



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 19, 2026 – 03:39 PM UTC

PDB ID : 6OXA / pdb_00006oxa
Title : Dimeric E.coli YoeB bound to Thermus thermophilus 70S pre-cleavage (AAU)
Authors : Pavelich, I.J.; Hoffer, E.D.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2019-05-13
Resolution : 3.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

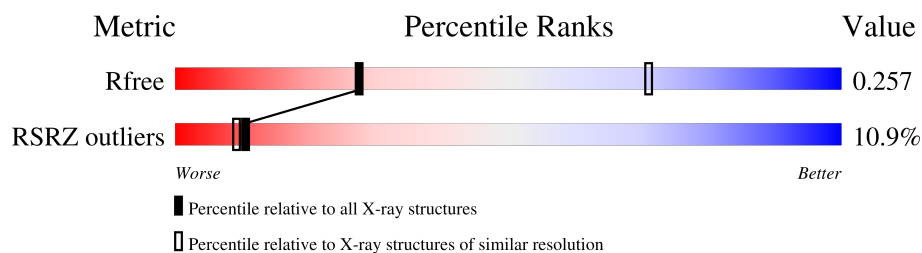
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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
57	MG	QA	1637	-	-	-	X
57	MG	RA	3001	-	-	-	X
57	MG	RA	3126	-	-	-	X
57	MG	RQ	201	-	-	-	X
57	MG	XA	1710	-	-	-	X
57	MG	XD	302	-	-	-	X
57	MG	YA	3096	-	-	-	X
57	MG	YD	302	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 298432 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 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1510	Total	C	N	O	P	0	0	0
			32452	14444	6009	10489	1510			
1	XA	1507	Total	C	N	O	P	0	0	0
			32389	14416	5999	10467	1507			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	235	Total	C	N	O	S	0	0	0
			1907	1217	342	343	5			
2	XB	236	Total	C	N	O	S	0	0	0
			1915	1223	343	344	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	QC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	XC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			
8	XH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	QI	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	XI	126	Total	C	N	O		0	0	0
			998	633	193	172				

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	XJ	96	Total	C	N	O	S	0	0	0
			777	487	153	136	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	XK	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	QM	120	Total	C	N	O	S	0	0	0
			955	591	197	165	2			
12	XM	119	Total	C	N	O	S	0	0	0
			946	585	195	164	2			

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
14	XO	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 15 is a protein called 30S ribosomal protein S16.

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

- Molecule 16 is a protein called 30S ribosomal protein S17.

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

- Molecule 17 is a protein called 30S ribosomal protein S18.

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

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
18	XS	83	Total	C	N	O	S	0	0	0
			656	418	123	113	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

- Molecule 20 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	QU	25	Total	C	N	O	0	0	0
			217	134	52	31			
20	XU	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 21 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	QV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
21	QW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
21	XV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
21	XW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QX	20	Total	C	N	O	P	0	0	0
			435	198	87	131	19			
22	XX	20	Total	C	N	O	P	0	0	0
			435	198	87	131	19			

- Molecule 23 is a protein called Addiction module toxin, Txe/YoeB family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QY	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
23	QZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
23	XY	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
23	XZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			
24	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 26 is a protein called 50S ribosomal protein L30.

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

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			
27	Y4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
28	Y5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
29	Y6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	R7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
30	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

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

- Molecule 32 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	RA	2891	Total	C	N	O	P	0	0	0
			62266	27713	11649	20014	2890			
32	YA	2875	Total	C	N	O	P	0	0	0
			61921	27560	11583	19904	2874			

- Molecule 33 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	RB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			
33	YB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			

- Molecule 34 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
34	YD	274	Total	C	N	O	S	0	0	0
			2135	1347	426	359	3			

- Molecule 35 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
35	YE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 36 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
36	YG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 37 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
37	YH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 38 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
38	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 39 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
39	YN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 40 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
40	YO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 41 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	YP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 42 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
42	YQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 43 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RR	117	Total	C	N	O		0	0	0
			960	599	202	159				
43	YR	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 44 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RS	111	Total	C	N	O		0	0	0
			882	556	176	150				
44	YS	111	Total	C	N	O		0	0	0
			882	556	176	150				

- Molecule 45 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
45	YT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 46 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	RU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
46	YU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 47 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	RV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
47	YV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 48 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	RW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
48	YW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 49 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	RX	92	Total	C	N	O	0	0	0
			725	471	131	123			
49	YX	92	Total	C	N	O	0	0	0
			725	471	131	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	RY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			
50	YY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			

- Molecule 51 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	XL	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			
51	QL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 52 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	Y1	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			
52	R1	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			

- Molecule 53 is a protein called 50S ribosomal protein L35.

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

- Molecule 54 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	YF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
54	RF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 55 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			
55	YZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

- Molecule 56 is a RNA chain called CCPuro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	ZA	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
56	ZB	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	94	Total	Mg	0	0
			94	94		

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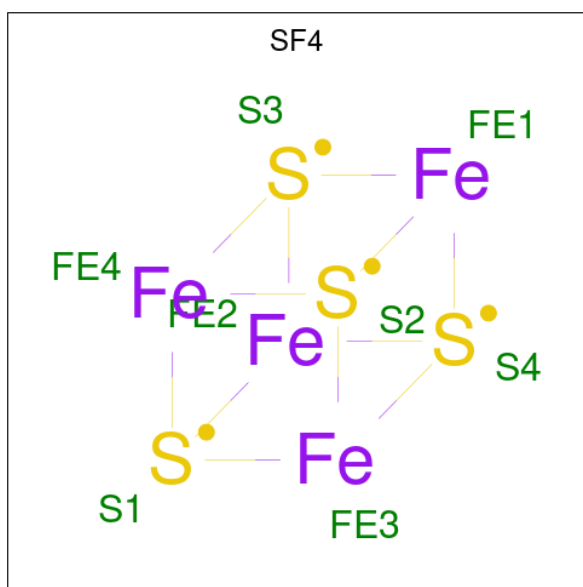
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QD	2	Total 2	Mg 2	0	0
57	QE	1	Total 1	Mg 1	0	0
57	QF	1	Total 1	Mg 1	0	0
57	QV	3	Total 3	Mg 3	0	0
57	QX	1	Total 1	Mg 1	0	0
57	R0	1	Total 1	Mg 1	0	0
57	RA	302	Total 302	Mg 302	0	0
57	RB	3	Total 3	Mg 3	0	0
57	RD	1	Total 1	Mg 1	0	0
57	RE	1	Total 1	Mg 1	0	0
57	RN	1	Total 1	Mg 1	0	0
57	RO	1	Total 1	Mg 1	0	0
57	RP	2	Total 2	Mg 2	0	0
57	RQ	2	Total 2	Mg 2	0	0
57	RR	2	Total 2	Mg 2	0	0
57	RY	1	Total 1	Mg 1	0	0
57	XA	116	Total 116	Mg 116	0	0
57	XD	1	Total 1	Mg 1	0	0
57	XE	1	Total 1	Mg 1	0	0
57	XF	1	Total 1	Mg 1	0	0
57	XL	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	XM	1	Total 1	Mg 1	0	0
57	XV	3	Total 3	Mg 3	0	0
57	Y0	2	Total 2	Mg 2	0	0
57	Y3	1	Total 1	Mg 1	0	0
57	Y9	1	Total 1	Mg 1	0	0
57	YA	326	Total 326	Mg 326	0	0
57	YB	5	Total 5	Mg 5	0	0
57	YF	1	Total 1	Mg 1	0	0
57	YG	1	Total 1	Mg 1	0	0
57	YO	1	Total 1	Mg 1	0	0
57	YD	5	Total 5	Mg 5	0	0
57	YQ	3	Total 3	Mg 3	0	0
57	YV	1	Total 1	Mg 1	0	0
57	YE	5	Total 5	Mg 5	0	0
57	R8	1	Total 1	Mg 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	QD	1	Total	Fe	S	0	0
			8	4	4		
58	XD	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	QN	1	Total	Zn	0	0
			1	1		
59	R4	1	Total	Zn	0	0
			1	1		
59	R5	1	Total	Zn	0	0
			1	1		
59	R6	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		
59	Y4	1	Total	Zn	0	0
			1	1		
59	Y6	1	Total	Zn	0	0
			1	1		

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

3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	212.79Å 453.08Å 608.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.59 – 3.25 146.59 – 3.25	Depositor EDS
% Data completeness (in resolution range)	93.4 (146.59-3.25) 93.4 (146.59-3.25)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.229 , 0.256 0.230 , 0.257	Depositor DCC
R_{free} test set	41088 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 75.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	298432	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.35% 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](#)

8 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	$\# Z > 2$
22	OMU	QX	21	1,22	19,22,23	1.81	4 (21%)	25,31,34	2.19	9 (36%)
56	PPU	ZB	76	56,32	37,40,41	1.20	5 (13%)	47,57,60	2.08	13 (27%)
22	A2M	XX	20	22	22,25,26	1.48	5 (22%)	30,36,39	2.10	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PPU	ZA	76	56,32	37,40,41	1.61	7 (18%)	47,57,60	2.23	16 (34%)
22	A2M	QX	20	22	22,25,26	1.55	4 (18%)	30,36,39	2.06	6 (20%)
22	A2M	QX	19	22	22,25,26	1.54	4 (18%)	30,36,39	2.12	10 (33%)
22	A2M	XX	19	22	22,25,26	1.47	5 (22%)	30,36,39	2.10	10 (33%)
22	OMU	XX	21	1,22	19,22,23	1.23	3 (15%)	25,31,34	1.80	5 (20%)

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
22	OMU	QX	21	1,22	-	2/9/27/28	0/2/2/2
56	PPU	ZB	76	56,32	-	6/25/43/44	0/4/4/4
22	A2M	XX	20	22	-	2/9/27/28	0/3/3/3
56	PPU	ZA	76	56,32	-	4/25/43/44	0/4/4/4
22	A2M	QX	20	22	-	1/9/27/28	0/3/3/3
22	A2M	QX	19	22	-	0/9/27/28	0/3/3/3
22	A2M	XX	19	22	-	2/9/27/28	0/3/3/3
22	OMU	XX	21	1,22	-	2/9/27/28	0/2/2/2

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QX	20	A2M	C5-C4	4.86	1.47	1.39
22	QX	19	A2M	C5-C4	4.82	1.47	1.39
22	XX	20	A2M	C5-C4	4.40	1.46	1.39
22	XX	19	A2M	C5-C4	4.35	1.46	1.39
56	ZB	76	PPU	C5-C4	4.33	1.46	1.39

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	QX	20	A2M	C5-C4-N3	-6.40	117.91	126.72
22	XX	20	A2M	C5-C4-N3	-6.08	118.34	126.72
22	QX	19	A2M	C5-C4-N3	-5.90	118.60	126.72
56	ZB	76	PPU	C5-C4-N3	-5.83	118.69	126.72
22	XX	19	A2M	C5-C4-N3	-5.57	119.05	126.72

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	XX	21	OMU	C3'-C4'-C5'-O5'
22	XX	21	OMU	O4'-C4'-C5'-O5'
56	ZA	76	PPU	C4'-C3'-N3'-C
56	ZB	76	PPU	C5-C6-N6-C10
22	QX	21	OMU	O4'-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 906 ligands modelled in this entry, 904 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	SF4	XD	301	4	0,12,12	-	-	-		
58	SF4	QD	301	4	0,12,12	-	-	-		

