



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 12:41 AM UTC

PDB ID : 6OTR / pdb_00006otr
Title : Dimeric E.coli YoeB bound to Thermus thermophilus 70S post-cleavage (AAU)
Authors : Pavelich, I.P.; Hoffer, E.D.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2019-05-03
Resolution : 3.12 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

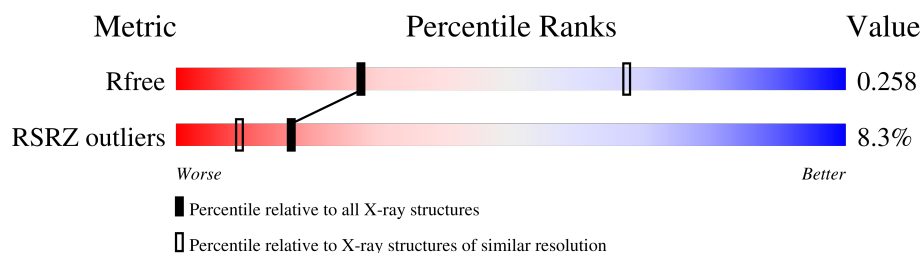
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.12 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	1816 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

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	1603	-	-	-	X
57	MG	QA	1609	-	-	-	X
57	MG	QA	1614	-	-	-	X
57	MG	QA	1618	-	-	-	X
57	MG	QA	1628	-	-	-	X
57	MG	QA	1630	-	-	-	X
57	MG	QA	1632	-	-	-	X
57	MG	QA	1638	-	-	-	X
57	MG	QA	1640	-	-	-	X
57	MG	QA	1643	-	-	-	X
57	MG	QA	1651	-	-	-	X
57	MG	QA	1655	-	-	-	X
57	MG	QA	1659	-	-	-	X
57	MG	QA	1676	-	-	-	X
57	MG	QA	1679	-	-	-	X
57	MG	QA	1680	-	-	-	X
57	MG	QA	1681	-	-	-	X
57	MG	QA	1682	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	QA	1687	-	-	-	X
57	MG	QE	201	-	-	-	X
57	MG	RA	3001	-	-	-	X
57	MG	RA	3138	-	-	-	X
57	MG	RA	3178	-	-	-	X
57	MG	RA	3262	-	-	-	X
57	MG	RA	3268	-	-	-	X
57	MG	RA	3273	-	-	-	X
57	MG	RA	3276	-	-	-	X
57	MG	RA	3277	-	-	-	X
57	MG	RA	3278	-	-	-	X
57	MG	RA	3283	-	-	-	X
57	MG	RA	3284	-	-	-	X
57	MG	RA	3287	-	-	-	X
57	MG	RA	3290	-	-	-	X
57	MG	RA	3294	-	-	-	X
57	MG	XA	1609	-	-	-	X
57	MG	XA	1613	-	-	-	X
57	MG	XA	1619	-	-	-	X
57	MG	XA	1636	-	-	-	X
57	MG	XA	1670	-	-	-	X
57	MG	XA	1681	-	-	-	X
57	MG	XA	1690	-	-	-	X
57	MG	XA	1692	-	-	-	X
57	MG	XA	1694	-	-	-	X
57	MG	XA	1696	-	-	-	X
57	MG	XA	1701	-	-	-	X
57	MG	XA	1704	-	-	-	X
57	MG	YA	3159	-	-	-	X
57	MG	YA	3192	-	-	-	X
57	MG	YA	3284	-	-	-	X
57	MG	YA	3286	-	-	-	X
57	MG	YA	3290	-	-	-	X
57	MG	YA	3293	-	-	-	X
57	MG	YA	3294	-	-	-	X
57	MG	YA	3297	-	-	-	X
57	MG	YA	3302	-	-	-	X
57	MG	YA	3303	-	-	-	X
57	MG	YA	3305	-	-	-	X
57	MG	YA	3312	-	-	-	X
57	MG	YA	3314	-	-	-	X
57	MG	YA	3316	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3318	-	-	-	X
57	MG	YA	3319	-	-	-	X
57	MG	YA	3329	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 298517 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			

Continued on next page...

Continued from previous page...

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 S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

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

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

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

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	XS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein Thx.

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

- Molecule 22 is a RNA chain called tRNA-fMet.

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

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	17	Total	C	N	O	P	0	0	0
			370	167	77	110	16			
23	XX	17	Total	C	N	O	P	0	0	0
			370	167	77	110	16			

- Molecule 24 is a protein called Addiction module toxin, Txe/YoeB family.

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

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			

Continued on next page...

Continued from previous page...

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

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
26	Y1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
27	Y2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 28 is a protein called 50S ribosomal protein L30.

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

- Molecule 29 is a protein called 50S ribosomal protein L31.

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

- Molecule 30 is a protein called 50S ribosomal protein L32.

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

- Molecule 31 is a protein called 50S ribosomal protein L33.

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

- Molecule 32 is a protein called 50S ribosomal protein L34.

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

- Molecule 33 is a protein called 50S ribosomal protein L35.

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

- Molecule 34 is a protein called 50S ribosomal protein L36.

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

- Molecule 35 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RA	2891	Total	C	N	O	P	0	0	0
			62266	27713	11649	20014	2890			
35	YA	2878	Total	C	N	O	P	0	0	0
			61981	27587	11589	19928	2877			

- Molecule 36 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
36	YB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 37 is a protein called 50S ribosomal protein L2.

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

- Molecule 38 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
38	YE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 39 is a protein called 50S ribosomal protein L4.

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

- Molecule 40 is a protein called 50S ribosomal protein L5.

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

- Molecule 41 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	YH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			

- Molecule 42 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RI	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
42	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 43 is a protein called 50S ribosomal protein L13.

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

- Molecule 44 is a protein called 50S ribosomal protein L14.

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

- Molecule 45 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
45	YP	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 46 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	RQ	139	Total	C	N	O	S	0	0	0
			1107	707	209	184	7			
46	YQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 47 is a protein called 50S ribosomal protein L17.

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

- Molecule 48 is a protein called 50S ribosomal protein L18.

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

- Molecule 49 is a protein called 50S ribosomal protein L19.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L21.

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

- Molecule 52 is a protein called 50S ribosomal protein L22.

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

- Molecule 53 is a protein called 50S ribosomal protein L23.

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

- Molecule 54 is a protein called 50S ribosomal protein L24.

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

- 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	87	Total	Mg	0	0
			87	87		

Continued on next page...

Continued from previous page...

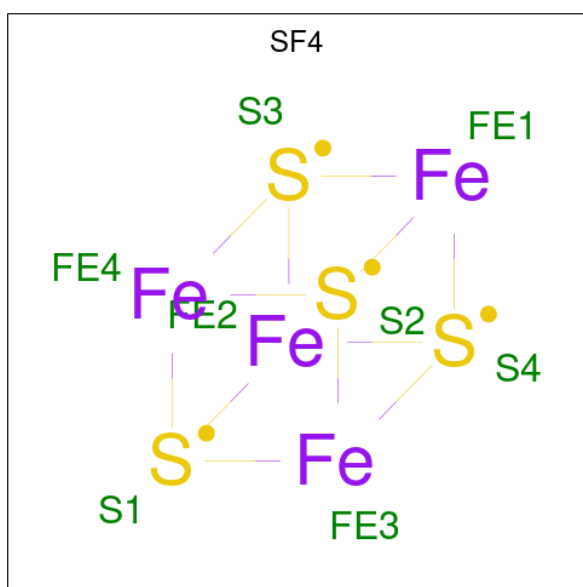
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QE	1	Total 1	Mg 1	0	0
57	QV	3	Total 3	Mg 3	0	0
57	R0	2	Total 2	Mg 2	0	0
57	R5	1	Total 1	Mg 1	0	0
57	RA	305	Total 305	Mg 305	0	0
57	RB	3	Total 3	Mg 3	0	0
57	RD	1	Total 1	Mg 1	0	0
57	RE	2	Total 2	Mg 2	0	0
57	RN	1	Total 1	Mg 1	0	0
57	RO	1	Total 1	Mg 1	0	0
57	RP	1	Total 1	Mg 1	0	0
57	RQ	1	Total 1	Mg 1	0	0
57	RR	1	Total 1	Mg 1	0	0
57	XA	106	Total 106	Mg 106	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
57	XV	4	Total 4	Mg 4	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	Y9	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YA	329	Total 329	Mg 329	0	0
57	YB	6	Total 6	Mg 6	0	0
57	YD	2	Total 2	Mg 2	0	0
57	YE	4	Total 4	Mg 4	0	0
57	YG	1	Total 1	Mg 1	0	0
57	YO	1	Total 1	Mg 1	0	0
57	YP	1	Total 1	Mg 1	0	0
57	YQ	1	Total 1	Mg 1	0	0
57	YR	1	Total 1	Mg 1	0	0
57	YS	1	Total 1	Mg 1	0	0
57	YV	1	Total 1	Mg 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

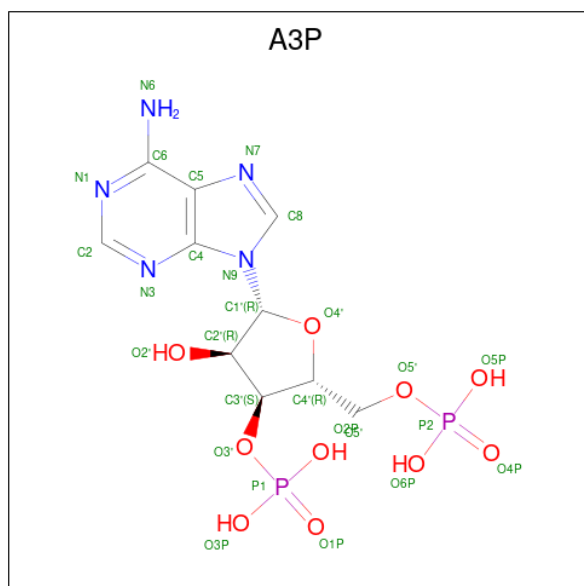


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	QD	1	Total	Fe	S	0	0
			8	4	4		
58	XD	1	Total	Fe	S	0	0
			8	4	4		

- 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	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	Y6	1	Total	Zn	0	0
			1	1		

- Molecule 60 is ADENOSINE-3'-5'-DIPHOSPHATE (CCD ID: A3P) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
60	QX	1	Total 26	C 10	N 5	O 9	P 2	0	0
60	XX	1	Total 26	C 10	N 5	O 9	P 2	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	213.36Å 451.70Å 607.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.15 – 3.12 146.15 – 3.12	Depositor EDS
% Data completeness (in resolution range)	98.6 (146.15-3.12) 98.6 (146.15-3.12)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.232 , 0.257 0.233 , 0.258	Depositor DCC
R_{free} test set	47520 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	62.4	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	298517	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% 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	$\# Z > 2$
56	PPU	ZB	3	56,35	37,40,41	1.30	4 (10%)	47,57,60	2.04	13 (27%)
56	PPU	ZA	3	56,35	37,40,41	1.32	4 (10%)	47,57,60	2.08	14 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PPU	ZB	3	56,35	-	3/25/43/44	0/4/4/4
56	PPU	ZA	3	56,35	-	4/25/43/44	0/4/4/4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	ZA	3	PPU	C5-C4	5.12	1.48	1.39
56	ZB	3	PPU	C5-C4	5.08	1.48	1.39
56	ZB	3	PPU	C5-C6	3.24	1.49	1.41
56	ZA	3	PPU	C5-C6	3.23	1.49	1.41
56	ZA	3	PPU	C6-N6	2.13	1.42	1.36

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	ZA	3	PPU	C5-C4-N3	-5.72	118.83	126.72
56	ZB	3	PPU	C5-C4-N3	-5.68	118.89	126.72
56	ZB	3	PPU	C2-N1-C6	4.53	122.90	111.83
56	ZA	3	PPU	C2-N1-C6	4.49	122.79	111.83
56	ZA	3	PPU	N3-C4-N9	4.33	134.53	127.17

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	ZB	3	PPU	CE1-CZ-OC-CM
56	ZB	3	PPU	CE2-CZ-OC-CM
56	ZA	3	PPU	CE1-CZ-OC-CM
56	ZA	3	PPU	CE2-CZ-OC-CM
56	ZA	3	PPU	C5-C6-N6-C9

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 883 ligands modelled in this entry, 879 are monoatomic - leaving 4 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	QD	301	4	0,12,12	-	-	-		
60	A3P	QX	101	23	25,28,29	3.29	9 (36%)	37,42,45	2.17	10 (27%)
58	SF4	XD	301	4	0,12,12	-	-	-		
60	A3P	XX	101	23	25,28,29	3.33	8 (32%)	37,42,45	2.19	12 (32%)

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	QD	301	4	-	-	0/6/5/5
60	A3P	QX	101	23	-	2/12/30/31	0/3/3/3
60	A3P	XX	101	23	-	1/12/30/31	0/3/3/3
58	SF4	XD	301	4	-	-	0/6/5/5

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	XX	101	A3P	O4'-C1'	10.82	1.67	1.42
60	QX	101	A3P	O4'-C1'	10.54	1.66	1.42
60	XX	101	A3P	C2'-C1'	-6.65	1.32	1.53
60	QX	101	A3P	C2'-C1'	-6.55	1.32	1.53
60	QX	101	A3P	O4'-C4'	-6.34	1.30	1.45

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	QX	101	A3P	C5-C4-N3	-6.34	117.99	126.72
60	XX	101	A3P	C5-C4-N3	-6.21	118.16	126.72
60	XX	101	A3P	N3-C2-N1	-5.01	120.99	128.58
60	QX	101	A3P	N3-C2-N1	-4.87	121.22	128.58
60	XX	101	A3P	C2-N3-C4	4.29	122.30	111.83

There are no chirality outliers.

