



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:16 AM UTC

PDB ID : 5EL7 / pdb_00005el7
Title : Structure of T. thermophilus 70S ribosome complex with mRNA and tRNA^{Lys} in the A-site with a U-U mismatch in the second position and antibiotic paromomycin
Authors : Rozov, A.; Demeshkina, N.; Khusainov, I.; Yusupov, M.; Yusupova, G.
Deposited on : 2015-11-04
Resolution : 3.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.48.1

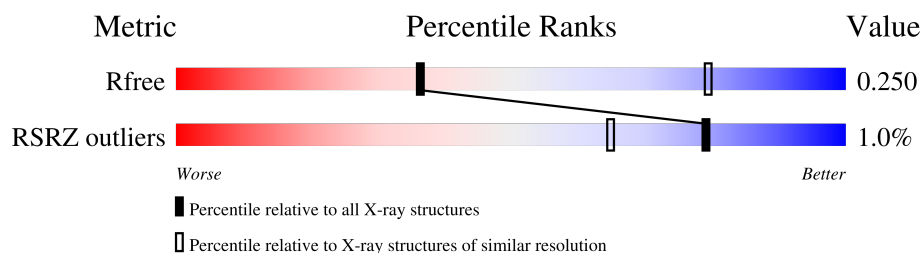
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	164625	2168 (3.20-3.12)
RSRZ outliers	164620	2169 (3.20-3.12)

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	13	1625	-	-	-	X
57	MG	13	1659	-	-	-	X
57	MG	14	3035	-	-	-	X
57	MG	14	3170	-	-	-	X
57	MG	1H	3211	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296184 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	13	1496	Total	C	N	O	P	0	0	0
			32157	14313	5960	10388	1496			
1	1G	1506	Total	C	N	O	P	0	0	0
			32368	14408	5999	10456	1505			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
13	1542	G	-	expression tag	GB 55771382
13	1543	C	-	expression tag	GB 55771382
13	1544	U	-	expression tag	GB 55771382
1G	1542	G	-	expression tag	GB 55771382
1G	1543	C	-	expression tag	GB 55771382
1G	1544	U	-	expression tag	GB 55771382

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	231	Total	C	N	O	S	0	0	0
			1874	1199	334	336	5			
2	12	210	Total	C	N	O	S	0	0	0
			1721	1100	309	308	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2E	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	22	196	Total	C	N	O	S	0	0	0
			1541	975	298	267	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3E	207	Total	C	N	O	S	0	0	0
			1690	1058	336	289	7			
4	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	148	Total	C	N	O	S	0	0	0
			1134	718	215	197	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5E	100	Total	C	N	O	S	0	0	0
			837	528	154	152	3			
6	52	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	154	Total	C	N	O	S	0	0	0
			1242	770	250	216	6			
7	62	139	Total	C	N	O	S	0	0	0
			1115	692	222	195	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7E	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			
8	72	137	Total	C	N	O	S	0	0	0
			1107	700	214	191	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	8E	126	Total	C	N	O		0	0	0
			1000	634	196	170				

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	82	121	Total	C	N	O	0	0	0
			953	605	186	162			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	91	Total	C	N	O	S	0	0	0
			734	459	144	130	1			
10	1A	80	Total	C	N	O		0	0	0
			646	403	129	114				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	111	Total	C	N	O	S	0	0	0
			823	512	154	154	3			
11	2A	113	Total	C	N	O	S	0	0	0
			835	520	156	156	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	3I	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			
12	3A	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	4I	119	Total	C	N	O	S	0	0	0
			942	582	194	164	2			
13	4A	111	Total	C	N	O	S	0	0	0
			893	552	183	156	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			
14	5A	59	Total	C	N	O	S	0	0	0
			486	309	103	70	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			
15	6A	88	Total	C	N	O	S	0	0	0
			733	459	147	125	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
16	7A	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	8I	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	8A	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	68	Total	C	N	O	0	0	0
			549	352	105	92			
18	9A	67	Total	C	N	O	0	0	0
			544	349	104	91			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	81	Total	C	N	O	S	0	0	0
			654	417	122	113	2			
19	AA	62	Total	C	N	O	S	0	0	0
			481	306	85	88	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	97	Total	C	N	O	S	0	0	0
			746	461	157	126	2			
20	BA	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1F	23	Total	C	N	O		0	0	0
			199	122	48	29				
21	1B	22	Total	C	N	O		0	0	0
			188	116	44	28				