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
58	SF4	XD	301	4	-	-	0/6/5/5
58	SF4	QD	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1510/1521 (99%)	0.23	41 (2%) 56 38	44, 86, 196, 383	0
1	XA	1507/1521 (99%)	0.09	40 (2%) 56 38	34, 75, 177, 475	0
2	QB	235/256 (91%)	0.84	21 (8%) 15 12	58, 118, 181, 243	0
2	XB	236/256 (92%)	0.98	30 (12%) 8 6	53, 108, 176, 224	0
3	QC	205/239 (85%)	1.00	18 (8%) 15 12	67, 114, 167, 195	0
3	XC	205/239 (85%)	0.70	8 (3%) 43 29	51, 88, 139, 192	0
4	QD	208/209 (99%)	1.02	29 (13%) 6 5	44, 79, 119, 165	0
4	XD	208/209 (99%)	1.09	35 (16%) 4 4	42, 78, 119, 205	0
5	QE	151/162 (93%)	1.09	20 (13%) 7 6	45, 79, 122, 166	0
5	XE	151/162 (93%)	0.79	12 (7%) 18 14	39, 70, 119, 208	0
6	QF	101/101 (100%)	0.79	4 (3%) 42 28	53, 90, 121, 159	0
6	XF	101/101 (100%)	0.87	12 (11%) 9 8	44, 82, 116, 238	0
7	QG	155/156 (99%)	1.18	27 (17%) 4 4	76, 113, 152, 223	0
7	XG	155/156 (99%)	1.29	35 (22%) 2 2	58, 98, 152, 174	0
8	QH	137/138 (99%)	1.14	22 (16%) 4 4	48, 83, 119, 136	0
8	XH	137/138 (99%)	0.83	13 (9%) 14 11	40, 79, 119, 154	0
9	QI	127/128 (99%)	1.34	28 (22%) 2 2	80, 133, 168, 206	0
9	XI	126/128 (98%)	1.55	29 (23%) 2 2	60, 110, 158, 181	0
10	QJ	99/105 (94%)	1.88	37 (37%) 1 1	88, 136, 195, 218	0
10	XJ	96/105 (91%)	1.41	21 (21%) 2 2	62, 122, 189, 238	0
11	QK	119/129 (92%)	1.31	26 (21%) 2 2	41, 93, 148, 208	0
11	XK	116/129 (89%)	1.07	16 (13%) 6 5	46, 80, 122, 180	0
12	QM	120/126 (95%)	1.49	29 (24%) 2 2	67, 119, 180, 215	0
12	XM	119/126 (94%)	1.30	28 (23%) 2 2	55, 99, 146, 265	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QN	60/61 (98%)	2.09	24 (40%) 1 1	66, 114, 161, 194	0
13	XN	60/61 (98%)	1.42	17 (28%) 1 1	57, 91, 132, 201	0
14	QO	88/89 (98%)	0.99	10 (11%) 10 9	49, 87, 131, 146	0
14	XO	87/89 (97%)	0.64	3 (3%) 48 32	47, 75, 122, 143	0
15	QP	84/88 (95%)	0.98	7 (8%) 17 13	50, 79, 125, 202	0
15	XP	84/88 (95%)	1.02	9 (10%) 11 9	51, 80, 121, 198	0
16	QQ	100/105 (95%)	1.13	16 (16%) 5 4	51, 78, 118, 144	0
16	XQ	100/105 (95%)	0.74	8 (8%) 18 14	49, 81, 109, 143	0
17	QR	70/88 (79%)	0.84	6 (8%) 16 13	56, 95, 138, 180	0
17	XR	70/88 (79%)	0.68	4 (5%) 29 20	39, 76, 125, 148	0
18	QS	83/93 (89%)	1.85	32 (38%) 1 1	87, 133, 189, 224	0
18	XS	83/93 (89%)	1.03	12 (14%) 6 5	64, 96, 157, 174	0
19	QT	99/106 (93%)	1.32	19 (19%) 3 3	61, 96, 160, 220	0
19	XT	99/106 (93%)	1.41	24 (24%) 2 2	55, 93, 163, 203	0
20	QU	25/27 (92%)	2.41	12 (48%) 0 0	86, 117, 154, 187	0
20	XU	25/27 (92%)	2.55	12 (48%) 0 0	73, 104, 134, 150	0
21	QV	77/77 (100%)	0.15	3 (3%) 43 29	49, 95, 154, 202	0
21	QW	77/77 (100%)	1.20	9 (11%) 9 8	68, 198, 300, 360	0
21	XV	77/77 (100%)	0.06	2 (2%) 57 38	40, 81, 134, 208	0
21	XW	77/77 (100%)	1.10	13 (16%) 4 4	78, 237, 321, 383	0
22	QX	17/22 (77%)	1.97	8 (47%) 0 0	55, 210, 302, 312	0
22	XX	17/22 (77%)	2.67	12 (70%) 0 0	47, 206, 295, 330	0
23	QY	84/84 (100%)	1.27	17 (20%) 3 2	49, 83, 128, 162	0
23	QZ	84/84 (100%)	0.68	5 (5%) 27 19	73, 122, 172, 216	0
23	XY	84/84 (100%)	1.03	11 (13%) 7 6	36, 70, 108, 121	0
23	XZ	84/84 (100%)	1.07	12 (14%) 6 5	69, 108, 153, 213	0
24	R0	81/85 (95%)	1.26	15 (18%) 3 3	45, 66, 98, 144	0
24	Y0	82/85 (96%)	1.34	21 (25%) 1 2	38, 63, 105, 111	0
25	R2	69/72 (95%)	0.84	6 (8%) 16 12	38, 89, 166, 200	0
25	Y2	69/72 (95%)	1.08	12 (17%) 4 4	39, 71, 125, 264	0
26	R3	59/60 (98%)	1.13	9 (15%) 5 5	44, 72, 125, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
26	Y3	59/60 (98%)	1.08	9 (15%) 5 5	44, 74, 122, 162	0
27	R4	69/71 (97%)	1.90	27 (39%) 1 1	106, 159, 243, 324	0
27	Y4	69/71 (97%)	1.07	13 (18%) 3 3	82, 133, 191, 238	0
28	R5	59/60 (98%)	0.75	2 (3%) 48 32	35, 66, 139, 176	0
28	Y5	59/60 (98%)	1.44	14 (23%) 2 2	28, 76, 152, 166	0
29	R6	53/54 (98%)	1.40	14 (26%) 1 1	74, 109, 153, 159	0
29	Y6	53/54 (98%)	0.96	6 (11%) 10 9	71, 97, 153, 195	0
30	R7	47/49 (95%)	0.73	6 (12%) 7 6	27, 46, 79, 139	0
30	Y7	48/49 (97%)	0.87	5 (10%) 11 9	25, 43, 112, 140	0
31	R9	37/37 (100%)	1.88	14 (37%) 1 1	87, 124, 155, 209	0
31	Y9	37/37 (100%)	1.56	10 (27%) 1 1	75, 116, 153, 158	0
32	RA	2891/2915 (99%)	0.01	78 (2%) 56 38	24, 63, 207, 475	0
32	YA	2875/2915 (98%)	-0.06	62 (2%) 62 43	19, 58, 247, 435	0
33	RB	120/124 (96%)	0.39	3 (2%) 58 39	58, 103, 141, 194	0
33	YB	120/124 (96%)	0.14	2 (1%) 69 50	57, 83, 120, 191	0
34	RD	272/276 (98%)	1.11	43 (15%) 5 4	26, 62, 110, 239	0
34	YD	274/276 (99%)	0.57	16 (5%) 29 19	13, 44, 80, 120	0
35	RE	205/206 (99%)	1.33	47 (22%) 2 2	31, 79, 154, 219	0
35	YE	204/206 (99%)	0.90	19 (9%) 14 11	31, 67, 122, 155	0
36	RG	181/182 (99%)	1.35	40 (22%) 2 2	72, 113, 153, 188	0
36	YG	181/182 (99%)	0.99	18 (9%) 13 10	53, 98, 147, 195	0
37	RH	174/180 (96%)	1.62	51 (29%) 1 1	94, 147, 219, 276	0
37	YH	174/180 (96%)	1.63	49 (28%) 1 1	60, 124, 195, 262	0
38	RI	146/148 (98%)	1.83	54 (36%) 1 1	59, 115, 160, 186	0
38	YI	146/148 (98%)	1.53	40 (27%) 1 1	44, 98, 151, 201	0
39	RN	138/140 (98%)	1.71	45 (32%) 1 1	46, 80, 138, 218	0
39	YN	138/140 (98%)	1.39	32 (23%) 2 2	47, 81, 138, 181	0
40	RO	122/122 (100%)	0.87	9 (7%) 20 15	35, 72, 107, 130	0
40	YO	122/122 (100%)	0.64	6 (4%) 35 23	34, 61, 91, 120	0
41	RP	150/150 (100%)	1.25	32 (21%) 2 2	30, 77, 140, 258	0
41	YP	149/150 (99%)	0.94	19 (12%) 7 6	33, 61, 103, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
42	RQ	141/141 (100%)	1.64	43 (30%) 1 1	37, 80, 141, 230	0
42	YQ	141/141 (100%)	0.73	8 (5%) 29 20	37, 69, 110, 233	0
43	RR	117/118 (99%)	0.80	8 (6%) 23 16	38, 68, 106, 164	0
43	YR	117/118 (99%)	1.29	17 (14%) 6 5	41, 65, 107, 161	0
44	RS	111/112 (99%)	1.54	34 (30%) 1 1	64, 107, 160, 226	0
44	YS	111/112 (99%)	1.32	24 (21%) 2 2	46, 78, 123, 204	0
45	RT	137/146 (93%)	1.35	30 (21%) 2 2	53, 85, 141, 206	0
45	YT	137/146 (93%)	1.02	20 (14%) 6 5	40, 79, 148, 229	0
46	RU	117/118 (99%)	1.02	18 (15%) 5 5	30, 62, 123, 192	0
46	YU	117/118 (99%)	1.10	17 (14%) 6 5	36, 69, 117, 168	0
47	RV	101/101 (100%)	1.28	26 (25%) 1 1	37, 79, 138, 251	0
47	YV	101/101 (100%)	1.50	28 (27%) 1 1	33, 86, 143, 218	0
48	RW	113/113 (100%)	0.59	8 (7%) 22 16	31, 58, 112, 209	0
48	YW	113/113 (100%)	0.65	9 (7%) 18 14	34, 62, 122, 209	0
49	RX	92/96 (95%)	1.06	13 (14%) 6 5	37, 72, 114, 146	0
49	YX	92/96 (95%)	0.63	6 (6%) 25 17	31, 62, 99, 125	0
50	RY	107/110 (97%)	1.72	36 (33%) 1 1	39, 84, 133, 166	0
50	YY	107/110 (97%)	1.19	18 (16%) 4 4	35, 92, 141, 173	0
51	QL	125/132 (94%)	1.20	25 (20%) 3 2	44, 74, 124, 180	0
51	XL	122/132 (92%)	0.85	19 (15%) 5 4	32, 64, 102, 125	0
52	R1	94/98 (95%)	1.86	41 (43%) 0 1	32, 76, 156, 196	0
52	Y1	93/98 (94%)	1.50	25 (26%) 1 1	29, 57, 118, 129	0
53	R8	64/65 (98%)	1.12	11 (17%) 4 4	35, 58, 105, 158	0
53	Y8	64/65 (98%)	1.71	25 (39%) 1 1	35, 63, 100, 210	0
54	RF	202/210 (96%)	0.69	18 (8%) 15 12	24, 57, 114, 193	0
54	YF	202/210 (96%)	0.76	16 (7%) 18 14	25, 64, 135, 185	0
55	RZ	183/206 (88%)	1.15	26 (14%) 6 5	65, 111, 154, 191	0
55	YZ	183/206 (88%)	1.08	21 (11%) 9 8	59, 102, 146, 177	0
56	ZA	2/3 (66%)	-0.06	0 100 100	47, 47, 47, 49	0
56	ZB	2/3 (66%)	0.38	0 100 100	54, 54, 54, 63	0
All	All	21359/21942 (97%)	0.67	2326 (10%) 10 9	13, 79, 174, 475	0

The worst 5 of 2326 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	QK	129	SER	10.4
34	RD	34	VAL	9.4
38	YI	15	VAL	8.8
27	R4	24	THR	8.7
37	YH	17	VAL	8.5

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
22	OMU	QX	21	21/22	0.91	0.15	41,76,85,86	0
22	A2M	XX	19	23/24	0.92	0.14	65,85,93,95	0
22	A2M	QX	20	23/24	0.92	0.12	71,74,83,87	0
22	A2M	QX	19	23/24	0.92	0.16	55,86,89,89	0
56	PPU	ZA	76	37/38	0.94	0.14	38,63,68,70	0
56	PPU	ZB	76	37/38	0.94	0.12	42,50,59,64	0
22	A2M	XX	20	23/24	0.95	0.10	60,66,73,77	0
22	OMU	XX	21	21/22	0.95	0.11	66,73,83,96	0

