56	OHX	CA	3282	7/7	1.00	0.03	79,83,97,109	0
56	OHX	DA	1734	7/7	1.00	0.03	102,105,122,149	1
56	OHX	AA	3425	7/7	1.00	0.04	45,61,75,79	0
56	OHX	AA	3417	7/7	1.00	0.06	68,72,82,103	0
56	OHX	CF	301	7/7	1.00	0.07	54,58,79,92	0
56	OHX	CA	3275	7/7	1.00	0.04	56,80,112,114	1
56	OHX	AA	3418	7/7	1.00	0.06	39,61,82,95	0
56	OHX	AA	3419	7/7	1.00	0.05	67,75,91,95	0
56	OHX	AF	303	7/7	1.00	0.07	45,52,58,77	0
56	OHX	CA	3271	7/7	1.00	0.09	67,82,101,115	0
55	MG	AA	3194	1/1	1.00	0.04	26,26,26,26	0
56	OHX	CA	3281	7/7	1.00	0.06	101,105,126,132	0

5.5 Other polymers ⓘ

There are no such residues in this entry.