- Molecule 22 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	69	Total	C	N	O	P	S	0	0	0
			1477	662	257	488	69	1			
22	1L	73	Total	C	N	O	P	S	0	0	0
			1563	700	271	518	73	1			

- Molecule 23 is a RNA chain called E. coli tRNA^{fMet}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P	S	0	0	0
			1646	735	298	535	77	1			
23	2L	77	Total	C	N	O	P	S	0	0	0
			1646	735	298	535	77	1			

- Molecule 24 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	76	Total	C	N	O	P	0	0	0
			1611	721	281	534	75			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	20	Total	C	N	O	P	0	0	0
			439	197	91	131	20			
25	4L	19	Total	C	N	O	P	0	0	0
			417	187	86	125	19			

- Molecule 26 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2833	Total	C	N	O	P	0	0	0
			61028	27159	11418	19618	2833			
26	14	2861	Total	C	N	O	P	0	0	0
			61630	27429	11535	19806	2860			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	UNK	conflict	GB 55771382
1H	654A	A	G	conflict	GB 55771382
1H	654E	C	G	conflict	GB 55771382
1H	654P	G	C	conflict	GB 55771382
1H	654T	A	C	conflict	GB 55771382
1H	1058	U	G	conflict	GB 55771382
1H	1080	A	C	conflict	GB 55771382
14	158	U	UNK	conflict	GB 55771382
14	654A	A	G	conflict	GB 55771382
14	654E	C	G	conflict	GB 55771382
14	654P	G	C	conflict	GB 55771382
14	654T	A	C	conflict	GB 55771382
14	1058	U	G	conflict	GB 55771382
14	1080	A	C	conflict	GB 55771382

- Molecule 27 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	16	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
27	1J	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 28 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	133	Total	C	N	O	S	0	0	0
			1033	651	194	187	1			
28	79	57	Total	C	N	O		0	0	0
			456	283	91	82				

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	11	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			
29	19	274	Total	C	N	O	S	0	0	0
			2125	1341	422	359	3			

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	21	203	Total	C	N	O	S	0	0	0
			1558	985	298	269	6			
30	29	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 31 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
31	39	204	Total	C	N	O	S	0	0	0
			1602	1022	299	279	2			

- Molecule 32 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
32	49	179	Total	C	N	O	S	0	0	0
			1458	931	266	257	4			

- Molecule 33 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	171	Total	C	N	O	S	0	0	0
			1312	832	246	233	1			
33	59	74	Total	C	N	O	S	0	0	0
			573	359	117	97				

- Molecule 34 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	69	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
35	15	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			
36	25	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	78	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			
37	35	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	88	141	Total	C	N	O	S	0	0	0
			1113	709	210	187	7			
38	45	138	Total	C	N	O	S	0	0	0
			1099	702	208	183	6			

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
39	55	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	A8	111	Total	C	N	O	0	0	0
			875	550	176	149			
40	65	110	Total	C	N	O	0	0	0
			876	553	175	148			

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B8	133	Total	C	N	O	S	0	0	0
			1109	691	228	189	1			
41	75	133	Total	C	N	O	S	0	0	0
			1109	691	228	189	1			

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	C8	115	Total	C	N	O	S	0	0	0
			950	603	199	147	1			
42	85	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	D8	100	Total	C	N	O	S	0	0	0
			774	499	141	133	1			
43	95	100	Total	C	N	O	S	0	0	0
			774	499	141	133	1			

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	E8	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			
44	A5	113	Total	C	N	O	S	0	0	0
			899	566	177	154	2			