5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
57	MG	RQ	201	1/1	-0.29	0.50	181,181,181,181	0
57	MG	QA	1617	1/1	-0.09	0.27	71,71,71,71	0
57	MG	YA	3180	1/1	-0.06	0.37	105,105,105,105	0
57	MG	YA	3108	1/1	0.10	0.24	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3058	1/1	0.10	0.23	98,98,98,98	0
57	MG	YA	3164	1/1	0.12	0.22	64,64,64,64	0
57	MG	YA	3184	1/1	0.15	0.30	84,84,84,84	0
57	MG	RA	3074	1/1	0.16	0.31	55,55,55,55	0
57	MG	RA	3126	1/1	0.25	0.41	57,57,57,57	0
57	MG	XA	1634	1/1	0.27	0.22	51,51,51,51	0
57	MG	RA	3174	1/1	0.30	0.39	88,88,88,88	0
57	MG	YA	3170	1/1	0.30	0.22	50,50,50,50	0
57	MG	YA	3096	1/1	0.32	0.41	94,94,94,94	0
57	MG	QA	1604	1/1	0.36	0.28	97,97,97,97	0
57	MG	YA	3154	1/1	0.37	0.15	80,80,80,80	0
57	MG	YA	3159	1/1	0.37	0.32	91,91,91,91	0
57	MG	XA	1603	1/1	0.38	0.31	51,51,51,51	0
57	MG	XA	1614	1/1	0.38	0.27	36,36,36,36	0
57	MG	RA	3111	1/1	0.42	0.18	70,70,70,70	0
57	MG	QA	1637	1/1	0.43	0.48	104,104,104,104	0
57	MG	RA	3170	1/1	0.44	0.19	38,38,38,38	0
57	MG	R0	101	1/1	0.45	0.31	58,58,58,58	0
57	MG	RA	3050	1/1	0.45	0.26	30,30,30,30	0
57	MG	RY	201	1/1	0.48	0.38	59,59,59,59	0
57	MG	YA	3080	1/1	0.48	0.22	38,38,38,38	0
57	MG	YA	3112	1/1	0.48	0.28	39,39,39,39	0
57	MG	RA	3129	1/1	0.49	0.20	56,56,56,56	0
57	MG	RA	3133	1/1	0.50	0.28	63,63,63,63	0
57	MG	YA	3125	1/1	0.50	0.13	58,58,58,58	0
57	MG	RA	3178	1/1	0.51	0.17	50,50,50,50	0
57	MG	RA	3165	1/1	0.51	0.21	75,75,75,75	0
57	MG	YE	304	1/1	0.51	0.36	95,95,95,95	0
57	MG	YA	3172	1/1	0.52	0.18	56,56,56,56	0
57	MG	QA	1622	1/1	0.52	0.17	47,47,47,47	0
57	MG	RA	3097	1/1	0.52	0.22	32,32,32,32	0
57	MG	RA	3180	1/1	0.52	0.21	54,54,54,54	0
57	MG	RA	3188	1/1	0.53	0.25	59,59,59,59	0
57	MG	YA	3142	1/1	0.53	0.32	40,40,40,40	0
57	MG	RA	3160	1/1	0.54	0.21	56,56,56,56	0
57	MG	XA	1605	1/1	0.54	0.17	52,52,52,52	0
57	MG	XA	1710	1/1	0.54	0.41	70,70,70,70	0
57	MG	RA	3190	1/1	0.55	0.32	56,56,56,56	0
57	MG	QA	1692	1/1	0.56	0.16	72,72,72,72	0
57	MG	YA	3115	1/1	0.56	0.32	56,56,56,56	0
57	MG	RA	3293	1/1	0.56	0.26	82,82,82,82	0
57	MG	RA	3150	1/1	0.56	0.21	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1625	1/1	0.56	0.20	52,52,52,52	0
57	MG	XA	1636	1/1	0.56	0.28	53,53,53,53	0
57	MG	RA	3161	1/1	0.57	0.12	70,70,70,70	0
57	MG	QA	1638	1/1	0.57	0.25	65,65,65,65	0
57	MG	RA	3136	1/1	0.57	0.16	58,58,58,58	0
57	MG	QA	1610	1/1	0.58	0.16	68,68,68,68	0
57	MG	YA	3312	1/1	0.58	0.24	62,62,62,62	0
57	MG	YO	201	1/1	0.58	0.26	65,65,65,65	0
57	MG	RN	201	1/1	0.58	0.16	42,42,42,42	0
57	MG	XA	1626	1/1	0.59	0.16	64,64,64,64	0
57	MG	RA	3166	1/1	0.59	0.26	61,61,61,61	0
57	MG	RA	3153	1/1	0.60	0.21	13,13,13,13	0
57	MG	YA	3051	1/1	0.61	0.25	47,47,47,47	0
57	MG	QA	1647	1/1	0.62	0.15	68,68,68,68	0
57	MG	QA	1691	1/1	0.62	0.19	61,61,61,61	0
57	MG	RA	3298	1/1	0.62	0.16	26,26,26,26	0
57	MG	YA	3243	1/1	0.62	0.26	47,47,47,47	0
57	MG	YA	3289	1/1	0.62	0.15	53,53,53,53	0
57	MG	XA	1638	1/1	0.62	0.25	56,56,56,56	0
57	MG	RA	3300	1/1	0.62	0.21	21,21,21,21	0
57	MG	RA	3156	1/1	0.62	0.26	32,32,32,32	0
59	ZN	R4	101	1/1	0.62	0.14	193,193,193,193	0
57	MG	XD	302	1/1	0.63	0.55	92,92,92,92	0
57	MG	YA	3004	1/1	0.63	0.24	27,27,27,27	0
57	MG	YA	3144	1/1	0.63	0.18	48,48,48,48	0
57	MG	RA	3059	1/1	0.63	0.20	21,21,21,21	0
57	MG	QA	1632	1/1	0.64	0.18	67,67,67,67	0
57	MG	YA	3088	1/1	0.64	0.17	51,51,51,51	0
57	MG	YA	3185	1/1	0.64	0.19	44,44,44,44	0
57	MG	RA	3268	1/1	0.65	0.16	48,48,48,48	0
57	MG	RA	3141	1/1	0.65	0.26	29,29,29,29	0
57	MG	RA	3098	1/1	0.66	0.22	35,35,35,35	0
57	MG	XL	201	1/1	0.66	0.18	60,60,60,60	0
57	MG	QA	1680	1/1	0.66	0.24	86,86,86,86	0
57	MG	YA	3295	1/1	0.66	0.17	55,55,55,55	0
57	MG	RA	3186	1/1	0.66	0.25	70,70,70,70	0
57	MG	QA	1603	1/1	0.66	0.16	72,72,72,72	0
57	MG	YE	302	1/1	0.66	0.34	90,90,90,90	0
57	MG	XA	1694	1/1	0.66	0.27	49,49,49,49	0
57	MG	RA	3162	1/1	0.66	0.30	70,70,70,70	0
57	MG	YV	201	1/1	0.67	0.23	84,84,84,84	0
57	MG	YA	3186	1/1	0.67	0.15	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3001	1/1	0.67	0.48	66,66,66,66	0
57	MG	RA	3157	1/1	0.67	0.13	36,36,36,36	0
57	MG	YA	3315	1/1	0.68	0.21	42,42,42,42	0
57	MG	RA	3094	1/1	0.68	0.17	49,49,49,49	0
57	MG	RA	3125	1/1	0.68	0.21	41,41,41,41	0
57	MG	YA	3174	1/1	0.69	0.28	59,59,59,59	0
57	MG	RA	3151	1/1	0.69	0.20	83,83,83,83	0
57	MG	RA	3026	1/1	0.69	0.31	74,74,74,74	0
57	MG	YA	3100	1/1	0.69	0.24	42,42,42,42	0
57	MG	YA	3124	1/1	0.69	0.26	51,51,51,51	0
57	MG	RA	3209	1/1	0.70	0.22	39,39,39,39	0
57	MG	RA	3155	1/1	0.70	0.19	56,56,56,56	0
57	MG	XA	1610	1/1	0.70	0.23	50,50,50,50	0
57	MG	XA	1693	1/1	0.70	0.09	44,44,44,44	0
57	MG	RA	3128	1/1	0.70	0.23	47,47,47,47	0
57	MG	RA	3104	1/1	0.70	0.22	50,50,50,50	0
57	MG	YA	3131	1/1	0.71	0.26	45,45,45,45	0
57	MG	RA	3137	1/1	0.71	0.25	35,35,35,35	0
57	MG	YA	3248	1/1	0.71	0.14	27,27,27,27	0
57	MG	YA	3001	1/1	0.71	0.20	52,52,52,52	0
59	ZN	R5	101	1/1	0.71	0.33	137,137,137,137	0
57	MG	XA	1615	1/1	0.72	0.12	44,44,44,44	0
57	MG	YA	3138	1/1	0.72	0.11	49,49,49,49	0
57	MG	QA	1646	1/1	0.72	0.36	64,64,64,64	0
57	MG	YA	3297	1/1	0.72	0.11	65,65,65,65	0
57	MG	XA	1632	1/1	0.72	0.15	65,65,65,65	0
57	MG	RA	3131	1/1	0.72	0.25	47,47,47,47	0
57	MG	RA	3118	1/1	0.73	0.31	59,59,59,59	0
57	MG	YA	3122	1/1	0.73	0.15	40,40,40,40	0
57	MG	YA	3017	1/1	0.73	0.18	27,27,27,27	0
57	MG	QA	1693	1/1	0.73	0.18	50,50,50,50	0
57	MG	YA	3128	1/1	0.73	0.18	38,38,38,38	0
57	MG	RR	202	1/1	0.73	0.26	47,47,47,47	0
57	MG	YE	303	1/1	0.73	0.22	24,24,24,24	0
57	MG	QA	1689	1/1	0.73	0.14	42,42,42,42	0
57	MG	YA	3140	1/1	0.73	0.20	85,85,85,85	0
57	MG	YA	3296	1/1	0.73	0.24	54,54,54,54	0
57	MG	RA	3084	1/1	0.74	0.16	56,56,56,56	0
57	MG	XA	1705	1/1	0.74	0.23	54,54,54,54	0
57	MG	XA	1709	1/1	0.74	0.22	48,48,48,48	0
57	MG	YA	3105	1/1	0.74	0.33	53,53,53,53	0
57	MG	YA	3279	1/1	0.74	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1677	1/1	0.74	0.08	39,39,39,39	0
57	MG	XA	1639	1/1	0.74	0.18	44,44,44,44	0
57	MG	YA	3063	1/1	0.74	0.19	32,32,32,32	0
57	MG	QA	1667	1/1	0.74	0.10	52,52,52,52	0
57	MG	YA	3145	1/1	0.75	0.10	48,48,48,48	0
57	MG	YA	3319	1/1	0.75	0.20	13,13,13,13	0
57	MG	YA	3173	1/1	0.75	0.24	40,40,40,40	0
57	MG	RA	3093	1/1	0.75	0.22	48,48,48,48	0
57	MG	QA	1608	1/1	0.75	0.22	30,30,30,30	0
57	MG	YA	3160	1/1	0.75	0.21	43,43,43,43	0
57	MG	RA	3068	1/1	0.75	0.23	22,22,22,22	0
57	MG	RA	3090	1/1	0.75	0.24	64,64,64,64	0
57	MG	YA	3224	1/1	0.75	0.23	56,56,56,56	0
57	MG	RA	3051	1/1	0.76	0.32	45,45,45,45	0
57	MG	RA	3032	1/1	0.76	0.10	17,17,17,17	0
57	MG	YA	3110	1/1	0.76	0.10	20,20,20,20	0
57	MG	QA	1682	1/1	0.76	0.17	72,72,72,72	0
57	MG	RA	3139	1/1	0.76	0.16	53,53,53,53	0
57	MG	RA	3176	1/1	0.77	0.13	47,47,47,47	0
