



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 11:20 AM UTC

PDB ID : 5VPP / pdb_00005vpp
Title : The 70S P-site tRNA SufA6 complex
Authors : Hong, S.; Sunita, S.; Dunkle, J.A.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2017-05-05
Resolution : 3.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

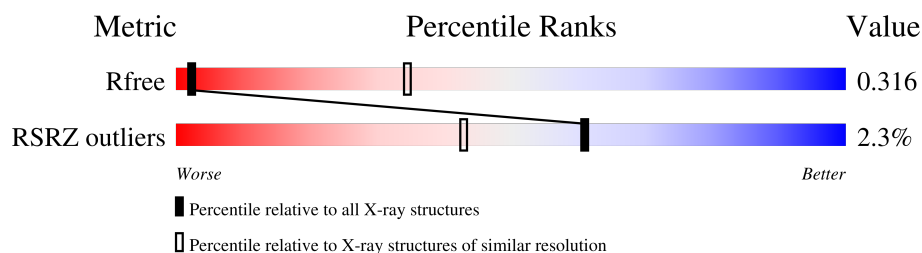
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1270 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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
54	MG	QA	1611	-	-	-	X
54	MG	QA	1621	-	-	-	X
54	MG	QA	1634	-	-	-	X
54	MG	QA	1638	-	-	-	X
54	MG	QA	1648	-	-	-	X
54	MG	QA	1668	-	-	-	X
54	MG	QA	1673	-	-	-	X
54	MG	QA	1695	-	-	-	X
54	MG	QP	101	-	-	-	X
54	MG	QP	102	-	-	-	X
54	MG	RA	3026	-	-	-	X
54	MG	RA	3033	-	-	-	X
54	MG	RA	3043	-	-	-	X
54	MG	RA	3071	-	-	-	X
54	MG	RA	3126	-	-	-	X
54	MG	RA	3130	-	-	-	X
54	MG	RA	3151	-	-	-	X
54	MG	RA	3160	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	RA	3162	-	-	-	X
54	MG	RA	3176	-	-	-	X
54	MG	RA	3201	-	-	-	X
54	MG	RA	3206	-	-	-	X
54	MG	RA	3215	-	-	-	X
54	MG	RA	3222	-	-	-	X
54	MG	RA	3230	-	-	-	X
54	MG	RA	3233	-	-	-	X
54	MG	RA	3259	-	-	-	X
54	MG	RA	3260	-	-	-	X
54	MG	RA	3295	-	-	-	X
54	MG	RA	3301	-	-	-	X
54	MG	RA	3305	-	-	-	X
54	MG	RA	3323	-	-	-	X
54	MG	RA	3335	-	-	-	X
54	MG	RA	3337	-	-	-	X
54	MG	RA	3346	-	-	-	X
54	MG	RA	3357	-	-	-	X
54	MG	RA	3437	-	-	-	X
54	MG	RA	3451	-	-	-	X
54	MG	RA	3479	-	-	-	X
54	MG	RA	3485	-	-	-	X
54	MG	RB	204	-	-	-	X
54	MG	RB	206	-	-	-	X
54	MG	RB	207	-	-	-	X
54	MG	XA	1644	-	-	-	X
54	MG	XA	1677	-	-	-	X
54	MG	XA	1684	-	-	-	X
54	MG	XA	1699	-	-	-	X
54	MG	YA	3610	-	-	-	X
54	MG	YA	3614	-	-	-	X
54	MG	YA	3617	-	-	-	X
54	MG	YA	3618	-	-	-	X
54	MG	YA	3625	-	-	-	X
54	MG	YA	3636	-	-	-	X
54	MG	YA	3640	-	-	-	X
54	MG	YA	3646	-	-	-	X
54	MG	YA	3650	-	-	-	X
54	MG	YA	3658	-	-	-	X
54	MG	YA	3668	-	-	-	X
54	MG	YA	3671	-	-	-	X
54	MG	YA	3686	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	YA	3687	-	-	-	X
54	MG	YA	3698	-	-	-	X
54	MG	YA	3731	-	-	-	X
54	MG	YA	3737	-	-	-	X
54	MG	YA	3741	-	-	-	X
54	MG	YA	3759	-	-	-	X
54	MG	YA	3760	-	-	-	X
54	MG	YA	3761	-	-	-	X
54	MG	YA	3767	-	-	-	X
54	MG	YA	3772	-	-	-	X
54	MG	YA	3776	-	-	-	X
54	MG	YA	3794	-	-	-	X
54	MG	YA	3796	-	-	-	X
54	MG	YA	3806	-	-	-	X
54	MG	YA	3809	-	-	-	X
54	MG	YA	3816	-	-	-	X
54	MG	YA	3823	-	-	-	X
54	MG	YA	3832	-	-	-	X
54	MG	YA	3848	-	-	-	X
54	MG	YA	3854	-	-	-	X
54	MG	YA	3858	-	-	-	X
54	MG	YA	3869	-	-	-	X
54	MG	YA	3874	-	-	-	X
54	MG	YA	3888	-	-	-	X
54	MG	YA	3891	-	-	-	X
54	MG	YA	3901	-	-	-	X
54	MG	YA	3917	-	-	-	X
54	MG	YA	3921	-	-	-	X
54	MG	YA	3947	-	-	-	X
54	MG	YA	3948	-	-	-	X
54	MG	YA	3956	-	-	-	X
54	MG	YA	3959	-	-	-	X
54	MG	YB	205	-	-	-	X
54	MG	YB	206	-	-	-	X
54	MG	YD	302	-	-	-	X

2 Entry composition [i](#)

There are 55 unique types of molecules in this entry. The entry contains 291660 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 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	RA	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			
1	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	RB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
2	YB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
3	YD	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	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
4	YE	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	RF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
5	YF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	RG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
6	YG	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	RH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
7	YH	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	RI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
8	YI	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	RN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
9	YN	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	RO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	YO	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	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
11	YP	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	RQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	YQ	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	RR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	YR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	RS	111	Total	C	N	O	0	0	0
			882	556	176	150			
14	YS	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	RT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
15	YT	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	RU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
16	YU	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	RV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
17	YV	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	RW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
18	YW	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	RX	92	Total	C	N	O	0	0	0
			725	471	131	123			
19	YX	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	RY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
20	YY	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	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			
21	YZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	R0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			
22	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
23	Y1	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	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
24	Y2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	R3	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	Y3	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			
27	Y6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
28	Y7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	R8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
29	Y8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	R9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
30	Y9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 31 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	QB	235	Total	C	N	O	S	0	0	0
			1909	1218	342	344	5			
31	XB	235	Total	C	N	O	S	0	0	0
			1909	1218	342	344	5			

- Molecule 32 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	QC	207	Total	C	N	O	S	0	0	0
			1620	1022	315	282	1			
32	XC	207	Total	C	N	O	S	0	0	0
			1620	1022	315	282	1			

- Molecule 33 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	QD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
33	XD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 34 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	QE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
34	XE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 35 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	QF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
35	XF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 36 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	QG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
36	XG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 37 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	QH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
37	XH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 38 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	QI	127	Total	C	N	O	S	0	0	0
			1010	639	197	174				
38	XI	127	Total	C	N	O	S	0	0	0
			1010	639	197	174				

- Molecule 39 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	QJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			
39	XJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 40 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	QK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
40	XK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 41 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	QL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
41	XL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 42 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	QM	114	Total	C	N	O	S	0	0	0
			914	565	189	158	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	XM	114	Total	C	N	O	S	0	0	0
			914	565	189	158	2			

- Molecule 43 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	QN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
43	XN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 44 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
44	XO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 45 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	QP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
45	XP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 46 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	QQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
46	XQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 47 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	QR	70	Total	C	N	O	0	0	0
			574	367	112	95			
47	XR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 48 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	QT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
48	XT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 49 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	QA	1511	Total	C	N	O	P	0	0	0
			32472	14454	6013	10495	1510			
49	XA	1515	Total	C	N	O	P	0	0	0
			32554	14491	6024	10525	1514			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QA	458C	G	C	conflict	GB 55771382
XA	458C	G	C	conflict	GB 55771382

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	XS	79	Total	C	N	O	S	0	0	0
			633	405	115	111	2			
50	QS	79	Total	C	N	O	S	0	0	0
			633	405	115	111	2			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	R4	34	Total	C	N	O	S	0	0	0
			262	169	43	48	2			
51	Y4	46	Total	C	N	O	S	0	0	0
			357	229	59	64	5			

- Molecule 52 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	XX	19	Total	C	N	O	P	0	0	0
			409	184	81	126	18			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	QX	19	Total	C	N	O	P	0	0	0
			409	184	81	126	18			

- Molecule 53 is a RNA chain called P-site tRNA SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	XV	78	Total	C	N	O	P	0	0	0
			1670	744	300	548	78			
53	QV	78	Total	C	N	O	P	0	0	0
			1670	744	300	548	78			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XV	38	1MG	-	insertion	GB 1151176235
QV	38	1MG	-	insertion	GB 1151176235

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	RA	562	Total	Mg	0	0
			562	562		
54	RB	15	Total	Mg	0	0
			15	15		
54	RD	10	Total	Mg	0	0
			10	10		
54	RE	7	Total	Mg	0	0
			7	7		
54	RF	4	Total	Mg	0	0
			4	4		
54	RI	1	Total	Mg	0	0
			1	1		
54	RO	2	Total	Mg	0	0
			2	2		
54	RQ	2	Total	Mg	0	0
			2	2		
54	RR	3	Total	Mg	0	0
			3	3		
54	RT	3	Total	Mg	0	0
			3	3		
54	RU	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	RX	2	Total 2	Mg 2	0	0
54	RY	1	Total 1	Mg 1	0	0
54	R0	2	Total 2	Mg 2	0	0
54	R1	3	Total 3	Mg 3	0	0
54	R3	1	Total 1	Mg 1	0	0
54	R6	1	Total 1	Mg 1	0	0
54	R8	3	Total 3	Mg 3	0	0
54	YA	379	Total 379	Mg 379	0	0
54	YB	10	Total 10	Mg 10	0	0
54	YD	4	Total 4	Mg 4	0	0
54	YE	5	Total 5	Mg 5	0	0
54	YI	1	Total 1	Mg 1	0	0
54	YP	1	Total 1	Mg 1	0	0
54	YQ	1	Total 1	Mg 1	0	0
54	YR	1	Total 1	Mg 1	0	0
54	YT	2	Total 2	Mg 2	0	0
54	YU	1	Total 1	Mg 1	0	0
54	YX	1	Total 1	Mg 1	0	0
54	YY	1	Total 1	Mg 1	0	0
54	Y0	1	Total 1	Mg 1	0	0
54	Y1	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	Y8	1	Total 1	Mg 1	0	0
54	QC	1	Total 1	Mg 1	0	0
54	QD	3	Total 3	Mg 3	0	0
54	QE	1	Total 1	Mg 1	0	0
54	QL	3	Total 3	Mg 3	0	0
54	QP	2	Total 2	Mg 2	0	0
54	QQ	2	Total 2	Mg 2	0	0
54	QT	2	Total 2	Mg 2	0	0
54	QA	131	Total 131	Mg 131	0	0
54	XC	1	Total 1	Mg 1	0	0
54	XD	1	Total 1	Mg 1	0	0
54	XE	1	Total 1	Mg 1	0	0
54	XK	1	Total 1	Mg 1	0	0
54	XL	2	Total 2	Mg 2	0	0
54	XM	1	Total 1	Mg 1	0	0
54	XO	1	Total 1	Mg 1	0	0
54	XP	1	Total 1	Mg 1	0	0
54	XA	128	Total 128	Mg 128	0	0

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	Y9	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QD	2	Total 2	Zn 2	0	0
55	XD	1	Total 1	Zn 1	0	0

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	210.75Å 450.05Å 626.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.60 – 3.90 16.60 – 3.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (16.60-3.90) 96.8 (16.60-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.88Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	(Not available) , (Not available) 0.272 , 0.316	Depositor DCC
R_{free} test set	23266 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å ²)	128.1	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	291660	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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](#)

2 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	$\# Z > 2$
53	1MG	XV	38	53	23,26,27	1.19	3 (13%)	33,39,42	1.78	5 (15%)
53	1MG	QV	38	53	23,26,27	1.17	3 (13%)	33,39,42	1.77	5 (15%)

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
53	1MG	XV	38	53	-	3/7/25/26	0/3/3/3
53	1MG	QV	38	53	-	3/7/25/26	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	XV	38	1MG	C5-C4	3.02	1.47	1.38
53	QV	38	1MG	C5-C4	3.02	1.47	1.38
53	XV	38	1MG	C5-N7	-2.54	1.34	1.39
53	QV	38	1MG	C5-N7	-2.47	1.34	1.39
53	XV	38	1MG	C2-N1	2.26	1.41	1.37
53	QV	38	1MG	C2-N1	2.20	1.41	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	QV	38	1MG	C5-C4-N3	-5.71	119.31	128.39
53	XV	38	1MG	C5-C4-N3	-5.70	119.32	128.39
53	XV	38	1MG	C2-N3-C4	4.50	122.10	111.98
53	QV	38	1MG	C2-N3-C4	4.50	122.08	111.98
53	QV	38	1MG	N9-C4-N3	4.33	134.61	125.95
53	XV	38	1MG	N9-C4-N3	4.33	134.61	125.95
53	QV	38	1MG	C6-C5-N7	2.45	134.79	129.36
53	XV	38	1MG	C6-C5-N7	2.44	134.79	129.36
53	QV	38	1MG	C4-C5-N7	-2.42	106.83	110.67
53	XV	38	1MG	C4-C5-N7	-2.41	106.86	110.67

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	XV	38	1MG	C4'-C5'-O5'-P
53	QV	38	1MG	C4'-C5'-O5'-P
53	XV	38	1MG	O4'-C4'-C5'-O5'
53	QV	38	1MG	O4'-C4'-C5'-O5'
53	XV	38	1MG	C3'-C4'-C5'-O5'
53	QV	38	1MG	C3'-C4'-C5'-O5'

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 1319 ligands modelled in this entry, 1319 are monoatomic - leaving 0 for Mogul analysis.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	RA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	RA	1052:C	O3'	1053:C	P	3.18