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	F8	95	Total	C	N	O	S	0	0	0
			743	482	134	126	1			
45	B5	94	Total	C	N	O	S	0	0	0
			735	477	133	125				

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	G8	105	Total	C	N	O	S	0	0	0
			796	513	150	128	5			
46	C5	104	Total	C	N	O	S	0	0	0
			794	510	152	127	5			

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	H8	171	Total	C	N	O	S	0	0	0
			1373	876	247	247	3			
47	D5	132	Total	C	N	O	S	0	0	0
			1074	691	193	188	2			

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	I8	76	Total	C	N	O	S	0	0	0
			606	376	128	101	1			
48	E5	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	J8	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			
49	F5	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	K8	68	Total	C	N	O	S	0	0	0
			568	352	115	100	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	G5	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	L8	58	Total	C	N	O		0	0	0
			459	293	89	77				
51	H5	58	Total	C	N	O		0	0	0
			459	293	89	77				

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M8	47	Total	C	N	O	S	0	0	0
			366	234	61	66	5			

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	N8	48	Total	C	N	O	S	0	0	0
			369	229	75	60	5			
53	J5	56	Total	C	N	O	S	0	0	0
			434	272	87	70	5			

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	P8	47	Total	C	N	O	S	0	0	0
			401	246	99	54	2			
54	L5	47	Total	C	N	O	S	0	0	0
			401	246	99	54	2			

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	Q8	64	Total	C	N	O	S	0	0	0
			516	331	102	81	2			
55	M5	64	Total	C	N	O	S	0	0	0
			516	331	102	81	2			

- Molecule 56 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	3L	75	Total	C	N	O	P	0	0	0
			1601	717	280	530	74			

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

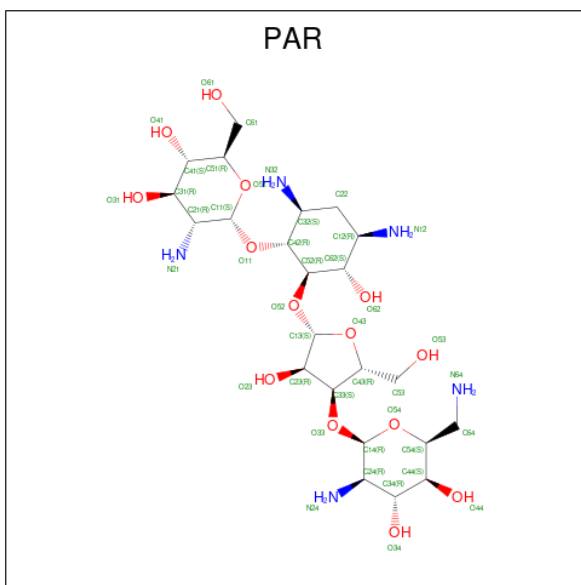
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	13	150	Total	Mg	0	0
			150	150		
57	5E	1	Total	Mg	0	0
			1	1		
57	1I	1	Total	Mg	0	0
			1	1		
57	3I	1	Total	Mg	0	0
			1	1		
57	5I	1	Total	Mg	0	0
			1	1		
57	BI	1	Total	Mg	0	0
			1	1		
57	2K	3	Total	Mg	0	0
			3	3		
57	1H	502	Total	Mg	0	0
			502	502		
57	16	12	Total	Mg	0	0
			12	12		
57	11	3	Total	Mg	0	0
			3	3		
57	21	3	Total	Mg	0	0
			3	3		
57	31	1	Total	Mg	0	0
			1	1		
57	41	2	Total	Mg	0	0
			2	2		
57	78	1	Total	Mg	0	0
			1	1		
57	88	1	Total	Mg	0	0
			1	1		
57	I8	1	Total	Mg	0	0
			1	1		
57	L8	1	Total	Mg	0	0
			1	1		
57	P8	1	Total	Mg	0	0
			1	1		
57	Q8	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