57	MG	RA	3121	1/1	0.77	0.17	47,47,47,47	0
57	MG	XA	1618	1/1	0.77	0.16	40,40,40,40	0
57	MG	YA	3150	1/1	0.77	0.11	13,13,13,13	0
57	MG	RA	3232	1/1	0.77	0.13	50,50,50,50	0
57	MG	RA	3245	1/1	0.77	0.17	48,48,48,48	0
57	MG	YQ	3001	1/1	0.77	0.23	59,59,59,59	0
57	MG	QA	1628	1/1	0.77	0.21	35,35,35,35	0
57	MG	RA	3278	1/1	0.77	0.15	45,45,45,45	0
57	MG	YA	3268	1/1	0.77	0.23	42,42,42,42	0
57	MG	RA	3067	1/1	0.77	0.22	23,23,23,23	0
57	MG	YA	3002	1/1	0.77	0.12	47,47,47,47	0
57	MG	RA	3078	1/1	0.77	0.28	32,32,32,32	0
57	MG	XA	1643	1/1	0.78	0.14	61,61,61,61	0
57	MG	YD	302	1/1	0.78	0.50	126,126,126,126	0
57	MG	XA	1625	1/1	0.78	0.09	37,37,37,37	0
57	MG	RA	3106	1/1	0.78	0.27	43,43,43,43	0
57	MG	YA	3162	1/1	0.78	0.18	55,55,55,55	0
57	MG	YA	3308	1/1	0.78	0.10	57,57,57,57	0
57	MG	RA	3244	1/1	0.78	0.18	60,60,60,60	0
57	MG	XA	1633	1/1	0.78	0.16	33,33,33,33	0
57	MG	YA	3284	1/1	0.78	0.21	48,48,48,48	0
57	MG	RA	3189	1/1	0.79	0.18	84,84,84,84	0
57	MG	YA	3177	1/1	0.79	0.14	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1627	1/1	0.79	0.10	69,69,69,69	0
57	MG	YE	301	1/1	0.79	0.27	82,82,82,82	0
57	MG	RA	3142	1/1	0.79	0.13	42,42,42,42	0
57	MG	RA	3053	1/1	0.79	0.18	56,56,56,56	0
57	MG	YA	3317	1/1	0.79	0.19	24,24,24,24	0
57	MG	QA	1630	1/1	0.79	0.17	44,44,44,44	0
57	MG	RA	3064	1/1	0.79	0.21	19,19,19,19	0
57	MG	YA	3301	1/1	0.80	0.21	53,53,53,53	0
57	MG	QA	1612	1/1	0.80	0.11	41,41,41,41	0
57	MG	RA	3246	1/1	0.80	0.28	36,36,36,36	0
57	MG	RA	3182	1/1	0.80	0.18	46,46,46,46	0
57	MG	RA	3109	1/1	0.80	0.18	31,31,31,31	0
57	MG	YA	3015	1/1	0.80	0.22	22,22,22,22	0
57	MG	RA	3290	1/1	0.80	0.11	61,61,61,61	0
57	MG	XA	1647	1/1	0.80	0.30	69,69,69,69	0
57	MG	QA	1635	1/1	0.80	0.09	33,33,33,33	0
57	MG	RA	3112	1/1	0.80	0.26	49,49,49,49	0
57	MG	QA	1679	1/1	0.80	0.22	74,74,74,74	0
57	MG	YA	3286	1/1	0.80	0.16	40,40,40,40	0
57	MG	RA	3018	1/1	0.80	0.15	18,18,18,18	0
57	MG	QA	1623	1/1	0.80	0.12	39,39,39,39	0
57	MG	YA	3176	1/1	0.80	0.19	45,45,45,45	0
57	MG	RA	3060	1/1	0.80	0.24	39,39,39,39	0
57	MG	RA	3004	1/1	0.81	0.12	17,17,17,17	0
57	MG	RA	3005	1/1	0.81	0.15	41,41,41,41	0
57	MG	RA	3107	1/1	0.81	0.24	37,37,37,37	0
57	MG	YA	3179	1/1	0.81	0.20	41,41,41,41	0
57	MG	YA	3309	1/1	0.81	0.26	49,49,49,49	0
57	MG	RA	3058	1/1	0.81	0.11	21,21,21,21	0
57	MG	RA	3088	1/1	0.81	0.13	27,27,27,27	0
57	MG	QA	1666	1/1	0.81	0.20	36,36,36,36	0
57	MG	RA	3019	1/1	0.81	0.20	18,18,18,18	0
57	MG	YB	201	1/1	0.81	0.19	29,29,29,29	0
57	MG	QA	1694	1/1	0.81	0.10	55,55,55,55	0
57	MG	YA	3155	1/1	0.81	0.30	75,75,75,75	0
57	MG	RA	3301	1/1	0.81	0.13	49,49,49,49	0
57	MG	RA	3191	1/1	0.81	0.30	68,68,68,68	0
57	MG	YA	3003	1/1	0.81	0.17	41,41,41,41	0
57	MG	RA	3122	1/1	0.81	0.13	47,47,47,47	0
57	MG	RA	3228	1/1	0.81	0.20	38,38,38,38	0
57	MG	QA	1629	1/1	0.81	0.19	55,55,55,55	0
57	MG	YA	3292	1/1	0.81	0.19	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1636	1/1	0.81	0.21	44,44,44,44	0
57	MG	YA	3183	1/1	0.82	0.13	73,73,73,73	0
57	MG	YA	3303	1/1	0.82	0.19	60,60,60,60	0
57	MG	RA	3140	1/1	0.82	0.13	42,42,42,42	0
57	MG	RA	3163	1/1	0.82	0.19	53,53,53,53	0
57	MG	YA	3006	1/1	0.82	0.22	40,40,40,40	0
57	MG	RA	3082	1/1	0.82	0.15	47,47,47,47	0
57	MG	RA	3252	1/1	0.82	0.18	46,46,46,46	0
57	MG	YA	3246	1/1	0.82	0.12	29,29,29,29	0
57	MG	YA	3021	1/1	0.82	0.19	41,41,41,41	0
57	MG	RA	3179	1/1	0.82	0.17	52,52,52,52	0
57	MG	RQ	202	1/1	0.82	0.35	75,75,75,75	0
57	MG	QF	301	1/1	0.82	0.10	37,37,37,37	0
57	MG	XA	1714	1/1	0.82	0.17	57,57,57,57	0
57	MG	RA	3285	1/1	0.82	0.26	50,50,50,50	0
57	MG	YA	3141	1/1	0.82	0.31	53,53,53,53	0
57	MG	RA	3286	1/1	0.82	0.32	55,55,55,55	0
57	MG	RA	3146	1/1	0.82	0.20	38,38,38,38	0
57	MG	RA	3173	1/1	0.82	0.18	50,50,50,50	0
57	MG	YA	3298	1/1	0.82	0.20	51,51,51,51	0
57	MG	YG	201	1/1	0.83	0.12	41,41,41,41	0
57	MG	YA	3163	1/1	0.83	0.25	53,53,53,53	0
57	MG	XA	1689	1/1	0.83	0.10	37,37,37,37	0
57	MG	RA	3103	1/1	0.83	0.13	22,22,22,22	0
57	MG	YA	3153	1/1	0.83	0.25	52,52,52,52	0
57	MG	RA	3263	1/1	0.83	0.19	45,45,45,45	0
57	MG	RA	3144	1/1	0.83	0.11	58,58,58,58	0
57	MG	YA	3294	1/1	0.83	0.20	40,40,40,40	0
57	MG	XA	1646	1/1	0.83	0.07	30,30,30,30	0
57	MG	YA	3039	1/1	0.83	0.19	43,43,43,43	0
57	MG	RA	3193	1/1	0.83	0.24	19,19,19,19	0
59	ZN	Y4	101	1/1	0.83	0.17	276,276,276,276	0
57	MG	XA	1669	1/1	0.84	0.14	31,31,31,31	0
57	MG	RA	3080	1/1	0.84	0.24	18,18,18,18	0
57	MG	XA	1629	1/1	0.84	0.13	25,25,25,25	0
57	MG	RA	3226	1/1	0.84	0.26	51,51,51,51	0
57	MG	XA	1696	1/1	0.84	0.17	44,44,44,44	0
57	MG	XA	1699	1/1	0.84	0.10	44,44,44,44	0
57	MG	YA	3137	1/1	0.84	0.18	26,26,26,26	0
57	MG	RA	3102	1/1	0.84	0.20	46,46,46,46	0
57	MG	XA	1706	1/1	0.84	0.15	66,66,66,66	0
57	MG	RA	3138	1/1	0.84	0.21	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3313	1/1	0.84	0.08	40,40,40,40	0
57	MG	YA	3065	1/1	0.84	0.21	23,23,23,23	0
57	MG	YA	3316	1/1	0.84	0.14	75,75,75,75	0
57	MG	YA	3078	1/1	0.84	0.26	16,16,16,16	0
57	MG	YA	3189	1/1	0.84	0.22	26,26,26,26	0
57	MG	YA	3199	1/1	0.84	0.24	21,21,21,21	0
57	MG	YB	205	1/1	0.84	0.18	53,53,53,53	0
57	MG	YA	3215	1/1	0.84	0.19	28,28,28,28	0
57	MG	RA	3092	1/1	0.84	0.14	28,28,28,28	0
57	MG	YA	3237	1/1	0.84	0.12	28,28,28,28	0
57	MG	XA	1712	1/1	0.84	0.20	56,56,56,56	0
57	MG	RA	3044	1/1	0.84	0.23	40,40,40,40	0
57	MG	YA	3099	1/1	0.84	0.20	13,13,13,13	0
57	MG	QA	1620	1/1	0.84	0.08	31,31,31,31	0
57	MG	QA	1641	1/1	0.84	0.12	54,54,54,54	0
57	MG	XA	1645	1/1	0.84	0.19	43,43,43,43	0
57	MG	R8	101	1/1	0.84	0.18	55,55,55,55	0
57	MG	RA	3134	1/1	0.84	0.15	36,36,36,36	0
57	MG	RA	3145	1/1	0.84	0.24	51,51,51,51	0
57	MG	YA	3114	1/1	0.84	0.21	25,25,25,25	0
57	MG	XA	1688	1/1	0.85	0.17	41,41,41,41	0
57	MG	Y0	101	1/1	0.85	0.09	15,15,15,15	0
57	MG	Y3	101	1/1	0.85	0.17	33,33,33,33	0
57	MG	RA	3003	1/1	0.85	0.21	60,60,60,60	0
57	MG	RA	3192	1/1	0.85	0.23	54,54,54,54	0
57	MG	YA	3311	1/1	0.85	0.29	62,62,62,62	0
57	MG	YA	3146	1/1	0.85	0.12	73,73,73,73	0
57	MG	RP	202	1/1	0.85	0.22	49,49,49,49	0
57	MG	YA	3314	1/1	0.85	0.13	31,31,31,31	0
57	MG	RA	3248	1/1	0.85	0.19	56,56,56,56	0
57	MG	XA	1642	1/1	0.85	0.10	61,61,61,61	0
57	MG	YA	3109	1/1	0.85	0.13	22,22,22,22	0
57	MG	XA	1704	1/1	0.85	0.13	40,40,40,40	0
57	MG	YA	3244	1/1	0.85	0.11	24,24,24,24	0
57	MG	RA	3100	1/1	0.85	0.31	50,50,50,50	0
57	MG	RA	3233	1/1	0.85	0.22	45,45,45,45	0
57	MG	YA	3024	1/1	0.85	0.16	75,75,75,75	0
57	MG	YD	301	1/1	0.85	0.26	90,90,90,90	0
57	MG	YA	3277	1/1	0.85	0.17	32,32,32,32	0
57	MG	YD	305	1/1	0.85	0.57	50,50,50,50	0
57	MG	YA	3030	1/1	0.85	0.14	25,25,25,25	0
57	MG	YA	3166	1/1	0.85	0.20	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3297	1/1	0.85	0.19	31,31,31,31	0
57	MG	QA	1658	1/1	0.85	0.15	42,42,42,42	0