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	RA	2882/2915 (98%)	0.18	66 (2%) 61 43	94, 115, 163, 199	0
1	YA	2883/2915 (98%)	0.40	99 (3%) 48 34	91, 101, 157, 189	0
2	RB	120/122 (98%)	0.31	1 (0%) 82 64	111, 133, 146, 156	0
2	YB	120/122 (98%)	0.09	0 100 100	92, 110, 128, 155	0
3	RD	272/276 (98%)	0.06	2 (0%) 84 67	92, 110, 128, 149	0
3	YD	272/276 (98%)	0.35	10 (3%) 45 32	91, 103, 121, 147	0
4	RE	205/206 (99%)	0.11	5 (2%) 59 42	93, 122, 141, 157	0
4	YE	205/206 (99%)	0.22	3 (1%) 72 50	91, 103, 128, 170	0
5	RF	202/210 (96%)	-0.10	1 (0%) 87 72	96, 119, 138, 160	0
5	YF	202/210 (96%)	0.16	3 (1%) 72 50	90, 101, 130, 153	0
6	RG	181/182 (99%)	0.35	5 (2%) 55 38	114, 142, 165, 174	0
6	YG	181/182 (99%)	0.21	4 (2%) 62 44	99, 129, 155, 168	0
7	RH	170/180 (94%)	0.03	0 100 100	99, 141, 162, 191	0
7	YH	170/180 (94%)	0.17	2 (1%) 76 55	94, 108, 134, 148	0
8	RI	146/148 (98%)	-0.05	0 100 100	113, 132, 147, 158	0
8	YI	146/148 (98%)	0.24	4 (2%) 56 39	98, 130, 155, 167	0
9	RN	138/140 (98%)	-0.07	3 (2%) 62 44	97, 122, 141, 156	0
9	YN	138/140 (98%)	0.19	1 (0%) 84 67	91, 101, 125, 158	0
10	RO	122/122 (100%)	-0.05	0 100 100	94, 116, 137, 144	0
10	YO	122/122 (100%)	0.02	1 (0%) 82 64	92, 102, 120, 138	0
11	RP	150/150 (100%)	-0.05	2 (1%) 75 54	96, 122, 144, 169	0
11	YP	150/150 (100%)	0.23	3 (2%) 65 45	92, 105, 134, 168	0
12	RQ	141/141 (100%)	0.00	0 100 100	98, 124, 144, 157	0
12	YQ	141/141 (100%)	0.05	1 (0%) 84 67	91, 106, 132, 154	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	RR	118/118 (100%)	0.02	2 (1%) 69 48	93, 109, 129, 148	0
13	YR	118/118 (100%)	0.34	3 (2%) 58 41	92, 103, 120, 129	0
14	RS	111/112 (99%)	0.07	1 (0%) 81 62	108, 130, 150, 161	0
14	YS	111/112 (99%)	-0.09	0 100 100	93, 107, 133, 158	0
15	RT	137/146 (93%)	-0.12	0 100 100	101, 123, 146, 172	0
15	YT	137/146 (93%)	0.03	2 (1%) 72 50	96, 109, 139, 158	0
16	RU	117/118 (99%)	0.04	2 (1%) 69 48	94, 116, 143, 151	0
16	YU	117/118 (99%)	0.50	5 (4%) 40 30	91, 99, 116, 164	0
17	RV	101/101 (100%)	-0.18	0 100 100	96, 125, 146, 160	0
17	YV	101/101 (100%)	0.12	3 (2%) 52 36	91, 101, 124, 162	0
18	RW	113/113 (100%)	0.05	2 (1%) 67 47	92, 105, 126, 155	0
18	YW	113/113 (100%)	0.16	0 100 100	90, 97, 115, 147	0
19	RX	92/96 (95%)	-0.07	0 100 100	93, 108, 130, 140	0
19	YX	92/96 (95%)	0.21	1 (1%) 78 57	91, 98, 116, 130	0
20	RY	102/110 (92%)	0.17	0 100 100	98, 124, 148, 166	0
20	YY	102/110 (92%)	0.23	2 (1%) 65 45	92, 109, 132, 146	0
21	RZ	183/206 (88%)	0.33	6 (3%) 49 34	107, 139, 160, 168	0
21	YZ	183/206 (88%)	0.07	2 (1%) 78 57	94, 112, 147, 167	0
22	R0	82/85 (96%)	0.08	2 (2%) 59 42	95, 120, 158, 175	0
22	Y0	82/85 (96%)	0.23	1 (1%) 76 55	92, 103, 140, 172	0
23	R1	97/98 (98%)	-0.02	0 100 100	98, 116, 139, 165	0
23	Y1	97/98 (98%)	0.23	0 100 100	92, 105, 133, 149	0
24	R2	69/72 (95%)	-0.11	0 100 100	96, 117, 135, 164	0
24	Y2	69/72 (95%)	0.37	2 (2%) 53 37	92, 107, 130, 138	0
25	R3	59/60 (98%)	-0.06	0 100 100	105, 124, 145, 158	0
25	Y3	59/60 (98%)	0.07	2 (3%) 48 34	91, 102, 122, 129	0
26	R5	59/60 (98%)	0.46	5 (8%) 16 17	93, 113, 147, 160	0
26	Y5	59/60 (98%)	0.79	2 (3%) 48 34	91, 104, 152, 161	0
27	R6	49/54 (90%)	0.48	1 (2%) 65 45	100, 128, 156, 170	0
27	Y6	49/54 (90%)	0.66	4 (8%) 17 18	95, 116, 146, 154	0
28	R7	49/49 (100%)	0.22	2 (4%) 41 31	91, 106, 125, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	Y7	49/49 (100%)	0.46	2 (4%) 41 31	91, 96, 117, 147	0
29	R8	64/65 (98%)	-0.04	0 100 100	100, 117, 133, 140	0
29	Y8	64/65 (98%)	0.27	1 (1%) 70 49	93, 103, 123, 139	0
30	R9	37/37 (100%)	0.47	2 (5%) 31 25	111, 125, 144, 167	0
30	Y9	37/37 (100%)	0.44	3 (8%) 18 18	91, 104, 129, 129	0
31	QB	235/256 (91%)	0.28	6 (2%) 57 40	112, 142, 167, 180	0
31	XB	235/256 (91%)	0.15	3 (1%) 75 54	105, 139, 163, 179	0
32	QC	207/239 (86%)	0.22	2 (0%) 79 59	115, 147, 163, 187	0
32	XC	207/239 (86%)	0.19	2 (0%) 79 59	112, 143, 164, 185	0
33	QD	208/209 (99%)	0.37	9 (4%) 40 30	109, 138, 161, 176	0
33	XD	208/209 (99%)	0.31	6 (2%) 53 37	107, 138, 158, 170	0
34	QE	151/162 (93%)	0.34	4 (2%) 57 40	112, 141, 163, 173	0
34	XE	151/162 (93%)	0.16	2 (1%) 75 54	98, 128, 152, 160	0
35	QF	101/101 (100%)	0.14	0 100 100	109, 139, 163, 170	0
35	XF	101/101 (100%)	0.13	0 100 100	102, 131, 154, 165	0
36	QG	155/156 (99%)	0.37	3 (1%) 66 46	123, 148, 171, 188	0
36	XG	155/156 (99%)	0.32	3 (1%) 66 46	120, 149, 166, 170	0
37	QH	138/138 (100%)	0.18	2 (1%) 73 52	103, 136, 159, 171	0
37	XH	138/138 (100%)	0.15	1 (0%) 84 67	108, 133, 154, 175	0
38	QI	127/128 (99%)	0.57	6 (4%) 36 28	128, 150, 167, 175	0
38	XI	127/128 (99%)	0.38	2 (1%) 70 49	112, 146, 167, 173	0
39	QJ	99/105 (94%)	0.56	4 (4%) 42 31	129, 152, 167, 175	0
39	XJ	99/105 (94%)	0.54	3 (3%) 52 36	111, 152, 167, 175	0
40	QK	119/129 (92%)	0.36	2 (1%) 69 48	105, 140, 158, 176	0
40	XK	119/129 (92%)	0.33	4 (3%) 48 34	98, 133, 156, 185	0
41	QL	125/132 (94%)	0.60	9 (7%) 21 20	106, 141, 162, 181	0
41	XL	125/132 (94%)	0.53	9 (7%) 21 20	100, 133, 156, 166	0
42	QM	114/126 (90%)	0.47	4 (3%) 47 33	115, 152, 177, 189	0
42	XM	114/126 (90%)	0.35	2 (1%) 67 47	112, 150, 169, 180	0
43	QN	60/61 (98%)	0.66	2 (3%) 49 34	133, 149, 169, 174	0
43	XN	60/61 (98%)	0.49	2 (3%) 49 34	117, 150, 164, 171	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	QO	88/89 (98%)	0.01	1 (1%) 78 57	96, 129, 150, 157	0
44	XO	88/89 (98%)	0.21	1 (1%) 78 57	104, 127, 150, 160	0
45	QP	84/88 (95%)	0.43	4 (4%) 35 27	103, 138, 166, 173	0
45	XP	84/88 (95%)	0.45	7 (8%) 17 18	104, 136, 156, 164	0
46	QQ	100/105 (95%)	0.18	1 (1%) 79 59	108, 132, 153, 161	0
46	XQ	100/105 (95%)	0.21	2 (2%) 65 45	105, 129, 151, 161	0
47	QR	70/88 (79%)	0.01	1 (1%) 73 52	113, 132, 151, 158	0
47	XR	70/88 (79%)	0.09	0 100 100	101, 130, 151, 167	0
48	QT	99/106 (93%)	0.12	1 (1%) 79 59	107, 131, 155, 163	0
48	XT	99/106 (93%)	0.08	1 (1%) 79 59	102, 129, 154, 168	0
49	QA	1511/1521 (99%)	0.40	40 (2%) 57 40	102, 135, 167, 186	0
49	XA	1515/1521 (99%)	0.31	38 (2%) 58 41	96, 130, 164, 192	0
50	QS	79/93 (84%)	0.63	4 (5%) 33 26	133, 155, 173, 185	0
50	XS	79/93 (84%)	0.42	1 (1%) 75 54	121, 152, 169, 174	0
51	R4	34/71 (47%)	0.31	0 100 100	113, 153, 169, 176	0
51	Y4	46/71 (64%)	0.28	2 (4%) 40 30	110, 145, 171, 184	0
52	QX	19/19 (100%)	0.87	0 100 100	135, 162, 170, 174	0
52	XX	19/19 (100%)	0.49	0 100 100	135, 156, 175, 178	0
53	QV	77/78 (98%)	0.88	2 (2%) 57 40	121, 158, 174, 187	0
53	XV	77/78 (98%)	0.65	2 (2%) 57 40	97, 153, 174, 194	0
All	All	20753/21384 (97%)	0.26	476 (2%) 61 43	90, 122, 161, 199	0

All (476) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	Y5	2	ALA	10.8
33	QD	25	ARG	8.3
6	YG	43	LEU	6.2
30	Y9	1	MET	6.0
27	Y6	42	TRP	5.8
7	YH	2	SER	5.5
1	YA	883	G	5.3
37	XH	4	ASP	5.2
4	YE	187	ALA	5.1
1	YA	1303	G	4.9

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Mol	Chain	Res	Type	RSRZ
1	YA	2892	A	4.8
1	RA	1089	G	4.7
1	RA	882	G	4.7
27	R6	42	TRP	4.5
38	QI	109	VAL	4.5
1	RA	1055	G	4.5
1	RA	2182	G	4.5
1	YA	2173	A	4.4
8	YI	65	ALA	4.4
6	RG	42	GLY	4.3
33	XD	22	LYS	4.3
32	XC	2	GLY	4.2
1	YA	2112	G	4.2
41	QL	85	ILE	4.2
49	QA	1365	G	4.2
13	YR	1	MET	4.1
32	QC	195	VAL	4.1
1	RA	1087	G	4.1
1	RA	2892	A	4.1
1	YA	1536	A	4.1
43	XN	30	ALA	4.1
49	XA	266	G	4.0
4	YE	159	HIS	4.0
1	YA	1082	U	3.8
48	XT	15	ARG	3.8
1	YA	892	G	3.8
26	Y5	50	GLY	3.8
13	RR	106	GLY	3.7
1	YA	882	G	3.7
1	YA	1534	G	3.7
49	XA	993	G	3.7
31	XB	29	ALA	3.7
33	QD	32	ALA	3.7
1	RA	1086	A	3.6
1	RA	1536	A	3.6
1	YA	1063	G	3.6
1	YA	2125	G	3.6
1	RA	1069	A	3.6
42	QM	97	PRO	3.6
33	QD	26	CYS	3.5
1	YA	2119	A	3.5
21	YZ	144	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
45	QP	15	PRO	3.5
39	XJ	55	LYS	3.5
41	QL	67	THR	3.5
49	QA	1276	G	3.4
33	QD	22	LYS	3.4
8	YI	90	GLY	3.4
1	YA	2166	G	3.4
1	YA	2178	C	3.4
22	R0	34	GLY	3.4
1	RA	1076	C	3.4
1	YA	2174	C	3.3
34	QE	34	VAL	3.3
9	RN	57	ALA	3.3
1	RA	1099	G	3.3
1	YA	2155	G	3.3
49	QA	971	G	3.3
49	QA	1118	C	3.3
1	YA	1314	C	3.3
1	RA	2125	G	3.3
1	YA	2795	G	3.3
49	QA	1129	C	3.2
1	YA	1062	G	3.2
49	XA	345	C	3.2
45	QP	30	GLY	3.2
49	XA	1238	A	3.2
1	YA	2133	G	3.2
1	RA	1082	U	3.2
26	R5	2	ALA	3.2
1	RA	2792	G	3.1
46	XQ	16	GLN	3.1
41	XL	30	ALA	3.1
1	RA	1236	G	3.1
1	RA	2141	G	3.1
33	XD	25	ARG	3.1
1	YA	888	C	3.1
1	YA	2179	C	3.1
4	RE	187	ALA	3.1
41	XL	58	VAL	3.1
49	QA	1128	C	3.1
49	QA	1222	G	3.1
49	XA	971	G	3.1
4	RE	143	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
26	R5	54	GLY	3.1
49	QA	266	G	3.0
49	QA	1028(G)	G	3.0
1	RA	887	A	3.0
39	QJ	54	PHE	3.0
1	YA	884	C	3.0
13	YR	15	SER	3.0
25	Y3	9	VAL	3.0
49	QA	1181	G	3.0
4	YE	142	GLY	3.0
6	RG	39	ILE	3.0
49	XA	1016	A	3.0
1	YA	1612	C	3.0
3	YD	34	VAL	3.0
1	YA	2792	G	3.0
26	R5	10	LYS	3.0
1	RA	1090	U	3.0
1	RA	2119	A	2.9
1	RA	1075	C	2.9
20	YY	47	LYS	2.9
1	YA	2056	G	2.9
49	XA	346	G	2.9
1	YA	2779	U	2.9
22	Y0	6	GLY	2.9
48	QT	106	ALA	2.9
1	YA	457	A	2.9
1	YA	2000	G	2.9
41	XL	56	ALA	2.9
51	Y4	36	CYS	2.9
27	Y6	20	ASN	2.9
38	QI	12	GLU	2.9
49	XA	195	A	2.8
1	YA	787	U	2.8
1	YA	2111	C	2.8
1	YA	2124	G	2.8
21	RZ	25	PRO	2.8
3	YD	243	GLY	2.8
47	QR	81	PHE	2.8
49	QA	1269	A	2.8
26	R5	3	LYS	2.8
1	RA	361	G	2.8
1	RA	1071	G	2.8

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Mol	Chain	Res	Type	RSRZ
1	YA	2801	A	2.8
49	XA	1256	A	2.8
45	QP	68	ASP	2.8
49	QA	429	U	2.8
49	XA	1024	G	2.8
1	RA	2801	A	2.8
16	YU	2	PRO	2.8
27	Y6	22	ALA	2.8
6	RG	126	ASP	2.7
30	R9	1	MET	2.7
24	Y2	72	ALA	2.7
1	RA	2115	G	2.7
1	YA	981	A	2.7
49	QA	1363	A	2.7
34	QE	41	VAL	2.7
38	QI	123	PRO	2.7
50	XS	34	TRP	2.7
1	RA	2149	G	2.7
1	YA	1093	G	2.7
3	RD	235	GLY	2.7
18	RW	61	ASN	2.7
22	R0	7	LEU	2.7
31	QB	118	LEU	2.7
42	XM	105	THR	2.7
45	QP	69	THR	2.7
41	QL	118	SER	2.7
1	YA	573	G	2.7
1	YA	1094	U	2.7
49	QA	1182	G	2.7
28	Y7	1	MET	2.7
1	YA	1060	U	2.6
42	QM	86	CYS	2.6
49	XA	1304	G	2.6
26	R5	45	VAL	2.6
32	XC	195	VAL	2.6
28	Y7	49	ARG	2.6
7	YH	82	GLY	2.6
37	QH	61	VAL	2.6
1	YA	890	A	2.6
1	RA	2144	U	2.6
21	RZ	41	LEU	2.6
42	XM	90	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
11	RP	61	ARG	2.6
21	YZ	79	ARG	2.6
38	QI	118	LYS	2.6
1	RA	1072	C	2.6
1	RA	2143	C	2.6
1	YA	2137	C	2.6
16	RU	2	PRO	2.6
9	RN	31	ALA	2.6
31	QB	113	HIS	2.6
1	YA	878	A	2.6
34	QE	100	VAL	2.6
41	QL	119	LYS	2.6
5	RF	134	GLY	2.6
1	YA	2168	G	2.6
39	XJ	48	THR	2.6
10	YO	28	SER	2.6
1	YA	2108	C	2.6
1	RA	1098	A	2.6
6	YG	88	ILE	2.5
33	QD	135	LEU	2.5
6	RG	87	PRO	2.5
38	QI	15	ALA	2.5
49	QA	1139	G	2.5
53	XV	9	G	2.5
40	XK	88	GLY	2.5
1	RA	2161	C	2.5
1	YA	2175	C	2.5
41	QL	6	THR	2.5
49	XA	1129	C	2.5
49	XA	1149	C	2.5
1	YA	1096	A	2.5
36	QG	2	ALA	2.5
32	QC	2	GLY	2.5
38	XI	109	VAL	2.5
1	RA	892	G	2.5
49	XA	1356	G	2.5
1	RA	888	C	2.5
1	YA	1076	C	2.5
4	RE	204	ALA	2.5
1	RA	2173	A	2.5
21	RZ	39	VAL	2.5
41	XL	49	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
8	YI	88	ILE	2.5
43	QN	2	ALA	2.5
11	YP	71	VAL	2.5
1	RA	2680	C	2.5
1	YA	997	G	2.5
49	XA	581	G	2.5
49	XA	758	G	2.5
53	XV	54	G	2.5
1	RA	1088	A	2.5
49	XA	1239	A	2.5
3	YD	50	THR	2.5
36	XG	120	ILE	2.4
11	YP	55	ARG	2.4
42	QM	24	GLY	2.4
1	YA	889	C	2.4
1	YA	2144	U	2.4
53	QV	8	U	2.4
1	RA	2147	G	2.4
1	RA	2158	A	2.4
1	YA	70	G	2.4
1	YA	2149	G	2.4
1	YA	2807	G	2.4
49	XA	1067	A	2.4
4	RE	77	ILE	2.4
45	XP	63	GLY	2.4
27	Y6	15	GLU	2.4
1	YA	1061	U	2.4
16	YU	28	ARG	2.4
31	QB	88	ALA	2.4
49	QA	194	C	2.4
49	QA	253	U	2.4
1	YA	1088	A	2.4
1	YA	2134	A	2.4
1	RA	2802	G	2.4
1	YA	2052	G	2.4
1	YA	2805	G	2.4
49	QA	1197	G	2.4
49	QA	1371	G	2.4
41	XL	117	ARG	2.4
36	XG	37	ASN	2.4
33	QD	152	SER	2.4
34	XE	47	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	YA	1535	U	2.4
16	YU	80	ILE	2.4
1	RA	2129	C	2.4
1	YA	2443	C	2.4
49	XA	1145	C	2.4
49	XA	978	A	2.4
33	QD	42	GLN	2.4
1	RA	1059	G	2.4
1	YA	465	G	2.4
49	QA	988	G	2.4
9	RN	49	GLY	2.4
36	QG	71	PRO	2.4
41	QL	94	PRO	2.4
1	RA	568	U	2.3
43	XN	49	HIS	2.3
3	YD	87	ASN	2.3
34	XE	77	PRO	2.3
16	RU	77	SER	2.3
1	RA	1048	A	2.3
1	YA	886	C	2.3
1	RA	2116	G	2.3
1	YA	1521	G	2.3
1	YA	2116	G	2.3
1	YA	2127	G	2.3
1	YA	2186	G	2.3
49	XA	1300	G	2.3
5	YF	8	GLN	2.3
31	QB	117	GLU	2.3
3	YD	234	GLY	2.3
17	YV	45	THR	2.3
1	RA	2134	A	2.3
1	YA	2142	C	2.3
1	YA	2602	A	2.3
49	QA	1287	A	2.3
49	XA	975	A	2.3
50	QS	16	LEU	2.3
40	XK	119	CYS	2.3
1	YA	879	G	2.3
1	YA	2447	G	2.3
49	QA	1047	G	2.3
49	XA	1371	G	2.3
33	XD	32	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
6	YG	41	GLN	2.3
39	XJ	61	GLU	2.3
6	YG	89	GLY	2.3
18	RW	112	GLY	2.3
41	QL	45	PRO	2.3
44	QO	22	THR	2.3
49	QA	1275	A	2.3
1	RA	2177	C	2.3
1	RA	2196	C	2.3
1	YA	1604	C	2.3
33	XD	12	CYS	2.3
3	YD	191	ALA	2.3
17	YV	36	PRO	2.3
42	QM	104	ARG	2.3
1	RA	2093	G	2.3
1	YA	450	G	2.3
1	YA	831	G	2.3
49	QA	1178	G	2.3
53	QV	9	G	2.3
6	RG	88	ILE	2.3
1	YA	887	A	2.3
49	XA	994	A	2.3
1	YA	1064	C	2.3
21	RZ	68	PRO	2.3
3	YD	99	ASP	2.3
45	XP	16	HIS	2.2
33	XD	31	CYS	2.2
1	RA	1106	G	2.2
1	YA	1059	G	2.2
1	YA	1087	G	2.2
1	YA	2162	G	2.2
49	QA	388	G	2.2
49	XA	1042	G	2.2
49	XA	68(O)	A	2.2
14	RS	86	ALA	2.2
21	RZ	7	ALA	2.2
1	YA	2107	C	2.2
1	YA	2164	C	2.2
46	QQ	17	LYS	2.2
49	XA	1539	C	2.2
41	XL	34	ARG	2.2
37	QH	2	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
5	YF	82	ILE	2.2
39	QJ	38	ILE	2.2
1	YA	2109	U	2.2
30	Y9	2	LYS	2.2
43	QN	61	TRP	2.2
1	RA	2127	G	2.2
1	YA	2106	G	2.2
19	YX	65	ARG	2.2
49	XA	966	G	2.2
49	XA	1011	G	2.2
15	YT	109	GLU	2.2
40	QK	47	VAL	2.2
50	QS	41	VAL	2.2
1	RA	2311	A	2.2
1	YA	2001	A	2.2
24	Y2	57	ILE	2.2
2	RB	108	C	2.2
49	QA	967	C	2.2
49	XA	1237	C	2.2
40	XK	61	ALA	2.2
41	QL	30	ALA	2.2
41	XL	94	PRO	2.2
1	YA	2132	U	2.2
49	XA	1542	U	2.2
44	XO	51	HIS	2.2
49	XA	1309	G	2.2
1	YA	2140	C	2.2
4	RE	139	GLY	2.2
45	XP	30	GLY	2.2
1	RA	1065	U	2.1
3	RD	48	ARG	2.1
12	YQ	141	GLN	2.1
30	R9	37	GLY	2.1
29	Y8	56	GLU	2.1
49	XA	1332	A	2.1
1	RA	2112	G	2.1
1	RA	2124	G	2.1
1	YA	2115	G	2.1
49	QA	1215	G	2.1
1	RA	2103	C	2.1
49	QA	856	C	2.1
49	QA	1200	C	2.1