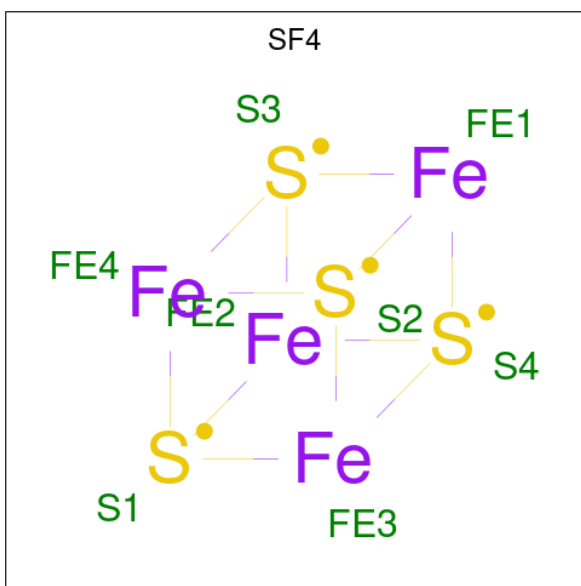
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1G	93	Total 93	Mg 93	0	0
57	7A	1	Total 1	Mg 1	0	0
57	2L	4	Total 4	Mg 4	0	0
57	14	454	Total 454	Mg 454	0	0
57	1J	6	Total 6	Mg 6	0	0
57	29	4	Total 4	Mg 4	0	0
57	39	2	Total 2	Mg 2	0	0
57	35	2	Total 2	Mg 2	0	0
57	45	3	Total 3	Mg 3	0	0
57	55	1	Total 1	Mg 1	0	0
57	85	1	Total 1	Mg 1	0	0
57	C5	1	Total 1	Mg 1	0	0
57	E5	1	Total 1	Mg 1	0	0
57	M5	1	Total 1	Mg 1	0	0

- Molecule 58 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	13	1	Total 42	C 23	N 5	O 14	0	0
58	1G	1	Total 42	C 23	N 5	O 14	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	3E	1	Total 8	Fe 4	S 4	0	0
59	32	1	Total 8	Fe 4	S 4	0	0

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	5I	1	Total Zn 1 1	0	0
60	G8	1	Total Zn 1 1	0	0
60	5A	1	Total Zn 1 1	0	0
60	C5	1	Total Zn 1 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	13	319	Total O 319 319	0	0
61	3E	3	Total O 3 3	0	0
61	4E	3	Total O 3 3	0	0
61	8E	1	Total O 1 1	0	0
61	1I	1	Total O 1 1	0	0
61	3I	3	Total O 3 3	0	0
61	5I	1	Total O 1 1	0	0
61	6I	2	Total O 2 2	0	0
61	8I	2	Total O 2 2	0	0
61	BI	5	Total O 5 5	0	0
61	1F	1	Total O 1 1	0	0
61	1K	1	Total O 1 1	0	0
61	2K	7	Total O 7 7	0	0
61	3K	1	Total O 1 1	0	0
61	4K	4	Total O 4 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1H	1158	Total 1158	O 1158	0	0
61	16	26	Total 26	O 26	0	0
61	11	12	Total 12	O 12	0	0
61	21	6	Total 6	O 6	0	0
61	31	9	Total 9	O 9	0	0
61	58	1	Total 1	O 1	0	0
61	78	6	Total 6	O 6	0	0
61	88	2	Total 2	O 2	0	0
61	C8	2	Total 2	O 2	0	0
61	E8	3	Total 3	O 3	0	0
61	F8	2	Total 2	O 2	0	0
61	G8	2	Total 2	O 2	0	0
61	I8	5	Total 5	O 5	0	0
61	J8	3	Total 3	O 3	0	0
61	K8	2	Total 2	O 2	0	0
61	L8	2	Total 2	O 2	0	0
61	P8	1	Total 1	O 1	0	0
61	Q8	9	Total 9	O 9	0	0
61	1G	226	Total 226	O 226	0	0
61	32	3	Total 3	O 3	0	0
61	42	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	3A	1	Total 1	O 1	0	0
61	6A	3	Total 3	O 3	0	0
61	8A	1	Total 1	O 1	0	0
61	BA	3	Total 3	O 3	0	0
61	2L	1	Total 1	O 1	0	0
61	4L	3	Total 3	O 3	0	0
61	14	1015	Total 1015	O 1015	0	0
61	1J	18	Total 18	O 18	0	0
61	19	12	Total 12	O 12	0	0
61	29	6	Total 6	O 6	0	0
61	39	8	Total 8	O 8	0	0
61	35	5	Total 5	O 5	0	0
61	55	1	Total 1	O 1	0	0
61	75	1	Total 1	O 1	0	0
61	85	2	Total 2	O 2	0	0
61	A5	2	Total 2	O 2	0	0
61	B5	1	Total 1	O 1	0	0
61	C5	4	Total 4	O 4	0	0
61	H5	3	Total 3	O 3	0	0
61	L5	2	Total 2	O 2	0	0
61	M5	10	Total 10	O 10	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	209.70Å 449.50Å 620.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.17 – 3.15 152.17 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (152.17-3.15) 91.9 (152.17-3.15)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.192 , 0.247 0.194 , 0.250	Depositor DCC
R_{free} test set	2000 reflections (0.20%)	wwPDB-VP
Wilson B-factor (Å ²)	80.1	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	296184	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% 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](#)