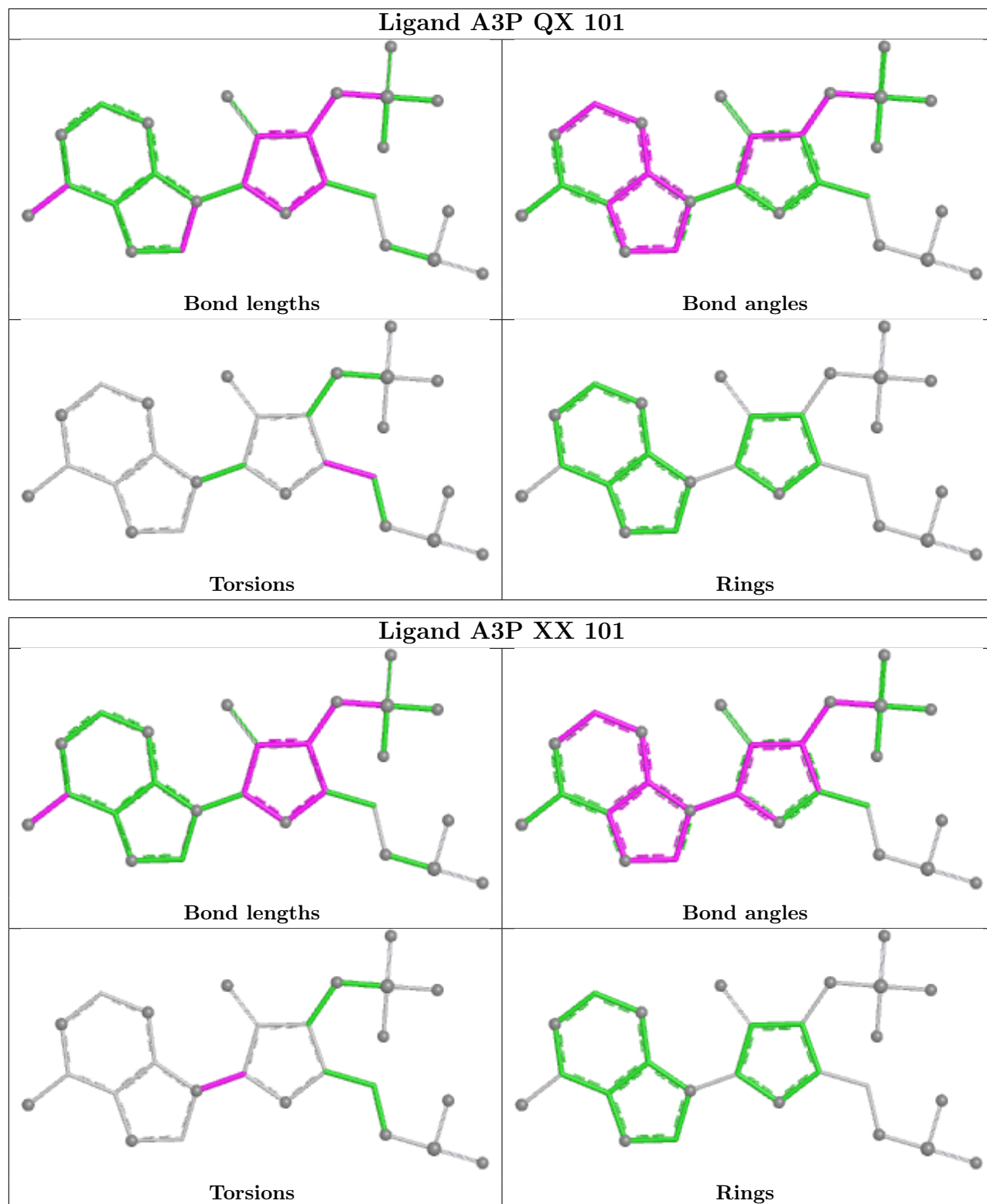
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	QX	101	A3P	O4'-C4'-C5'-O5'
60	QX	101	A3P	C3'-C4'-C5'-O5'
60	XX	101	A3P	O4'-C1'-N9-C8

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

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%)	0.37	65 (4%) 40 22	48, 83, 151, 349	0
1	XA	1507/1521 (99%)	0.28	62 (4%) 41 23	40, 76, 121, 310	0
2	QB	235/256 (91%)	1.05	30 (12%) 7 4	83, 117, 168, 203	0
2	XB	236/256 (92%)	0.92	26 (11%) 10 6	55, 99, 156, 185	0
3	QC	205/239 (85%)	1.11	28 (13%) 6 3	82, 107, 146, 165	0
3	XC	205/239 (85%)	0.98	24 (11%) 9 5	57, 85, 114, 145	0
4	QD	208/209 (99%)	0.49	3 (1%) 73 53	52, 72, 99, 110	0
4	XD	208/209 (99%)	0.80	18 (8%) 16 9	50, 72, 92, 119	0
5	QE	151/162 (93%)	0.86	11 (7%) 21 11	49, 74, 101, 148	0
5	XE	151/162 (93%)	0.57	8 (5%) 32 17	48, 65, 96, 134	0
6	QF	101/101 (100%)	0.72	5 (4%) 34 18	61, 85, 109, 126	0
6	XF	101/101 (100%)	0.38	1 (0%) 79 61	50, 74, 98, 133	0
7	QG	155/156 (99%)	1.44	35 (22%) 2 1	91, 115, 137, 158	0
7	XG	155/156 (99%)	0.94	19 (12%) 8 5	67, 91, 125, 144	0
8	QH	137/138 (99%)	0.76	7 (5%) 33 18	58, 79, 100, 118	0
8	XH	137/138 (99%)	0.77	9 (6%) 24 12	52, 71, 94, 125	0
9	QI	127/128 (99%)	1.26	26 (20%) 2 1	97, 130, 152, 170	0
9	XI	126/128 (98%)	1.40	23 (18%) 3 2	65, 102, 130, 137	0
10	QJ	99/105 (94%)	1.37	18 (18%) 3 2	107, 135, 177, 202	0
10	XJ	96/105 (91%)	1.59	29 (30%) 1 1	75, 115, 153, 171	0
11	QK	119/129 (92%)	1.60	29 (24%) 2 1	59, 93, 132, 181	0
11	XK	116/129 (89%)	0.59	3 (2%) 57 36	51, 72, 97, 144	0
12	QL	125/132 (94%)	0.71	9 (7%) 21 11	40, 62, 84, 170	0
12	XL	122/132 (92%)	0.53	7 (5%) 29 16	46, 56, 73, 96	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	120/126 (95%)	1.50	30 (25%) 2 1	83, 131, 157, 163	0
13	XM	119/126 (94%)	0.88	9 (7%) 20 10	67, 101, 120, 133	0
14	QN	60/61 (98%)	1.48	19 (31%) 1 1	85, 99, 136, 140	0
14	XN	60/61 (98%)	0.88	4 (6%) 24 12	65, 81, 106, 122	0
15	QO	88/89 (98%)	0.58	0 100 100	60, 77, 106, 118	0
15	XO	87/89 (97%)	0.66	1 (1%) 78 59	50, 71, 92, 96	0
16	QP	84/88 (95%)	1.00	12 (14%) 6 3	51, 74, 102, 145	0
16	XP	84/88 (95%)	0.80	6 (7%) 22 11	65, 78, 102, 158	0
17	QQ	100/105 (95%)	0.73	6 (6%) 27 15	48, 74, 100, 121	0
17	XQ	100/105 (95%)	0.55	4 (4%) 42 23	52, 73, 91, 100	0
18	QR	70/88 (79%)	0.64	2 (2%) 53 32	52, 90, 109, 126	0
18	XR	70/88 (79%)	0.55	2 (2%) 53 32	58, 75, 109, 133	0
19	QS	83/93 (89%)	1.13	12 (14%) 6 3	81, 136, 157, 164	0
19	XS	83/93 (89%)	0.86	7 (8%) 17 9	74, 98, 139, 152	0
20	QT	99/106 (93%)	1.24	17 (17%) 4 2	67, 88, 148, 170	0
20	XT	99/106 (93%)	1.13	18 (18%) 3 2	70, 96, 142, 174	0
21	QU	25/27 (92%)	1.70	10 (40%) 1 0	94, 125, 161, 170	0
21	XU	25/27 (92%)	1.31	6 (24%) 2 1	82, 102, 121, 153	0
22	QV	77/77 (100%)	0.43	1 (1%) 75 56	45, 102, 144, 212	0
22	QW	77/77 (100%)	1.79	28 (36%) 1 1	92, 188, 251, 253	0
22	XV	77/77 (100%)	0.68	3 (3%) 43 24	39, 86, 126, 155	0
22	XW	77/77 (100%)	2.00	32 (41%) 0 0	92, 232, 262, 271	0
23	QX	17/20 (85%)	2.40	10 (58%) 0 0	74, 190, 245, 247	0
23	XX	17/20 (85%)	2.35	9 (52%) 0 0	58, 174, 245, 248	0
24	QY	84/84 (100%)	0.83	8 (9%) 14 7	61, 87, 115, 169	0
24	QZ	84/84 (100%)	0.72	5 (5%) 27 15	98, 140, 171, 180	0
24	XY	84/84 (100%)	0.92	8 (9%) 14 7	50, 76, 104, 129	0
24	XZ	84/84 (100%)	1.36	17 (20%) 3 1	91, 138, 180, 184	0
25	R0	81/85 (95%)	0.50	3 (3%) 45 25	42, 58, 85, 91	0
25	Y0	82/85 (96%)	0.47	3 (3%) 45 25	41, 58, 80, 88	0
26	R1	97/98 (98%)	1.48	23 (23%) 2 1	37, 66, 132, 195	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
26	Y1	97/98 (98%)	0.56	5 (5%)	33 17	31, 51, 80, 88	0
27	R2	69/72 (95%)	0.73	5 (7%)	21 11	61, 83, 115, 145	0
27	Y2	69/72 (95%)	0.71	8 (11%)	9 5	43, 64, 82, 93	0
28	R3	59/60 (98%)	0.40	2 (3%)	48 28	49, 60, 107, 129	0
28	Y3	59/60 (98%)	0.55	4 (6%)	23 12	48, 65, 106, 139	0
29	R4	69/71 (97%)	1.80	26 (37%)	1 0	102, 160, 187, 232	0
29	Y4	69/71 (97%)	1.12	12 (17%)	4 2	78, 118, 162, 197	0
30	R5	59/60 (98%)	0.40	0	100 100	36, 63, 113, 140	0
30	Y5	59/60 (98%)	0.88	9 (15%)	5 2	43, 60, 117, 140	0
31	R6	53/54 (98%)	1.03	4 (7%)	20 11	77, 106, 138, 149	0
31	Y6	53/54 (98%)	1.12	7 (13%)	7 4	66, 86, 124, 132	0
32	R7	47/49 (95%)	0.57	6 (12%)	7 4	34, 41, 63, 108	0
32	Y7	48/49 (97%)	0.37	4 (8%)	17 9	23, 34, 70, 108	0
33	R8	64/65 (98%)	0.66	3 (4%)	36 19	35, 54, 71, 92	0
33	Y8	64/65 (98%)	0.75	4 (6%)	26 14	33, 52, 64, 77	0
34	R9	37/37 (100%)	1.90	12 (32%)	1 1	69, 108, 139, 149	0
34	Y9	37/37 (100%)	1.63	13 (35%)	1 1	81, 98, 123, 138	0
35	RA	2891/2915 (99%)	0.27	118 (4%)	41 23	28, 62, 147, 342	0
35	YA	2878/2915 (98%)	0.14	117 (4%)	41 23	23, 55, 136, 334	0
36	RB	122/124 (98%)	0.31	5 (4%)	41 23	64, 111, 132, 240	0
36	YB	122/124 (98%)	0.16	0	100 100	56, 84, 114, 250	0
37	RD	272/276 (98%)	0.67	20 (7%)	20 11	34, 54, 75, 98	0
37	YD	274/276 (99%)	0.23	5 (1%)	67 46	23, 39, 52, 67	0
38	RE	205/206 (99%)	0.92	24 (11%)	9 5	40, 74, 107, 132	0
38	YE	204/206 (99%)	0.70	12 (5%)	28 15	37, 65, 95, 128	0
39	RF	202/210 (96%)	0.34	4 (1%)	65 44	26, 47, 83, 94	0
39	YF	202/210 (96%)	0.51	10 (4%)	34 18	29, 59, 106, 122	0
40	RG	181/182 (99%)	1.01	14 (7%)	19 10	85, 117, 146, 168	0
40	YG	181/182 (99%)	1.31	38 (20%)	2 1	71, 100, 122, 141	0
41	RH	174/180 (96%)	1.65	54 (31%)	1 1	92, 134, 166, 238	0
41	YH	174/180 (96%)	1.49	49 (28%)	1 1	69, 106, 153, 171	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
42	RI	145/148 (97%)	1.27	26 (17%) 3 2	74, 98, 118, 137	0
42	YI	146/148 (98%)	1.06	17 (11%) 9 5	50, 92, 118, 132	0
43	RN	138/140 (98%)	1.27	22 (15%) 5 2	43, 76, 113, 146	0
43	YN	138/140 (98%)	0.96	15 (10%) 10 6	46, 71, 109, 142	0
44	RO	122/122 (100%)	0.54	4 (3%) 49 29	41, 65, 83, 99	0
44	YO	122/122 (100%)	0.53	5 (4%) 41 23	35, 56, 72, 90	0
45	RP	150/150 (100%)	1.11	22 (14%) 6 3	31, 70, 105, 182	0
45	YP	147/150 (98%)	0.65	12 (8%) 17 9	37, 58, 86, 107	0
46	RQ	139/141 (98%)	1.21	23 (16%) 4 2	36, 75, 98, 119	0
46	YQ	141/141 (100%)	0.44	3 (2%) 63 42	32, 60, 81, 106	0
47	RR	117/118 (99%)	0.69	8 (6%) 23 12	43, 65, 99, 125	0
47	YR	117/118 (99%)	0.85	12 (10%) 12 6	46, 60, 79, 115	0
48	RS	111/112 (99%)	1.36	25 (22%) 2 1	85, 105, 134, 179	0
48	YS	111/112 (99%)	0.64	8 (7%) 21 11	60, 74, 91, 108	0
49	RT	137/146 (93%)	0.89	17 (12%) 8 5	57, 77, 130, 162	0
49	YT	137/146 (93%)	0.84	16 (11%) 9 5	48, 68, 144, 248	0
50	RU	117/118 (99%)	0.33	2 (1%) 69 48	29, 53, 96, 150	0
50	YU	117/118 (99%)	0.78	11 (9%) 14 8	42, 63, 96, 123	0
51	RV	101/101 (100%)	0.39	2 (1%) 65 44	30, 71, 101, 112	0
51	YV	101/101 (100%)	1.06	15 (14%) 5 3	39, 83, 115, 164	0
52	RW	113/113 (100%)	0.56	5 (4%) 39 21	38, 54, 85, 163	0
52	YW	113/113 (100%)	0.64	11 (9%) 13 7	37, 56, 87, 184	0
53	RX	92/96 (95%)	0.56	5 (5%) 31 17	46, 66, 87, 94	0
53	YX	92/96 (95%)	0.15	2 (2%) 62 41	31, 51, 79, 91	0
54	RY	107/110 (97%)	1.65	31 (28%) 1 1	46, 74, 120, 147	0
54	YY	107/110 (97%)	0.76	9 (8%) 17 9	49, 77, 102, 120	0
55	RZ	183/206 (88%)	1.18	27 (14%) 5 3	82, 106, 128, 155	0
55	YZ	183/206 (88%)	0.63	7 (3%) 44 25	70, 95, 118, 133	0
56	ZA	2/3 (66%)	0.88	0 100 100	62, 62, 62, 65	0
56	ZB	2/3 (66%)	-0.14	0 100 100	39, 39, 39, 43	0
All	All	21368/21938 (97%)	0.62	1766 (8%) 17 9	23, 74, 144, 349	0