57	MG	YA	3290	1/1	0.85	0.12	53,53,53,53	0
57	MG	YA	3057	1/1	0.85	0.10	65,65,65,65	0
57	MG	XA	1661	1/1	0.85	0.20	39,39,39,39	0
57	MG	YA	3136	1/1	0.85	0.17	25,25,25,25	0
57	MG	RA	3270	1/1	0.85	0.10	56,56,56,56	0
57	MG	XA	1675	1/1	0.85	0.03	11,11,11,11	0
57	MG	QA	1684	1/1	0.86	0.13	52,52,52,52	0
57	MG	YA	3066	1/1	0.86	0.17	19,19,19,19	0
57	MG	YA	3182	1/1	0.86	0.15	39,39,39,39	0
57	MG	RA	3281	1/1	0.86	0.21	50,50,50,50	0
57	MG	RA	3065	1/1	0.86	0.13	37,37,37,37	0
57	MG	XA	1613	1/1	0.86	0.20	37,37,37,37	0
57	MG	YA	3143	1/1	0.86	0.10	54,54,54,54	0
57	MG	YA	3093	1/1	0.86	0.17	60,60,60,60	0
57	MG	YA	3198	1/1	0.86	0.19	39,39,39,39	0
57	MG	RA	3213	1/1	0.86	0.19	39,39,39,39	0
57	MG	YA	3203	1/1	0.86	0.16	38,38,38,38	0
57	MG	QA	1640	1/1	0.86	0.23	45,45,45,45	0
57	MG	YA	3148	1/1	0.86	0.07	41,41,41,41	0
57	MG	RA	3007	1/1	0.86	0.12	22,22,22,22	0
57	MG	YA	3104	1/1	0.86	0.28	46,46,46,46	0
57	MG	XA	1621	1/1	0.86	0.08	32,32,32,32	0
57	MG	QV	102	1/1	0.86	0.10	20,20,20,20	0
57	MG	YA	3157	1/1	0.86	0.15	31,31,31,31	0
57	MG	QA	1626	1/1	0.86	0.21	39,39,39,39	0
57	MG	RA	3184	1/1	0.86	0.18	59,59,59,59	0
57	MG	RA	3108	1/1	0.86	0.21	25,25,25,25	0
57	MG	YQ	3003	1/1	0.86	0.31	105,105,105,105	0
57	MG	XA	1698	1/1	0.86	0.16	51,51,51,51	0
57	MG	RA	3187	1/1	0.86	0.29	150,150,150,150	0
57	MG	RA	3096	1/1	0.86	0.32	53,53,53,53	0
57	MG	QA	1645	1/1	0.86	0.11	35,35,35,35	0
57	MG	XA	1637	1/1	0.86	0.14	25,25,25,25	0
57	MG	YA	3127	1/1	0.86	0.18	40,40,40,40	0
57	MG	RA	3149	1/1	0.86	0.11	12,12,12,12	0
57	MG	QA	1621	1/1	0.86	0.17	34,34,34,34	0
57	MG	RA	3113	1/1	0.86	0.26	58,58,58,58	0
57	MG	QA	1663	1/1	0.87	0.19	61,61,61,61	0
57	MG	RA	3071	1/1	0.87	0.17	59,59,59,59	0
57	MG	XA	1654	1/1	0.87	0.16	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3185	1/1	0.87	0.42	127,127,127,127	0
57	MG	RA	3072	1/1	0.87	0.20	14,14,14,14	0
57	MG	RA	3021	1/1	0.87	0.26	21,21,21,21	0
57	MG	RA	3243	1/1	0.87	0.23	48,48,48,48	0
57	MG	RA	3294	1/1	0.87	0.09	36,36,36,36	0
57	MG	YA	3018	1/1	0.87	0.12	19,19,19,19	0
57	MG	RA	3296	1/1	0.87	0.22	48,48,48,48	0
57	MG	QA	1616	1/1	0.87	0.09	28,28,28,28	0
57	MG	RA	3154	1/1	0.87	0.07	37,37,37,37	0
57	MG	RA	3127	1/1	0.87	0.15	28,28,28,28	0
57	MG	YA	3049	1/1	0.87	0.26	15,15,15,15	0
57	MG	YA	3050	1/1	0.87	0.20	44,44,44,44	0
57	MG	XA	1631	1/1	0.87	0.14	46,46,46,46	0
57	MG	YA	3134	1/1	0.87	0.12	64,64,64,64	0
57	MG	RA	3006	1/1	0.87	0.21	22,22,22,22	0
57	MG	RD	301	1/1	0.87	0.13	1,1,1,1	0
57	MG	YA	3059	1/1	0.87	0.26	26,26,26,26	0
57	MG	YA	3060	1/1	0.87	0.18	15,15,15,15	0
57	MG	YA	3323	1/1	0.87	0.24	34,34,34,34	0
57	MG	QD	302	1/1	0.87	0.21	64,64,64,64	0
57	MG	RO	201	1/1	0.87	0.17	51,51,51,51	0
57	MG	YA	3210	1/1	0.87	0.19	36,36,36,36	0
57	MG	RA	3011	1/1	0.87	0.25	24,24,24,24	0
57	MG	YA	3219	1/1	0.87	0.21	34,34,34,34	0
57	MG	YA	3072	1/1	0.87	0.25	29,29,29,29	0
57	MG	RA	3267	1/1	0.87	0.19	50,50,50,50	0
57	MG	RA	3202	1/1	0.87	0.22	34,34,34,34	0
57	MG	RR	201	1/1	0.87	0.13	25,25,25,25	0
57	MG	YA	3089	1/1	0.87	0.10	41,41,41,41	0
57	MG	YA	3090	1/1	0.87	0.14	29,29,29,29	0
57	MG	YA	3250	1/1	0.87	0.21	36,36,36,36	0
57	MG	YA	3253	1/1	0.87	0.18	32,32,32,32	0
57	MG	YA	3266	1/1	0.87	0.26	44,44,44,44	0
57	MG	QA	1687	1/1	0.87	0.26	70,70,70,70	0
57	MG	YA	3094	1/1	0.87	0.38	108,108,108,108	0
57	MG	RA	3274	1/1	0.87	0.21	48,48,48,48	0
57	MG	YA	3158	1/1	0.87	0.16	49,49,49,49	0
57	MG	QA	1676	1/1	0.88	0.09	47,47,47,47	0
57	MG	YA	3107	1/1	0.88	0.23	24,24,24,24	0
57	MG	YA	3306	1/1	0.88	0.29	67,67,67,67	0
57	MG	XA	1648	1/1	0.88	0.08	77,77,77,77	0
57	MG	RA	3110	1/1	0.88	0.32	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3214	1/1	0.88	0.17	33,33,33,33	0
57	MG	QA	1686	1/1	0.88	0.16	33,33,33,33	0
57	MG	YA	3111	1/1	0.88	0.21	39,39,39,39	0
57	MG	YA	3221	1/1	0.88	0.22	25,25,25,25	0
57	MG	QA	1643	1/1	0.88	0.17	27,27,27,27	0
57	MG	RA	3283	1/1	0.88	0.19	54,54,54,54	0
57	MG	QA	1619	1/1	0.88	0.09	25,25,25,25	0
57	MG	YA	3121	1/1	0.88	0.10	10,10,10,10	0
57	MG	RA	3114	1/1	0.88	0.17	33,33,33,33	0
57	MG	QA	1606	1/1	0.88	0.18	20,20,20,20	0
57	MG	QA	1633	1/1	0.88	0.10	48,48,48,48	0
57	MG	YA	3077	1/1	0.88	0.20	37,37,37,37	0
57	MG	YA	3257	1/1	0.88	0.16	43,43,43,43	0
57	MG	RA	3194	1/1	0.88	0.15	8,8,8,8	0
57	MG	YA	3129	1/1	0.88	0.19	48,48,48,48	0
57	MG	XA	1604	1/1	0.88	0.19	28,28,28,28	0
57	MG	YA	3133	1/1	0.88	0.19	37,37,37,37	0
57	MG	YQ	3002	1/1	0.88	0.42	96,96,96,96	0
57	MG	YA	3016	1/1	0.88	0.14	10,10,10,10	0
57	MG	RA	3042	1/1	0.88	0.21	23,23,23,23	0
57	MG	XA	1703	1/1	0.88	0.09	54,54,54,54	0
57	MG	YA	3092	1/1	0.88	0.20	31,31,31,31	0
57	MG	RA	3259	1/1	0.88	0.19	59,59,59,59	0
57	MG	RA	3164	1/1	0.88	0.08	30,30,30,30	0
57	MG	RA	3212	1/1	0.88	0.18	33,33,33,33	0
57	MG	YA	3035	1/1	0.88	0.20	21,21,21,21	0
57	MG	RA	3008	1/1	0.88	0.24	24,24,24,24	0
59	ZN	R9	101	1/1	0.88	0.26	110,110,110,110	0
57	MG	XA	1616	1/1	0.88	0.15	25,25,25,25	0
59	ZN	Y6	101	1/1	0.88	0.21	209,209,209,209	0
57	MG	RA	3196	1/1	0.89	0.18	17,17,17,17	0
57	MG	RA	3200	1/1	0.89	0.15	23,23,23,23	0
57	MG	YA	3299	1/1	0.89	0.22	50,50,50,50	0
57	MG	RA	3201	1/1	0.89	0.26	35,35,35,35	0
57	MG	RA	3183	1/1	0.89	0.20	21,21,21,21	0
57	MG	RA	3266	1/1	0.89	0.11	44,44,44,44	0
57	MG	YA	3307	1/1	0.89	0.14	43,43,43,43	0
57	MG	RA	3204	1/1	0.89	0.22	26,26,26,26	0
57	MG	YA	3103	1/1	0.89	0.15	55,55,55,55	0
57	MG	RA	3083	1/1	0.89	0.18	25,25,25,25	0
57	MG	YA	3031	1/1	0.89	0.23	9,9,9,9	0
57	MG	QV	101	1/1	0.89	0.20	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3220	1/1	0.89	0.21	35,35,35,35	0
57	MG	YA	3038	1/1	0.89	0.29	37,37,37,37	0
57	MG	QA	1609	1/1	0.89	0.20	45,45,45,45	0
57	MG	YA	3156	1/1	0.89	0.30	31,31,31,31	0
57	MG	YA	3240	1/1	0.89	0.09	31,31,31,31	0
57	MG	YA	3322	1/1	0.89	0.20	4,4,4,4	0
57	MG	YA	3046	1/1	0.89	0.16	19,19,19,19	0
57	MG	RA	3217	1/1	0.89	0.22	28,28,28,28	0
57	MG	YB	203	1/1	0.89	0.18	29,29,29,29	0
57	MG	RA	3171	1/1	0.89	0.16	38,38,38,38	0
57	MG	YA	3113	1/1	0.89	0.11	30,30,30,30	0
57	MG	QA	1642	1/1	0.89	0.08	45,45,45,45	0
57	MG	YA	3251	1/1	0.89	0.17	52,52,52,52	0
57	MG	RA	3158	1/1	0.89	0.13	29,29,29,29	0
57	MG	RA	3147	1/1	0.89	0.24	30,30,30,30	0
57	MG	RA	3287	1/1	0.89	0.11	45,45,45,45	0
57	MG	YA	3267	1/1	0.89	0.15	36,36,36,36	0
57	MG	RA	3237	1/1	0.89	0.22	26,26,26,26	0
57	MG	YA	3272	1/1	0.89	0.23	38,38,38,38	0
57	MG	XF	301	1/1	0.89	0.11	47,47,47,47	0
57	MG	RA	3238	1/1	0.89	0.15	32,32,32,32	0
57	MG	QA	1670	1/1	0.89	0.15	34,34,34,34	0
57	MG	XA	1658	1/1	0.89	0.17	27,27,27,27	0
57	MG	RA	3116	1/1	0.89	0.18	44,44,44,44	0
57	MG	RA	3061	1/1	0.89	0.19	28,28,28,28	0
57	MG	XA	1670	1/1	0.89	0.24	40,40,40,40	0
57	MG	XA	1674	1/1	0.89	0.23	41,41,41,41	0