23 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	PSU	1K	55	22	18,21,22	1.21	1 (5%)	21,30,33	1.97	4 (19%)
22	5MU	1L	54	22	19,22,23	3.97	5 (26%)	27,32,35	3.29	9 (33%)
23	PSU	2K	56	23	18,21,22	1.20	2 (11%)	21,30,33	2.04	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PSU	1L	55	22	18,21,22	1.14	1 (5%)	21,30,33	1.83	5 (23%)
23	4SU	2L	8	23	18,21,22	1.92	3 (16%)	25,30,33	2.78	5 (20%)
24	PSU	3K	39	24	18,21,22	1.32	1 (5%)	21,30,33	1.87	4 (19%)
22	T6A	1K	37	22	26,34,35	2.29	6 (23%)	28,49,52	2.79	9 (32%)
22	5MU	1K	54	22	19,22,23	3.86	5 (26%)	27,32,35	3.19	10 (37%)
22	T6A	1L	37	22	26,34,35	2.04	6 (23%)	28,49,52	2.61	9 (32%)
22	PSU	1K	39	22	18,21,22	1.14	2 (11%)	21,30,33	1.85	5 (23%)
56	PSU	3L	39	56	18,21,22	1.18	2 (11%)	21,30,33	2.11	6 (28%)
23	G7M	2L	47	23	20,26,27	2.39	6 (30%)	16,39,42	1.03	1 (6%)
23	OMC	2K	33	23	19,22,23	1.80	3 (15%)	25,31,34	0.82	0
23	OMC	2L	33	23	19,22,23	1.95	4 (21%)	25,31,34	1.09	1 (4%)
23	4SU	2K	8	23	18,21,22	1.99	5 (27%)	25,30,33	2.64	5 (20%)
23	5MU	2K	55	23	19,22,23	3.87	5 (26%)	27,32,35	3.42	6 (22%)
23	5MU	2L	55	23	19,22,23	3.99	5 (26%)	27,32,35	3.43	11 (40%)
23	PSU	2L	56	23	18,21,22	1.10	1 (5%)	21,30,33	1.92	5 (23%)
22	U8U	1L	34	25,22	20,24,25	2.45	7 (35%)	22,34,37	1.13	3 (13%)
22	PSU	1L	39	22	18,21,22	1.04	1 (5%)	21,30,33	1.85	3 (14%)
56	T6A	3L	37	56	26,34,35	1.93	5 (19%)	28,49,52	2.43	11 (39%)
23	G7M	2K	47	23	20,26,27	2.41	6 (30%)	16,39,42	0.84	1 (6%)
22	U8U	1K	34	25,22	20,24,25	2.37	6 (30%)	22,34,37	0.96	1 (4%)