The worst 5 of 1766 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	QK	129	SER	13.6
26	R1	95	LEU	9.5
26	R1	96	LYS	8.6
34	R9	1	MET	8.0
54	RY	62	GLU	8.0

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
56	PPU	ZA	3	37/38	0.93	0.14	32,40,48,51	0
56	PPU	ZB	3	37/38	0.93	0.12	21,34,43,48	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
57	MG	YA	3305	1/1	-0.26	0.47	74,74,74,74	0
57	MG	QA	1614	1/1	-0.15	0.48	116,116,116,116	0
57	MG	YB	205	1/1	-0.15	0.18	120,120,120,120	0
57	MG	XA	1704	1/1	-0.01	0.50	47,47,47,47	0
57	MG	QA	1686	1/1	0.03	0.23	139,139,139,139	0
57	MG	YA	3289	1/1	0.08	0.29	88,88,88,88	0
57	MG	XA	1692	1/1	0.14	0.44	104,104,104,104	0
57	MG	RA	3269	1/1	0.19	0.35	99,99,99,99	0
57	MG	RA	3278	1/1	0.21	0.48	99,99,99,99	0
57	MG	QA	1681	1/1	0.22	0.57	162,162,162,162	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3280	1/1	0.24	0.34	124,124,124,124	0
57	MG	XA	1686	1/1	0.25	0.23	126,126,126,126	0
57	MG	QA	1638	1/1	0.28	0.57	133,133,133,133	0
57	MG	YA	3307	1/1	0.29	0.37	96,96,96,96	0
57	MG	XA	1687	1/1	0.29	0.21	144,144,144,144	0
57	MG	YA	3316	1/1	0.30	0.46	125,125,125,125	0
57	MG	RA	3272	1/1	0.30	0.34	128,128,128,128	0
57	MG	XA	1691	1/1	0.31	0.31	90,90,90,90	0
57	MG	RA	3263	1/1	0.31	0.21	86,86,86,86	0
57	MG	YA	3285	1/1	0.32	0.37	58,58,58,58	0
57	MG	YA	3136	1/1	0.32	0.35	89,89,89,89	0
57	MG	QA	1680	1/1	0.33	0.52	95,95,95,95	0
57	MG	QA	1603	1/1	0.33	0.55	102,102,102,102	0
57	MG	QA	1659	1/1	0.34	0.41	100,100,100,100	0
57	MG	YA	3318	1/1	0.35	0.42	87,87,87,87	0
57	MG	RA	3277	1/1	0.38	0.54	122,122,122,122	0
57	MG	XA	1631	1/1	0.39	0.37	112,112,112,112	0
57	MG	QA	1687	1/1	0.42	0.54	126,126,126,126	0
57	MG	RA	3297	1/1	0.42	0.12	62,62,62,62	0
57	MG	YA	3308	1/1	0.43	0.29	119,119,119,119	0
57	MG	R5	101	1/1	0.44	0.33	102,102,102,102	0
57	MG	QE	201	1/1	0.45	0.46	109,109,109,109	0
57	MG	QA	1683	1/1	0.45	0.37	105,105,105,105	0
57	MG	QA	1643	1/1	0.46	0.46	105,105,105,105	0
57	MG	XA	1702	1/1	0.46	0.30	111,111,111,111	0
57	MG	XA	1690	1/1	0.46	0.43	83,83,83,83	0
57	MG	YA	3320	1/1	0.46	0.23	85,85,85,85	0
57	MG	QA	1679	1/1	0.46	0.45	126,126,126,126	0
57	MG	XA	1636	1/1	0.47	0.57	102,102,102,102	0
57	MG	XA	1696	1/1	0.47	0.70	64,64,64,64	0
57	MG	XA	1698	1/1	0.47	0.30	134,134,134,134	0
57	MG	RA	3276	1/1	0.48	0.51	136,136,136,136	0
57	MG	QA	1618	1/1	0.49	0.55	105,105,105,105	0
57	MG	RA	3265	1/1	0.49	0.39	192,192,192,192	0
57	MG	XA	1685	1/1	0.50	0.19	87,87,87,87	0
57	MG	QA	1682	1/1	0.50	0.46	109,109,109,109	0
57	MG	XA	1700	1/1	0.50	0.23	154,154,154,154	0
57	MG	QA	1677	1/1	0.51	0.18	119,119,119,119	0
57	MG	XA	1613	1/1	0.51	0.51	83,83,83,83	0
57	MG	YA	3317	1/1	0.51	0.21	147,147,147,147	0
57	MG	RA	3287	1/1	0.52	0.58	171,171,171,171	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3264	1/1	0.52	0.36	125,125,125,125	0
57	MG	QA	1639	1/1	0.52	0.29	86,86,86,86	0
57	MG	QA	1655	1/1	0.54	0.48	108,108,108,108	0
57	MG	QA	1676	1/1	0.55	0.67	132,132,132,132	0
57	MG	YA	3184	1/1	0.56	0.21	68,68,68,68	0
57	MG	RA	3284	1/1	0.57	0.57	29,29,29,29	0
57	MG	XA	1701	1/1	0.57	0.45	145,145,145,145	0
57	MG	RA	3292	1/1	0.57	0.28	73,73,73,73	0
57	MG	RA	3296	1/1	0.57	0.25	46,46,46,46	0
57	MG	YA	3319	1/1	0.58	0.79	42,42,42,42	0
57	MG	QA	1633	1/1	0.59	0.33	91,91,91,91	0
57	MG	RA	3290	1/1	0.59	0.49	73,73,73,73	0
57	MG	QA	1637	1/1	0.59	0.27	88,88,88,88	0
57	MG	RA	3294	1/1	0.59	0.62	123,123,123,123	0
57	MG	XA	1670	1/1	0.59	0.51	85,85,85,85	0
57	MG	RA	3285	1/1	0.59	0.20	50,50,50,50	0
57	MG	YA	3192	1/1	0.60	0.62	93,93,93,93	0
57	MG	RA	3270	1/1	0.61	0.26	116,116,116,116	0
57	MG	XA	1703	1/1	0.62	0.17	182,182,182,182	0
57	MG	XA	1669	1/1	0.62	0.38	73,73,73,73	0
57	MG	YA	3302	1/1	0.62	0.58	116,116,116,116	0
57	MG	RA	3262	1/1	0.62	0.41	102,102,102,102	0
57	MG	XA	1695	1/1	0.62	0.37	96,96,96,96	0
57	MG	QA	1626	1/1	0.62	0.27	122,122,122,122	0
57	MG	RA	3283	1/1	0.63	0.54	99,99,99,99	0
57	MG	QA	1651	1/1	0.63	0.78	98,98,98,98	0
57	MG	XA	1697	1/1	0.63	0.13	127,127,127,127	0
57	MG	YA	3100	1/1	0.64	0.33	87,87,87,87	0
57	MG	YA	3314	1/1	0.64	0.53	39,39,39,39	0
57	MG	QA	1640	1/1	0.64	0.43	104,104,104,104	0
57	MG	RA	3138	1/1	0.64	0.51	120,120,120,120	0
57	MG	QA	1622	1/1	0.65	0.18	58,58,58,58	0
57	MG	XA	1651	1/1	0.65	0.39	59,59,59,59	0
57	MG	RA	3150	1/1	0.65	0.14	56,56,56,56	0
57	MG	XD	302	1/1	0.65	0.14	63,63,63,63	0
57	MG	YA	3313	1/1	0.65	0.37	96,96,96,96	0
57	MG	YA	3321	1/1	0.65	0.25	92,92,92,92	0
57	MG	RA	3268	1/1	0.65	0.64	130,130,130,130	0
57	MG	QA	1663	1/1	0.66	0.37	80,80,80,80	0
57	MG	RA	3293	1/1	0.67	0.26	140,140,140,140	0
57	MG	XA	1678	1/1	0.67	0.28	73,73,73,73	0
57	MG	YA	3110	1/1	0.67	0.16	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1679	1/1	0.67	0.40	98,98,98,98	0
57	MG	XA	1641	1/1	0.67	0.29	80,80,80,80	0
57	MG	RA	3271	1/1	0.67	0.35	84,84,84,84	0
57	MG	QA	1649	1/1	0.67	0.38	94,94,94,94	0
57	MG	XA	1609	1/1	0.68	0.48	61,61,61,61	0
57	MG	RA	3288	1/1	0.68	0.13	96,96,96,96	0
57	MG	RA	3181	1/1	0.69	0.19	61,61,61,61	0
57	MG	RA	3273	1/1	0.69	0.70	56,56,56,56	0
57	MG	QA	1657	1/1	0.69	0.33	66,66,66,66	0
57	MG	QA	1615	1/1	0.69	0.19	69,69,69,69	0
57	MG	YA	3312	1/1	0.69	0.52	118,118,118,118	0
57	MG	XA	1633	1/1	0.69	0.28	59,59,59,59	0
57	MG	YA	3294	1/1	0.69	0.55	152,152,152,152	0
57	MG	XA	1624	1/1	0.70	0.30	76,76,76,76	0
57	MG	YA	3297	1/1	0.70	1.18	63,63,63,63	0
57	MG	RA	3261	1/1	0.70	0.37	118,118,118,118	0
57	MG	QA	1647	1/1	0.70	0.31	105,105,105,105	0
57	MG	QA	1684	1/1	0.71	0.34	104,104,104,104	0
57	MG	YA	3311	1/1	0.71	0.28	131,131,131,131	0
57	MG	XA	1654	1/1	0.71	0.25	44,44,44,44	0
57	MG	YA	3286	1/1	0.71	0.53	145,145,145,145	0
57	MG	RA	3185	1/1	0.72	0.23	74,74,74,74	0
57	MG	RA	3001	1/1	0.72	0.61	161,161,161,161	0
57	MG	RA	3162	1/1	0.72	0.21	49,49,49,49	0
57	MG	XA	1705	1/1	0.72	0.18	81,81,81,81	0
57	MG	QA	1630	1/1	0.72	0.44	74,74,74,74	0
57	MG	RA	3295	1/1	0.73	0.33	95,95,95,95	0
57	MG	RA	3235	1/1	0.73	0.16	33,33,33,33	0
57	MG	YA	3290	1/1	0.73	0.87	55,55,55,55	0
57	MG	YA	3281	1/1	0.73	0.32	27,27,27,27	0
57	MG	YA	3171	1/1	0.73	0.23	48,48,48,48	0
57	MG	YB	206	1/1	0.73	0.21	142,142,142,142	0
57	MG	RE	301	1/1	0.74	0.25	57,57,57,57	0
57	MG	RA	3174	1/1	0.74	0.39	58,58,58,58	0
57	MG	RA	3178	1/1	0.74	0.42	73,73,73,73	0
57	MG	YA	3329	1/1	0.74	0.49	49,49,49,49	0
57	MG	RA	3286	1/1	0.74	0.35	132,132,132,132	0
57	MG	QA	1624	1/1	0.74	0.21	63,63,63,63	0
57	MG	YE	302	1/1	0.74	0.29	59,59,59,59	0
57	MG	RA	3282	1/1	0.75	0.35	115,115,115,115	0
57	MG	XA	1638	1/1	0.75	0.34	59,59,59,59	0
57	MG	QA	1631	1/1	0.75	0.32	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3284	1/1	0.75	0.49	134,134,134,134	0
57	MG	YA	3298	1/1	0.75	0.26	50,50,50,50	0
57	MG	XA	1642	1/1	0.75	0.22	79,79,79,79	0
57	MG	YA	3303	1/1	0.75	0.42	132,132,132,132	0
57	MG	XA	1694	1/1	0.75	0.42	159,159,159,159	0
57	MG	YA	3273	1/1	0.76	0.16	37,37,37,37	0
57	MG	YA	3299	1/1	0.76	0.31	54,54,54,54	0
57	MG	XA	1706	1/1	0.76	0.18	104,104,104,104	0
57	MG	XA	1699	1/1	0.76	0.34	106,106,106,106	0
57	MG	YA	3304	1/1	0.76	0.36	118,118,118,118	0
57	MG	XA	1681	1/1	0.76	0.44	77,77,77,77	0
57	MG	QA	1685	1/1	0.76	0.30	117,117,117,117	0
57	MG	QA	1644	1/1	0.76	0.18	82,82,82,82	0
57	MG	XA	1644	1/1	0.76	0.32	71,71,71,71	0
57	MG	XA	1646	1/1	0.76	0.35	78,78,78,78	0
57	MG	RA	3075	1/1	0.76	0.26	48,48,48,48	0
57	MG	QA	1632	1/1	0.77	0.40	71,71,71,71	0
57	MG	QA	1628	1/1	0.77	0.76	82,82,82,82	0
57	MG	RA	3281	1/1	0.77	0.26	121,121,121,121	0
57	MG	YA	3326	1/1	0.77	0.27	59,59,59,59	0
57	MG	YA	3293	1/1	0.77	0.42	130,130,130,130	0
57	MG	XA	1688	1/1	0.77	0.33	112,112,112,112	0
57	MG	YA	3159	1/1	0.77	0.50	73,73,73,73	0
57	MG	RA	3184	1/1	0.77	0.12	60,60,60,60	0
57	MG	QA	1661	1/1	0.78	0.38	71,71,71,71	0
57	MG	QA	1609	1/1	0.78	0.51	60,60,60,60	0
57	MG	YA	3052	1/1	0.78	0.19	41,41,41,41	0
57	MG	YA	3177	1/1	0.78	0.16	45,45,45,45	0
57	MG	YA	3094	1/1	0.78	0.18	41,41,41,41	0
57	MG	RA	3135	1/1	0.78	0.26	49,49,49,49	0
57	MG	YA	3267	1/1	0.78	0.27	48,48,48,48	0
57	MG	QA	1645	1/1	0.78	0.17	71,71,71,71	0
57	MG	YA	3265	1/1	0.79	0.25	46,46,46,46	0
57	MG	QA	1650	1/1	0.79	0.20	81,81,81,81	0
57	MG	RA	3188	1/1	0.79	0.14	48,48,48,48	0
57	MG	RA	3266	1/1	0.79	0.39	102,102,102,102	0
57	MG	XA	1619	1/1	0.79	0.47	61,61,61,61	0
57	MG	QA	1604	1/1	0.79	0.29	73,73,73,73	0
57	MG	YA	3117	1/1	0.79	0.26	38,38,38,38	0
57	MG	YE	304	1/1	0.79	0.14	58,58,58,58	0
57	MG	RA	3189	1/1	0.80	0.32	55,55,55,55	0
57	MG	QA	1616	1/1	0.80	0.14	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3275	1/1	0.80	0.29	162,162,162,162	0
57	MG	RA	3245	1/1	0.80	0.27	43,43,43,43	0
57	MG	YA	3292	1/1	0.80	0.28	123,123,123,123	0
57	MG	YA	3158	1/1	0.80	0.07	37,37,37,37	0
57	MG	RA	3256	1/1	0.80	0.27	44,44,44,44	0
57	MG	RA	3129	1/1	0.80	0.08	35,35,35,35	0
57	MG	XA	1637	1/1	0.80	0.36	72,72,72,72	0
57	MG	QA	1634	1/1	0.80	0.28	51,51,51,51	0
57	MG	XA	1680	1/1	0.80	0.29	59,59,59,59	0
57	MG	YA	3025	1/1	0.80	0.33	73,73,73,73	0
57	MG	YA	3040	1/1	0.80	0.21	28,28,28,28	0
57	MG	QA	1678	1/1	0.80	0.13	93,93,93,93	0
57	MG	YA	3083	1/1	0.80	0.11	28,28,28,28	0
57	MG	XA	1611	1/1	0.80	0.15	63,63,63,63	0
57	MG	YA	3229	1/1	0.81	0.28	39,39,39,39	0
57	MG	XA	1635	1/1	0.81	0.20	62,62,62,62	0
57	MG	RA	3098	1/1	0.81	0.18	29,29,29,29	0
57	MG	YA	3041	1/1	0.81	0.35	48,48,48,48	0
57	MG	YA	3296	1/1	0.81	0.36	182,182,182,182	0
57	MG	QA	1602	1/1	0.81	0.59	76,76,76,76	0
57	MG	RA	3038	1/1	0.81	0.28	22,22,22,22	0
57	MG	QA	1673	1/1	0.81	0.16	55,55,55,55	0
57	MG	XA	1661	1/1	0.81	0.44	87,87,87,87	0
57	MG	XA	1683	1/1	0.81	0.30	74,74,74,74	0