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Mol	Chain	Res	Type	RSRZ
45	XP	29	ASP	2.1
36	QG	75	VAL	2.1
21	RZ	104	PHE	2.1
34	QE	47	LYS	2.1
38	QI	72	GLY	2.1
1	YA	1026	U	2.1
3	YD	133	LEU	2.1
15	YT	114	LEU	2.1
49	XA	429	U	2.1
13	YR	2	ARG	2.1
45	XP	84	ALA	2.1
33	XD	113	SER	2.1
40	QK	29	ILE	2.1
5	YF	57	VAL	2.1
9	YN	46	VAL	2.1
46	XQ	73	VAL	2.1
49	QA	978	A	2.1
31	XB	203	GLY	2.1
31	QB	202	PRO	2.1
1	RA	2162	G	2.1
1	RA	2891	G	2.1
49	XA	1291	G	2.1
1	YA	574	C	2.1
40	XK	26	ASN	2.1
45	XP	14	ASN	2.1
1	RA	1094	U	2.1
8	YI	107	VAL	2.1
11	RP	71	VAL	2.1
31	QB	112	VAL	2.1
16	YU	38	THR	2.1
45	XP	75	ARG	2.1
39	QJ	94	VAL	2.1
1	RA	1043	C	2.1
1	RA	1049	C	2.1
1	YA	2183	C	2.1
49	QA	1237	C	2.1
49	XA	1200	C	2.1
1	RA	883	G	2.1
1	YA	2147	G	2.1
1	YA	2152	G	2.1
1	YA	2154	G	2.1
1	YA	2454	G	2.1

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Mol	Chain	Res	Type	RSRZ
3	YD	230	ASP	2.1
28	R7	49	ARG	2.1
25	Y3	25	ALA	2.1
31	XB	70	PHE	2.1
41	XL	32	PHE	2.1
1	YA	2114	A	2.0
1	YA	2629	A	2.0
49	QA	1236	A	2.0
17	YV	78	LYS	2.0
13	RR	27	SER	2.0
50	QS	4	SER	2.0
1	YA	2794	C	2.0
38	XI	14	VAL	2.0
49	QA	1362(A)	C	2.0
1	RA	1093	G	2.0
1	RA	2155	G	2.0
1	YA	2891	G	2.0
28	R7	1	MET	2.0
49	QA	1177	G	2.0
49	QA	1233	G	2.0
49	XA	1181	G	2.0
49	XA	1198	G	2.0
41	QL	35	GLY	2.0
41	XL	5	PRO	2.0
36	XG	33	ASP	2.0
39	QJ	18	ALA	2.0
50	QS	15	LEU	2.0
1	RA	1057	A	2.0
1	YA	654	A	2.0
30	Y9	25	VAL	2.0
33	QD	8	VAL	2.0
49	QA	563	A	2.0
49	QA	968	A	2.0
49	QA	1396	A	2.0
3	YD	55	GLY	2.0
11	YP	53	GLY	2.0
16	YU	34	LYS	2.0
20	YY	95	LYS	2.0
33	QD	57	ARG	2.0
1	RA	885	C	2.0
1	RA	1064	C	2.0
1	RA	2175	C	2.0

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Mol	Chain	Res	Type	RSRZ
1	YA	1957	C	2.0
49	QA	1172	C	2.0
49	QA	1199	U	2.0
51	Y4	35	VAL	2.0