57	MG	RA	3119	1/1	0.89	0.17	33,33,33,33	0
57	MG	YA	3010	1/1	0.89	0.30	38,38,38,38	0
57	MG	YA	3288	1/1	0.90	0.18	44,44,44,44	0
57	MG	RA	3284	1/1	0.90	0.28	54,54,54,54	0
57	MG	QA	1665	1/1	0.90	0.12	44,44,44,44	0
57	MG	RA	3239	1/1	0.90	0.28	44,44,44,44	0
57	MG	YA	3293	1/1	0.90	0.17	47,47,47,47	0
57	MG	RA	3159	1/1	0.90	0.14	26,26,26,26	0
57	MG	XA	1607	1/1	0.90	0.18	21,21,21,21	0
57	MG	QA	1671	1/1	0.90	0.07	38,38,38,38	0
57	MG	RA	3132	1/1	0.90	0.10	36,36,36,36	0
57	MG	XE	201	1/1	0.90	0.09	47,47,47,47	0
57	MG	YA	3132	1/1	0.90	0.14	27,27,27,27	0
57	MG	XA	1650	1/1	0.90	0.15	24,24,24,24	0
57	MG	XA	1653	1/1	0.90	0.18	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3305	1/1	0.90	0.19	42,42,42,42	0
57	MG	RA	3047	1/1	0.90	0.13	11,11,11,11	0
57	MG	YA	3190	1/1	0.90	0.20	23,23,23,23	0
57	MG	QA	1672	1/1	0.90	0.21	40,40,40,40	0
57	MG	YA	3087	1/1	0.90	0.21	10,10,10,10	0
57	MG	YA	3139	1/1	0.90	0.27	40,40,40,40	0
57	MG	RA	3207	1/1	0.90	0.23	30,30,30,30	0
57	MG	YA	3212	1/1	0.90	0.19	34,34,34,34	0
57	MG	XA	1667	1/1	0.90	0.24	43,43,43,43	0
57	MG	XA	1617	1/1	0.90	0.15	21,21,21,21	0
57	MG	YA	3216	1/1	0.90	0.19	44,44,44,44	0
57	MG	YA	3217	1/1	0.90	0.18	27,27,27,27	0
57	MG	YA	3091	1/1	0.90	0.26	39,39,39,39	0
57	MG	RA	3208	1/1	0.90	0.14	29,29,29,29	0
57	MG	XA	1673	1/1	0.90	0.17	41,41,41,41	0
57	MG	QA	1639	1/1	0.90	0.19	52,52,52,52	0
57	MG	YA	3225	1/1	0.90	0.07	19,19,19,19	0
57	MG	RA	3264	1/1	0.90	0.33	55,55,55,55	0
57	MG	YF	301	1/1	0.90	0.09	45,45,45,45	0
57	MG	XA	1683	1/1	0.90	0.14	45,45,45,45	0
57	MG	XA	1684	1/1	0.90	0.23	42,42,42,42	0
57	MG	RB	203	1/1	0.90	0.23	46,46,46,46	0
57	MG	QA	1685	1/1	0.90	0.11	42,42,42,42	0
57	MG	XA	1691	1/1	0.90	0.24	43,43,43,43	0
57	MG	RA	3152	1/1	0.90	0.17	24,24,24,24	0
57	MG	RA	3169	1/1	0.90	0.15	38,38,38,38	0
57	MG	RA	3055	1/1	0.90	0.21	4,4,4,4	0
57	MG	XA	1697	1/1	0.90	0.15	56,56,56,56	0
57	MG	YA	3262	1/1	0.90	0.39	36,36,36,36	0
57	MG	RA	3031	1/1	0.90	0.18	16,16,16,16	0
57	MG	YA	3042	1/1	0.90	0.11	27,27,27,27	0
57	MG	QA	1602	1/1	0.90	0.18	27,27,27,27	0
57	MG	YA	3270	1/1	0.90	0.36	45,45,45,45	0
57	MG	RA	3079	1/1	0.90	0.15	26,26,26,26	0
57	MG	YA	3167	1/1	0.90	0.15	49,49,49,49	0
57	MG	YA	3169	1/1	0.90	0.25	51,51,51,51	0
57	MG	RA	3035	1/1	0.90	0.16	17,17,17,17	0
57	MG	YA	3120	1/1	0.90	0.15	32,32,32,32	0
57	MG	QA	1675	1/1	0.91	0.14	24,24,24,24	0
57	MG	YA	3023	1/1	0.91	0.20	21,21,21,21	0
57	MG	QA	1690	1/1	0.91	0.30	57,57,57,57	0
57	MG	RA	3115	1/1	0.91	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3203	1/1	0.91	0.27	61,61,61,61	0
57	MG	QA	1601	1/1	0.91	0.19	17,17,17,17	0
57	MG	YA	3102	1/1	0.91	0.22	15,15,15,15	0
57	MG	RA	3168	1/1	0.91	0.13	54,54,54,54	0
57	MG	RA	3117	1/1	0.91	0.19	20,20,20,20	0
57	MG	XA	1649	1/1	0.91	0.23	59,59,59,59	0
57	MG	RA	3250	1/1	0.91	0.10	45,45,45,45	0
57	MG	YA	3274	1/1	0.91	0.18	37,37,37,37	0
57	MG	XA	1651	1/1	0.91	0.24	22,22,22,22	0
57	MG	QA	1650	1/1	0.91	0.12	21,21,21,21	0
57	MG	YA	3281	1/1	0.91	0.22	37,37,37,37	0
57	MG	RA	3254	1/1	0.91	0.16	43,43,43,43	0
57	MG	YA	3285	1/1	0.91	0.17	38,38,38,38	0
57	MG	RA	3255	1/1	0.91	0.13	42,42,42,42	0
57	MG	RA	3257	1/1	0.91	0.09	25,25,25,25	0
57	MG	RA	3025	1/1	0.91	0.32	30,30,30,30	0
57	MG	RA	3172	1/1	0.91	0.14	45,45,45,45	0
57	MG	QA	1651	1/1	0.91	0.15	26,26,26,26	0
57	MG	YA	3119	1/1	0.91	0.29	22,22,22,22	0
57	MG	XA	1628	1/1	0.91	0.07	54,54,54,54	0
57	MG	RA	3225	1/1	0.91	0.22	13,13,13,13	0
57	MG	XA	1630	1/1	0.91	0.15	32,32,32,32	0
57	MG	XA	1682	1/1	0.91	0.20	36,36,36,36	0
57	MG	RA	3135	1/1	0.91	0.13	31,31,31,31	0
57	MG	RA	3175	1/1	0.91	0.28	61,61,61,61	0
57	MG	YE	305	1/1	0.91	0.20	27,27,27,27	0
57	MG	RA	3148	1/1	0.91	0.09	46,46,46,46	0
57	MG	YA	3302	1/1	0.91	0.16	50,50,50,50	0
57	MG	RA	3273	1/1	0.91	0.12	54,54,54,54	0
57	MG	RA	3076	1/1	0.91	0.11	28,28,28,28	0
57	MG	RA	3275	1/1	0.91	0.11	34,34,34,34	0
57	MG	QA	1656	1/1	0.91	0.12	28,28,28,28	0
57	MG	XA	1692	1/1	0.92	0.16	51,51,51,51	0
57	MG	YA	3037	1/1	0.92	0.18	7,7,7,7	0
57	MG	QA	1652	1/1	0.92	0.19	43,43,43,43	0
57	MG	QA	1668	1/1	0.92	0.07	37,37,37,37	0
57	MG	RA	3242	1/1	0.92	0.20	42,42,42,42	0
57	MG	RA	3027	1/1	0.92	0.16	3,3,3,3	0
57	MG	XA	1641	1/1	0.92	0.16	22,22,22,22	0
57	MG	RA	3054	1/1	0.92	0.14	22,22,22,22	0
57	MG	RA	3028	1/1	0.92	0.16	45,45,45,45	0
57	MG	XA	1606	1/1	0.92	0.17	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1655	1/1	0.92	0.17	30,30,30,30	0
57	MG	YA	3195	1/1	0.92	0.17	21,21,21,21	0
57	MG	YA	3130	1/1	0.92	0.16	29,29,29,29	0
57	MG	QA	1624	1/1	0.92	0.07	45,45,45,45	0
57	MG	XA	1708	1/1	0.92	0.13	36,36,36,36	0
57	MG	YA	3062	1/1	0.92	0.10	31,31,31,31	0
57	MG	RA	3249	1/1	0.92	0.22	42,42,42,42	0
57	MG	RA	3292	1/1	0.92	0.18	44,44,44,44	0
57	MG	XA	1711	1/1	0.92	0.10	29,29,29,29	0
57	MG	RA	3210	1/1	0.92	0.22	33,33,33,33	0
57	MG	YA	3076	1/1	0.92	0.14	5,5,5,5	0
57	MG	RA	3014	1/1	0.92	0.15	17,17,17,17	0
57	MG	XA	1652	1/1	0.92	0.19	23,23,23,23	0
57	MG	RA	3036	1/1	0.92	0.15	19,19,19,19	0
57	MG	YA	3085	1/1	0.92	0.17	24,24,24,24	0
57	MG	RA	3215	1/1	0.92	0.18	30,30,30,30	0
57	MG	YA	3230	1/1	0.92	0.12	28,28,28,28	0
57	MG	XA	1655	1/1	0.92	0.17	15,15,15,15	0
57	MG	XV	102	1/1	0.92	0.18	33,33,33,33	0
57	MG	YA	3325	1/1	0.92	0.14	49,49,49,49	0
57	MG	XA	1620	1/1	0.92	0.21	34,34,34,34	0
57	MG	RA	3216	1/1	0.92	0.24	28,28,28,28	0
57	MG	YA	3152	1/1	0.92	0.12	20,20,20,20	0
57	MG	XA	1666	1/1	0.92	0.21	32,32,32,32	0
57	MG	YA	3249	1/1	0.92	0.20	51,51,51,51	0
57	MG	XA	1622	1/1	0.92	0.20	36,36,36,36	0
57	MG	XA	1623	1/1	0.92	0.15	23,23,23,23	0
57	MG	RA	3063	1/1	0.92	0.10	25,25,25,25	0
57	MG	YD	304	1/1	0.92	0.29	117,117,117,117	0
57	MG	RA	3218	1/1	0.92	0.19	28,28,28,28	0
57	MG	XA	1627	1/1	0.92	0.22	25,25,25,25	0
57	MG	YA	3101	1/1	0.92	0.17	30,30,30,30	0
57	MG	YA	3013	1/1	0.92	0.21	21,21,21,21	0
57	MG	RA	3037	1/1	0.92	0.16	22,22,22,22	0
57	MG	QA	1657	1/1	0.92	0.27	41,41,41,41	0
57	MG	YA	3271	1/1	0.92	0.30	52,52,52,52	0
57	MG	RA	3066	1/1	0.92	0.12	49,49,49,49	0
57	MG	QA	1688	1/1	0.92	0.15	48,48,48,48	0
57	MG	XA	1685	1/1	0.92	0.12	52,52,52,52	0
57	MG	XA	1686	1/1	0.92	0.14	44,44,44,44	0
57	MG	RA	3199	1/1	0.92	0.26	26,26,26,26	0
57	MG	YA	3283	1/1	0.92	0.25	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3025	1/1	0.92	0.19	9,9,9,9	0
57	MG	RA	3236	1/1	0.92	0.16	27,27,27,27	0
57	MG	QA	1681	1/1	0.92	0.15	36,36,36,36	0
57	MG	YA	3048	1/1	0.93	0.20	17,17,17,17	0
57	MG	XA	1668	1/1	0.93	0.08	23,23,23,23	0
57	MG	RA	3279	1/1	0.93	0.12	48,48,48,48	0
57	MG	YA	3181	1/1	0.93	0.19	102,102,102,102	0
57	MG	XA	1716	1/1	0.93	0.20	39,39,39,39	0
57	MG	YA	3123	1/1	0.93	0.21	20,20,20,20	0
57	MG	RA	3280	1/1	0.93	0.24	51,51,51,51	0
57	MG	RA	3081	1/1	0.93	0.12	22,22,22,22	0