57	MG	Y5	3001	1/1	0.82	0.10	33,33,33,33	0
57	MG	QA	1641	1/1	0.82	0.41	65,65,65,65	0
57	MG	QA	1662	1/1	0.82	0.49	59,59,59,59	0
57	MG	RA	3118	1/1	0.82	0.34	43,43,43,43	0
57	MG	YA	3288	1/1	0.82	0.33	207,207,207,207	0
57	MG	XA	1693	1/1	0.82	0.38	139,139,139,139	0
57	MG	RO	201	1/1	0.82	0.15	54,54,54,54	0
57	MG	XA	1630	1/1	0.82	0.36	80,80,80,80	0
57	MG	RA	3058	1/1	0.82	0.14	39,39,39,39	0
57	MG	XA	1677	1/1	0.82	0.28	50,50,50,50	0
57	MG	XA	1610	1/1	0.82	0.31	58,58,58,58	0
57	MG	YA	3133	1/1	0.82	0.21	45,45,45,45	0
57	MG	RA	3128	1/1	0.83	0.29	49,49,49,49	0
57	MG	RA	3156	1/1	0.83	0.11	39,39,39,39	0
57	MG	XA	1682	1/1	0.83	0.31	57,57,57,57	0
57	MG	QA	1617	1/1	0.83	0.24	73,73,73,73	0
57	MG	XA	1655	1/1	0.83	0.29	47,47,47,47	0
57	MG	YA	3148	1/1	0.83	0.17	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3133	1/1	0.83	0.15	37,37,37,37	0
57	MG	RA	3111	1/1	0.83	0.09	36,36,36,36	0
57	MG	QA	1601	1/1	0.83	0.40	52,52,52,52	0
57	MG	YA	3306	1/1	0.83	0.27	45,45,45,45	0
57	MG	RN	201	1/1	0.83	0.20	51,51,51,51	0
57	MG	RA	3248	1/1	0.83	0.21	27,27,27,27	0
57	MG	YA	3185	1/1	0.83	0.51	87,87,87,87	0
57	MG	XA	1645	1/1	0.83	0.22	53,53,53,53	0
57	MG	YR	201	1/1	0.83	0.22	59,59,59,59	0
57	MG	YA	3310	1/1	0.84	0.39	159,159,159,159	0
57	MG	XA	1666	1/1	0.84	0.63	76,76,76,76	0
57	MG	RA	3217	1/1	0.84	0.29	47,47,47,47	0
57	MG	QA	1658	1/1	0.84	0.32	48,48,48,48	0
57	MG	RA	3147	1/1	0.84	0.10	54,54,54,54	0
57	MG	RA	3291	1/1	0.84	0.40	105,105,105,105	0
57	MG	RA	3101	1/1	0.84	0.23	27,27,27,27	0
57	MG	XA	1662	1/1	0.84	0.36	46,46,46,46	0
57	MG	YA	3309	1/1	0.84	0.30	144,144,144,144	0
57	MG	QA	1646	1/1	0.85	0.36	52,52,52,52	0
57	MG	XA	1627	1/1	0.85	0.21	100,100,100,100	0
57	MG	YA	3050	1/1	0.85	0.27	27,27,27,27	0
57	MG	RA	3159	1/1	0.85	0.19	24,24,24,24	0
57	MG	XA	1664	1/1	0.85	0.40	48,48,48,48	0
57	MG	YA	3091	1/1	0.85	0.12	40,40,40,40	0
57	MG	RA	3134	1/1	0.85	0.22	51,51,51,51	0
57	MG	QA	1636	1/1	0.85	0.33	56,56,56,56	0
57	MG	YA	3102	1/1	0.85	0.25	39,39,39,39	0
57	MG	QA	1619	1/1	0.85	0.31	66,66,66,66	0
57	MG	QA	1623	1/1	0.85	0.22	45,45,45,45	0
57	MG	QA	1671	1/1	0.85	0.35	55,55,55,55	0
57	MG	XA	1689	1/1	0.85	0.35	137,137,137,137	0
57	MG	QA	1613	1/1	0.86	0.29	59,59,59,59	0
57	MG	RA	3003	1/1	0.86	0.25	61,61,61,61	0
57	MG	RA	3259	1/1	0.86	0.27	44,44,44,44	0
57	MG	RP	201	1/1	0.86	0.22	32,32,32,32	0
57	MG	YA	3152	1/1	0.86	0.30	58,58,58,58	0
57	MG	XA	1603	1/1	0.86	0.25	70,70,70,70	0
57	MG	RA	3119	1/1	0.86	0.31	48,48,48,48	0
57	MG	QA	1648	1/1	0.86	0.26	65,65,65,65	0
57	MG	RA	3144	1/1	0.86	0.13	51,51,51,51	0
57	MG	XA	1640	1/1	0.86	0.35	59,59,59,59	0
57	MG	RA	3050	1/1	0.86	0.27	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1615	1/1	0.86	0.14	37,37,37,37	0
57	MG	RA	3237	1/1	0.86	0.20	41,41,41,41	0
57	MG	RA	3149	1/1	0.86	0.14	43,43,43,43	0
57	MG	QA	1669	1/1	0.87	0.16	47,47,47,47	0
57	MG	QA	1605	1/1	0.87	0.12	67,67,67,67	0
57	MG	QA	1672	1/1	0.87	0.29	62,62,62,62	0
57	MG	RA	3121	1/1	0.87	0.17	59,59,59,59	0
57	MG	RA	3154	1/1	0.87	0.15	46,46,46,46	0
57	MG	RA	3238	1/1	0.87	0.16	22,22,22,22	0
57	MG	RA	3070	1/1	0.87	0.27	24,24,24,24	0
57	MG	YA	3243	1/1	0.87	0.29	38,38,38,38	0
57	MG	QA	1610	1/1	0.87	0.32	58,58,58,58	0
57	MG	RA	3077	1/1	0.87	0.24	35,35,35,35	0
57	MG	RA	3090	1/1	0.87	0.22	60,60,60,60	0
57	MG	RA	3002	1/1	0.87	0.15	18,18,18,18	0
57	MG	RA	3279	1/1	0.87	0.28	126,126,126,126	0
57	MG	RA	3137	1/1	0.87	0.27	32,32,32,32	0
57	MG	YE	301	1/1	0.87	0.24	51,51,51,51	0
57	MG	RA	3183	1/1	0.87	0.17	47,47,47,47	0
57	MG	QA	1629	1/1	0.87	0.24	111,111,111,111	0
57	MG	RA	3139	1/1	0.87	0.26	45,45,45,45	0
60	A3P	QX	101	26/27	0.87	0.15	53,80,86,88	0
57	MG	XA	1648	1/1	0.88	0.26	100,100,100,100	0
57	MG	RA	3221	1/1	0.88	0.13	29,29,29,29	0
57	MG	YA	3268	1/1	0.88	0.10	44,44,44,44	0
57	MG	YA	3269	1/1	0.88	0.18	41,41,41,41	0
57	MG	RA	3113	1/1	0.88	0.17	41,41,41,41	0
57	MG	RA	3117	1/1	0.88	0.20	21,21,21,21	0
57	MG	YA	3001	1/1	0.88	0.30	29,29,29,29	0
57	MG	XA	1659	1/1	0.88	0.26	51,51,51,51	0
57	MG	RA	3289	1/1	0.88	0.36	191,191,191,191	0
57	MG	YA	3154	1/1	0.88	0.16	23,23,23,23	0
57	MG	RA	3186	1/1	0.88	0.21	138,138,138,138	0
57	MG	RA	3053	1/1	0.88	0.18	30,30,30,30	0
57	MG	YA	3162	1/1	0.88	0.20	44,44,44,44	0
57	MG	YA	3164	1/1	0.88	0.32	52,52,52,52	0
57	MG	QA	1620	1/1	0.88	0.36	46,46,46,46	0
57	MG	YA	3295	1/1	0.88	0.15	99,99,99,99	0
57	MG	YA	3071	1/1	0.88	0.24	15,15,15,15	0
57	MG	XA	1667	1/1	0.88	0.21	32,32,32,32	0
57	MG	XA	1602	1/1	0.88	0.46	46,46,46,46	0
57	MG	YA	3092	1/1	0.88	0.09	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3216	1/1	0.88	0.15	33,33,33,33	0
57	MG	QA	1627	1/1	0.88	0.10	44,44,44,44	0
57	MG	RA	3258	1/1	0.88	0.08	37,37,37,37	0
57	MG	YA	3262	1/1	0.88	0.11	24,24,24,24	0
57	MG	YA	3301	1/1	0.89	0.37	112,112,112,112	0
57	MG	YA	3231	1/1	0.89	0.20	29,29,29,29	0
57	MG	RA	3216	1/1	0.89	0.13	24,24,24,24	0
57	MG	YA	3256	1/1	0.89	0.27	39,39,39,39	0
57	MG	QA	1621	1/1	0.89	0.40	78,78,78,78	0
57	MG	YA	3141	1/1	0.89	0.32	43,43,43,43	0
57	MG	XA	1674	1/1	0.89	0.35	59,59,59,59	0
57	MG	R0	101	1/1	0.89	0.40	57,57,57,57	0
57	MG	RA	3164	1/1	0.89	0.07	48,48,48,48	0
57	MG	YA	3155	1/1	0.89	0.16	32,32,32,32	0
57	MG	YA	3278	1/1	0.89	0.08	23,23,23,23	0
57	MG	XA	1616	1/1	0.89	0.28	44,44,44,44	0
57	MG	YA	3283	1/1	0.89	0.13	30,30,30,30	0
57	MG	XA	1639	1/1	0.89	0.20	44,44,44,44	0
57	MG	YA	3161	1/1	0.89	0.14	46,46,46,46	0
57	MG	RA	3141	1/1	0.89	0.18	31,31,31,31	0
57	MG	YA	3287	1/1	0.89	0.25	141,141,141,141	0
57	MG	RA	3123	1/1	0.89	0.27	26,26,26,26	0
57	MG	YA	3170	1/1	0.89	0.18	48,48,48,48	0
57	MG	YA	3098	1/1	0.89	0.31	39,39,39,39	0
57	MG	YA	3323	1/1	0.89	0.07	25,25,25,25	0
57	MG	XL	201	1/1	0.89	0.13	43,43,43,43	0
57	MG	RA	3240	1/1	0.89	0.31	40,40,40,40	0
57	MG	YB	204	1/1	0.89	0.33	149,149,149,149	0
57	MG	RA	3145	1/1	0.89	0.15	34,34,34,34	0
57	MG	YA	3187	1/1	0.89	0.08	40,40,40,40	0
57	MG	YA	3114	1/1	0.89	0.18	35,35,35,35	0
57	MG	RA	3197	1/1	0.89	0.18	13,13,13,13	0
57	MG	YA	3222	1/1	0.89	0.14	19,19,19,19	0
57	MG	YG	201	1/1	0.89	0.11	42,42,42,42	0
57	MG	YA	3118	1/1	0.89	0.17	46,46,46,46	0
57	MG	YV	201	1/1	0.89	0.09	44,44,44,44	0
57	MG	YA	3300	1/1	0.89	0.18	45,45,45,45	0
57	MG	RA	3227	1/1	0.90	0.12	20,20,20,20	0
57	MG	YA	3195	1/1	0.90	0.20	18,18,18,18	0
57	MG	RA	3228	1/1	0.90	0.20	29,29,29,29	0
57	MG	YA	3217	1/1	0.90	0.22	28,28,28,28	0
57	MG	XA	1601	1/1	0.90	0.25	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3112	1/1	0.90	0.19	36,36,36,36	0
57	MG	RA	3046	1/1	0.90	0.20	19,19,19,19	0
57	MG	XA	1605	1/1	0.90	0.13	40,40,40,40	0
57	MG	YA	3255	1/1	0.90	0.21	24,24,24,24	0
57	MG	XA	1643	1/1	0.90	0.15	31,31,31,31	0
57	MG	YA	3127	1/1	0.90	0.11	32,32,32,32	0
57	MG	XA	1606	1/1	0.90	0.31	40,40,40,40	0
57	MG	YA	3135	1/1	0.90	0.22	38,38,38,38	0
57	MG	QA	1668	1/1	0.90	0.21	48,48,48,48	0
57	MG	YA	3140	1/1	0.90	0.10	37,37,37,37	0
57	MG	YA	3270	1/1	0.90	0.18	37,37,37,37	0
57	MG	RA	3082	1/1	0.90	0.10	21,21,21,21	0
57	MG	QA	1606	1/1	0.90	0.26	57,57,57,57	0
57	MG	RA	3247	1/1	0.90	0.25	41,41,41,41	0
57	MG	RA	3274	1/1	0.90	0.26	116,116,116,116	0
57	MG	YA	3039	1/1	0.90	0.19	6,6,6,6	0
57	MG	RA	3009	1/1	0.90	0.28	28,28,28,28	0
57	MG	RA	3160	1/1	0.90	0.07	37,37,37,37	0
57	MG	RA	3060	1/1	0.90	0.18	17,17,17,17	0
57	MG	RA	3107	1/1	0.90	0.31	49,49,49,49	0
57	MG	YA	3065	1/1	0.90	0.10	32,32,32,32	0
57	MG	RA	3210	1/1	0.90	0.32	28,28,28,28	0
57	MG	YA	3291	1/1	0.90	0.29	232,232,232,232	0
57	MG	RA	3172	1/1	0.90	0.31	60,60,60,60	0
57	MG	YA	3174	1/1	0.90	0.09	25,25,25,25	0
57	MG	RA	3301	1/1	0.90	0.20	56,56,56,56	0
57	MG	QA	1665	1/1	0.90	0.28	61,61,61,61	0
57	MG	YO	201	1/1	0.90	0.29	51,51,51,51	0
57	MG	YA	3093	1/1	0.90	0.16	44,44,44,44	0
57	MG	RA	3175	1/1	0.90	0.07	48,48,48,48	0
57	MG	YA	3189	1/1	0.90	0.17	48,48,48,48	0
60	A3P	XX	101	26/27	0.90	0.12	51,53,58,61	0
57	MG	RA	3251	1/1	0.91	0.06	24,24,24,24	0
57	MG	RA	3253	1/1	0.91	0.28	34,34,34,34	0
57	MG	YA	3054	1/1	0.91	0.26	12,12,12,12	0
57	MG	RA	3254	1/1	0.91	0.31	151,151,151,151	0
57	MG	YA	3183	1/1	0.91	0.13	33,33,33,33	0
57	MG	YA	3066	1/1	0.91	0.26	24,24,24,24	0
57	MG	RA	3095	1/1	0.91	0.19	60,60,60,60	0
57	MG	YA	3076	1/1	0.91	0.26	20,20,20,20	0
57	MG	YA	3078	1/1	0.91	0.19	28,28,28,28	0
57	MG	RA	3190	1/1	0.91	0.23	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1650	1/1	0.91	0.23	37,37,37,37	0
57	MG	RA	3191	1/1	0.91	0.31	66,66,66,66	0
57	MG	RA	3260	1/1	0.91	0.17	50,50,50,50	0
57	MG	RA	3195	1/1	0.91	0.29	42,42,42,42	0
57	MG	YA	3096	1/1	0.91	0.12	52,52,52,52	0
57	MG	RA	3017	1/1	0.91	0.14	14,14,14,14	0
57	MG	YA	3241	1/1	0.91	0.15	26,26,26,26	0
57	MG	XA	1660	1/1	0.91	0.22	37,37,37,37	0
57	MG	YA	3249	1/1	0.91	0.08	25,25,25,25	0
57	MG	RA	3165	1/1	0.91	0.29	60,60,60,60	0
57	MG	RA	3171	1/1	0.91	0.08	33,33,33,33	0
57	MG	YA	3258	1/1	0.91	0.26	36,36,36,36	0
57	MG	RA	3100	1/1	0.91	0.24	47,47,47,47	0
57	MG	XA	1621	1/1	0.91	0.28	47,47,47,47	0
57	MG	RA	3220	1/1	0.91	0.16	27,27,27,27	0
57	MG	RA	3173	1/1	0.91	0.23	39,39,39,39	0
57	MG	QA	1674	1/1	0.91	0.20	58,58,58,58	0
57	MG	RA	3074	1/1	0.91	0.18	21,21,21,21	0
57	MG	RA	3109	1/1	0.91	0.23	34,34,34,34	0
57	MG	YA	3275	1/1	0.91	0.25	38,38,38,38	0
57	MG	YA	3276	1/1	0.91	0.22	36,36,36,36	0
57	MG	QA	1642	1/1	0.91	0.23	43,43,43,43	0
57	MG	QA	1611	1/1	0.91	0.17	55,55,55,55	0
57	MG	XV	104	1/1	0.91	0.22	32,32,32,32	0
57	MG	RA	3239	1/1	0.91	0.23	39,39,39,39	0
57	MG	RB	201	1/1	0.91	0.24	36,36,36,36	0
57	MG	YA	3003	1/1	0.91	0.29	49,49,49,49	0
57	MG	YA	3156	1/1	0.91	0.14	21,21,21,21	0