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
53	1MG	QV	38	24/25	0.58	0.11	139,172,202,204	0
53	1MG	XV	38	24/25	0.61	0.11	108,152,169,192	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
54	MG	QA	1724	1/1	-0.43	0.19	160,160,160,160	0
54	MG	QA	1657	1/1	-0.33	0.21	90,90,90,90	0
54	MG	XA	1674	1/1	-0.21	0.14	90,90,90,90	0
54	MG	XA	1714	1/1	-0.20	0.18	90,90,90,90	0
54	MG	RT	201	1/1	-0.16	0.22	144,144,144,144	0
54	MG	RA	3427	1/1	-0.15	0.17	176,176,176,176	0
54	MG	RA	3298	1/1	-0.13	0.28	106,106,106,106	0
54	MG	XA	1709	1/1	-0.10	0.22	94,94,94,94	0
54	MG	YA	3876	1/1	-0.09	0.16	138,138,138,138	0
54	MG	QA	1663	1/1	-0.07	0.28	95,95,95,95	0
54	MG	RA	3347	1/1	-0.05	0.28	94,94,94,94	0
54	MG	QA	1677	1/1	-0.04	0.23	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	XA	1677	1/1	-0.03	0.59	99,99,99,99	0
54	MG	RA	3100	1/1	0.01	0.38	90,90,90,90	0
54	MG	RA	3380	1/1	0.02	0.11	148,148,148,148	0
54	MG	QA	1616	1/1	0.02	0.25	156,156,156,156	0
54	MG	RA	3535	1/1	0.03	0.11	92,92,92,92	0
54	MG	QA	1693	1/1	0.03	0.15	123,123,123,123	0
54	MG	QA	1709	1/1	0.03	0.24	97,97,97,97	0
54	MG	YA	3670	1/1	0.03	0.20	110,110,110,110	0
54	MG	XA	1711	1/1	0.06	0.18	156,156,156,156	0
54	MG	QL	201	1/1	0.06	0.11	188,188,188,188	0
54	MG	R3	101	1/1	0.07	0.23	170,170,170,170	0
54	MG	YA	3766	1/1	0.07	0.25	90,90,90,90	0
54	MG	QA	1668	1/1	0.08	0.42	90,90,90,90	0
54	MG	YA	3832	1/1	0.10	0.56	96,96,96,96	0
54	MG	QA	1715	1/1	0.10	0.27	95,95,95,95	0
54	MG	QA	1721	1/1	0.10	0.13	128,128,128,128	0
54	MG	YA	3836	1/1	0.10	0.33	90,90,90,90	0
54	MG	QA	1727	1/1	0.10	0.12	182,182,182,182	0
54	MG	YA	3942	1/1	0.11	0.35	90,90,90,90	0
54	MG	YA	3648	1/1	0.12	0.23	151,151,151,151	0
54	MG	RI	201	1/1	0.12	0.27	161,161,161,161	0
54	MG	RA	3039	1/1	0.13	0.24	96,96,96,96	0
54	MG	YA	3704	1/1	0.14	0.28	91,91,91,91	0
54	MG	Y0	101	1/1	0.14	0.28	96,96,96,96	0
54	MG	YA	3737	1/1	0.14	0.54	90,90,90,90	0
54	MG	QP	101	1/1	0.14	0.41	120,120,120,120	0
54	MG	RA	3135	1/1	0.15	0.21	90,90,90,90	0
54	MG	QE	201	1/1	0.15	0.10	166,166,166,166	0
54	MG	YA	3776	1/1	0.15	0.52	90,90,90,90	0
54	MG	RA	3361	1/1	0.15	0.16	136,136,136,136	0
54	MG	QA	1725	1/1	0.16	0.17	106,106,106,106	0
54	MG	YA	3879	1/1	0.16	0.15	153,153,153,153	0
54	MG	XA	1611	1/1	0.16	0.40	110,110,110,110	0
54	MG	RA	3129	1/1	0.16	0.29	96,96,96,96	0
54	MG	XA	1669	1/1	0.17	0.27	118,118,118,118	0
54	MG	RA	3546	1/1	0.17	0.17	106,106,106,106	0
54	MG	YA	3709	1/1	0.17	0.33	90,90,90,90	0
54	MG	QA	1611	1/1	0.17	0.43	114,114,114,114	0
54	MG	RA	3247	1/1	0.17	0.14	99,99,99,99	0
54	MG	XA	1623	1/1	0.17	0.14	125,125,125,125	0
54	MG	YA	3974	1/1	0.18	0.15	94,94,94,94	0
54	MG	RA	3166	1/1	0.18	0.33	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	QA	1645	1/1	0.19	0.23	92,92,92,92	0
54	MG	RA	3043	1/1	0.19	0.41	90,90,90,90	0
54	MG	XA	1624	1/1	0.19	0.14	141,141,141,141	0
54	MG	YA	3679	1/1	0.20	0.24	90,90,90,90	0
54	MG	YA	3943	1/1	0.20	0.11	133,133,133,133	0
54	MG	YA	3828	1/1	0.20	0.27	90,90,90,90	0
54	MG	YA	3783	1/1	0.21	0.21	151,151,151,151	0
54	MG	RA	3413	1/1	0.21	0.21	136,136,136,136	0
54	MG	RA	3553	1/1	0.22	0.19	90,90,90,90	0
54	MG	QC	301	1/1	0.22	0.15	154,154,154,154	0
54	MG	YA	3814	1/1	0.22	0.22	92,92,92,92	0
54	MG	YA	3910	1/1	0.22	0.26	91,91,91,91	0
54	MG	RA	3466	1/1	0.22	0.20	128,128,128,128	0
54	MG	RA	3025	1/1	0.22	0.37	90,90,90,90	0
54	MG	RA	3113	1/1	0.22	0.22	97,97,97,97	0
54	MG	XA	1668	1/1	0.23	0.32	172,172,172,172	0
54	MG	YI	201	1/1	0.24	0.18	104,104,104,104	0
54	MG	RA	3279	1/1	0.25	0.17	148,148,148,148	0
54	MG	XA	1629	1/1	0.25	0.23	164,164,164,164	0
54	MG	RA	3437	1/1	0.25	1.05	134,134,134,134	0
54	MG	RA	3561	1/1	0.26	0.40	92,92,92,92	0
54	MG	XA	1703	1/1	0.27	0.14	91,91,91,91	0
54	MG	YA	3874	1/1	0.27	0.41	90,90,90,90	0
54	MG	QA	1669	1/1	0.27	0.17	97,97,97,97	0
54	MG	R1	102	1/1	0.27	0.15	149,149,149,149	0
54	MG	YA	3891	1/1	0.28	0.51	90,90,90,90	0
54	MG	RA	3185	1/1	0.28	0.21	129,129,129,129	0
54	MG	RA	3066	1/1	0.29	0.26	100,100,100,100	0
54	MG	YA	3698	1/1	0.30	0.45	91,91,91,91	0
54	MG	RA	3525	1/1	0.30	0.14	100,100,100,100	0
54	MG	YA	3787	1/1	0.30	0.28	90,90,90,90	0
54	MG	YA	3653	1/1	0.30	0.28	106,106,106,106	0
54	MG	RA	3171	1/1	0.30	0.24	92,92,92,92	0
54	MG	RA	3286	1/1	0.30	0.19	90,90,90,90	0
54	MG	RA	3312	1/1	0.31	0.34	113,113,113,113	0
54	MG	YA	3953	1/1	0.31	0.23	125,125,125,125	0
54	MG	RA	3248	1/1	0.31	0.20	90,90,90,90	0
54	MG	YA	3724	1/1	0.31	0.17	97,97,97,97	0
54	MG	YA	3854	1/1	0.32	0.64	90,90,90,90	0
54	MG	RA	3246	1/1	0.32	0.31	90,90,90,90	0
54	MG	YA	3755	1/1	0.32	0.26	90,90,90,90	0
54	MG	XA	1700	1/1	0.32	0.11	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	YA	3613	1/1	0.33	0.25	90,90,90,90	0
54	MG	RA	3418	1/1	0.33	0.20	134,134,134,134	0
54	MG	RA	3449	1/1	0.33	0.39	90,90,90,90	0
54	MG	RA	3180	1/1	0.33	0.29	90,90,90,90	0
54	MG	QA	1652	1/1	0.33	0.25	91,91,91,91	0
54	MG	YA	3671	1/1	0.33	0.40	90,90,90,90	0
54	MG	QA	1706	1/1	0.34	0.08	94,94,94,94	0
54	MG	YA	3774	1/1	0.34	0.27	90,90,90,90	0
54	MG	RE	306	1/1	0.34	0.15	90,90,90,90	0
54	MG	QA	1618	1/1	0.34	0.09	96,96,96,96	0
54	MG	QA	1640	1/1	0.34	0.19	97,97,97,97	0
54	MG	RA	3545	1/1	0.35	0.21	93,93,93,93	0
54	MG	R0	102	1/1	0.35	0.18	103,103,103,103	0
54	MG	QA	1625	1/1	0.35	0.33	98,98,98,98	0
54	MG	RA	3301	1/1	0.35	0.47	90,90,90,90	0
54	MG	QA	1628	1/1	0.36	0.16	92,92,92,92	0
54	MG	QA	1700	1/1	0.36	0.39	90,90,90,90	0
54	MG	YA	3794	1/1	0.37	0.48	168,168,168,168	0
54	MG	RD	303	1/1	0.37	0.37	90,90,90,90	0
54	MG	RA	3032	1/1	0.37	0.13	94,94,94,94	0
54	MG	QA	1620	1/1	0.37	0.22	96,96,96,96	0
54	MG	RA	3159	1/1	0.38	0.24	98,98,98,98	0
54	MG	RA	3087	1/1	0.38	0.16	174,174,174,174	0
54	MG	QA	1711	1/1	0.38	0.35	92,92,92,92	0
54	MG	RA	3299	1/1	0.38	0.18	90,90,90,90	0
54	MG	RA	3125	1/1	0.38	0.29	90,90,90,90	0
54	MG	QA	1664	1/1	0.38	0.11	114,114,114,114	0
54	MG	QA	1705	1/1	0.38	0.23	90,90,90,90	0
54	MG	RA	3384	1/1	0.39	0.23	97,97,97,97	0
54	MG	RA	3539	1/1	0.39	0.24	90,90,90,90	0
54	MG	YA	3703	1/1	0.39	0.33	90,90,90,90	0
54	MG	QA	1690	1/1	0.39	0.26	103,103,103,103	0
54	MG	YA	3615	1/1	0.39	0.35	90,90,90,90	0
54	MG	YA	3769	1/1	0.39	0.37	90,90,90,90	0
54	MG	YA	3625	1/1	0.39	0.61	125,125,125,125	0
54	MG	XA	1723	1/1	0.39	0.22	96,96,96,96	0
54	MG	QA	1638	1/1	0.40	0.40	90,90,90,90	0
54	MG	YA	3731	1/1	0.40	0.61	90,90,90,90	0
54	MG	RA	3005	1/1	0.40	0.20	95,95,95,95	0
54	MG	RA	3223	1/1	0.41	0.18	106,106,106,106	0
54	MG	RA	3558	1/1	0.41	0.38	90,90,90,90	0
54	MG	XA	1652	1/1	0.41	0.18	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	YA	3967	1/1	0.41	0.25	135,135,135,135	0
54	MG	RA	3162	1/1	0.41	0.70	90,90,90,90	0
54	MG	RA	3329	1/1	0.41	0.22	91,91,91,91	0
54	MG	XA	1676	1/1	0.41	0.34	90,90,90,90	0
54	MG	RA	3297	1/1	0.42	0.18	136,136,136,136	0
54	MG	YA	3612	1/1	0.42	0.33	90,90,90,90	0
54	MG	YA	3846	1/1	0.42	0.15	94,94,94,94	0
54	MG	RB	205	1/1	0.42	0.18	179,179,179,179	0
54	MG	RA	3196	1/1	0.42	0.17	107,107,107,107	0
54	MG	RA	3370	1/1	0.42	0.23	127,127,127,127	0
54	MG	XA	1688	1/1	0.42	0.17	92,92,92,92	0
54	MG	YA	3685	1/1	0.42	0.32	90,90,90,90	0
54	MG	YA	3747	1/1	0.42	0.26	90,90,90,90	0
54	MG	YA	3643	1/1	0.42	0.35	90,90,90,90	0
54	MG	YA	3760	1/1	0.42	0.44	90,90,90,90	0
54	MG	XA	1627	1/1	0.42	0.13	94,94,94,94	0
54	MG	QA	1655	1/1	0.42	0.12	102,102,102,102	0
54	MG	YA	3707	1/1	0.43	0.23	94,94,94,94	0
54	MG	RA	3036	1/1	0.43	0.16	144,144,144,144	0
54	MG	RA	3451	1/1	0.43	0.41	90,90,90,90	0
54	MG	RB	212	1/1	0.43	0.25	99,99,99,99	0
54	MG	RA	3337	1/1	0.44	0.74	90,90,90,90	0
54	MG	YA	3921	1/1	0.44	0.44	90,90,90,90	0
54	MG	QA	1666	1/1	0.44	0.17	91,91,91,91	0
54	MG	RA	3228	1/1	0.44	0.10	145,145,145,145	0
54	MG	RA	3253	1/1	0.44	0.31	90,90,90,90	0
54	MG	RA	3428	1/1	0.44	0.37	102,102,102,102	0
54	MG	YA	3765	1/1	0.45	0.37	90,90,90,90	0
54	MG	RA	3270	1/1	0.45	0.36	90,90,90,90	0
54	MG	YA	3935	1/1	0.45	0.20	90,90,90,90	0
54	MG	RA	3452	1/1	0.45	0.27	110,110,110,110	0
54	MG	QA	1631	1/1	0.45	0.18	95,95,95,95	0
54	MG	XA	1653	1/1	0.45	0.16	91,91,91,91	0
54	MG	YA	3905	1/1	0.46	0.21	90,90,90,90	0
54	MG	RA	3342	1/1	0.46	0.14	90,90,90,90	0
54	MG	RA	3323	1/1	0.46	0.58	90,90,90,90	0
54	MG	RA	3415	1/1	0.46	0.24	100,100,100,100	0
54	MG	YD	302	1/1	0.46	0.42	90,90,90,90	0
54	MG	QA	1603	1/1	0.46	0.19	98,98,98,98	0
54	MG	QA	1609	1/1	0.46	0.22	90,90,90,90	0
54	MG	YE	304	1/1	0.46	0.21	118,118,118,118	0
54	MG	QA	1681	1/1	0.46	0.14	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	RA	3350	1/1	0.46	0.14	90,90,90,90	0
54	MG	XA	1638	1/1	0.47	0.20	91,91,91,91	0
54	MG	RA	3400	1/1	0.47	0.37	93,93,93,93	0
54	MG	RA	3339	1/1	0.47	0.21	130,130,130,130	0
54	MG	RA	3481	1/1	0.48	0.20	90,90,90,90	0
54	MG	YA	3919	1/1	0.48	0.18	90,90,90,90	0
54	MG	RA	3503	1/1	0.48	0.36	94,94,94,94	0
54	MG	YA	3923	1/1	0.48	0.28	94,94,94,94	0
54	MG	QA	1696	1/1	0.48	0.21	129,129,129,129	0
54	MG	QA	1606	1/1	0.48	0.14	94,94,94,94	0
54	MG	RA	3059	1/1	0.48	0.20	97,97,97,97	0
54	MG	RF	301	1/1	0.49	0.17	115,115,115,115	0
54	MG	RA	3303	1/1	0.49	0.17	145,145,145,145	0
54	MG	RA	3041	1/1	0.49	0.25	181,181,181,181	0
54	MG	RA	3215	1/1	0.49	0.44	90,90,90,90	0
54	MG	RA	3386	1/1	0.49	0.13	100,100,100,100	0
54	MG	RA	3392	1/1	0.49	0.21	108,108,108,108	0
54	MG	YA	3692	1/1	0.49	0.30	94,94,94,94	0
54	MG	YA	3902	1/1	0.49	0.20	93,93,93,93	0
54	MG	YA	3604	1/1	0.49	0.19	131,131,131,131	0
54	MG	YA	3700	1/1	0.49	0.25	90,90,90,90	0
54	MG	RB	206	1/1	0.49	0.78	178,178,178,178	0
54	MG	RA	3447	1/1	0.49	0.31	100,100,100,100	0
54	MG	RA	3230	1/1	0.49	0.46	91,91,91,91	0
54	MG	RE	303	1/1	0.49	0.14	127,127,127,127	0
54	MG	RA	3249	1/1	0.49	0.12	140,140,140,140	0
54	MG	QA	1612	1/1	0.49	0.13	90,90,90,90	0
54	MG	YA	3644	1/1	0.49	0.35	173,173,173,173	0
54	MG	QA	1708	1/1	0.50	0.20	95,95,95,95	0
54	MG	XA	1689	1/1	0.50	0.21	182,182,182,182	0
54	MG	YA	3817	1/1	0.50	0.15	90,90,90,90	0
54	MG	YA	3687	1/1	0.50	0.40	90,90,90,90	0
54	MG	RA	3111	1/1	0.50	0.11	90,90,90,90	0
54	MG	RA	3441	1/1	0.50	0.13	90,90,90,90	0
54	MG	RA	3306	1/1	0.50	0.29	92,92,92,92	0
54	MG	YA	3710	1/1	0.50	0.28	158,158,158,158	0
54	MG	RA	3192	1/1	0.51	0.18	92,92,92,92	0
54	MG	YA	3835	1/1	0.51	0.22	90,90,90,90	0
54	MG	RA	3396	1/1	0.51	0.22	113,113,113,113	0
54	MG	XA	1699	1/1	0.51	0.43	90,90,90,90	0
54	MG	RA	3335	1/1	0.51	0.50	121,121,121,121	0
54	MG	Y1	101	1/1	0.51	0.14	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	YA	3958	1/1	0.51	0.27	90,90,90,90	0
54	MG	YA	3922	1/1	0.51	0.40	90,90,90,90	0
54	MG	RA	3038	1/1	0.51	0.13	171,171,171,171	0
54	MG	QA	1680	1/1	0.51	0.14	151,151,151,151	0
54	MG	YA	3899	1/1	0.52	0.32	90,90,90,90	0
54	MG	RA	3331	1/1	0.52	0.17	110,110,110,110	0
54	MG	RA	3376	1/1	0.52	0.33	93,93,93,93	0
54	MG	RA	3362	1/1	0.52	0.20	120,120,120,120	0
54	MG	YA	3603	1/1	0.52	0.14	98,98,98,98	0
54	MG	QA	1660	1/1	0.53	0.35	96,96,96,96	0
54	MG	RA	3470	1/1	0.53	0.19	124,124,124,124	0
54	MG	YB	204	1/1	0.53	0.13	158,158,158,158	0
54	MG	RA	3155	1/1	0.54	0.18	90,90,90,90	0
54	MG	YA	3693	1/1	0.54	0.18	94,94,94,94	0
54	MG	RA	3273	1/1	0.54	0.20	90,90,90,90	0
54	MG	YA	3761	1/1	0.54	1.04	90,90,90,90	0
54	MG	XA	1690	1/1	0.54	0.21	125,125,125,125	0
54	MG	YA	3859	1/1	0.54	0.29	92,92,92,92	0
54	MG	RA	3294	1/1	0.55	0.21	120,120,120,120	0
54	MG	YA	3833	1/1	0.55	0.22	137,137,137,137	0
54	MG	YA	3885	1/1	0.55	0.24	93,93,93,93	0
54	MG	RA	3283	1/1	0.55	0.34	91,91,91,91	0
54	MG	YA	3978	1/1	0.55	0.20	90,90,90,90	0
54	MG	XA	1719	1/1	0.55	0.15	114,114,114,114	0
54	MG	YA	3778	1/1	0.55	0.18	191,191,191,191	0
54	MG	RA	3562	1/1	0.56	0.17	90,90,90,90	0
54	MG	RA	3346	1/1	0.56	0.54	96,96,96,96	0
54	MG	YA	3750	1/1	0.56	0.31	90,90,90,90	0
54	MG	QA	1622	1/1	0.56	0.24	114,114,114,114	0
54	MG	YA	3779	1/1	0.56	0.18	90,90,90,90	0
54	MG	QD	303	1/1	0.56	0.15	128,128,128,128	0
54	MG	RA	3319	1/1	0.56	0.22	90,90,90,90	0
54	MG	RA	3023	1/1	0.56	0.24	100,100,100,100	0
54	MG	YA	3969	1/1	0.56	0.12	94,94,94,94	0
54	MG	RA	3516	1/1	0.56	0.33	90,90,90,90	0
54	MG	QA	1648	1/1	0.56	0.59	127,127,127,127	0
54	MG	RD	307	1/1	0.56	0.11	93,93,93,93	0
54	MG	XA	1631	1/1	0.56	0.09	91,91,91,91	0
54	MG	RA	3262	1/1	0.56	0.39	99,99,99,99	0
54	MG	RA	3214	1/1	0.56	0.23	90,90,90,90	0