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	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
22	5MU	1L	54	22	-	0/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
22	PSU	1L	55	22	-	3/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	0/7/25/26	0/2/2/2
24	PSU	3K	39	24	-	3/7/25/26	0/2/2/2
22	T6A	1K	37	22	-	5/19/41/42	0/3/3/3
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
22	T6A	1L	37	22	-	7/19/41/42	0/3/3/3
22	PSU	1K	39	22	-	2/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PSU	3L	39	56	-	2/7/25/26	0/2/2/2
23	G7M	2L	47	23	-	2/3/25/26	0/3/3/3
23	OMC	2K	33	23	-	0/9/27/28	0/2/2/2
23	OMC	2L	33	23	-	1/9/27/28	0/2/2/2
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	1/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
22	U8U	1L	34	25,22	-	3/10/28/29	0/2/2/2
22	PSU	1L	39	22	-	2/7/25/26	0/2/2/2
56	T6A	3L	37	56	-	11/19/41/42	0/3/3/3
23	G7M	2K	47	23	-	1/3/25/26	0/3/3/3
22	U8U	1K	34	25,22	-	2/10/28/29	0/2/2/2

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1L	54	5MU	C2-N1	12.87	1.58	1.38
23	2L	55	5MU	C2-N1	12.85	1.58	1.38
23	2K	55	5MU	C2-N1	12.78	1.58	1.38
22	1K	54	5MU	C2-N1	12.28	1.57	1.38
22	1L	54	5MU	C4-N3	-6.20	1.27	1.38
23	2L	55	5MU	C4-N3	-6.09	1.27	1.38
22	1K	54	5MU	C4-N3	-6.09	1.27	1.38
23	2K	55	5MU	C2-N3	6.07	1.48	1.38
22	1K	37	T6A	C10-N11	6.05	1.52	1.35
23	2L	8	4SU	C5-C4	6.00	1.49	1.42
56	3L	37	T6A	C10-N6	5.97	1.50	1.37
22	1K	37	T6A	C10-N6	5.95	1.50	1.37
23	2K	8	4SU	C5-C4	5.95	1.49	1.42
23	2L	55	5MU	C2-N3	5.90	1.48	1.38
22	1L	34	U8U	C2-S2	-5.77	1.58	1.67
22	1L	54	5MU	C2-N3	5.73	1.47	1.38
22	1K	54	5MU	C2-N3	5.72	1.47	1.38
22	1L	54	5MU	C6-N1	5.62	1.47	1.38
22	1L	37	T6A	C10-N6	5.62	1.49	1.37
23	2L	55	5MU	C6-N1	5.60	1.47	1.38
23	2K	55	5MU	C4-N3	-5.58	1.28	1.38
23	2L	55	5MU	C4-C5	5.50	1.53	1.44
22	1K	54	5MU	C6-N1	5.48	1.47	1.38
23	2K	47	G7M	C2-N3	5.45	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2K	55	5MU	C6-N1	5.33	1.47	1.38
22	1K	34	U8U	C6-C5	5.24	1.49	1.35
22	1L	34	U8U	C6-C5	5.22	1.49	1.35
22	1K	54	5MU	C4-C5	5.21	1.53	1.44
22	1L	37	T6A	C10-N11	5.21	1.49	1.35