57	MG	YA	3005	1/1	0.91	0.27	48,48,48,48	0
57	MG	QA	1670	1/1	0.91	0.22	46,46,46,46	0
57	MG	RA	3115	1/1	0.91	0.10	28,28,28,28	0
57	MG	RA	3011	1/1	0.91	0.17	20,20,20,20	0
57	MG	RA	3161	1/1	0.91	0.21	70,70,70,70	0
57	MG	QA	1635	1/1	0.92	0.18	52,52,52,52	0
57	MG	YA	3176	1/1	0.92	0.07	32,32,32,32	0
57	MG	RA	3300	1/1	0.92	0.22	31,31,31,31	0
57	MG	RA	3204	1/1	0.92	0.26	25,25,25,25	0
57	MG	YA	3095	1/1	0.92	0.12	67,67,67,67	0
57	MG	RA	3303	1/1	0.92	0.19	22,22,22,22	0
57	MG	RA	3208	1/1	0.92	0.23	25,25,25,25	0
57	MG	RA	3163	1/1	0.92	0.10	30,30,30,30	0
57	MG	QV	101	1/1	0.92	0.17	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3193	1/1	0.92	0.20	12,12,12,12	0
57	MG	YA	3194	1/1	0.92	0.14	11,11,11,11	0
57	MG	RA	3042	1/1	0.92	0.08	21,21,21,21	0
57	MG	RA	3136	1/1	0.92	0.11	30,30,30,30	0
57	MG	YA	3115	1/1	0.92	0.15	46,46,46,46	0
57	MG	RR	201	1/1	0.92	0.17	19,19,19,19	0
57	MG	YA	3226	1/1	0.92	0.15	27,27,27,27	0
57	MG	YA	3014	1/1	0.92	0.27	22,22,22,22	0
57	MG	YA	3121	1/1	0.92	0.34	34,34,34,34	0
57	MG	YA	3235	1/1	0.92	0.25	39,39,39,39	0
57	MG	YA	3236	1/1	0.92	0.22	36,36,36,36	0
57	MG	YA	3238	1/1	0.92	0.21	32,32,32,32	0
57	MG	YA	3024	1/1	0.92	0.27	21,21,21,21	0
57	MG	YA	3132	1/1	0.92	0.23	41,41,41,41	0
57	MG	YA	3244	1/1	0.92	0.25	34,34,34,34	0
57	MG	RA	3076	1/1	0.92	0.14	21,21,21,21	0
57	MG	YA	3251	1/1	0.92	0.14	38,38,38,38	0
57	MG	YA	3028	1/1	0.92	0.23	16,16,16,16	0
57	MG	RA	3255	1/1	0.92	0.31	54,54,54,54	0
57	MG	YA	3137	1/1	0.92	0.07	21,21,21,21	0
57	MG	YA	3261	1/1	0.92	0.25	39,39,39,39	0
57	MG	RA	3222	1/1	0.92	0.26	30,30,30,30	0
57	MG	RA	3223	1/1	0.92	0.17	28,28,28,28	0
57	MG	YA	3143	1/1	0.92	0.17	36,36,36,36	0
57	MG	XA	1668	1/1	0.92	0.31	58,58,58,58	0
57	MG	YA	3149	1/1	0.92	0.21	29,29,29,29	0
57	MG	RA	3124	1/1	0.92	0.21	19,19,19,19	0
57	MG	RA	3125	1/1	0.92	0.26	50,50,50,50	0
57	MG	YA	3060	1/1	0.92	0.10	30,30,30,30	0
57	MG	XA	1671	1/1	0.92	0.39	59,59,59,59	0
57	MG	YA	3157	1/1	0.92	0.22	42,42,42,42	0
57	MG	XA	1672	1/1	0.92	0.15	81,81,81,81	0
57	MG	XA	1673	1/1	0.92	0.14	58,58,58,58	0
57	MG	QA	1664	1/1	0.92	0.37	49,49,49,49	0
57	MG	XA	1676	1/1	0.92	0.12	52,52,52,52	0
57	MG	RA	3192	1/1	0.92	0.25	16,16,16,16	0
57	MG	YA	3089	1/1	0.92	0.19	22,22,22,22	0
57	MG	RA	3068	1/1	0.92	0.19	21,21,21,21	0
57	MG	YA	3012	1/1	0.93	0.14	15,15,15,15	0
57	MG	YA	3013	1/1	0.93	0.17	10,10,10,10	0
57	MG	YA	3142	1/1	0.93	0.32	64,64,64,64	0
57	MG	RA	3045	1/1	0.93	0.26	19,19,19,19	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3015	1/1	0.93	0.17	9,9,9,9	0
57	MG	YA	3016	1/1	0.93	0.24	24,24,24,24	0
57	MG	RB	202	1/1	0.93	0.18	33,33,33,33	0
57	MG	RA	3198	1/1	0.93	0.17	14,14,14,14	0
57	MG	RA	3170	1/1	0.93	0.14	29,29,29,29	0
57	MG	YA	3033	1/1	0.93	0.21	15,15,15,15	0
57	MG	RA	3205	1/1	0.93	0.20	18,18,18,18	0
57	MG	RA	3015	1/1	0.93	0.32	17,17,17,17	0
57	MG	QA	1675	1/1	0.93	0.27	52,52,52,52	0
57	MG	YA	3049	1/1	0.93	0.12	13,13,13,13	0
57	MG	XA	1684	1/1	0.93	0.33	52,52,52,52	0
57	MG	YA	3051	1/1	0.93	0.27	18,18,18,18	0
57	MG	YA	3169	1/1	0.93	0.23	29,29,29,29	0
57	MG	RA	3211	1/1	0.93	0.30	33,33,33,33	0
57	MG	RA	3079	1/1	0.93	0.14	23,23,23,23	0
57	MG	RA	3019	1/1	0.93	0.23	19,19,19,19	0
57	MG	YA	3064	1/1	0.93	0.10	16,16,16,16	0
57	MG	RA	3034	1/1	0.93	0.23	15,15,15,15	0
57	MG	QV	102	1/1	0.93	0.15	18,18,18,18	0
57	MG	XA	1607	1/1	0.93	0.25	31,31,31,31	0
57	MG	YA	3072	1/1	0.93	0.12	18,18,18,18	0
57	MG	XA	1649	1/1	0.93	0.19	31,31,31,31	0
57	MG	RA	3096	1/1	0.93	0.29	45,45,45,45	0
57	MG	RA	3063	1/1	0.93	0.06	17,17,17,17	0
57	MG	RA	3225	1/1	0.93	0.19	45,45,45,45	0
57	MG	RA	3039	1/1	0.93	0.20	15,15,15,15	0
57	MG	XA	1656	1/1	0.93	0.29	41,41,41,41	0
57	MG	YA	3204	1/1	0.93	0.10	27,27,27,27	0
57	MG	YA	3214	1/1	0.93	0.23	31,31,31,31	0
57	MG	RA	3155	1/1	0.93	0.25	33,33,33,33	0
57	MG	QA	1608	1/1	0.93	0.44	49,49,49,49	0
57	MG	YA	3219	1/1	0.93	0.26	25,25,25,25	0
57	MG	XA	1617	1/1	0.93	0.33	66,66,66,66	0
57	MG	RA	3103	1/1	0.93	0.17	29,29,29,29	0
57	MG	YA	3315	1/1	0.93	0.27	205,205,205,205	0
57	MG	XA	1663	1/1	0.93	0.27	33,33,33,33	0
57	MG	XA	1620	1/1	0.93	0.07	35,35,35,35	0
57	MG	XA	1665	1/1	0.93	0.32	44,44,44,44	0
57	MG	YA	3108	1/1	0.93	0.19	23,23,23,23	0
57	MG	RA	3105	1/1	0.93	0.15	24,24,24,24	0
57	MG	YA	3239	1/1	0.93	0.29	33,33,33,33	0
57	MG	YA	3113	1/1	0.93	0.25	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3325	1/1	0.93	0.12	28,28,28,28	0
57	MG	XA	1623	1/1	0.93	0.14	44,44,44,44	0
57	MG	YA	3327	1/1	0.93	0.15	12,12,12,12	0
57	MG	YA	3328	1/1	0.93	0.08	50,50,50,50	0
57	MG	RA	3071	1/1	0.93	0.10	19,19,19,19	0
57	MG	YB	201	1/1	0.93	0.17	20,20,20,20	0
57	MG	YA	3116	1/1	0.93	0.18	18,18,18,18	0
57	MG	XA	1625	1/1	0.93	0.07	51,51,51,51	0
57	MG	YA	3253	1/1	0.93	0.14	37,37,37,37	0
57	MG	YD	301	1/1	0.93	0.11	23,23,23,23	0
57	MG	RA	3108	1/1	0.93	0.25	25,25,25,25	0
57	MG	XV	102	1/1	0.93	0.06	14,14,14,14	0
57	MG	YA	3125	1/1	0.93	0.15	12,12,12,12	0
57	MG	XA	1628	1/1	0.93	0.38	52,52,52,52	0
57	MG	RA	3241	1/1	0.93	0.24	43,43,43,43	0
57	MG	YQ	201	1/1	0.93	0.12	52,52,52,52	0
57	MG	RA	3044	1/1	0.93	0.27	29,29,29,29	0
57	MG	XA	1632	1/1	0.93	0.23	36,36,36,36	0
57	MG	RA	3110	1/1	0.93	0.22	21,21,21,21	0
57	MG	YA	3007	1/1	0.93	0.24	14,14,14,14	0
57	MG	YA	3153	1/1	0.94	0.26	38,38,38,38	0
57	MG	YA	3266	1/1	0.94	0.13	22,22,22,22	0
57	MG	QA	1625	1/1	0.94	0.11	42,42,42,42	0
57	MG	RA	3091	1/1	0.94	0.08	44,44,44,44	0
57	MG	YA	3075	1/1	0.94	0.22	20,20,20,20	0
57	MG	RA	3116	1/1	0.94	0.25	51,51,51,51	0
57	MG	XV	103	1/1	0.94	0.19	13,13,13,13	0
57	MG	XA	1612	1/1	0.94	0.24	39,39,39,39	0
57	MG	RA	3092	1/1	0.94	0.18	29,29,29,29	0
57	MG	RA	3094	1/1	0.94	0.16	24,24,24,24	0
57	MG	RA	3012	1/1	0.94	0.14	20,20,20,20	0
57	MG	YA	3167	1/1	0.94	0.24	34,34,34,34	0
57	MG	YA	3168	1/1	0.94	0.12	32,32,32,32	0
57	MG	YA	3004	1/1	0.94	0.18	12,12,12,12	0
57	MG	RA	3153	1/1	0.94	0.06	24,24,24,24	0
57	MG	XA	1653	1/1	0.94	0.28	33,33,33,33	0
57	MG	QA	1652	1/1	0.94	0.22	38,38,38,38	0
57	MG	YA	3097	1/1	0.94	0.21	33,33,33,33	0
57	MG	RA	3069	1/1	0.94	0.18	21,21,21,21	0
57	MG	YA	3180	1/1	0.94	0.10	23,23,23,23	0
57	MG	YA	3181	1/1	0.94	0.22	11,11,11,11	0
57	MG	YA	3182	1/1	0.94	0.18	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3099	1/1	0.94	0.21	16,16,16,16	0
57	MG	QA	1667	1/1	0.94	0.29	54,54,54,54	0
57	MG	YA	3103	1/1	0.94	0.14	21,21,21,21	0
57	MG	RA	3006	1/1	0.94	0.17	12,12,12,12	0
57	MG	YA	3188	1/1	0.94	0.11	65,65,65,65	0
57	MG	YA	3022	1/1	0.94	0.11	19,19,19,19	0
57	MG	YA	3190	1/1	0.94	0.11	61,61,61,61	0
57	MG	YA	3111	1/1	0.94	0.24	38,38,38,38	0
57	MG	RA	3021	1/1	0.94	0.22	22,22,22,22	0
57	MG	RA	3132	1/1	0.94	0.19	44,44,44,44	0
57	MG	RA	3023	1/1	0.94	0.27	19,19,19,19	0
57	MG	YA	3196	1/1	0.94	0.19	14,14,14,14	0
57	MG	YA	3198	1/1	0.94	0.12	11,11,11,11	0
57	MG	YA	3201	1/1	0.94	0.28	24,24,24,24	0
57	MG	YA	3202	1/1	0.94	0.23	31,31,31,31	0
57	MG	RA	3052	1/1	0.94	0.07	35,35,35,35	0
57	MG	YA	3206	1/1	0.94	0.24	19,19,19,19	0
57	MG	YA	3207	1/1	0.94	0.25	24,24,24,24	0
57	MG	YA	3209	1/1	0.94	0.23	35,35,35,35	0
57	MG	YA	3211	1/1	0.94	0.30	26,26,26,26	0
57	MG	YA	3037	1/1	0.94	0.19	20,20,20,20	0
57	MG	YA	3215	1/1	0.94	0.06	12,12,12,12	0
57	MG	RA	3199	1/1	0.94	0.27	17,17,17,17	0
57	MG	YA	3119	1/1	0.94	0.16	16,16,16,16	0
57	MG	RA	3250	1/1	0.94	0.36	39,39,39,39	0
57	MG	YA	3123	1/1	0.94	0.10	19,19,19,19	0
57	MG	YA	3223	1/1	0.94	0.20	26,26,26,26	0
57	MG	RA	3200	1/1	0.94	0.22	19,19,19,19	0
57	MG	YA	3046	1/1	0.94	0.23	15,15,15,15	0
57	MG	YA	3131	1/1	0.94	0.12	21,21,21,21	0
57	MG	YA	3048	1/1	0.94	0.17	21,21,21,21	0
57	MG	RA	3032	1/1	0.94	0.19	14,14,14,14	0
57	MG	YA	3237	1/1	0.94	0.20	34,34,34,34	0
57	MG	YA	3134	1/1	0.94	0.19	38,38,38,38	0
57	MG	RA	3169	1/1	0.94	0.15	32,32,32,32	0
57	MG	RA	3207	1/1	0.94	0.26	19,19,19,19	0
57	MG	RA	3055	1/1	0.94	0.14	31,31,31,31	0
57	MG	XA	1604	1/1	0.94	0.18	45,45,45,45	0
57	MG	YA	3247	1/1	0.94	0.20	36,36,36,36	0
57	MG	RA	3080	1/1	0.94	0.20	8,8,8,8	0
57	MG	YA	3062	1/1	0.94	0.18	13,13,13,13	0
57	MG	YE	303	1/1	0.94	0.18	16,16,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3252	1/1	0.94	0.07	21,21,21,21	0
57	MG	QA	1612	1/1	0.94	0.22	50,50,50,50	0
57	MG	YA	3145	1/1	0.94	0.07	56,56,56,56	0
57	MG	XA	1675	1/1	0.94	0.13	57,57,57,57	0
57	MG	RA	3088	1/1	0.94	0.14	13,13,13,13	0
57	MG	YA	3150	1/1	0.94	0.31	20,20,20,20	0
57	MG	YA	3069	1/1	0.94	0.16	18,18,18,18	0
57	MG	YA	3264	1/1	0.94	0.27	39,39,39,39	0
57	MG	YA	3084	1/1	0.95	0.20	21,21,21,21	0
57	MG	RA	3257	1/1	0.95	0.21	30,30,30,30	0
57	MG	YA	3090	1/1	0.95	0.19	7,7,7,7	0
57	MG	YA	3144	1/1	0.95	0.34	33,33,33,33	0
57	MG	QA	1654	1/1	0.95	0.12	47,47,47,47	0
57	MG	YA	3147	1/1	0.95	0.09	18,18,18,18	0
57	MG	YA	3212	1/1	0.95	0.07	16,16,16,16	0
57	MG	RA	3177	1/1	0.95	0.10	34,34,34,34	0
57	MG	RA	3212	1/1	0.95	0.26	33,33,33,33	0
57	MG	YA	3035	1/1	0.95	0.20	13,13,13,13	0
57	MG	RA	3214	1/1	0.95	0.07	18,18,18,18	0
57	MG	XA	1634	1/1	0.95	0.26	50,50,50,50	0
57	MG	YA	3220	1/1	0.95	0.14	29,29,29,29	0
57	MG	RA	3030	1/1	0.95	0.08	14,14,14,14	0
57	MG	XF	201	1/1	0.95	0.11	46,46,46,46	0
57	MG	YA	3225	1/1	0.95	0.25	28,28,28,28	0
57	MG	YA	3043	1/1	0.95	0.17	20,20,20,20	0
57	MG	YA	3101	1/1	0.95	0.19	32,32,32,32	0
57	MG	RA	3114	1/1	0.95	0.07	15,15,15,15	0
57	MG	YA	3233	1/1	0.95	0.05	16,16,16,16	0
57	MG	YA	3047	1/1	0.95	0.25	20,20,20,20	0
57	MG	YA	3105	1/1	0.95	0.06	34,34,34,34	0
57	MG	YA	3106	1/1	0.95	0.12	23,23,23,23	0
57	MG	YA	3163	1/1	0.95	0.09	55,55,55,55	0
57	MG	RA	3242	1/1	0.95	0.12	26,26,26,26	0
57	MG	YA	3109	1/1	0.95	0.13	26,26,26,26	0
57	MG	RA	3089	1/1	0.95	0.14	1,1,1,1	0