57	MG	RA	3039	1/1	0.93	0.17	15,15,15,15	0
57	MG	XA	1602	1/1	0.93	0.25	28,28,28,28	0
57	MG	XA	1678	1/1	0.93	0.08	33,33,33,33	0
57	MG	XA	1635	1/1	0.93	0.17	30,30,30,30	0
57	MG	QA	1669	1/1	0.93	0.10	26,26,26,26	0
57	MG	RA	3123	1/1	0.93	0.17	12,12,12,12	0
57	MG	YA	3300	1/1	0.93	0.18	46,46,46,46	0
57	MG	YA	3068	1/1	0.93	0.20	4,4,4,4	0
57	MG	RA	3002	1/1	0.93	0.14	15,15,15,15	0
57	MG	RA	3143	1/1	0.93	0.12	23,23,23,23	0
57	MG	QA	1613	1/1	0.93	0.08	43,43,43,43	0
57	MG	YA	3005	1/1	0.93	0.21	91,91,91,91	0
57	MG	RA	3013	1/1	0.93	0.16	19,19,19,19	0
57	MG	YA	3008	1/1	0.93	0.18	4,4,4,4	0
57	MG	YA	3086	1/1	0.93	0.17	23,23,23,23	0
57	MG	YA	3310	1/1	0.93	0.25	52,52,52,52	0
57	MG	YA	3009	1/1	0.93	0.20	25,25,25,25	0
57	MG	XA	1690	1/1	0.93	0.16	41,41,41,41	0
57	MG	XA	1612	1/1	0.93	0.16	28,28,28,28	0
57	MG	RA	3091	1/1	0.93	0.11	42,42,42,42	0
57	MG	YA	3226	1/1	0.93	0.23	34,34,34,34	0
57	MG	QA	1644	1/1	0.93	0.06	44,44,44,44	0
57	MG	YA	3235	1/1	0.93	0.14	24,24,24,24	0
57	MG	RA	3015	1/1	0.93	0.22	3,3,3,3	0
57	MG	YA	3149	1/1	0.93	0.17	46,46,46,46	0
57	MG	YA	3242	1/1	0.93	0.18	40,40,40,40	0
57	MG	XA	1695	1/1	0.93	0.08	29,29,29,29	0
57	MG	RA	3016	1/1	0.93	0.20	17,17,17,17	0
57	MG	YA	3022	1/1	0.93	0.18	22,22,22,22	0
57	MG	YA	3098	1/1	0.93	0.24	47,47,47,47	0
57	MG	RA	3241	1/1	0.93	0.15	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3033	1/1	0.93	0.10	29,29,29,29	0
57	MG	RA	3271	1/1	0.93	0.07	41,41,41,41	0
57	MG	YA	3029	1/1	0.93	0.13	21,21,21,21	0
57	MG	YA	3254	1/1	0.93	0.16	27,27,27,27	0
57	MG	YA	3256	1/1	0.93	0.17	40,40,40,40	0
57	MG	RB	202	1/1	0.93	0.25	42,42,42,42	0
57	MG	YA	3258	1/1	0.93	0.16	36,36,36,36	0
57	MG	RA	3272	1/1	0.93	0.11	66,66,66,66	0
57	MG	YA	3034	1/1	0.93	0.13	17,17,17,17	0
57	MG	RA	3017	1/1	0.93	0.20	1,1,1,1	0
57	MG	YA	3036	1/1	0.93	0.14	30,30,30,30	0
57	MG	QA	1683	1/1	0.93	0.05	40,40,40,40	0
57	MG	QA	1653	1/1	0.93	0.14	33,33,33,33	0
57	MG	RP	201	1/1	0.93	0.08	15,15,15,15	0
57	MG	RA	3276	1/1	0.93	0.25	56,56,56,56	0
57	MG	YA	3043	1/1	0.93	0.18	20,20,20,20	0
57	MG	RA	3038	1/1	0.93	0.15	27,27,27,27	0
57	MG	YA	3280	1/1	0.93	0.45	69,69,69,69	0
59	ZN	R6	101	1/1	0.93	0.11	223,223,223,223	0
57	MG	YA	3047	1/1	0.93	0.18	12,12,12,12	0
57	MG	YA	3282	1/1	0.93	0.17	48,48,48,48	0
57	MG	YA	3117	1/1	0.93	0.20	27,27,27,27	0
57	MG	YA	3207	1/1	0.94	0.12	19,19,19,19	0
57	MG	RA	3214	1/1	0.94	0.21	19,19,19,19	0
57	MG	XA	1660	1/1	0.94	0.15	45,45,45,45	0
57	MG	RA	3052	1/1	0.94	0.16	5,5,5,5	0
57	MG	QA	1660	1/1	0.94	0.24	37,37,37,37	0
57	MG	RA	3130	1/1	0.94	0.13	19,19,19,19	0
57	MG	YA	3007	1/1	0.94	0.14	1,1,1,1	0
57	MG	YA	3052	1/1	0.94	0.16	3,3,3,3	0
57	MG	QA	1662	1/1	0.94	0.23	41,41,41,41	0
57	MG	XA	1702	1/1	0.94	0.12	29,29,29,29	0
57	MG	RA	3221	1/1	0.94	0.17	42,42,42,42	0
57	MG	YA	3012	1/1	0.94	0.12	12,12,12,12	0
57	MG	YA	3061	1/1	0.94	0.07	13,13,13,13	0
57	MG	XA	1640	1/1	0.94	0.07	40,40,40,40	0
57	MG	RA	3022	1/1	0.94	0.16	25,25,25,25	0
57	MG	RA	3069	1/1	0.94	0.24	23,23,23,23	0
57	MG	XA	1707	1/1	0.94	0.07	49,49,49,49	0
57	MG	YA	3118	1/1	0.94	0.11	23,23,23,23	0
57	MG	RA	3086	1/1	0.94	0.14	27,27,27,27	0
57	MG	YA	3165	1/1	0.94	0.16	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3071	1/1	0.94	0.14	35,35,35,35	0
57	MG	YA	3247	1/1	0.94	0.12	48,48,48,48	0
57	MG	XA	1677	1/1	0.94	0.24	41,41,41,41	0
57	MG	YA	3168	1/1	0.94	0.21	53,53,53,53	0
57	MG	YA	3073	1/1	0.94	0.23	19,19,19,19	0
57	MG	YA	3075	1/1	0.94	0.17	21,21,21,21	0
57	MG	XA	1644	1/1	0.94	0.12	29,29,29,29	0
57	MG	XA	1680	1/1	0.94	0.10	42,42,42,42	0
57	MG	RA	3070	1/1	0.94	0.18	16,16,16,16	0
57	MG	RA	3261	1/1	0.94	0.10	37,37,37,37	0
57	MG	YA	3027	1/1	0.94	0.23	21,21,21,21	0
57	MG	YA	3260	1/1	0.94	0.13	32,32,32,32	0
57	MG	RA	3023	1/1	0.94	0.21	40,40,40,40	0
57	MG	RA	3167	1/1	0.94	0.15	38,38,38,38	0
57	MG	RA	3045	1/1	0.94	0.15	16,16,16,16	0
57	MG	RA	3046	1/1	0.94	0.15	11,11,11,11	0
57	MG	YA	3269	1/1	0.94	0.33	49,49,49,49	0
57	MG	RA	3124	1/1	0.94	0.19	28,28,28,28	0
57	MG	YA	3135	1/1	0.94	0.17	38,38,38,38	0
57	MG	XV	101	1/1	0.94	0.23	30,30,30,30	0
57	MG	QA	1631	1/1	0.94	0.22	62,62,62,62	0
57	MG	YA	3275	1/1	0.94	0.10	36,36,36,36	0
57	MG	RA	3211	1/1	0.94	0.23	38,38,38,38	0
57	MG	QV	103	1/1	0.94	0.07	2,2,2,2	0
57	MG	YA	3193	1/1	0.94	0.16	16,16,16,16	0
57	MG	YA	3194	1/1	0.94	0.15	27,27,27,27	0
57	MG	Y9	101	1/1	0.94	0.11	73,73,73,73	0
57	MG	YA	3097	1/1	0.94	0.17	31,31,31,31	0
57	MG	QA	1664	1/1	0.94	0.14	44,44,44,44	0
57	MG	YA	3200	1/1	0.94	0.11	28,28,28,28	0
57	MG	YA	3201	1/1	0.94	0.11	36,36,36,36	0
57	MG	YA	3287	1/1	0.94	0.18	39,39,39,39	0
57	MG	YA	3202	1/1	0.94	0.10	26,26,26,26	0
57	MG	YA	3045	1/1	0.94	0.22	17,17,17,17	0
57	MG	YA	3206	1/1	0.94	0.22	27,27,27,27	0
57	MG	RA	3195	1/1	0.95	0.22	14,14,14,14	0
57	MG	RA	3043	1/1	0.95	0.17	15,15,15,15	0
57	MG	YA	3178	1/1	0.95	0.12	41,41,41,41	0
57	MG	YA	3245	1/1	0.95	0.15	30,30,30,30	0
57	MG	RA	3260	1/1	0.95	0.05	29,29,29,29	0
57	MG	YA	3014	1/1	0.95	0.16	1,1,1,1	0
57	MG	YA	3053	1/1	0.95	0.16	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3054	1/1	0.95	0.19	15,15,15,15	0
57	MG	YA	3055	1/1	0.95	0.20	13,13,13,13	0
57	MG	XA	1624	1/1	0.95	0.11	28,28,28,28	0
57	MG	RA	3197	1/1	0.95	0.21	15,15,15,15	0
57	MG	XA	1713	1/1	0.95	0.15	24,24,24,24	0
57	MG	QA	1674	1/1	0.95	0.09	40,40,40,40	0
57	MG	XA	1687	1/1	0.95	0.16	25,25,25,25	0
57	MG	RA	3095	1/1	0.95	0.11	35,35,35,35	0
57	MG	YA	3147	1/1	0.95	0.12	16,16,16,16	0
57	MG	YA	3261	1/1	0.95	0.18	20,20,20,20	0
57	MG	RA	3062	1/1	0.95	0.12	7,7,7,7	0
57	MG	YA	3263	1/1	0.95	0.41	52,52,52,52	0
57	MG	YA	3320	1/1	0.95	0.21	10,10,10,10	0
57	MG	YA	3321	1/1	0.95	0.12	19,19,19,19	0
57	MG	YA	3064	1/1	0.95	0.13	12,12,12,12	0
57	MG	XA	1601	1/1	0.95	0.13	13,13,13,13	0
57	MG	YA	3324	1/1	0.95	0.19	6,6,6,6	0
57	MG	RA	3120	1/1	0.95	0.10	4,4,4,4	0
57	MG	YA	3026	1/1	0.95	0.14	15,15,15,15	0
57	MG	XM	201	1/1	0.95	0.08	49,49,49,49	0
57	MG	QX	101	1/1	0.95	0.21	31,31,31,31	0
57	MG	YA	3205	1/1	0.95	0.23	25,25,25,25	0
57	MG	YA	3116	1/1	0.95	0.09	26,26,26,26	0
57	MG	QA	1634	1/1	0.95	0.20	44,44,44,44	0
57	MG	YA	3209	1/1	0.95	0.11	31,31,31,31	0
57	MG	XV	103	1/1	0.95	0.09	25,25,25,25	0
57	MG	YA	3032	1/1	0.95	0.18	16,16,16,16	0
57	MG	RA	3223	1/1	0.95	0.10	26,26,26,26	0
57	MG	YA	3161	1/1	0.95	0.13	35,35,35,35	0
57	MG	RA	3205	1/1	0.95	0.17	21,21,21,21	0
57	MG	QA	1654	1/1	0.95	0.12	28,28,28,28	0
57	MG	YA	3082	1/1	0.95	0.12	25,25,25,25	0
57	MG	RA	3056	1/1	0.95	0.13	21,21,21,21	0
57	MG	RA	3251	1/1	0.95	0.20	44,44,44,44	0
57	MG	RA	3302	1/1	0.95	0.06	38,38,38,38	0
57	MG	RB	201	1/1	0.95	0.16	29,29,29,29	0
57	MG	RA	3230	1/1	0.95	0.17	22,22,22,22	0