54	MG	YA	3924	1/1	0.56	0.30	90,90,90,90	0
54	MG	YA	3666	1/1	0.57	0.26	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	RA	3526	1/1	0.57	0.21	100,100,100,100	0
54	MG	QL	202	1/1	0.57	0.18	113,113,113,113	0
54	MG	RA	3123	1/1	0.57	0.17	94,94,94,94	0
54	MG	RA	3510	1/1	0.57	0.24	125,125,125,125	0
54	MG	XA	1664	1/1	0.57	0.17	90,90,90,90	0
54	MG	RO	201	1/1	0.57	0.14	103,103,103,103	0
54	MG	YA	3686	1/1	0.57	0.54	90,90,90,90	0
54	MG	RA	3011	1/1	0.57	0.30	96,96,96,96	0
54	MG	YA	3880	1/1	0.57	0.20	95,95,95,95	0
54	MG	RA	3238	1/1	0.57	0.13	113,113,113,113	0
54	MG	RA	3356	1/1	0.58	0.22	109,109,109,109	0
54	MG	YA	3793	1/1	0.58	0.14	98,98,98,98	0
54	MG	YA	3881	1/1	0.58	0.34	90,90,90,90	0
54	MG	RA	3381	1/1	0.58	0.25	95,95,95,95	0
54	MG	YA	3809	1/1	0.58	0.58	90,90,90,90	0
54	MG	RA	3509	1/1	0.58	0.28	132,132,132,132	0
54	MG	RA	3366	1/1	0.58	0.13	99,99,99,99	0
54	MG	RA	3430	1/1	0.58	0.19	90,90,90,90	0
54	MG	YA	3944	1/1	0.58	0.17	101,101,101,101	0
54	MG	YA	3909	1/1	0.58	0.18	90,90,90,90	0
54	MG	RA	3518	1/1	0.58	0.21	109,109,109,109	0
54	MG	YA	3966	1/1	0.58	0.17	90,90,90,90	0
54	MG	RA	3499	1/1	0.59	0.09	92,92,92,92	0
54	MG	RA	3173	1/1	0.59	0.24	90,90,90,90	0
54	MG	YA	3617	1/1	0.59	0.46	90,90,90,90	0
54	MG	RA	3229	1/1	0.59	0.09	144,144,144,144	0
54	MG	RA	3394	1/1	0.59	0.19	100,100,100,100	0
54	MG	XA	1706	1/1	0.59	0.29	112,112,112,112	0
54	MG	RA	3148	1/1	0.59	0.35	90,90,90,90	0
54	MG	RA	3288	1/1	0.59	0.27	90,90,90,90	0
54	MG	RA	3550	1/1	0.59	0.22	94,94,94,94	0
54	MG	YA	3654	1/1	0.59	0.30	90,90,90,90	0
54	MG	YA	3901	1/1	0.59	0.44	94,94,94,94	0
54	MG	YA	3743	1/1	0.60	0.39	90,90,90,90	0
54	MG	QA	1704	1/1	0.60	0.15	98,98,98,98	0
54	MG	YA	3865	1/1	0.60	0.36	152,152,152,152	0
54	MG	YA	3744	1/1	0.60	0.25	90,90,90,90	0
54	MG	XA	1697	1/1	0.60	0.28	95,95,95,95	0
54	MG	YB	208	1/1	0.60	0.36	90,90,90,90	0
54	MG	RA	3048	1/1	0.60	0.25	90,90,90,90	0
54	MG	RA	3515	1/1	0.60	0.23	90,90,90,90	0
54	MG	RA	3131	1/1	0.60	0.19	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	RA	3393	1/1	0.60	0.07	91,91,91,91	0
54	MG	YA	3851	1/1	0.60	0.29	90,90,90,90	0
54	MG	QA	1614	1/1	0.60	0.23	95,95,95,95	0
54	MG	RA	3336	1/1	0.60	0.22	90,90,90,90	0
54	MG	YA	3897	1/1	0.60	0.24	90,90,90,90	0
54	MG	YA	3929	1/1	0.61	0.10	94,94,94,94	0
54	MG	QA	1719	1/1	0.61	0.17	92,92,92,92	0
54	MG	R0	101	1/1	0.61	0.40	92,92,92,92	0
54	MG	RA	3468	1/1	0.61	0.28	121,121,121,121	0
54	MG	QA	1674	1/1	0.61	0.14	90,90,90,90	0
54	MG	RA	3074	1/1	0.61	0.24	90,90,90,90	0
54	MG	XE	201	1/1	0.61	0.18	95,95,95,95	0
54	MG	XO	101	1/1	0.61	0.13	147,147,147,147	0
54	MG	QA	1678	1/1	0.61	0.09	91,91,91,91	0
54	MG	QA	1661	1/1	0.61	0.10	106,106,106,106	0
54	MG	RA	3411	1/1	0.61	0.14	90,90,90,90	0
54	MG	RA	3397	1/1	0.61	0.20	94,94,94,94	0
54	MG	YE	301	1/1	0.62	0.26	90,90,90,90	0
54	MG	RA	3517	1/1	0.62	0.25	120,120,120,120	0
54	MG	RA	3450	1/1	0.62	0.25	90,90,90,90	0
54	MG	RA	3015	1/1	0.62	0.17	93,93,93,93	0
54	MG	RA	3130	1/1	0.62	1.03	90,90,90,90	0
54	MG	YA	3665	1/1	0.62	0.40	90,90,90,90	0
54	MG	QD	302	1/1	0.62	0.08	96,96,96,96	0
54	MG	XA	1610	1/1	0.62	0.07	90,90,90,90	0
54	MG	YA	3690	1/1	0.62	0.12	90,90,90,90	0
54	MG	YA	3884	1/1	0.62	0.18	90,90,90,90	0
54	MG	RA	3045	1/1	0.62	0.26	111,111,111,111	0
54	MG	RA	3500	1/1	0.62	0.18	94,94,94,94	0
54	MG	RA	3014	1/1	0.63	0.23	90,90,90,90	0
54	MG	YA	3838	1/1	0.63	0.13	158,158,158,158	0
54	MG	RA	3264	1/1	0.63	0.28	90,90,90,90	0
54	MG	YA	3850	1/1	0.63	0.23	90,90,90,90	0
54	MG	QA	1665	1/1	0.63	0.12	96,96,96,96	0
54	MG	YA	3734	1/1	0.63	0.30	93,93,93,93	0
54	MG	RA	3201	1/1	0.63	0.61	90,90,90,90	0
54	MG	QA	1632	1/1	0.63	0.14	133,133,133,133	0
54	MG	RA	3363	1/1	0.63	0.10	90,90,90,90	0
54	MG	RA	3233	1/1	0.63	0.42	90,90,90,90	0
54	MG	RB	207	1/1	0.63	0.71	262,262,262,262	0
54	MG	YA	3945	1/1	0.63	0.11	90,90,90,90	0
54	MG	RA	3385	1/1	0.63	0.19	170,170,170,170	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	YA	3754	1/1	0.63	0.23	93,93,93,93	0
54	MG	YA	3723	1/1	0.63	0.30	90,90,90,90	0
54	MG	YE	303	1/1	0.64	0.13	98,98,98,98	0
54	MG	RA	3002	1/1	0.64	0.11	133,133,133,133	0
54	MG	RA	3121	1/1	0.64	0.23	90,90,90,90	0
54	MG	XA	1620	1/1	0.64	0.36	90,90,90,90	0
54	MG	RA	3033	1/1	0.64	0.65	90,90,90,90	0
54	MG	XA	1670	1/1	0.64	0.17	91,91,91,91	0
54	MG	RA	3020	1/1	0.64	0.16	119,119,119,119	0
54	MG	YA	3640	1/1	0.64	0.49	90,90,90,90	0
54	MG	RA	3138	1/1	0.64	0.34	90,90,90,90	0
54	MG	RA	3555	1/1	0.64	0.30	90,90,90,90	0
54	MG	RA	3390	1/1	0.64	0.34	152,152,152,152	0
54	MG	XA	1613	1/1	0.65	0.39	90,90,90,90	0
54	MG	RA	3431	1/1	0.65	0.15	137,137,137,137	0
54	MG	YA	3763	1/1	0.65	0.22	91,91,91,91	0
54	MG	YA	3619	1/1	0.65	0.14	146,146,146,146	0
54	MG	RA	3259	1/1	0.65	0.43	90,90,90,90	0
54	MG	YA	3932	1/1	0.65	0.18	90,90,90,90	0
54	MG	YA	3637	1/1	0.65	0.37	98,98,98,98	0
54	MG	YA	3941	1/1	0.65	0.14	103,103,103,103	0
54	MG	QA	1621	1/1	0.65	0.45	93,93,93,93	0
54	MG	RA	3314	1/1	0.65	0.12	187,187,187,187	0
54	MG	QA	1694	1/1	0.65	0.12	129,129,129,129	0
54	MG	RA	3107	1/1	0.65	0.27	116,116,116,116	0
54	MG	YA	3917	1/1	0.65	0.59	90,90,90,90	0
54	MG	RA	3022	1/1	0.65	0.28	90,90,90,90	0
54	MG	RA	3026	1/1	0.65	0.58	94,94,94,94	0
54	MG	YA	3638	1/1	0.66	0.33	90,90,90,90	0
54	MG	RA	3271	1/1	0.66	0.17	98,98,98,98	0
54	MG	YA	3933	1/1	0.66	0.07	107,107,107,107	0
54	MG	RA	3467	1/1	0.66	0.23	90,90,90,90	0
54	MG	YA	3711	1/1	0.66	0.20	90,90,90,90	0
54	MG	RB	202	1/1	0.66	0.26	99,99,99,99	0
54	MG	YA	3861	1/1	0.66	0.32	107,107,107,107	0
54	MG	RA	3146	1/1	0.66	0.16	130,130,130,130	0
54	MG	RA	3044	1/1	0.66	0.28	140,140,140,140	0
54	MG	RA	3429	1/1	0.66	0.26	183,183,183,183	0
54	MG	RA	3315	1/1	0.66	0.12	113,113,113,113	0
54	MG	YA	3738	1/1	0.66	0.12	102,102,102,102	0
54	MG	RA	3389	1/1	0.66	0.14	109,109,109,109	0
54	MG	RA	3434	1/1	0.66	0.07	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	YA	3972	1/1	0.66	0.20	126,126,126,126	0
54	MG	R1	103	1/1	0.66	0.11	113,113,113,113	0
54	MG	YA	3927	1/1	0.66	0.26	90,90,90,90	0
54	MG	YR	201	1/1	0.67	0.15	112,112,112,112	0
54	MG	YA	3912	1/1	0.67	0.14	123,123,123,123	0
54	MG	YA	3741	1/1	0.67	0.69	90,90,90,90	0
54	MG	RA	3313	1/1	0.67	0.11	90,90,90,90	0
54	MG	YA	3962	1/1	0.67	0.26	100,100,100,100	0
54	MG	RA	3145	1/1	0.67	0.29	90,90,90,90	0
54	MG	RA	3332	1/1	0.67	0.14	104,104,104,104	0
54	MG	RA	3126	1/1	0.67	0.53	121,121,121,121	0
54	MG	YA	3714	1/1	0.67	0.38	90,90,90,90	0
54	MG	QA	1686	1/1	0.67	0.20	93,93,93,93	0
54	MG	YA	3845	1/1	0.67	0.36	90,90,90,90	0
54	MG	YA	3784	1/1	0.67	0.20	121,121,121,121	0
54	MG	YA	3655	1/1	0.67	0.39	90,90,90,90	0
54	MG	RA	3195	1/1	0.67	0.26	94,94,94,94	0
54	MG	QA	1698	1/1	0.67	0.38	90,90,90,90	0
54	MG	RA	3158	1/1	0.67	0.36	118,118,118,118	0
54	MG	XA	1626	1/1	0.67	0.37	90,90,90,90	0
54	MG	RO	202	1/1	0.67	0.08	108,108,108,108	0
54	MG	XA	1628	1/1	0.67	0.24	114,114,114,114	0
54	MG	YA	3611	1/1	0.67	0.34	90,90,90,90	0
54	MG	RA	3541	1/1	0.67	0.19	90,90,90,90	0
54	MG	YA	3867	1/1	0.67	0.35	90,90,90,90	0
54	MG	RA	3213	1/1	0.68	0.17	90,90,90,90	0
54	MG	RA	3269	1/1	0.68	0.22	117,117,117,117	0
54	MG	RA	3504	1/1	0.68	0.25	256,256,256,256	0
54	MG	RA	3086	1/1	0.68	0.12	131,131,131,131	0
54	MG	RA	3160	1/1	0.68	0.60	90,90,90,90	0
54	MG	YA	3668	1/1	0.68	0.47	90,90,90,90	0
54	MG	RA	3405	1/1	0.68	0.17	90,90,90,90	0
54	MG	QQ	202	1/1	0.68	0.24	167,167,167,167	0
54	MG	XA	1625	1/1	0.68	0.17	174,174,174,174	0
54	MG	YA	3758	1/1	0.68	0.22	90,90,90,90	0
54	MG	XA	1698	1/1	0.68	0.29	90,90,90,90	0
54	MG	YA	3842	1/1	0.68	0.18	95,95,95,95	0
54	MG	RA	3071	1/1	0.68	0.46	90,90,90,90	0
54	MG	QA	1646	1/1	0.68	0.14	107,107,107,107	0
54	MG	YA	3646	1/1	0.68	0.75	90,90,90,90	0
54	MG	QA	1723	1/1	0.68	0.12	149,149,149,149	0
54	MG	XA	1651	1/1	0.68	0.17	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	YA	3847	1/1	0.68	0.26	90,90,90,90	0
54	MG	RA	3334	1/1	0.68	0.14	95,95,95,95	0
54	MG	YA	3739	1/1	0.68	0.18	95,95,95,95	0
54	MG	RA	3351	1/1	0.69	0.13	90,90,90,90	0
54	MG	RA	3210	1/1	0.69	0.18	123,123,123,123	0
54	MG	XA	1660	1/1	0.69	0.19	90,90,90,90	0
54	MG	RD	301	1/1	0.69	0.21	124,124,124,124	0
54	MG	QA	1673	1/1	0.69	0.66	90,90,90,90	0
54	MG	RA	3021	1/1	0.69	0.20	112,112,112,112	0
54	MG	QA	1676	1/1	0.69	0.36	90,90,90,90	0
54	MG	YA	3607	1/1	0.69	0.30	90,90,90,90	0
54	MG	QA	1630	1/1	0.69	0.32	120,120,120,120	0
54	MG	YA	3790	1/1	0.69	0.21	90,90,90,90	0
54	MG	RA	3120	1/1	0.69	0.35	96,96,96,96	0
54	MG	RA	3419	1/1	0.69	0.17	142,142,142,142	0
54	MG	YA	3914	1/1	0.69	0.26	90,90,90,90	0
54	MG	RA	3250	1/1	0.69	0.10	121,121,121,121	0
54	MG	RA	3338	1/1	0.69	0.10	129,129,129,129	0
54	MG	YA	3873	1/1	0.69	0.27	91,91,91,91	0
54	MG	RA	3031	1/1	0.69	0.10	122,122,122,122	0
54	MG	RA	3257	1/1	0.69	0.14	102,102,102,102	0
54	MG	YA	3672	1/1	0.69	0.12	100,100,100,100	0
54	MG	RA	3522	1/1	0.69	0.16	145,145,145,145	0
54	MG	RA	3222	1/1	0.69	0.49	134,134,134,134	0
54	MG	RB	204	1/1	0.69	0.54	158,158,158,158	0
54	MG	RA	3305	1/1	0.69	0.55	93,93,93,93	0
54	MG	RA	3056	1/1	0.69	0.30	116,116,116,116	0
54	MG	RA	3457	1/1	0.70	0.28	90,90,90,90	0
54	MG	RA	3096	1/1	0.70	0.15	98,98,98,98	0
54	MG	XA	1691	1/1	0.70	0.09	121,121,121,121	0
54	MG	YA	3618	1/1	0.70	0.41	90,90,90,90	0
54	MG	RA	3035	1/1	0.70	0.17	94,94,94,94	0
54	MG	QA	1688	1/1	0.70	0.09	173,173,173,173	0
54	MG	YA	3886	1/1	0.70	0.22	162,162,162,162	0
54	MG	YB	205	1/1	0.70	0.50	97,97,97,97	0
54	MG	QL	203	1/1	0.70	0.13	126,126,126,126	0
54	MG	YB	207	1/1	0.70	0.19	109,109,109,109	0
54	MG	XA	1644	1/1	0.70	0.41	91,91,91,91	0
54	MG	XA	1684	1/1	0.70	0.77	90,90,90,90	0
54	MG	XA	1687	1/1	0.70	0.08	91,91,91,91	0
54	MG	YA	3759	1/1	0.70	0.52	90,90,90,90	0
54	MG	YA	3827	1/1	0.71	0.14	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	YA	3888	1/1	0.71	0.41	90,90,90,90	0
54	MG	RA	3465	1/1	0.71	0.31	90,90,90,90	0
54	MG	YA	3895	1/1	0.71	0.35	90,90,90,90	0
54	MG	RA	3265	1/1	0.71	0.30	90,90,90,90	0
54	MG	RA	3085	1/1	0.71	0.10	126,126,126,126	0
54	MG	YA	3652	1/1	0.71	0.34	90,90,90,90	0
54	MG	YA	3682	1/1	0.71	0.22	90,90,90,90	0
54	MG	YB	201	1/1	0.71	0.19	90,90,90,90	0
54	MG	YA	3632	1/1	0.71	0.20	91,91,91,91	0
54	MG	YA	3636	1/1	0.71	0.56	113,113,113,113	0
54	MG	RA	3295	1/1	0.71	0.46	108,108,108,108	0
54	MG	QA	1679	1/1	0.71	0.09	108,108,108,108	0
54	MG	QT	201	1/1	0.71	0.36	205,205,205,205	0
54	MG	RA	3544	1/1	0.71	0.11	90,90,90,90	0
54	MG	YA	3813	1/1	0.71	0.39	111,111,111,111	0
54	MG	RA	3052	1/1	0.71	0.20	98,98,98,98	0
54	MG	YA	3947	1/1	0.71	0.43	90,90,90,90	0
54	MG	RA	3193	1/1	0.71	0.11	91,91,91,91	0
54	MG	YA	3956	1/1	0.71	0.45	93,93,93,93	0
54	MG	RA	3268	1/1	0.72	0.39	90,90,90,90	0
54	MG	QA	1656	1/1	0.72	0.21	90,90,90,90	0
54	MG	YA	3614	1/1	0.72	0.56	90,90,90,90	0
54	MG	YA	3796	1/1	0.72	0.90	90,90,90,90	0
54	MG	RA	3199	1/1	0.72	0.26	148,148,148,148	0
54	MG	YA	3725	1/1	0.72	0.33	92,92,92,92	0
54	MG	YA	3925	1/1	0.72	0.38	90,90,90,90	0
54	MG	QA	1635	1/1	0.72	0.24	102,102,102,102	0
54	MG	RA	3076	1/1	0.72	0.26	92,92,92,92	0
54	MG	RA	3549	1/1	0.72	0.18	121,121,121,121	0
54	MG	YA	3868	1/1	0.72	0.38	154,154,154,154	0
54	MG	RA	3485	1/1	0.72	0.51	90,90,90,90	0
54	MG	RA	3399	1/1	0.72	0.14	158,158,158,158	0
54	MG	YA	3918	1/1	0.72	0.24	90,90,90,90	0
54	MG	RA	3047	1/1	0.73	0.12	93,93,93,93	0
54	MG	RA	3019	1/1	0.73	0.39	132,132,132,132	0
54	MG	YA	3649	1/1	0.73	0.32	90,90,90,90	0
54	MG	RA	3486	1/1	0.73	0.20	90,90,90,90	0
54	MG	RA	3200	1/1	0.73	0.30	90,90,90,90	0
54	MG	RA	3219	1/1	0.73	0.29	112,112,112,112	0
54	MG	YA	3896	1/1	0.73	0.14	93,93,93,93	0
54	MG	RA	3175	1/1	0.73	0.15	97,97,97,97	0
54	MG	XA	1675	1/1	0.73	0.27	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	QA	1726	1/1	0.73	0.28	195,195,195,195	0
54	MG	YA	3898	1/1	0.73	0.29	145,145,145,145	0
54	MG	YA	3745	1/1	0.73	0.26	90,90,90,90	0
54	MG	QA	1629	1/1	0.73	0.11	105,105,105,105	0
54	MG	YA	3658	1/1	0.73	0.43	90,90,90,90	0
54	MG	YA	3858	1/1	0.73	0.74	90,90,90,90	0
54	MG	RA	3369	1/1	0.73	0.13	113,113,113,113	0
54	MG	RA	3412	1/1	0.73	0.36	90,90,90,90	0
54	MG	YA	3862	1/1	0.73	0.32	164,164,164,164	0
54	MG	RA	3206	1/1	0.73	0.41	134,134,134,134	0
54	MG	RB	214	1/1	0.73	0.28	106,106,106,106	0
54	MG	RA	3277	1/1	0.73	0.13	92,92,92,92	0