57	MG	RA	3127	1/1	0.95	0.19	39,39,39,39	0
57	MG	YA	3246	1/1	0.95	0.24	40,40,40,40	0
57	MG	YA	3112	1/1	0.95	0.08	34,34,34,34	0
57	MG	RA	3267	1/1	0.95	0.44	192,192,192,192	0
57	MG	YA	3173	1/1	0.95	0.24	36,36,36,36	0
57	MG	RE	302	1/1	0.95	0.15	20,20,20,20	0
57	MG	YA	3053	1/1	0.95	0.17	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1618	1/1	0.95	0.31	35,35,35,35	0
57	MG	YA	3179	1/1	0.95	0.10	25,25,25,25	0
57	MG	RA	3078	1/1	0.95	0.15	14,14,14,14	0
57	MG	YA	3324	1/1	0.95	0.15	13,13,13,13	0
57	MG	YA	3061	1/1	0.95	0.07	17,17,17,17	0
57	MG	RA	3040	1/1	0.95	0.23	12,12,12,12	0
57	MG	RA	3142	1/1	0.95	0.11	42,42,42,42	0
57	MG	YA	3008	1/1	0.95	0.23	8,8,8,8	0
57	MG	YA	3011	1/1	0.95	0.09	11,11,11,11	0
57	MG	YA	3067	1/1	0.95	0.14	22,22,22,22	0
57	MG	YB	202	1/1	0.95	0.18	23,23,23,23	0
57	MG	YB	203	1/1	0.95	0.17	35,35,35,35	0
57	MG	YA	3129	1/1	0.95	0.13	19,19,19,19	0
57	MG	RA	3035	1/1	0.95	0.20	16,16,16,16	0
57	MG	RA	3093	1/1	0.95	0.30	45,45,45,45	0
57	MG	YA	3272	1/1	0.95	0.25	31,31,31,31	0
57	MG	YA	3191	1/1	0.95	0.18	34,34,34,34	0
57	MG	RA	3231	1/1	0.95	0.21	21,21,21,21	0
57	MG	XA	1626	1/1	0.95	0.51	58,58,58,58	0
57	MG	YA	3277	1/1	0.95	0.12	21,21,21,21	0
57	MG	RA	3233	1/1	0.95	0.12	28,28,28,28	0
57	MG	YA	3280	1/1	0.95	0.23	26,26,26,26	0
57	MG	YP	201	1/1	0.95	0.08	22,22,22,22	0
57	MG	XA	1652	1/1	0.95	0.41	40,40,40,40	0
57	MG	YA	3282	1/1	0.95	0.29	26,26,26,26	0
57	MG	YA	3081	1/1	0.95	0.25	20,20,20,20	0
59	ZN	R6	101	1/1	0.95	0.12	137,137,137,137	0
59	ZN	Y6	101	1/1	0.95	0.09	121,121,121,121	0
57	MG	YA	3138	1/1	0.95	0.10	20,20,20,20	0
57	MG	YA	3023	1/1	0.95	0.21	18,18,18,18	0
57	MG	RA	3047	1/1	0.96	0.14	10,10,10,10	0
57	MG	YA	3205	1/1	0.96	0.27	27,27,27,27	0
57	MG	YA	3010	1/1	0.96	0.27	31,31,31,31	0
57	MG	RA	3168	1/1	0.96	0.08	11,11,11,11	0
57	MG	RA	3049	1/1	0.96	0.18	23,23,23,23	0
57	MG	YA	3210	1/1	0.96	0.17	20,20,20,20	0
57	MG	RA	3072	1/1	0.96	0.18	22,22,22,22	0
57	MG	YA	3086	1/1	0.96	0.16	21,21,21,21	0
57	MG	RA	3073	1/1	0.96	0.06	21,21,21,21	0
57	MG	R0	102	1/1	0.96	0.22	22,22,22,22	0
57	MG	XA	1647	1/1	0.96	0.07	131,131,131,131	0
57	MG	RA	3036	1/1	0.96	0.17	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3218	1/1	0.96	0.19	15,15,15,15	0
57	MG	XA	1608	1/1	0.96	0.33	30,30,30,30	0
57	MG	RA	3249	1/1	0.96	0.07	31,31,31,31	0
57	MG	RA	3209	1/1	0.96	0.19	31,31,31,31	0
57	MG	RA	3146	1/1	0.96	0.31	37,37,37,37	0
57	MG	RA	3014	1/1	0.96	0.11	5,5,5,5	0
57	MG	YA	3034	1/1	0.96	0.13	7,7,7,7	0
57	MG	YA	3227	1/1	0.96	0.25	26,26,26,26	0
57	MG	YA	3099	1/1	0.96	0.16	22,22,22,22	0
57	MG	RA	3176	1/1	0.96	0.28	13,13,13,13	0
57	MG	YA	3232	1/1	0.96	0.08	21,21,21,21	0
57	MG	RA	3054	1/1	0.96	0.27	13,13,13,13	0
57	MG	YA	3234	1/1	0.96	0.21	39,39,39,39	0
57	MG	YA	3160	1/1	0.96	0.19	23,23,23,23	0
57	MG	RA	3024	1/1	0.96	0.13	31,31,31,31	0
57	MG	RA	3027	1/1	0.96	0.20	22,22,22,22	0
57	MG	YA	3104	1/1	0.96	0.14	16,16,16,16	0
57	MG	RA	3219	1/1	0.96	0.17	25,25,25,25	0
57	MG	YA	3240	1/1	0.96	0.11	21,21,21,21	0
57	MG	YA	3166	1/1	0.96	0.04	31,31,31,31	0
57	MG	RA	3059	1/1	0.96	0.12	10,10,10,10	0
57	MG	YA	3107	1/1	0.96	0.27	34,34,34,34	0
57	MG	YA	3245	1/1	0.96	0.27	40,40,40,40	0
57	MG	QA	1607	1/1	0.96	0.32	43,43,43,43	0
57	MG	RA	3131	1/1	0.96	0.11	17,17,17,17	0
57	MG	RA	3157	1/1	0.96	0.18	40,40,40,40	0
57	MG	RA	3158	1/1	0.96	0.08	17,17,17,17	0
57	MG	YA	3322	1/1	0.96	0.15	55,55,55,55	0
57	MG	RA	3226	1/1	0.96	0.18	27,27,27,27	0
57	MG	RA	3299	1/1	0.96	0.07	17,17,17,17	0
57	MG	YA	3254	1/1	0.96	0.18	28,28,28,28	0
57	MG	RA	3083	1/1	0.96	0.20	16,16,16,16	0
57	MG	QA	1653	1/1	0.96	0.41	58,58,58,58	0
57	MG	YA	3257	1/1	0.96	0.10	28,28,28,28	0
57	MG	XE	201	1/1	0.96	0.16	37,37,37,37	0
57	MG	YA	3259	1/1	0.96	0.06	30,30,30,30	0
57	MG	YA	3057	1/1	0.96	0.18	14,14,14,14	0
57	MG	YA	3058	1/1	0.96	0.25	6,6,6,6	0
57	MG	RA	3229	1/1	0.96	0.05	22,22,22,22	0
57	MG	YA	3120	1/1	0.96	0.24	38,38,38,38	0
57	MG	RA	3304	1/1	0.96	0.05	21,21,21,21	0
57	MG	YA	3122	1/1	0.96	0.08	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3230	1/1	0.96	0.09	19,19,19,19	0
57	MG	YA	3124	1/1	0.96	0.06	37,37,37,37	0
57	MG	RA	3064	1/1	0.96	0.21	9,9,9,9	0
57	MG	YA	3271	1/1	0.96	0.11	31,31,31,31	0
57	MG	RB	203	1/1	0.96	0.22	38,38,38,38	0
57	MG	RA	3232	1/1	0.96	0.14	22,22,22,22	0
57	MG	YA	3274	1/1	0.96	0.30	37,37,37,37	0
57	MG	RA	3065	1/1	0.96	0.07	20,20,20,20	0
57	MG	RA	3234	1/1	0.96	0.22	35,35,35,35	0
57	MG	YA	3070	1/1	0.96	0.09	14,14,14,14	0
57	MG	RA	3194	1/1	0.96	0.23	19,19,19,19	0
57	MG	RA	3033	1/1	0.96	0.13	1,1,1,1	0
57	MG	YA	3073	1/1	0.96	0.16	22,22,22,22	0
57	MG	QA	1656	1/1	0.96	0.29	41,41,41,41	0
57	MG	YA	3197	1/1	0.97	0.05	14,14,14,14	0
57	MG	YA	3126	1/1	0.97	0.23	33,33,33,33	0
57	MG	YA	3199	1/1	0.97	0.21	16,16,16,16	0
57	MG	YA	3200	1/1	0.97	0.17	10,10,10,10	0
57	MG	RA	3029	1/1	0.97	0.18	12,12,12,12	0
57	MG	RA	3066	1/1	0.97	0.11	23,23,23,23	0
57	MG	YA	3203	1/1	0.97	0.34	34,34,34,34	0
57	MG	YA	3130	1/1	0.97	0.19	41,41,41,41	0
57	MG	XA	1622	1/1	0.97	0.33	45,45,45,45	0
57	MG	YA	3068	1/1	0.97	0.17	14,14,14,14	0
57	MG	RA	3218	1/1	0.97	0.20	31,31,31,31	0
57	MG	RA	3005	1/1	0.97	0.06	11,11,11,11	0
57	MG	RA	3179	1/1	0.97	0.15	32,32,32,32	0
57	MG	QA	1660	1/1	0.97	0.32	53,53,53,53	0
57	MG	RA	3182	1/1	0.97	0.24	12,12,12,12	0
57	MG	YA	3074	1/1	0.97	0.06	15,15,15,15	0
57	MG	RA	3048	1/1	0.97	0.20	8,8,8,8	0
57	MG	XA	1629	1/1	0.97	0.25	48,48,48,48	0
57	MG	YA	3077	1/1	0.97	0.25	26,26,26,26	0
57	MG	RA	3302	1/1	0.97	0.15	25,25,25,25	0
57	MG	YA	3079	1/1	0.97	0.14	10,10,10,10	0
57	MG	YA	3080	1/1	0.97	0.20	31,31,31,31	0
57	MG	RA	3224	1/1	0.97	0.23	21,21,21,21	0
57	MG	YA	3082	1/1	0.97	0.20	18,18,18,18	0
57	MG	YA	3224	1/1	0.97	0.26	29,29,29,29	0
57	MG	RA	3151	1/1	0.97	0.11	16,16,16,16	0
57	MG	RA	3305	1/1	0.97	0.28	93,93,93,93	0
57	MG	YA	3085	1/1	0.97	0.10	10,10,10,10	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3228	1/1	0.97	0.05	16,16,16,16	0
57	MG	RA	3152	1/1	0.97	0.20	9,9,9,9	0
57	MG	YA	3230	1/1	0.97	0.19	24,24,24,24	0
57	MG	YA	3088	1/1	0.97	0.11	15,15,15,15	0
57	MG	RA	3007	1/1	0.97	0.20	3,3,3,3	0
57	MG	RA	3187	1/1	0.97	0.09	14,14,14,14	0
57	MG	YA	3017	1/1	0.97	0.26	26,26,26,26	0
57	MG	YA	3019	1/1	0.97	0.04	4,4,4,4	0
57	MG	YA	3020	1/1	0.97	0.18	3,3,3,3	0
57	MG	RD	301	1/1	0.97	0.10	23,23,23,23	0
57	MG	RA	3122	1/1	0.97	0.06	24,24,24,24	0
57	MG	RA	3018	1/1	0.97	0.05	15,15,15,15	0
57	MG	RA	3097	1/1	0.97	0.26	25,25,25,25	0
57	MG	YA	3027	1/1	0.97	0.10	10,10,10,10	0
57	MG	RA	3051	1/1	0.97	0.22	7,7,7,7	0
57	MG	RA	3008	1/1	0.97	0.24	23,23,23,23	0
57	MG	RQ	201	1/1	0.97	0.15	43,43,43,43	0
57	MG	RA	3020	1/1	0.97	0.11	18,18,18,18	0
57	MG	RA	3037	1/1	0.97	0.09	20,20,20,20	0
57	MG	YA	3248	1/1	0.97	0.18	27,27,27,27	0
57	MG	RA	3102	1/1	0.97	0.11	26,26,26,26	0
57	MG	YA	3250	1/1	0.97	0.27	37,37,37,37	0
57	MG	YA	3172	1/1	0.97	0.20	39,39,39,39	0
57	MG	QA	1666	1/1	0.97	0.28	50,50,50,50	0
57	MG	RA	3104	1/1	0.97	0.15	23,23,23,23	0
57	MG	RA	3056	1/1	0.97	0.32	19,19,19,19	0
57	MG	RA	3201	1/1	0.97	0.08	13,13,13,13	0
57	MG	YA	3178	1/1	0.97	0.14	39,39,39,39	0
57	MG	RA	3022	1/1	0.97	0.21	18,18,18,18	0
57	MG	QV	103	1/1	0.97	0.04	8,8,8,8	0
57	MG	RA	3246	1/1	0.97	0.17	23,23,23,23	0
57	MG	RA	3081	1/1	0.97	0.16	10,10,10,10	0
57	MG	YD	302	1/1	0.97	0.16	30,30,30,30	0
57	MG	RA	3004	1/1	0.97	0.31	25,25,25,25	0
57	MG	YA	3263	1/1	0.97	0.35	44,44,44,44	0
57	MG	RA	3061	1/1	0.97	0.15	13,13,13,13	0
57	MG	XA	1658	1/1	0.97	0.19	35,35,35,35	0
57	MG	RA	3084	1/1	0.97	0.06	22,22,22,22	0
57	MG	YA	3055	1/1	0.97	0.15	20,20,20,20	0
57	MG	YA	3056	1/1	0.97	0.25	13,13,13,13	0
57	MG	XA	1614	1/1	0.97	0.12	39,39,39,39	0
57	MG	RA	3043	1/1	0.97	0.07	15,15,15,15	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YS	201	1/1	0.97	0.31	205,205,205,205	0
57	MG	RA	3252	1/1	0.97	0.20	41,41,41,41	0
59	ZN	QN	101	1/1	0.97	0.06	79,79,79,79	0
57	MG	RA	3143	1/1	0.97	0.19	31,31,31,31	0
57	MG	RA	3013	1/1	0.97	0.24	11,11,11,11	0
57	MG	YA	3063	1/1	0.97	0.15	6,6,6,6	0
57	MG	RA	3215	1/1	0.97	0.16	21,21,21,21	0
57	MG	RA	3243	1/1	0.98	0.26	44,44,44,44	0
57	MG	YA	3087	1/1	0.98	0.06	8,8,8,8	0
57	MG	YA	3009	1/1	0.98	0.13	20,20,20,20	0
57	MG	YA	3128	1/1	0.98	0.04	13,13,13,13	0
57	MG	RA	3244	1/1	0.98	0.14	32,32,32,32	0
57	MG	YA	3221	1/1	0.98	0.29	32,32,32,32	0
57	MG	RA	3166	1/1	0.98	0.03	21,21,21,21	0
57	MG	XA	1657	1/1	0.98	0.14	37,37,37,37	0
57	MG	RA	3202	1/1	0.98	0.21	22,22,22,22	0
57	MG	RA	3167	1/1	0.98	0.04	21,21,21,21	0
57	MG	RA	3067	1/1	0.98	0.17	15,15,15,15	0
57	MG	RA	3025	1/1	0.98	0.27	16,16,16,16	0
57	MG	RA	3041	1/1	0.98	0.12	17,17,17,17	0
57	MG	YA	3018	1/1	0.98	0.08	12,12,12,12	0
57	MG	RA	3140	1/1	0.98	0.04	17,17,17,17	0
57	MG	YA	3139	1/1	0.98	0.12	12,12,12,12	0
57	MG	RA	3126	1/1	0.98	0.10	30,30,30,30	0
57	MG	YA	3279	1/1	0.98	0.04	15,15,15,15	0
57	MG	YA	3021	1/1	0.98	0.14	14,14,14,14	0
57	MG	RA	3031	1/1	0.98	0.05	11,11,11,11	0
57	MG	RA	3062	1/1	0.98	0.15	13,13,13,13	0
57	MG	XV	101	1/1	0.98	0.25	25,25,25,25	0
57	MG	RA	3010	1/1	0.98	0.12	11,11,11,11	0
57	MG	YA	3146	1/1	0.98	0.06	14,14,14,14	0
57	MG	RA	3193	1/1	0.98	0.22	13,13,13,13	0
57	MG	RA	3028	1/1	0.98	0.10	6,6,6,6	0
57	MG	YA	3029	1/1	0.98	0.08	9,9,9,9	0
57	MG	YA	3030	1/1	0.98	0.14	14,14,14,14	0
57	MG	YA	3151	1/1	0.98	0.04	14,14,14,14	0
57	MG	YA	3031	1/1	0.98	0.07	15,15,15,15	0
57	MG	YA	3032	1/1	0.98	0.10	13,13,13,13	0
57	MG	RA	3057	1/1	0.98	0.15	14,14,14,14	0
57	MG	Y9	101	1/1	0.98	0.04	53,53,53,53	0
57	MG	RA	3196	1/1	0.98	0.15	11,11,11,11	0
57	MG	YA	3036	1/1	0.98	0.16	15,15,15,15	0