57	MG	YA	3228	1/1	0.95	0.24	24,24,24,24	0
57	MG	RA	3277	1/1	0.95	0.08	59,59,59,59	0
57	MG	YA	3231	1/1	0.95	0.09	24,24,24,24	0
57	MG	RA	3253	1/1	0.95	0.10	29,29,29,29	0
57	MG	RA	3048	1/1	0.95	0.09	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	ZN	XN	101	1/1	0.95	0.10	64,64,64,64	0
57	MG	YA	3238	1/1	0.95	0.09	16,16,16,16	0
57	MG	QA	1673	1/1	0.95	0.13	48,48,48,48	0
57	MG	QA	1648	1/1	0.96	0.14	28,28,28,28	0
57	MG	QA	1659	1/1	0.96	0.20	37,37,37,37	0
57	MG	XA	1662	1/1	0.96	0.12	58,58,58,58	0
57	MG	YA	3291	1/1	0.96	0.17	37,37,37,37	0
57	MG	YA	3222	1/1	0.96	0.19	23,23,23,23	0
57	MG	YA	3020	1/1	0.96	0.16	26,26,26,26	0
57	MG	YA	3067	1/1	0.96	0.14	22,22,22,22	0
57	MG	RE	301	1/1	0.96	0.18	15,15,15,15	0
57	MG	YA	3227	1/1	0.96	0.23	37,37,37,37	0
57	MG	YA	3070	1/1	0.96	0.12	26,26,26,26	0
57	MG	YA	3229	1/1	0.96	0.10	17,17,17,17	0
57	MG	RA	3075	1/1	0.96	0.12	7,7,7,7	0
57	MG	RA	3219	1/1	0.96	0.05	20,20,20,20	0
57	MG	YA	3234	1/1	0.96	0.18	24,24,24,24	0
57	MG	RA	3247	1/1	0.96	0.25	41,41,41,41	0
57	MG	YA	3236	1/1	0.96	0.22	31,31,31,31	0
57	MG	RA	3034	1/1	0.96	0.19	14,14,14,14	0
57	MG	YA	3171	1/1	0.96	0.46	35,35,35,35	0
57	MG	YA	3239	1/1	0.96	0.17	36,36,36,36	0
57	MG	XA	1672	1/1	0.96	0.17	21,21,21,21	0
57	MG	YA	3126	1/1	0.96	0.06	30,30,30,30	0
57	MG	RA	3222	1/1	0.96	0.15	22,22,22,22	0
57	MG	RA	3077	1/1	0.96	0.16	15,15,15,15	0
57	MG	QA	1618	1/1	0.96	0.23	24,24,24,24	0
57	MG	RA	3282	1/1	0.96	0.14	37,37,37,37	0
57	MG	YA	3084	1/1	0.96	0.10	24,24,24,24	0
57	MG	RA	3049	1/1	0.96	0.19	6,6,6,6	0
57	MG	YA	3033	1/1	0.96	0.18	15,15,15,15	0
57	MG	RA	3227	1/1	0.96	0.16	29,29,29,29	0
57	MG	YA	3318	1/1	0.96	0.17	9,9,9,9	0
57	MG	RA	3024	1/1	0.96	0.18	16,16,16,16	0
57	MG	YA	3252	1/1	0.96	0.18	33,33,33,33	0
57	MG	QA	1611	1/1	0.96	0.14	39,39,39,39	0
57	MG	RA	3231	1/1	0.96	0.20	27,27,27,27	0
57	MG	RA	3289	1/1	0.96	0.18	42,42,42,42	0
57	MG	RA	3101	1/1	0.96	0.19	10,10,10,10	0
57	MG	RA	3291	1/1	0.96	0.24	50,50,50,50	0
57	MG	Y0	102	1/1	0.96	0.17	13,13,13,13	0
57	MG	YB	202	1/1	0.96	0.14	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1608	1/1	0.96	0.21	18,18,18,18	0
57	MG	YB	204	1/1	0.96	0.04	41,41,41,41	0
57	MG	XA	1609	1/1	0.96	0.12	15,15,15,15	0
57	MG	YA	3197	1/1	0.96	0.10	21,21,21,21	0
57	MG	YA	3264	1/1	0.96	0.23	39,39,39,39	0
57	MG	RA	3010	1/1	0.96	0.14	12,12,12,12	0
57	MG	RA	3234	1/1	0.96	0.06	34,34,34,34	0
57	MG	RA	3235	1/1	0.96	0.24	36,36,36,36	0
57	MG	QD	303	1/1	0.96	0.06	58,58,58,58	0
57	MG	RA	3265	1/1	0.96	0.13	26,26,26,26	0
57	MG	RA	3041	1/1	0.96	0.15	3,3,3,3	0
57	MG	YA	3204	1/1	0.96	0.16	16,16,16,16	0
57	MG	YA	3273	1/1	0.96	0.04	39,39,39,39	0
57	MG	RA	3299	1/1	0.96	0.08	22,22,22,22	0
57	MG	YA	3151	1/1	0.96	0.14	28,28,28,28	0
57	MG	YA	3276	1/1	0.96	0.24	46,46,46,46	0
57	MG	RA	3012	1/1	0.96	0.10	25,25,25,25	0
57	MG	YA	3278	1/1	0.96	0.10	45,45,45,45	0
57	MG	YA	3208	1/1	0.96	0.15	20,20,20,20	0
57	MG	RA	3029	1/1	0.96	0.21	16,16,16,16	0
59	ZN	QN	101	1/1	0.96	0.13	59,59,59,59	0
57	MG	RA	3240	1/1	0.96	0.11	35,35,35,35	0
57	MG	YA	3211	1/1	0.96	0.24	36,36,36,36	0
57	MG	YA	3011	1/1	0.96	0.09	20,20,20,20	0
57	MG	XA	1700	1/1	0.96	0.19	36,36,36,36	0
57	MG	XA	1701	1/1	0.96	0.09	40,40,40,40	0
57	MG	RA	3089	1/1	0.96	0.16	4,4,4,4	0
57	MG	RA	3020	1/1	0.96	0.06	12,12,12,12	0
57	MG	YA	3265	1/1	0.97	0.30	62,62,62,62	0
57	MG	YA	3218	1/1	0.97	0.14	30,30,30,30	0
57	MG	QA	1649	1/1	0.97	0.06	26,26,26,26	0
57	MG	RA	3288	1/1	0.97	0.17	38,38,38,38	0
57	MG	YA	3079	1/1	0.97	0.13	1,1,1,1	0
57	MG	YA	3019	1/1	0.97	0.15	6,6,6,6	0
57	MG	YA	3081	1/1	0.97	0.14	27,27,27,27	0
57	MG	RA	3256	1/1	0.97	0.32	49,49,49,49	0
57	MG	YA	3083	1/1	0.97	0.13	17,17,17,17	0
57	MG	QA	1678	1/1	0.97	0.06	39,39,39,39	0
57	MG	RA	3258	1/1	0.97	0.26	51,51,51,51	0
57	MG	YA	3187	1/1	0.97	0.17	12,12,12,12	0
57	MG	YA	3188	1/1	0.97	0.18	5,5,5,5	0
57	MG	RA	3220	1/1	0.97	0.09	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3232	1/1	0.97	0.09	17,17,17,17	0
57	MG	YA	3326	1/1	0.97	0.16	21,21,21,21	0
57	MG	YA	3233	1/1	0.97	0.16	26,26,26,26	0
57	MG	RA	3105	1/1	0.97	0.13	37,37,37,37	0
57	MG	YA	3191	1/1	0.97	0.17	5,5,5,5	0
57	MG	YA	3192	1/1	0.97	0.24	13,13,13,13	0
57	MG	QA	1605	1/1	0.97	0.10	29,29,29,29	0
57	MG	YA	3056	1/1	0.97	0.09	15,15,15,15	0
57	MG	XA	1679	1/1	0.97	0.12	28,28,28,28	0
57	MG	YA	3196	1/1	0.97	0.24	26,26,26,26	0
57	MG	RA	3295	1/1	0.97	0.22	22,22,22,22	0
57	MG	XA	1681	1/1	0.97	0.19	32,32,32,32	0
57	MG	YD	303	1/1	0.97	0.08	31,31,31,31	0
57	MG	RA	3262	1/1	0.97	0.22	37,37,37,37	0
57	MG	RA	3040	1/1	0.97	0.16	23,23,23,23	0
57	MG	XA	1656	1/1	0.97	0.10	29,29,29,29	0
57	MG	RA	3224	1/1	0.97	0.12	19,19,19,19	0
57	MG	XA	1659	1/1	0.97	0.22	31,31,31,31	0
57	MG	RA	3181	1/1	0.97	0.13	26,26,26,26	0
57	MG	QA	1614	1/1	0.97	0.07	43,43,43,43	0
57	MG	QA	1615	1/1	0.97	0.14	46,46,46,46	0
57	MG	XA	1663	1/1	0.97	0.22	24,24,24,24	0
57	MG	XA	1715	1/1	0.97	0.21	45,45,45,45	0
57	MG	YA	3040	1/1	0.97	0.15	6,6,6,6	0
57	MG	XA	1665	1/1	0.97	0.26	24,24,24,24	0
57	MG	YA	3106	1/1	0.97	0.10	13,13,13,13	0
57	MG	RA	3057	1/1	0.97	0.16	16,16,16,16	0
57	MG	YA	3259	1/1	0.97	0.12	36,36,36,36	0
57	MG	YA	3213	1/1	0.97	0.18	17,17,17,17	0
57	MG	YA	3074	1/1	0.97	0.12	20,20,20,20	0
57	MG	YA	3175	1/1	0.97	0.10	15,15,15,15	0
57	MG	RA	3269	1/1	0.97	0.14	31,31,31,31	0
57	MG	QA	1661	1/1	0.97	0.09	16,16,16,16	0
57	MG	QE	201	1/1	0.98	0.13	31,31,31,31	0
57	MG	XA	1664	1/1	0.98	0.08	34,34,34,34	0
57	MG	XA	1611	1/1	0.98	0.04	35,35,35,35	0
57	MG	YA	3041	1/1	0.98	0.09	1,1,1,1	0
57	MG	RA	3198	1/1	0.98	0.19	15,15,15,15	0
57	MG	RA	3229	1/1	0.98	0.06	21,21,21,21	0
57	MG	YA	3044	1/1	0.98	0.07	5,5,5,5	0
57	MG	YA	3241	1/1	0.98	0.19	25,25,25,25	0
57	MG	RA	3085	1/1	0.98	0.07	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3073	1/1	0.98	0.10	33,33,33,33	0
57	MG	RA	3099	1/1	0.98	0.15	4,4,4,4	0
57	MG	YA	3028	1/1	0.98	0.13	18,18,18,18	0
57	MG	YA	3069	1/1	0.98	0.20	17,17,17,17	0
57	MG	YA	3223	1/1	0.98	0.10	14,14,14,14	0
57	MG	XA	1671	1/1	0.98	0.24	26,26,26,26	0
57	MG	RA	3177	1/1	0.98	0.15	1,1,1,1	0
57	MG	XA	1657	1/1	0.98	0.06	8,8,8,8	0
57	MG	RA	3087	1/1	0.98	0.11	15,15,15,15	0
57	MG	YA	3095	1/1	0.98	0.14	25,25,25,25	0
57	MG	XA	1619	1/1	0.98	0.24	23,23,23,23	0
57	MG	XA	1676	1/1	0.98	0.20	26,26,26,26	0
57	MG	YA	3304	1/1	0.98	0.16	33,33,33,33	0
57	MG	RA	3009	1/1	0.98	0.17	7,7,7,7	0
57	MG	QA	1607	1/1	0.98	0.16	19,19,19,19	0
57	MG	RA	3206	1/1	0.98	0.19	30,30,30,30	0
57	MG	RA	3030	1/1	0.99	0.09	8,8,8,8	0
57	MG	YA	3255	1/1	0.99	0.19	30,30,30,30	0
58	SF4	QD	301	8/8	0.99	0.04	47,50,57,83	0
58	SF4	XD	301	8/8	0.99	0.06	29,44,75,86	0

5.5 Other polymers

There are no such residues in this entry.