54	MG	RA	3091	1/1	0.73	0.20	99,99,99,99	0
54	MG	QQ	201	1/1	0.73	0.08	106,106,106,106	0
54	MG	YA	3678	1/1	0.73	0.20	94,94,94,94	0
54	MG	RA	3471	1/1	0.73	0.16	90,90,90,90	0
54	MG	XA	1712	1/1	0.73	0.06	96,96,96,96	0
54	MG	RD	308	1/1	0.73	0.13	94,94,94,94	0
54	MG	RA	3479	1/1	0.73	0.54	154,154,154,154	0
54	MG	YA	3732	1/1	0.73	0.26	221,221,221,221	0
54	MG	YA	3848	1/1	0.74	0.45	90,90,90,90	0
54	MG	RE	305	1/1	0.74	0.27	91,91,91,91	0
54	MG	YA	3806	1/1	0.74	0.47	90,90,90,90	0
54	MG	RA	3024	1/1	0.74	0.14	156,156,156,156	0
54	MG	QA	1730	1/1	0.74	0.12	112,112,112,112	0
54	MG	YA	3736	1/1	0.74	0.27	90,90,90,90	0
54	MG	RA	3444	1/1	0.74	0.25	119,119,119,119	0
54	MG	RA	3426	1/1	0.74	0.16	90,90,90,90	0
54	MG	RA	3080	1/1	0.74	0.19	100,100,100,100	0
54	MG	QA	1653	1/1	0.74	0.14	95,95,95,95	0
54	MG	YA	3706	1/1	0.74	0.18	118,118,118,118	0
54	MG	YD	304	1/1	0.74	0.21	121,121,121,121	0
54	MG	RA	3290	1/1	0.74	0.09	153,153,153,153	0
54	MG	RA	3293	1/1	0.74	0.10	118,118,118,118	0
54	MG	YA	3869	1/1	0.74	0.74	90,90,90,90	0
54	MG	RA	3357	1/1	0.74	0.45	171,171,171,171	0
54	MG	YA	3650	1/1	0.74	0.77	155,155,155,155	0
54	MG	RA	3341	1/1	0.74	0.08	92,92,92,92	0
54	MG	YA	3916	1/1	0.74	0.31	91,91,91,91	0
54	MG	RA	3489	1/1	0.74	0.22	92,92,92,92	0
54	MG	XA	1640	1/1	0.74	0.05	126,126,126,126	0
54	MG	QA	1714	1/1	0.74	0.27	174,174,174,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	YA	3843	1/1	0.74	0.30	174,174,174,174	0
54	MG	RA	3492	1/1	0.74	0.24	92,92,92,92	0
54	MG	RA	3168	1/1	0.74	0.32	90,90,90,90	0
54	MG	RA	3266	1/1	0.74	0.31	90,90,90,90	0
54	MG	RA	3414	1/1	0.75	0.08	112,112,112,112	0
54	MG	YA	3635	1/1	0.75	0.21	152,152,152,152	0
54	MG	QA	1639	1/1	0.75	0.15	91,91,91,91	0
54	MG	RA	3009	1/1	0.75	0.18	91,91,91,91	0
54	MG	RA	3512	1/1	0.75	0.17	105,105,105,105	0
54	MG	RA	3274	1/1	0.75	0.14	90,90,90,90	0
54	MG	YA	3608	1/1	0.75	0.21	90,90,90,90	0
54	MG	YA	3931	1/1	0.75	0.17	122,122,122,122	0
54	MG	RA	3292	1/1	0.75	0.17	96,96,96,96	0
54	MG	RA	3316	1/1	0.75	0.13	92,92,92,92	0
54	MG	XA	1636	1/1	0.75	0.07	103,103,103,103	0
54	MG	RA	3178	1/1	0.75	0.19	94,94,94,94	0
54	MG	QA	1687	1/1	0.75	0.40	90,90,90,90	0
54	MG	RR	202	1/1	0.75	0.11	108,108,108,108	0
54	MG	RA	3114	1/1	0.75	0.27	90,90,90,90	0
54	MG	RA	3554	1/1	0.75	0.11	103,103,103,103	0
54	MG	RA	3501	1/1	0.75	0.37	90,90,90,90	0
54	MG	RA	3040	1/1	0.75	0.24	91,91,91,91	0
54	MG	XL	201	1/1	0.75	0.11	99,99,99,99	0
54	MG	QA	1697	1/1	0.75	0.37	116,116,116,116	0
54	MG	YA	3893	1/1	0.75	0.20	101,101,101,101	0
54	MG	RA	3004	1/1	0.75	0.36	109,109,109,109	0
54	MG	YA	3860	1/1	0.76	0.20	90,90,90,90	0
54	MG	YA	3647	1/1	0.76	0.17	115,115,115,115	0
54	MG	RA	3042	1/1	0.76	0.33	103,103,103,103	0
54	MG	RA	3242	1/1	0.76	0.24	94,94,94,94	0
54	MG	RA	3383	1/1	0.76	0.10	133,133,133,133	0
54	MG	YA	3610	1/1	0.76	0.46	90,90,90,90	0
54	MG	RA	3513	1/1	0.76	0.17	137,137,137,137	0
54	MG	QA	1604	1/1	0.76	0.25	158,158,158,158	0
54	MG	YA	3871	1/1	0.76	0.28	90,90,90,90	0
54	MG	YA	3977	1/1	0.76	0.19	90,90,90,90	0
54	MG	RA	3472	1/1	0.76	0.22	90,90,90,90	0
54	MG	RA	3069	1/1	0.76	0.05	90,90,90,90	0
54	MG	RE	307	1/1	0.76	0.24	90,90,90,90	0
54	MG	RA	3055	1/1	0.76	0.25	136,136,136,136	0
54	MG	QA	1670	1/1	0.76	0.14	94,94,94,94	0
54	MG	RA	3560	1/1	0.76	0.25	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	RA	3101	1/1	0.76	0.14	123,123,123,123	0
54	MG	RA	3310	1/1	0.76	0.11	92,92,92,92	0
54	MG	YA	3767	1/1	0.76	0.45	90,90,90,90	0
54	MG	RA	3116	1/1	0.76	0.13	90,90,90,90	0
54	MG	YA	3772	1/1	0.76	0.68	90,90,90,90	0
54	MG	RA	3164	1/1	0.76	0.18	90,90,90,90	0
54	MG	RA	3534	1/1	0.76	0.32	119,119,119,119	0
54	MG	RA	3209	1/1	0.76	0.33	106,106,106,106	0
54	MG	R1	101	1/1	0.76	0.08	154,154,154,154	0
54	MG	QA	1634	1/1	0.76	0.59	99,99,99,99	0
54	MG	RA	3105	1/1	0.76	0.20	92,92,92,92	0
54	MG	RA	3340	1/1	0.76	0.14	97,97,97,97	0
54	MG	RA	3151	1/1	0.76	0.41	90,90,90,90	0
54	MG	QA	1695	1/1	0.76	0.57	131,131,131,131	0
54	MG	R6	101	1/1	0.76	0.28	159,159,159,159	0
54	MG	XA	1715	1/1	0.76	0.19	144,144,144,144	0
54	MG	RA	3260	1/1	0.76	0.43	90,90,90,90	0
54	MG	YA	3954	1/1	0.76	0.17	134,134,134,134	0
54	MG	RA	3254	1/1	0.77	0.23	149,149,149,149	0
54	MG	YA	3623	1/1	0.77	0.13	113,113,113,113	0
54	MG	RA	3498	1/1	0.77	0.24	90,90,90,90	0
54	MG	YA	3976	1/1	0.77	0.24	92,92,92,92	0
54	MG	RA	3289	1/1	0.77	0.26	94,94,94,94	0
54	MG	YA	3742	1/1	0.77	0.32	90,90,90,90	0
54	MG	YA	3634	1/1	0.77	0.15	93,93,93,93	0
54	MG	QA	1636	1/1	0.77	0.13	138,138,138,138	0
54	MG	XA	1648	1/1	0.77	0.14	95,95,95,95	0
54	MG	RA	3520	1/1	0.77	0.19	156,156,156,156	0
54	MG	RA	3464	1/1	0.77	0.12	105,105,105,105	0
54	MG	QA	1615	1/1	0.77	0.09	142,142,142,142	0
54	MG	YB	206	1/1	0.77	0.45	90,90,90,90	0
54	MG	XA	1707	1/1	0.77	0.15	134,134,134,134	0
54	MG	QA	1617	1/1	0.77	0.27	92,92,92,92	0
54	MG	RA	3240	1/1	0.77	0.11	91,91,91,91	0
54	MG	YA	3889	1/1	0.77	0.22	90,90,90,90	0
54	MG	RA	3202	1/1	0.77	0.22	90,90,90,90	0
54	MG	YA	3829	1/1	0.77	0.26	90,90,90,90	0
54	MG	YA	3791	1/1	0.77	0.20	132,132,132,132	0
54	MG	QA	1682	1/1	0.77	0.14	90,90,90,90	0
54	MG	RA	3211	1/1	0.78	0.27	92,92,92,92	0
54	MG	RA	3227	1/1	0.78	0.20	148,148,148,148	0
54	MG	QA	1675	1/1	0.78	0.12	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	RF	304	1/1	0.78	0.13	91,91,91,91	0
54	MG	YB	202	1/1	0.78	0.11	106,106,106,106	0
54	MG	YA	3959	1/1	0.78	0.53	111,111,111,111	0
54	MG	RA	3088	1/1	0.78	0.13	95,95,95,95	0
54	MG	YA	3721	1/1	0.78	0.35	90,90,90,90	0
54	MG	RA	3343	1/1	0.78	0.16	151,151,151,151	0
54	MG	RA	3058	1/1	0.78	0.15	122,122,122,122	0
54	MG	RA	3497	1/1	0.78	0.25	90,90,90,90	0
54	MG	YA	3948	1/1	0.78	0.50	90,90,90,90	0
54	MG	YA	3875	1/1	0.78	0.25	90,90,90,90	0
54	MG	XA	1682	1/1	0.78	0.25	90,90,90,90	0
54	MG	XP	101	1/1	0.78	0.15	208,208,208,208	0
54	MG	QA	1689	1/1	0.78	0.27	93,93,93,93	0
54	MG	XA	1645	1/1	0.78	0.10	99,99,99,99	0
54	MG	YQ	201	1/1	0.79	0.15	90,90,90,90	0
54	MG	QA	1605	1/1	0.79	0.19	90,90,90,90	0
54	MG	RA	3191	1/1	0.79	0.19	90,90,90,90	0
54	MG	RA	3439	1/1	0.79	0.13	100,100,100,100	0
54	MG	YA	3949	1/1	0.79	0.08	90,90,90,90	0
54	MG	RA	3136	1/1	0.79	0.21	139,139,139,139	0
54	MG	RA	3003	1/1	0.79	0.19	208,208,208,208	0
54	MG	YA	3841	1/1	0.79	0.36	90,90,90,90	0
54	MG	RA	3207	1/1	0.79	0.24	90,90,90,90	0
54	MG	RA	3176	1/1	0.79	0.60	90,90,90,90	0
54	MG	YA	3816	1/1	0.79	0.48	90,90,90,90	0
54	MG	QA	1650	1/1	0.79	0.10	141,141,141,141	0
54	MG	XA	1701	1/1	0.79	0.07	120,120,120,120	0
54	MG	XA	1654	1/1	0.79	0.12	97,97,97,97	0
54	MG	RA	3244	1/1	0.79	0.19	90,90,90,90	0
54	MG	XA	1663	1/1	0.79	0.16	90,90,90,90	0
54	MG	YA	3823	1/1	0.79	0.46	90,90,90,90	0
54	MG	XA	1710	1/1	0.79	0.19	129,129,129,129	0
54	MG	QP	102	1/1	0.79	0.91	145,145,145,145	0
54	MG	RA	3078	1/1	0.79	0.29	96,96,96,96	0
54	MG	RA	3118	1/1	0.79	0.19	90,90,90,90	0
54	MG	RA	3017	1/1	0.79	0.27	91,91,91,91	0
54	MG	QA	1718	1/1	0.79	0.21	205,205,205,205	0
54	MG	YA	3642	1/1	0.79	0.30	96,96,96,96	0
54	MG	RA	3037	1/1	0.80	0.31	124,124,124,124	0
54	MG	RA	3463	1/1	0.80	0.12	91,91,91,91	0
54	MG	QA	1731	1/1	0.80	0.25	98,98,98,98	0
54	MG	XD	302	1/1	0.80	0.11	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	RA	3536	1/1	0.80	0.27	114,114,114,114	0
54	MG	RA	3537	1/1	0.80	0.23	117,117,117,117	0
54	MG	RA	3425	1/1	0.80	0.06	133,133,133,133	0
54	MG	YA	3872	1/1	0.80	0.15	90,90,90,90	0
54	MG	XA	1603	1/1	0.80	0.21	90,90,90,90	0
54	MG	YA	3950	1/1	0.80	0.16	93,93,93,93	0
54	MG	XA	1680	1/1	0.80	0.14	159,159,159,159	0
54	MG	RA	3321	1/1	0.80	0.11	102,102,102,102	0
54	MG	YA	3641	1/1	0.80	0.10	93,93,93,93	0
54	MG	YA	3840	1/1	0.80	0.27	102,102,102,102	0
54	MG	RA	3079	1/1	0.80	0.15	93,93,93,93	0
54	MG	YA	3878	1/1	0.80	0.25	90,90,90,90	0
54	MG	RA	3179	1/1	0.80	0.24	172,172,172,172	0
54	MG	RB	210	1/1	0.80	0.23	217,217,217,217	0
54	MG	XA	1696	1/1	0.80	0.09	101,101,101,101	0
54	MG	RA	3051	1/1	0.80	0.14	145,145,145,145	0
54	MG	RT	202	1/1	0.80	0.19	141,141,141,141	0
54	MG	RA	3174	1/1	0.80	0.14	103,103,103,103	0
54	MG	YA	3807	1/1	0.80	0.16	90,90,90,90	0
54	MG	YA	3727	1/1	0.80	0.20	91,91,91,91	0
54	MG	QA	1633	1/1	0.80	0.14	90,90,90,90	0
54	MG	RA	3034	1/1	0.80	0.24	99,99,99,99	0
54	MG	XA	1641	1/1	0.80	0.10	90,90,90,90	0
54	MG	RA	3387	1/1	0.80	0.10	143,143,143,143	0
54	MG	QA	1720	1/1	0.80	0.14	137,137,137,137	0
54	MG	RA	3478	1/1	0.80	0.34	90,90,90,90	0
54	MG	RA	3453	1/1	0.80	0.21	90,90,90,90	0
54	MG	YA	3818	1/1	0.80	0.31	128,128,128,128	0
54	MG	YA	3696	1/1	0.80	0.22	93,93,93,93	0
54	MG	RA	3527	1/1	0.80	0.20	90,90,90,90	0
54	MG	XA	1658	1/1	0.80	0.15	117,117,117,117	0
54	MG	YA	3855	1/1	0.81	0.40	90,90,90,90	0
54	MG	XA	1686	1/1	0.81	0.10	158,158,158,158	0
54	MG	QA	1671	1/1	0.81	0.22	93,93,93,93	0
54	MG	YA	3979	1/1	0.81	0.12	119,119,119,119	0
54	MG	YA	3811	1/1	0.81	0.17	91,91,91,91	0
54	MG	YA	3877	1/1	0.81	0.11	92,92,92,92	0
54	MG	RA	3177	1/1	0.81	0.14	91,91,91,91	0
54	MG	XA	1602	1/1	0.81	0.31	162,162,162,162	0
54	MG	RA	3495	1/1	0.81	0.20	97,97,97,97	0
54	MG	RA	3505	1/1	0.81	0.11	92,92,92,92	0
54	MG	RA	3255	1/1	0.81	0.37	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	YA	3906	1/1	0.81	0.29	90,90,90,90	0
54	MG	RA	3143	1/1	0.81	0.13	90,90,90,90	0
54	MG	YA	3756	1/1	0.81	0.40	90,90,90,90	0
54	MG	YA	3963	1/1	0.81	0.13	91,91,91,91	0
54	MG	RA	3073	1/1	0.81	0.34	159,159,159,159	0
54	MG	XA	1708	1/1	0.81	0.08	133,133,133,133	0
54	MG	YA	3938	1/1	0.81	0.18	97,97,97,97	0
54	MG	YA	3620	1/1	0.81	0.15	95,95,95,95	0
54	MG	YA	3799	1/1	0.81	0.18	91,91,91,91	0
54	MG	RA	3070	1/1	0.81	0.26	90,90,90,90	0
54	MG	QA	1667	1/1	0.81	0.11	115,115,115,115	0
54	MG	RA	3302	1/1	0.81	0.19	98,98,98,98	0
54	MG	XA	1681	1/1	0.81	0.11	128,128,128,128	0
54	MG	XA	1721	1/1	0.81	0.30	143,143,143,143	0
54	MG	YA	3781	1/1	0.81	0.14	90,90,90,90	0
54	MG	XA	1665	1/1	0.82	0.18	92,92,92,92	0
54	MG	YA	3964	1/1	0.82	0.35	90,90,90,90	0
54	MG	RA	3436	1/1	0.82	0.13	113,113,113,113	0
54	MG	XA	1606	1/1	0.82	0.09	185,185,185,185	0
54	MG	RA	3543	1/1	0.82	0.21	139,139,139,139	0
54	MG	RA	3027	1/1	0.82	0.30	98,98,98,98	0
54	MG	RA	3438	1/1	0.82	0.16	126,126,126,126	0
54	MG	XA	1616	1/1	0.82	0.26	90,90,90,90	0
54	MG	YA	3712	1/1	0.82	0.32	90,90,90,90	0
54	MG	XA	1622	1/1	0.82	0.15	189,189,189,189	0
54	MG	YA	3975	1/1	0.82	0.52	90,90,90,90	0
54	MG	RA	3050	1/1	0.82	0.27	93,93,93,93	0
54	MG	YA	3719	1/1	0.82	0.24	90,90,90,90	0
54	MG	RA	3132	1/1	0.82	0.18	136,136,136,136	0
54	MG	RU	201	1/1	0.82	0.21	123,123,123,123	0
54	MG	YA	3903	1/1	0.82	0.31	90,90,90,90	0
54	MG	RY	201	1/1	0.82	0.19	100,100,100,100	0
54	MG	RA	3028	1/1	0.82	0.27	97,97,97,97	0
54	MG	XA	1635	1/1	0.82	0.09	102,102,102,102	0
54	MG	RA	3446	1/1	0.82	0.73	177,177,177,177	0
54	MG	XA	1637	1/1	0.82	0.09	137,137,137,137	0
54	MG	YA	3844	1/1	0.82	0.23	90,90,90,90	0
54	MG	RA	3368	1/1	0.82	0.05	93,93,93,93	0
54	MG	RA	3348	1/1	0.82	0.17	140,140,140,140	0
54	MG	XA	1702	1/1	0.82	0.08	144,144,144,144	0
54	MG	YD	301	1/1	0.82	0.23	90,90,90,90	0
54	MG	RA	3182	1/1	0.82	0.10	139,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	XA	1647	1/1	0.82	0.20	143,143,143,143	0
54	MG	QA	1729	1/1	0.82	0.09	94,94,94,94	0
54	MG	RA	3007	1/1	0.82	0.17	93,93,93,93	0
54	MG	RA	3507	1/1	0.82	0.34	90,90,90,90	0
54	MG	RA	3189	1/1	0.82	0.08	118,118,118,118	0
54	MG	YA	3662	1/1	0.82	0.14	108,108,108,108	0
54	MG	XA	1713	1/1	0.82	0.24	91,91,91,91	0
54	MG	XA	1656	1/1	0.82	0.18	90,90,90,90	0
54	MG	RA	3433	1/1	0.82	0.10	101,101,101,101	0
54	MG	RA	3053	1/1	0.82	0.22	90,90,90,90	0
54	MG	YA	3824	1/1	0.82	0.25	160,160,160,160	0
54	MG	XA	1601	1/1	0.82	0.17	166,166,166,166	0
54	MG	RA	3440	1/1	0.83	0.09	170,170,170,170	0
54	MG	YA	3810	1/1	0.83	0.42	90,90,90,90	0
54	MG	RA	3104	1/1	0.83	0.09	113,113,113,113	0
54	MG	YA	3616	1/1	0.83	0.25	139,139,139,139	0
54	MG	RA	3349	1/1	0.83	0.35	127,127,127,127	0
54	MG	RA	3082	1/1	0.83	0.08	140,140,140,140	0
54	MG	RA	3006	1/1	0.83	0.20	90,90,90,90	0
54	MG	YA	3771	1/1	0.83	0.18	109,109,109,109	0
54	MG	XA	1634	1/1	0.83	0.18	91,91,91,91	0
54	MG	RA	3256	1/1	0.83	0.31	126,126,126,126	0
54	MG	RA	3474	1/1	0.83	0.09	103,103,103,103	0
54	MG	RA	3232	1/1	0.83	0.38	90,90,90,90	0
54	MG	RA	3360	1/1	0.83	0.23	91,91,91,91	0