Continued on next page...

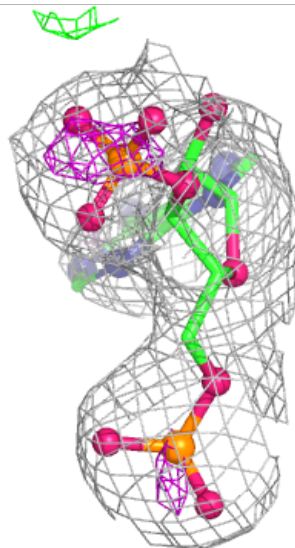
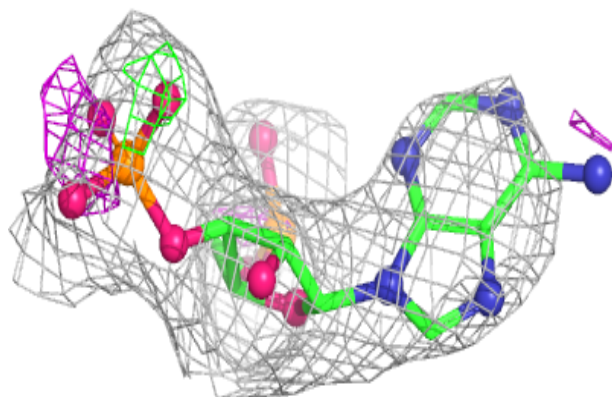
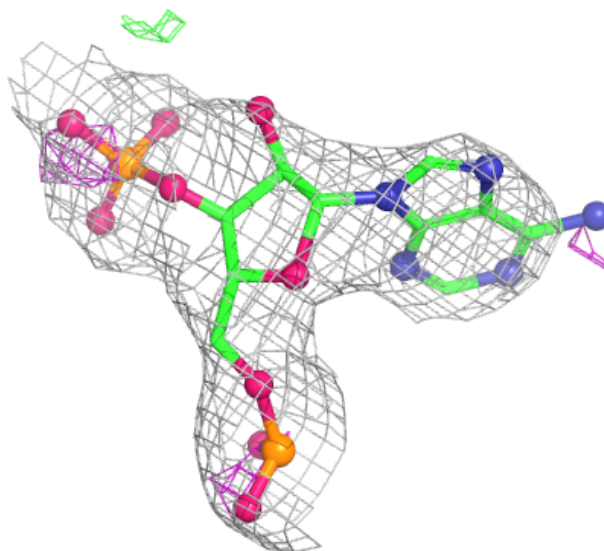
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3002	1/1	0.98	0.17	12,12,12,12	0
57	MG	YA	3038	1/1	0.98	0.09	17,17,17,17	0
57	MG	RA	3016	1/1	0.98	0.22	25,25,25,25	0
57	MG	RA	3120	1/1	0.98	0.14	22,22,22,22	0
57	MG	RA	3085	1/1	0.98	0.06	19,19,19,19	0
57	MG	YA	3042	1/1	0.98	0.12	14,14,14,14	0
58	SF4	XD	301	8/8	0.98	0.08	42,53,59,73	0
57	MG	YA	3006	1/1	0.98	0.10	10,10,10,10	0
57	MG	YA	3044	1/1	0.98	0.05	7,7,7,7	0
59	ZN	R9	101	1/1	0.98	0.06	132,132,132,132	0
57	MG	YA	3045	1/1	0.98	0.13	12,12,12,12	0
57	MG	YA	3260	1/1	0.98	0.10	32,32,32,32	0
57	MG	RA	3087	1/1	0.98	0.10	15,15,15,15	0
57	MG	YA	3242	1/1	0.99	0.15	30,30,30,30	0
57	MG	RA	3298	1/1	0.99	0.03	10,10,10,10	0
57	MG	YA	3175	1/1	0.99	0.20	13,13,13,13	0
57	MG	YA	3208	1/1	0.99	0.28	21,21,21,21	0
57	MG	RA	3148	1/1	0.99	0.05	13,13,13,13	0
57	MG	RA	3203	1/1	0.99	0.14	8,8,8,8	0
57	MG	YA	3059	1/1	0.99	0.07	10,10,10,10	0
57	MG	RA	3086	1/1	0.99	0.05	12,12,12,12	0
57	MG	YA	3213	1/1	0.99	0.06	13,13,13,13	0
57	MG	YA	3165	1/1	0.99	0.05	11,11,11,11	0
57	MG	RA	3213	1/1	0.99	0.04	15,15,15,15	0
57	MG	RA	3180	1/1	0.99	0.03	14,14,14,14	0
58	SF4	QD	301	8/8	0.99	0.04	49,54,67,76	0
57	MG	YA	3026	1/1	0.99	0.22	10,10,10,10	0
57	MG	RA	3206	1/1	0.99	0.25	19,19,19,19	0
57	MG	RA	3026	1/1	0.99	0.03	10,10,10,10	0
57	MG	YA	3186	1/1	0.99	0.04	18,18,18,18	0
57	MG	RA	3130	1/1	0.99	0.09	11,11,11,11	0
57	MG	RA	3236	1/1	0.99	0.25	26,26,26,26	0
57	MG	RA	3106	1/1	0.99	0.07	14,14,14,14	0
59	ZN	XN	101	1/1	1.00	0.02	68,68,68,68	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