22	1K	34	U8U	C2-S2	-5.09	1.59	1.67
23	2L	47	G7M	C2-N3	5.04	1.45	1.33
22	1L	54	5MU	C4-C5	5.03	1.53	1.44
56	3L	37	T6A	C10-N11	4.94	1.49	1.35
23	2K	47	G7M	C4-N3	4.83	1.48	1.37
22	1K	37	T6A	C6-C5	-4.82	1.37	1.44
23	2L	47	G7M	C2-N2	4.81	1.45	1.34
23	2K	47	G7M	C2-N2	4.81	1.45	1.34
23	2K	55	5MU	C4-C5	4.74	1.52	1.44
23	2L	47	G7M	C4-N3	4.70	1.48	1.37
23	2K	33	OMC	C2-N3	4.68	1.45	1.36
23	2L	33	OMC	C2-N3	4.61	1.45	1.36
24	3K	39	PSU	C6-C5	4.49	1.40	1.35
23	2L	33	OMC	C4-N4	4.47	1.44	1.33
22	1K	34	U8U	C2-N3	4.45	1.49	1.38
23	2K	33	OMC	C4-N4	4.36	1.44	1.33
22	1K	55	PSU	C6-C5	4.35	1.40	1.35
22	1L	34	U8U	C6-N1	4.31	1.45	1.38
22	1L	34	U8U	C2-N3	4.25	1.48	1.38
22	1K	34	U8U	C6-N1	4.24	1.45	1.38
23	2L	33	OMC	C5-C4	4.15	1.52	1.42
22	1L	37	T6A	C6-C5	-4.08	1.38	1.44
23	2K	56	PSU	C6-C5	3.90	1.39	1.35
23	2K	8	4SU	C2-N1	3.87	1.44	1.38
23	2L	47	G7M	C6-N1	3.87	1.43	1.37
22	1L	55	PSU	C6-C5	3.79	1.39	1.35
23	2K	33	OMC	C5-C4	3.70	1.51	1.42
23	2L	56	PSU	C6-C5	3.70	1.39	1.35
23	2K	47	G7M	C6-N1	3.67	1.43	1.37
56	3L	39	PSU	C6-C5	3.62	1.39	1.35
22	1K	39	PSU	C6-C5	3.57	1.39	1.35
23	2K	47	G7M	C5-C6	3.50	1.54	1.45
23	2L	8	4SU	C2-N1	3.47	1.43	1.38
22	1L	39	PSU	C6-C5	3.46	1.39	1.35
23	2L	47	G7M	C5-C6	3.18	1.53	1.45
23	2L	8	4SU	C6-N1	3.14	1.45	1.38
22	1L	34	U8U	C4-N3	3.09	1.44	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1K	34	U8U	C4-N3	2.98	1.44	1.38
23	2K	8	4SU	C6-N1	2.90	1.45	1.38
23	2L	47	G7M	C2-N1	2.86	1.44	1.37
23	2K	47	G7M	C2-N1	2.75	1.44	1.37
23	2L	33	OMC	C6-N1	2.75	1.44	1.38
22	1K	37	T6A	C2-N3	2.73	1.36	1.32
56	3L	37	T6A	ODB-C13	-2.58	1.22	1.30
22	1L	37	T6A	ODB-C13	-2.48	1.22	1.30
22	1L	34	U8U	O4-C4	-2.46	1.18	1.23
22	1L	37	T6A	C2-N3	2.39	1.35	1.32
22	1K	34	U8U	O4-C4	-2.38	1.19	1.23
56	3L	37	T6A	C2-N3	2.37	1.35	1.32
56	3L	37	T6A	C6-C5	-2.29	1.41	1.44
23	2K	8	4SU	C4-N3	2.28	1.40	1.37
22	1K	37	T6A	ODB-C13	-2.25	1.23	1.30
22	1L	34	U8U	C4-C5	2.18	1.50	1.45
23	2K	8	4SU	C2-N3	2.13	1.41	1.38
56	3L	39	PSU	O4'-C1'	-2.10	1.40	1.43
23	2K	56	PSU	C4-C5	-2.09	1.38	1.44
22	1K	37	T6A	C2-N1	2.05	1.37	1.33
22	1K	39	PSU	C4-C5	-2.03	1.38	1.44
22	1L	37	T6A	C2-N1	2.02	1.37	1.33