54	MG	QA	1728	1/1	0.83	0.11	92,92,92,92	0
54	MG	QT	202	1/1	0.83	0.06	112,112,112,112	0
54	MG	YA	3657	1/1	0.83	0.23	137,137,137,137	0
54	MG	YA	3601	1/1	0.83	0.17	111,111,111,111	0
54	MG	RA	3322	1/1	0.83	0.47	90,90,90,90	0
54	MG	YA	3870	1/1	0.83	0.42	90,90,90,90	0
54	MG	YA	3664	1/1	0.83	0.12	110,110,110,110	0
54	MG	RA	3110	1/1	0.83	0.24	90,90,90,90	0
54	MG	YA	3837	1/1	0.83	0.37	90,90,90,90	0
54	MG	RA	3093	1/1	0.83	0.17	100,100,100,100	0
54	MG	QA	1659	1/1	0.83	0.13	98,98,98,98	0
54	MG	RA	3460	1/1	0.83	0.43	146,146,146,146	0
54	MG	YA	3639	1/1	0.83	0.61	90,90,90,90	0
54	MG	YA	3713	1/1	0.83	0.12	90,90,90,90	0
54	MG	RR	201	1/1	0.83	0.27	131,131,131,131	0
54	MG	RA	3205	1/1	0.83	0.19	96,96,96,96	0
54	MG	XA	1666	1/1	0.83	0.53	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	XA	1614	1/1	0.83	0.18	126,126,126,126	0
54	MG	RA	3263	1/1	0.83	0.16	90,90,90,90	0
54	MG	XA	1720	1/1	0.83	0.13	169,169,169,169	0
54	MG	RA	3251	1/1	0.83	0.20	90,90,90,90	0
54	MG	YA	3965	1/1	0.83	0.18	90,90,90,90	0
54	MG	XA	1727	1/1	0.83	0.16	168,168,168,168	0
55	ZN	QD	305	1/1	0.83	0.14	338,338,338,338	0
54	MG	RA	3220	1/1	0.84	0.08	97,97,97,97	0
54	MG	YA	3853	1/1	0.84	0.20	105,105,105,105	0
54	MG	RA	3072	1/1	0.84	0.45	110,110,110,110	0
54	MG	RA	3285	1/1	0.84	0.16	90,90,90,90	0
54	MG	YA	3856	1/1	0.84	0.42	90,90,90,90	0
54	MG	RR	203	1/1	0.84	0.44	90,90,90,90	0
54	MG	YB	210	1/1	0.84	0.22	91,91,91,91	0
54	MG	RA	3364	1/1	0.84	0.17	144,144,144,144	0
54	MG	YA	3726	1/1	0.84	0.17	90,90,90,90	0
54	MG	XA	1617	1/1	0.84	0.11	97,97,97,97	0
54	MG	XA	1619	1/1	0.84	0.09	90,90,90,90	0
54	MG	YA	3961	1/1	0.84	0.22	93,93,93,93	0
54	MG	RA	3309	1/1	0.84	0.18	182,182,182,182	0
54	MG	RA	3157	1/1	0.84	0.20	90,90,90,90	0
54	MG	RD	309	1/1	0.84	0.54	189,189,189,189	0
54	MG	RE	301	1/1	0.84	0.16	121,121,121,121	0
54	MG	RA	3137	1/1	0.84	0.11	170,170,170,170	0
54	MG	RA	3353	1/1	0.84	0.13	90,90,90,90	0
54	MG	RA	3153	1/1	0.84	0.20	177,177,177,177	0
54	MG	RA	3186	1/1	0.84	0.14	140,140,140,140	0
54	MG	YA	3675	1/1	0.84	0.21	100,100,100,100	0
54	MG	RA	3258	1/1	0.84	0.24	90,90,90,90	0
54	MG	RA	3475	1/1	0.84	0.33	133,133,133,133	0
54	MG	QA	1623	1/1	0.84	0.10	118,118,118,118	0
54	MG	RA	3424	1/1	0.84	0.15	130,130,130,130	0
54	MG	RA	3524	1/1	0.84	0.12	138,138,138,138	0
54	MG	YA	3849	1/1	0.84	0.16	90,90,90,90	0
54	MG	YA	3716	1/1	0.84	0.24	90,90,90,90	0
54	MG	RA	3469	1/1	0.85	0.10	96,96,96,96	0
54	MG	QA	1651	1/1	0.85	0.18	94,94,94,94	0
54	MG	RA	3161	1/1	0.85	0.35	102,102,102,102	0
54	MG	YA	3801	1/1	0.85	0.34	94,94,94,94	0
54	MG	YA	3934	1/1	0.85	0.29	90,90,90,90	0
54	MG	RA	3029	1/1	0.85	0.10	97,97,97,97	0
54	MG	RA	3221	1/1	0.85	0.13	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	RX	101	1/1	0.85	0.16	93,93,93,93	0
54	MG	QA	1707	1/1	0.85	0.08	137,137,137,137	0
54	MG	XA	1683	1/1	0.85	0.17	109,109,109,109	0
54	MG	YA	3621	1/1	0.85	0.24	90,90,90,90	0
54	MG	RA	3060	1/1	0.85	0.16	157,157,157,157	0
54	MG	RA	3506	1/1	0.85	0.11	122,122,122,122	0
54	MG	YA	3630	1/1	0.85	0.16	130,130,130,130	0
54	MG	RA	3542	1/1	0.85	0.11	194,194,194,194	0
54	MG	QA	1716	1/1	0.85	0.30	158,158,158,158	0
54	MG	YA	3717	1/1	0.85	0.28	90,90,90,90	0
54	MG	RA	3064	1/1	0.85	0.09	142,142,142,142	0
54	MG	RA	3406	1/1	0.85	0.21	131,131,131,131	0
54	MG	YA	3722	1/1	0.85	0.57	90,90,90,90	0
54	MG	QA	1722	1/1	0.85	0.12	151,151,151,151	0
54	MG	RA	3224	1/1	0.85	0.09	96,96,96,96	0
54	MG	RA	3152	1/1	0.85	0.16	109,109,109,109	0
54	MG	QA	1626	1/1	0.85	0.13	121,121,121,121	0
54	MG	RA	3482	1/1	0.85	0.22	92,92,92,92	0
54	MG	XA	1704	1/1	0.85	0.16	96,96,96,96	0
54	MG	RA	3484	1/1	0.85	0.18	91,91,91,91	0
54	MG	RA	3282	1/1	0.85	0.25	97,97,97,97	0
54	MG	YA	3915	1/1	0.85	0.14	92,92,92,92	0
54	MG	XA	1650	1/1	0.85	0.18	138,138,138,138	0
54	MG	RA	3461	1/1	0.85	0.47	90,90,90,90	0
54	MG	YA	3606	1/1	0.85	0.37	201,201,201,201	0
54	MG	RA	3488	1/1	0.85	0.20	91,91,91,91	0
54	MG	YA	3735	1/1	0.85	0.24	90,90,90,90	0
54	MG	RA	3169	1/1	0.85	0.13	91,91,91,91	0
54	MG	QA	1637	1/1	0.85	0.08	91,91,91,91	0
54	MG	RA	3212	1/1	0.85	0.18	121,121,121,121	0
54	MG	RA	3030	1/1	0.85	0.35	90,90,90,90	0
54	MG	RA	3203	1/1	0.85	0.74	105,105,105,105	0
54	MG	RA	3330	1/1	0.85	0.09	92,92,92,92	0
54	MG	RB	203	1/1	0.85	0.18	165,165,165,165	0
54	MG	RA	3204	1/1	0.85	0.20	93,93,93,93	0
54	MG	XA	1633	1/1	0.86	0.09	109,109,109,109	0
54	MG	YA	3715	1/1	0.86	0.37	90,90,90,90	0
54	MG	YA	3683	1/1	0.86	0.49	90,90,90,90	0
54	MG	RB	208	1/1	0.86	0.14	178,178,178,178	0
54	MG	YA	3782	1/1	0.86	0.09	101,101,101,101	0
54	MG	RA	3328	1/1	0.86	0.07	110,110,110,110	0
54	MG	XK	201	1/1	0.86	0.10	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	RF	303	1/1	0.86	0.28	141,141,141,141	0
54	MG	XL	202	1/1	0.86	0.07	109,109,109,109	0
54	MG	XA	1694	1/1	0.86	0.10	104,104,104,104	0
54	MG	QA	1703	1/1	0.86	0.12	95,95,95,95	0
54	MG	RA	3245	1/1	0.86	0.21	92,92,92,92	0
54	MG	YA	3659	1/1	0.86	0.27	90,90,90,90	0
54	MG	RA	3388	1/1	0.86	0.17	95,95,95,95	0
54	MG	RA	3278	1/1	0.86	0.20	92,92,92,92	0
54	MG	RA	3099	1/1	0.86	0.25	97,97,97,97	0
54	MG	XA	1608	1/1	0.86	0.10	136,136,136,136	0
54	MG	YA	3960	1/1	0.86	0.07	90,90,90,90	0
54	MG	R8	103	1/1	0.86	0.25	97,97,97,97	0
54	MG	QA	1608	1/1	0.86	0.26	91,91,91,91	0
54	MG	XA	1659	1/1	0.86	0.44	93,93,93,93	0
54	MG	RA	3409	1/1	0.86	0.47	156,156,156,156	0
54	MG	YA	3839	1/1	0.86	0.14	90,90,90,90	0
54	MG	QA	1717	1/1	0.86	0.12	152,152,152,152	0
54	MG	RA	3308	1/1	0.86	0.15	129,129,129,129	0
54	MG	RA	3531	1/1	0.86	0.17	113,113,113,113	0
54	MG	QA	1649	1/1	0.86	0.18	94,94,94,94	0
54	MG	RD	310	1/1	0.86	0.08	150,150,150,150	0
54	MG	YA	3673	1/1	0.86	0.21	255,255,255,255	0
54	MG	XA	1717	1/1	0.86	0.11	145,145,145,145	0
54	MG	RA	3280	1/1	0.86	0.07	129,129,129,129	0
54	MG	RA	3367	1/1	0.86	0.08	160,160,160,160	0
54	MG	RA	3551	1/1	0.86	0.23	118,118,118,118	0
54	MG	YA	3681	1/1	0.86	0.16	120,120,120,120	0
54	MG	YA	3907	1/1	0.86	0.32	92,92,92,92	0
54	MG	XA	1728	1/1	0.86	0.55	90,90,90,90	0
54	MG	RA	3358	1/1	0.86	0.08	155,155,155,155	0
54	MG	YA	3753	1/1	0.87	0.27	90,90,90,90	0
54	MG	RA	3528	1/1	0.87	0.08	90,90,90,90	0
54	MG	YA	3968	1/1	0.87	0.07	90,90,90,90	0
54	MG	YA	3937	1/1	0.87	0.17	90,90,90,90	0
54	MG	RA	3016	1/1	0.87	0.10	93,93,93,93	0
54	MG	YA	3826	1/1	0.87	0.13	120,120,120,120	0
54	MG	RA	3141	1/1	0.87	0.21	267,267,267,267	0
54	MG	YA	3852	1/1	0.87	0.32	90,90,90,90	0
54	MG	YA	3609	1/1	0.87	0.49	90,90,90,90	0
54	MG	RA	3061	1/1	0.87	0.20	90,90,90,90	0
54	MG	YA	3680	1/1	0.87	0.16	90,90,90,90	0
54	MG	RA	3063	1/1	0.87	0.19	158,158,158,158	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	RF	302	1/1	0.87	0.12	232,232,232,232	0
54	MG	RA	3454	1/1	0.87	0.26	90,90,90,90	0
54	MG	RA	3557	1/1	0.87	0.19	154,154,154,154	0
54	MG	RA	3359	1/1	0.87	0.28	142,142,142,142	0
54	MG	XA	1673	1/1	0.87	0.48	90,90,90,90	0
54	MG	YA	3955	1/1	0.87	0.09	110,110,110,110	0
54	MG	RA	3521	1/1	0.87	0.09	158,158,158,158	0
54	MG	RA	3442	1/1	0.87	0.14	94,94,94,94	0
54	MG	YA	3866	1/1	0.87	0.08	110,110,110,110	0
54	MG	RA	3112	1/1	0.87	0.12	143,143,143,143	0
54	MG	XA	1716	1/1	0.87	0.16	99,99,99,99	0
54	MG	RA	3057	1/1	0.87	0.09	105,105,105,105	0
54	MG	XA	1718	1/1	0.87	0.33	90,90,90,90	0
54	MG	RA	3318	1/1	0.87	0.35	91,91,91,91	0
54	MG	QA	1641	1/1	0.87	0.06	118,118,118,118	0
54	MG	YA	3746	1/1	0.87	0.23	90,90,90,90	0
54	MG	RA	3183	1/1	0.87	0.25	95,95,95,95	0
54	MG	XA	1609	1/1	0.87	0.06	100,100,100,100	0
54	MG	YA	3622	1/1	0.87	0.33	90,90,90,90	0
54	MG	XA	1649	1/1	0.87	0.06	148,148,148,148	0
54	MG	YA	3798	1/1	0.88	0.40	90,90,90,90	0
54	MG	RA	3252	1/1	0.88	0.16	90,90,90,90	0
54	MG	YT	202	1/1	0.88	0.14	143,143,143,143	0
54	MG	RD	305	1/1	0.88	0.65	131,131,131,131	0
54	MG	RD	306	1/1	0.88	0.21	142,142,142,142	0
54	MG	XA	1685	1/1	0.88	0.11	115,115,115,115	0
54	MG	RA	3239	1/1	0.88	0.18	93,93,93,93	0
54	MG	YA	3808	1/1	0.88	0.20	90,90,90,90	0
54	MG	RA	3352	1/1	0.88	0.13	98,98,98,98	0
54	MG	RA	3187	1/1	0.88	0.10	143,143,143,143	0
54	MG	YA	3883	1/1	0.88	0.09	92,92,92,92	0
54	MG	RA	3115	1/1	0.88	0.15	173,173,173,173	0
54	MG	XA	1692	1/1	0.88	0.14	156,156,156,156	0
54	MG	RA	3084	1/1	0.88	0.20	121,121,121,121	0
54	MG	RE	302	1/1	0.88	0.05	141,141,141,141	0
54	MG	RA	3304	1/1	0.88	0.24	136,136,136,136	0
54	MG	RE	304	1/1	0.88	0.42	157,157,157,157	0
54	MG	QA	1685	1/1	0.88	0.07	178,178,178,178	0
54	MG	XA	1646	1/1	0.88	0.15	94,94,94,94	0
54	MG	RA	3508	1/1	0.88	0.12	98,98,98,98	0
54	MG	R8	102	1/1	0.88	0.06	118,118,118,118	0
54	MG	QA	1643	1/1	0.88	0.26	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	RA	3117	1/1	0.88	0.43	90,90,90,90	0
54	MG	RA	3010	1/1	0.88	0.48	92,92,92,92	0
54	MG	QA	1692	1/1	0.88	0.09	151,151,151,151	0
54	MG	RA	3538	1/1	0.88	0.22	93,93,93,93	0
54	MG	RA	3324	1/1	0.88	0.32	121,121,121,121	0
54	MG	RA	3487	1/1	0.88	0.13	91,91,91,91	0
54	MG	YA	3864	1/1	0.88	0.15	114,114,114,114	0
54	MG	RA	3097	1/1	0.88	0.10	90,90,90,90	0
54	MG	RA	3344	1/1	0.88	0.34	90,90,90,90	0
54	MG	QA	1699	1/1	0.88	0.10	90,90,90,90	0
54	MG	YA	3904	1/1	0.88	0.11	97,97,97,97	0
54	MG	QA	1613	1/1	0.88	0.10	147,147,147,147	0
54	MG	YA	3785	1/1	0.88	0.10	99,99,99,99	0
54	MG	RA	3217	1/1	0.88	0.25	138,138,138,138	0
54	MG	RA	3365	1/1	0.88	0.17	159,159,159,159	0
54	MG	YA	3908	1/1	0.88	0.20	90,90,90,90	0
54	MG	QA	1662	1/1	0.88	0.07	137,137,137,137	0
54	MG	RA	3098	1/1	0.88	0.36	90,90,90,90	0
54	MG	XA	1725	1/1	0.88	0.08	137,137,137,137	0
54	MG	RA	3198	1/1	0.88	0.14	120,120,120,120	0
54	MG	YA	3718	1/1	0.88	0.44	90,90,90,90	0
54	MG	RA	3083	1/1	0.88	0.11	92,92,92,92	0
54	MG	RA	3144	1/1	0.89	0.20	150,150,150,150	0
54	MG	QA	1654	1/1	0.89	0.08	96,96,96,96	0
54	MG	RA	3448	1/1	0.89	0.29	191,191,191,191	0
54	MG	YA	3882	1/1	0.89	0.15	95,95,95,95	0
54	MG	RA	3391	1/1	0.89	0.18	97,97,97,97	0
54	MG	YA	3749	1/1	0.89	0.22	134,134,134,134	0
54	MG	RA	3149	1/1	0.89	0.10	115,115,115,115	0
54	MG	YA	3857	1/1	0.89	0.21	90,90,90,90	0
54	MG	RA	3241	1/1	0.89	0.27	90,90,90,90	0
54	MG	RA	3382	1/1	0.89	0.28	90,90,90,90	0
54	MG	RA	3530	1/1	0.89	0.10	90,90,90,90	0
54	MG	RB	211	1/1	0.89	0.35	176,176,176,176	0
54	MG	QA	1627	1/1	0.89	0.06	132,132,132,132	0
54	MG	YA	3697	1/1	0.89	0.34	96,96,96,96	0
54	MG	YA	3795	1/1	0.89	0.11	98,98,98,98	0
54	MG	RA	3345	1/1	0.89	0.14	90,90,90,90	0
54	MG	YA	3699	1/1	0.89	0.29	91,91,91,91	0
54	MG	XA	1662	1/1	0.89	0.42	93,93,93,93	0
54	MG	YA	3973	1/1	0.89	0.34	101,101,101,101	0
54	MG	RA	3122	1/1	0.89	0.15	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	YA	3900	1/1	0.89	0.16	90,90,90,90	0
54	MG	YA	3936	1/1	0.89	0.13	98,98,98,98	0
54	MG	YA	3669	1/1	0.89	0.09	90,90,90,90	0
54	MG	RA	3276	1/1	0.89	0.29	144,144,144,144	0
54	MG	RA	3106	1/1	0.89	0.47	90,90,90,90	0
54	MG	XA	1672	1/1	0.89	0.08	130,130,130,130	0
54	MG	RA	3403	1/1	0.89	0.22	94,94,94,94	0
54	MG	RA	3237	1/1	0.89	0.13	90,90,90,90	0
54	MG	RA	3519	1/1	0.89	0.12	90,90,90,90	0
54	MG	RQ	201	1/1	0.89	0.08	113,113,113,113	0
54	MG	YA	3812	1/1	0.89	0.28	90,90,90,90	0
54	MG	XA	1679	1/1	0.89	0.15	123,123,123,123	0
54	MG	RA	3163	1/1	0.89	0.39	90,90,90,90	0
54	MG	RA	3373	1/1	0.89	0.14	108,108,108,108	0
54	MG	QA	1610	1/1	0.89	0.13	145,145,145,145	0
54	MG	YA	3605	1/1	0.89	0.39	245,245,245,245	0
54	MG	YA	3913	1/1	0.89	0.28	92,92,92,92	0
54	MG	YA	3628	1/1	0.89	0.55	130,130,130,130	0
54	MG	RA	3231	1/1	0.90	0.12	90,90,90,90	0
54	MG	RA	3216	1/1	0.90	0.21	92,92,92,92	0
54	MG	YA	3677	1/1	0.90	0.15	121,121,121,121	0
54	MG	YA	3651	1/1	0.90	0.31	91,91,91,91	0
54	MG	RA	3462	1/1	0.90	0.15	90,90,90,90	0
54	MG	RA	3296	1/1	0.90	0.10	96,96,96,96	0
54	MG	RA	3090	1/1	0.90	0.18	144,144,144,144	0
54	MG	RA	3378	1/1	0.90	0.05	107,107,107,107	0
54	MG	YA	3831	1/1	0.90	0.33	90,90,90,90	0
54	MG	RA	3267	1/1	0.90	0.13	104,104,104,104	0
54	MG	RA	3049	1/1	0.90	0.35	92,92,92,92	0
54	MG	XA	1604	1/1	0.90	0.07	130,130,130,130	0
54	MG	RA	3355	1/1	0.90	0.24	90,90,90,90	0
54	MG	XA	1607	1/1	0.90	0.27	90,90,90,90	0
54	MG	RA	3081	1/1	0.90	0.23	90,90,90,90	0
54	MG	YA	3805	1/1	0.90	0.10	163,163,163,163	0
54	MG	XA	1655	1/1	0.90	0.04	102,102,102,102	0
54	MG	YA	3863	1/1	0.90	0.23	90,90,90,90	0
54	MG	XA	1657	1/1	0.90	0.14	91,91,91,91	0