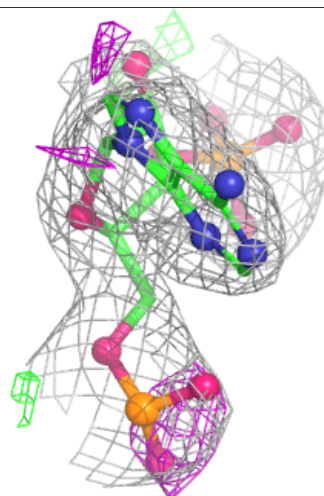
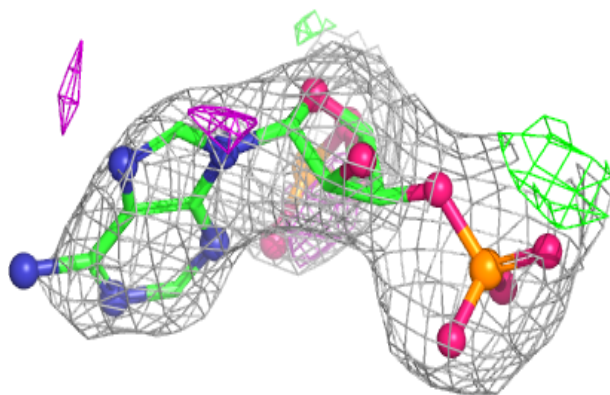
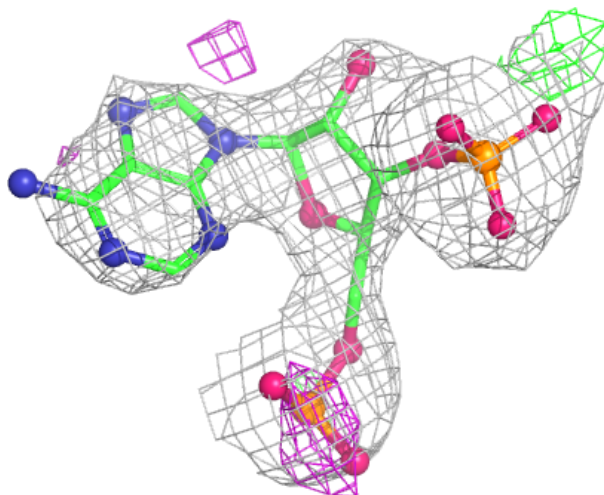
Electron density around A3P QX 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around A3P XX 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



5.5 Other polymers ⓘ

There are no such residues in this entry.