54	MG	YB	209	1/1	0.90	0.41	174,174,174,174	0
54	MG	XA	1612	1/1	0.90	0.08	125,125,125,125	0
54	MG	QA	1713	1/1	0.90	0.09	131,131,131,131	0
54	MG	RA	3395	1/1	0.90	0.27	91,91,91,91	0
54	MG	YA	3894	1/1	0.90	0.15	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	RA	3172	1/1	0.90	0.15	145,145,145,145	0
54	MG	XA	1618	1/1	0.90	0.08	134,134,134,134	0
54	MG	RA	3417	1/1	0.90	0.17	147,147,147,147	0
54	MG	QA	1644	1/1	0.90	0.79	90,90,90,90	0
54	MG	YA	3775	1/1	0.90	0.54	90,90,90,90	0
54	MG	RA	3062	1/1	0.90	0.17	90,90,90,90	0
54	MG	QA	1647	1/1	0.90	0.12	99,99,99,99	0
54	MG	YA	3645	1/1	0.90	0.42	90,90,90,90	0
54	MG	RA	3398	1/1	0.90	0.14	144,144,144,144	0
54	MG	RB	213	1/1	0.90	0.10	158,158,158,158	0
54	MG	YA	3752	1/1	0.90	0.47	138,138,138,138	0
54	MG	YA	3815	1/1	0.90	0.16	113,113,113,113	0
54	MG	XA	1722	1/1	0.90	0.09	91,91,91,91	0
54	MG	XA	1678	1/1	0.90	0.14	222,222,222,222	0
54	MG	YX	101	1/1	0.90	0.10	90,90,90,90	0
54	MG	YA	3626	1/1	0.90	0.22	90,90,90,90	0
54	MG	QA	1691	1/1	0.90	0.21	179,179,179,179	0
54	MG	YA	3970	1/1	0.90	0.15	90,90,90,90	0
54	MG	YA	3629	1/1	0.91	0.10	100,100,100,100	0
54	MG	YP	201	1/1	0.91	0.10	90,90,90,90	0
54	MG	RA	3275	1/1	0.91	0.18	128,128,128,128	0
54	MG	RA	3156	1/1	0.91	0.13	109,109,109,109	0
54	MG	YA	3946	1/1	0.91	0.11	97,97,97,97	0
54	MG	XC	301	1/1	0.91	0.07	138,138,138,138	0
54	MG	YA	3920	1/1	0.91	0.13	92,92,92,92	0
54	MG	QA	1642	1/1	0.91	0.08	131,131,131,131	0
54	MG	QA	1701	1/1	0.91	0.12	96,96,96,96	0
54	MG	XA	1632	1/1	0.91	0.07	152,152,152,152	0
54	MG	XA	1705	1/1	0.91	0.07	117,117,117,117	0
54	MG	YA	3762	1/1	0.91	0.38	90,90,90,90	0
54	MG	QA	1672	1/1	0.91	0.12	90,90,90,90	0
54	MG	RA	3181	1/1	0.91	0.18	90,90,90,90	0
54	MG	RA	3134	1/1	0.91	0.14	97,97,97,97	0
54	MG	RA	3291	1/1	0.91	0.11	138,138,138,138	0
54	MG	RA	3109	1/1	0.91	0.13	91,91,91,91	0
54	MG	YA	3926	1/1	0.91	0.10	95,95,95,95	0
54	MG	RA	3416	1/1	0.91	0.15	122,122,122,122	0
54	MG	RA	3077	1/1	0.91	0.14	96,96,96,96	0
54	MG	YA	3930	1/1	0.91	0.21	165,165,165,165	0
54	MG	RA	3281	1/1	0.91	0.50	90,90,90,90	0
54	MG	RA	3103	1/1	0.91	0.14	169,169,169,169	0
54	MG	QA	1684	1/1	0.91	0.44	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	YA	3821	1/1	0.91	0.23	90,90,90,90	0
54	MG	YA	3797	1/1	0.91	0.15	92,92,92,92	0
54	MG	YA	3676	1/1	0.91	0.14	177,177,177,177	0
54	MG	RA	3018	1/1	0.91	0.14	137,137,137,137	0
54	MG	QA	1601	1/1	0.91	0.14	93,93,93,93	0
54	MG	YA	3800	1/1	0.91	0.17	93,93,93,93	0
54	MG	XA	1726	1/1	0.91	0.29	93,93,93,93	0
54	MG	RA	3377	1/1	0.91	0.14	103,103,103,103	0
54	MG	RA	3147	1/1	0.91	0.15	94,94,94,94	0
55	ZN	Y9	101	1/1	0.91	0.07	140,140,140,140	0
54	MG	YA	3780	1/1	0.91	0.39	90,90,90,90	0
54	MG	RB	209	1/1	0.92	0.32	159,159,159,159	0
54	MG	YA	3819	1/1	0.92	0.08	90,90,90,90	0
54	MG	YA	3789	1/1	0.92	0.09	129,129,129,129	0
54	MG	RA	3124	1/1	0.92	0.20	93,93,93,93	0
54	MG	YA	3663	1/1	0.92	0.12	90,90,90,90	0
54	MG	RA	3001	1/1	0.92	0.16	90,90,90,90	0
54	MG	RA	3119	1/1	0.92	0.05	109,109,109,109	0
54	MG	RA	3272	1/1	0.92	0.26	90,90,90,90	0
54	MG	RA	3320	1/1	0.92	0.18	119,119,119,119	0
54	MG	RB	215	1/1	0.92	0.07	135,135,135,135	0
54	MG	YA	3890	1/1	0.92	0.21	90,90,90,90	0
54	MG	YA	3768	1/1	0.92	0.24	147,147,147,147	0
54	MG	YA	3892	1/1	0.92	0.19	90,90,90,90	0
54	MG	RA	3133	1/1	0.92	0.38	156,156,156,156	0
54	MG	YE	302	1/1	0.92	0.12	96,96,96,96	0
54	MG	RA	3300	1/1	0.92	0.15	139,139,139,139	0
54	MG	RA	3490	1/1	0.92	0.23	158,158,158,158	0
54	MG	YA	3804	1/1	0.92	0.35	90,90,90,90	0
54	MG	YA	3773	1/1	0.92	0.12	90,90,90,90	0
54	MG	YA	3720	1/1	0.92	0.12	90,90,90,90	0
54	MG	RA	3188	1/1	0.92	0.15	95,95,95,95	0
54	MG	YT	201	1/1	0.92	0.10	163,163,163,163	0
54	MG	YA	3748	1/1	0.92	0.15	90,90,90,90	0
54	MG	RA	3075	1/1	0.92	0.32	91,91,91,91	0
54	MG	QA	1658	1/1	0.92	0.23	90,90,90,90	0
54	MG	YY	201	1/1	0.92	0.19	90,90,90,90	0
54	MG	RA	3477	1/1	0.92	0.09	97,97,97,97	0
54	MG	YA	3701	1/1	0.92	0.39	90,90,90,90	0
54	MG	XM	201	1/1	0.92	0.10	180,180,180,180	0
54	MG	RA	3261	1/1	0.92	0.24	93,93,93,93	0
54	MG	RA	3371	1/1	0.92	0.06	144,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	RA	3372	1/1	0.92	0.12	130,130,130,130	0
54	MG	QD	304	1/1	0.92	0.06	142,142,142,142	0
54	MG	YA	3940	1/1	0.92	0.17	90,90,90,90	0
54	MG	YA	3602	1/1	0.92	0.16	132,132,132,132	0
54	MG	YA	3708	1/1	0.92	0.23	90,90,90,90	0
54	MG	YA	3786	1/1	0.92	0.14	101,101,101,101	0
54	MG	RA	3167	1/1	0.93	0.08	98,98,98,98	0
54	MG	RA	3493	1/1	0.93	0.08	90,90,90,90	0
54	MG	YE	305	1/1	0.93	0.27	90,90,90,90	0
54	MG	RA	3354	1/1	0.93	0.18	138,138,138,138	0
54	MG	RA	3128	1/1	0.93	0.14	131,131,131,131	0
54	MG	RA	3407	1/1	0.93	0.11	130,130,130,130	0
54	MG	YA	3684	1/1	0.93	0.28	90,90,90,90	0
54	MG	XA	1615	1/1	0.93	0.14	94,94,94,94	0
54	MG	RA	3473	1/1	0.93	0.08	90,90,90,90	0
54	MG	RA	3523	1/1	0.93	0.21	91,91,91,91	0
54	MG	YA	3633	1/1	0.93	0.08	90,90,90,90	0
54	MG	RA	3327	1/1	0.93	0.05	94,94,94,94	0
54	MG	RA	3410	1/1	0.93	0.19	97,97,97,97	0
54	MG	XA	1621	1/1	0.93	0.14	184,184,184,184	0
54	MG	RA	3197	1/1	0.93	0.19	95,95,95,95	0
54	MG	RA	3095	1/1	0.93	0.14	91,91,91,91	0
54	MG	RA	3234	1/1	0.93	0.38	90,90,90,90	0
54	MG	YA	3911	1/1	0.93	0.45	90,90,90,90	0
54	MG	RA	3529	1/1	0.93	0.27	106,106,106,106	0
54	MG	RA	3226	1/1	0.93	0.15	90,90,90,90	0
54	MG	RA	3317	1/1	0.93	0.14	92,92,92,92	0
54	MG	XA	1671	1/1	0.93	0.08	95,95,95,95	0
54	MG	RA	3533	1/1	0.93	0.17	95,95,95,95	0
54	MG	YA	3702	1/1	0.93	0.11	98,98,98,98	0
54	MG	YA	3733	1/1	0.93	0.11	90,90,90,90	0
54	MG	RA	3333	1/1	0.93	0.32	90,90,90,90	0
54	MG	YA	3952	1/1	0.93	0.07	97,97,97,97	0
54	MG	RA	3284	1/1	0.93	0.11	91,91,91,91	0
54	MG	YA	3830	1/1	0.93	0.11	95,95,95,95	0
54	MG	RA	3218	1/1	0.93	0.05	90,90,90,90	0
54	MG	RA	3307	1/1	0.93	0.17	126,126,126,126	0
54	MG	XA	1639	1/1	0.93	0.11	96,96,96,96	0
54	MG	RA	3443	1/1	0.93	0.05	109,109,109,109	0
54	MG	YD	303	1/1	0.93	0.12	99,99,99,99	0
54	MG	XA	1642	1/1	0.93	0.13	161,161,161,161	0
54	MG	RA	3170	1/1	0.93	0.12	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	XA	1605	1/1	0.93	0.12	123,123,123,123	0
54	MG	YA	3802	1/1	0.93	0.20	90,90,90,90	0
55	ZN	QD	301	1/1	0.93	0.07	131,131,131,131	0
54	MG	RA	3127	1/1	0.93	0.15	153,153,153,153	0
54	MG	XA	1695	1/1	0.94	0.37	90,90,90,90	0
54	MG	YA	3691	1/1	0.94	0.07	94,94,94,94	0
54	MG	RA	3540	1/1	0.94	0.05	96,96,96,96	0
54	MG	RA	3142	1/1	0.94	0.38	140,140,140,140	0
54	MG	RT	203	1/1	0.94	0.07	162,162,162,162	0
54	MG	YA	3820	1/1	0.94	0.43	90,90,90,90	0
54	MG	RA	3154	1/1	0.94	0.20	90,90,90,90	0
54	MG	YA	3822	1/1	0.94	0.46	90,90,90,90	0
54	MG	RA	3067	1/1	0.94	0.13	148,148,148,148	0
54	MG	RX	102	1/1	0.94	0.07	97,97,97,97	0
54	MG	XA	1630	1/1	0.94	0.10	127,127,127,127	0
54	MG	YA	3729	1/1	0.94	0.13	106,106,106,106	0
54	MG	RA	3108	1/1	0.94	0.05	94,94,94,94	0
54	MG	RA	3140	1/1	0.94	0.12	183,183,183,183	0
54	MG	RA	3190	1/1	0.94	0.09	148,148,148,148	0
54	MG	RA	3511	1/1	0.94	0.32	121,121,121,121	0
54	MG	QA	1602	1/1	0.94	0.16	90,90,90,90	0
54	MG	RA	3476	1/1	0.94	0.07	96,96,96,96	0
54	MG	RA	3208	1/1	0.94	0.07	94,94,94,94	0
54	MG	RA	3552	1/1	0.94	0.17	160,160,160,160	0
54	MG	YA	3834	1/1	0.94	0.07	97,97,97,97	0
54	MG	QA	1712	1/1	0.94	0.05	136,136,136,136	0
54	MG	RA	3514	1/1	0.94	0.17	125,125,125,125	0
54	MG	RA	3374	1/1	0.94	0.36	144,144,144,144	0
54	MG	RA	3375	1/1	0.94	0.12	136,136,136,136	0
54	MG	RA	3089	1/1	0.94	0.16	94,94,94,94	0
54	MG	RD	302	1/1	0.94	0.07	98,98,98,98	0
54	MG	YA	3627	1/1	0.94	0.42	90,90,90,90	0
54	MG	RA	3184	1/1	0.94	0.36	90,90,90,90	0
54	MG	RD	304	1/1	0.94	0.24	125,125,125,125	0
54	MG	YU	201	1/1	0.94	0.11	122,122,122,122	0
54	MG	RA	3483	1/1	0.94	0.07	90,90,90,90	0
54	MG	YA	3631	1/1	0.94	0.46	90,90,90,90	0
54	MG	RA	3325	1/1	0.94	0.12	93,93,93,93	0
54	MG	YA	3688	1/1	0.94	0.23	190,190,190,190	0
54	MG	RA	3420	1/1	0.94	0.20	126,126,126,126	0
55	ZN	XD	301	1/1	0.94	0.09	90,90,90,90	0
54	MG	R8	101	1/1	0.95	0.05	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	YA	3764	1/1	0.95	0.13	90,90,90,90	0
54	MG	RA	3008	1/1	0.95	0.13	118,118,118,118	0
54	MG	RA	3379	1/1	0.95	0.06	149,149,149,149	0
54	MG	YA	3674	1/1	0.95	0.05	130,130,130,130	0
54	MG	RA	3046	1/1	0.95	0.08	120,120,120,120	0
54	MG	RA	3532	1/1	0.95	0.07	133,133,133,133	0
54	MG	YA	3770	1/1	0.95	0.13	98,98,98,98	0
54	MG	YA	3694	1/1	0.95	0.10	101,101,101,101	0
54	MG	RA	3092	1/1	0.95	0.53	90,90,90,90	0
54	MG	YA	3660	1/1	0.95	0.27	90,90,90,90	0
54	MG	YA	3951	1/1	0.95	0.07	90,90,90,90	0
54	MG	RA	3556	1/1	0.95	0.05	96,96,96,96	0
54	MG	YA	3928	1/1	0.95	0.20	90,90,90,90	0
54	MG	RQ	202	1/1	0.95	0.10	134,134,134,134	0
54	MG	RA	3496	1/1	0.95	0.12	128,128,128,128	0
54	MG	YB	203	1/1	0.95	0.31	117,117,117,117	0
54	MG	YA	3777	1/1	0.95	0.09	120,120,120,120	0
54	MG	Y8	101	1/1	0.95	0.04	102,102,102,102	0
54	MG	YA	3957	1/1	0.95	0.46	112,112,112,112	0
54	MG	YA	3887	1/1	0.95	0.11	90,90,90,90	0
54	MG	YA	3757	1/1	0.95	0.22	132,132,132,132	0
54	MG	RA	3435	1/1	0.95	0.04	98,98,98,98	0
54	MG	QA	1619	1/1	0.95	0.09	153,153,153,153	0
54	MG	XA	1661	1/1	0.95	0.19	136,136,136,136	0
54	MG	RA	3194	1/1	0.95	0.12	90,90,90,90	0
54	MG	RA	3480	1/1	0.95	0.08	94,94,94,94	0
54	MG	RA	3459	1/1	0.95	0.08	125,125,125,125	0
54	MG	YA	3624	1/1	0.95	0.22	90,90,90,90	0
54	MG	QA	1624	1/1	0.95	0.13	147,147,147,147	0
54	MG	QA	1683	1/1	0.95	0.06	102,102,102,102	0
54	MG	YA	3751	1/1	0.96	0.11	90,90,90,90	0
54	MG	YA	3971	1/1	0.96	0.04	95,95,95,95	0
54	MG	RA	3421	1/1	0.96	0.29	178,178,178,178	0
54	MG	RA	3422	1/1	0.96	0.10	142,142,142,142	0
54	MG	YA	3689	1/1	0.96	0.17	90,90,90,90	0
54	MG	YA	3705	1/1	0.96	0.23	123,123,123,123	0
54	MG	RA	3456	1/1	0.96	0.05	93,93,93,93	0
54	MG	RA	3423	1/1	0.96	0.19	152,152,152,152	0
54	MG	YA	3939	1/1	0.96	0.14	92,92,92,92	0
54	MG	RA	3139	1/1	0.96	0.05	122,122,122,122	0
54	MG	RA	3326	1/1	0.96	0.11	113,113,113,113	0
54	MG	RA	3165	1/1	0.96	0.09	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	RA	3013	1/1	0.96	0.05	144,144,144,144	0
54	MG	RA	3401	1/1	0.96	0.07	157,157,157,157	0
54	MG	YA	3728	1/1	0.96	0.10	119,119,119,119	0
54	MG	RA	3150	1/1	0.96	0.09	94,94,94,94	0
54	MG	YA	3656	1/1	0.96	0.07	95,95,95,95	0
54	MG	RA	3054	1/1	0.96	0.15	98,98,98,98	0
54	MG	YA	3803	1/1	0.96	0.12	90,90,90,90	0
54	MG	RA	3559	1/1	0.96	0.61	173,173,173,173	0
54	MG	RB	201	1/1	0.97	0.16	127,127,127,127	0
54	MG	RA	3243	1/1	0.97	0.11	100,100,100,100	0
54	MG	RA	3094	1/1	0.97	0.10	95,95,95,95	0
54	MG	XA	1693	1/1	0.97	0.08	90,90,90,90	0
54	MG	YA	3730	1/1	0.97	0.31	188,188,188,188	0
54	MG	RA	3432	1/1	0.97	0.04	134,134,134,134	0
54	MG	RA	3408	1/1	0.97	0.19	90,90,90,90	0
54	MG	RA	3068	1/1	0.97	0.08	145,145,145,145	0
54	MG	RA	3102	1/1	0.97	0.07	148,148,148,148	0
54	MG	RA	3502	1/1	0.97	0.11	133,133,133,133	0
54	MG	QA	1702	1/1	0.97	0.09	141,141,141,141	0
54	MG	RA	3455	1/1	0.97	0.12	90,90,90,90	0
54	MG	RA	3445	1/1	0.97	0.13	175,175,175,175	0
54	MG	XA	1724	1/1	0.97	0.07	114,114,114,114	0
54	MG	RA	3402	1/1	0.97	0.22	101,101,101,101	0
54	MG	RA	3287	1/1	0.97	0.06	150,150,150,150	0
54	MG	XA	1643	1/1	0.97	0.05	133,133,133,133	0
54	MG	RA	3494	1/1	0.97	0.05	90,90,90,90	0
54	MG	YA	3695	1/1	0.97	0.11	91,91,91,91	0
54	MG	YA	3825	1/1	0.97	0.09	117,117,117,117	0
54	MG	QA	1710	1/1	0.97	0.07	120,120,120,120	0
54	MG	RA	3012	1/1	0.97	0.14	112,112,112,112	0
54	MG	YA	3740	1/1	0.98	0.06	101,101,101,101	0
54	MG	YA	3792	1/1	0.98	0.09	124,124,124,124	0
54	MG	RA	3404	1/1	0.98	0.04	124,124,124,124	0
54	MG	RA	3311	1/1	0.98	0.04	99,99,99,99	0
54	MG	YA	3661	1/1	0.98	0.28	135,135,135,135	0
54	MG	RA	3458	1/1	0.98	0.12	160,160,160,160	0
54	MG	RA	3225	1/1	0.98	0.07	142,142,142,142	0
54	MG	RA	3065	1/1	0.98	0.16	121,121,121,121	0
54	MG	RA	3547	1/1	0.98	0.04	99,99,99,99	0
54	MG	YA	3788	1/1	0.98	0.24	110,110,110,110	0
54	MG	RA	3548	1/1	0.98	0.04	103,103,103,103	0
54	MG	YA	3667	1/1	0.98	0.06	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	QA	1607	1/1	0.99	0.05	115,115,115,115	0
54	MG	RA	3236	1/1	0.99	0.04	98,98,98,98	0
54	MG	RA	3491	1/1	0.99	0.03	97,97,97,97	0
54	MG	RA	3235	1/1	0.99	0.04	104,104,104,104	0
54	MG	XA	1667	1/1	0.99	0.04	159,159,159,159	0

5.5 Other polymers [i](#)

There are no such residues in this entry.