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2K	55	5MU	C5-C4-N3	11.21	125.06	115.32
23	2L	55	5MU	C5-C4-N3	11.07	124.95	115.32
22	1L	54	5MU	C5-C4-N3	10.46	124.41	115.32
22	1K	54	5MU	C5-C4-N3	10.35	124.32	115.32
23	2L	8	4SU	C4-N3-C2	-9.10	118.59	127.31
23	2K	8	4SU	C4-N3-C2	-8.08	119.57	127.31
23	2L	8	4SU	C5-C4-N3	7.66	121.88	114.75
22	1K	37	T6A	N3-C2-N1	-7.55	118.42	128.67
22	1L	37	T6A	N3-C2-N1	-7.21	118.89	128.67
23	2L	55	5MU	C4-N3-C2	-6.74	118.51	127.34
23	2K	55	5MU	O4-C4-C5	-6.46	117.53	124.92
23	2K	55	5MU	C4-N3-C2	-6.44	118.89	127.34
22	1L	54	5MU	C4-N3-C2	-6.44	118.90	127.34
56	3L	37	T6A	N6-C10-N11	6.32	122.47	113.77
23	2K	55	5MU	C5-C6-N1	-6.24	116.53	123.31
22	1K	54	5MU	C4-N3-C2	-6.18	119.24	127.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	3L	37	T6A	N3-C2-N1	-6.11	120.38	128.67
23	2K	8	4SU	C5-C4-N3	6.03	120.36	114.75
22	1K	54	5MU	C5-C6-N1	-5.90	116.90	123.31
23	2L	55	5MU	C5-C6-N1	-5.83	116.98	123.31
22	1L	54	5MU	C6-C5-C4	5.80	122.80	118.02
22	1K	37	T6A	C2-N1-C6	5.76	121.07	116.60
22	1K	37	T6A	N6-C6-N1	5.73	125.16	118.71
22	1L	54	5MU	C5-C6-N1	-5.72	117.10	123.31
23	2K	8	4SU	C5-C4-S4	-5.70	117.79	124.31
56	3L	37	T6A	C2-N1-C6	5.56	120.92	116.60
23	2K	55	5MU	C6-C5-C4	5.48	122.54	118.02
22	1L	37	T6A	C2-N1-C6	5.44	120.82	116.60
22	1K	54	5MU	C6-C5-C4	5.41	122.48	118.02
23	2L	55	5MU	C6-C5-C4	5.35	122.43	118.02
56	3L	39	PSU	C4-N3-C2	-5.22	119.18	126.37
23	2K	56	PSU	N1-C2-N3	5.09	120.54	115.17
23	2L	55	5MU	O4-C4-C5	-5.05	119.14	124.92
22	1L	37	T6A	N6-C10-N11	5.02	120.67	113.77
22	1K	39	PSU	C4-N3-C2	-4.98	119.51	126.37
22	1L	54	5MU	O4-C4-C5	-4.96	119.25	124.92
22	1L	39	PSU	C4-N3-C2	-4.92	119.59	126.37
22	1K	55	PSU	N1-C2-N3	4.92	120.36	115.17
22	1K	54	5MU	O4-C4-C5	-4.83	119.39	124.92
23	2K	56	PSU	C4-N3-C2	-4.81	119.75	126.37
22	1K	37	T6A	N6-C10-N11	4.77	120.34	113.77
22	1K	37	T6A	C12-N11-C10	4.70	129.81	121.99
24	3K	39	PSU	N1-C2-N3	4.67	120.09	115.17
22	1L	37	T6A	C12-N11-C10	4.61	129.66	121.99
23	2L	55	5MU	C5M-C5-C6	-4.61	116.62	122.85
23	2L	8	4SU	N3-C2-N1	4.57	120.84	114.89
56	3L	39	PSU	N1-C2-N3	4.47	119.89	115.17
22	1K	55	PSU	C4-N3-C2	-4.42	120.28	126.37
22	1L	37	T6A	N6-C6-N1	4.40	123.66	118.71
22	1L	55	PSU	N1-C2-N3	4.40	119.81	115.17
22	1L	55	PSU	C4-N3-C2	-4.33	120.40	126.37
23	2K	55	5MU	C5M-C5-C6	-4.30	117.03	122.85
22	1K	39	PSU	N1-C2-N3	4.27	119.67	115.17
22	1L	39	PSU	N1-C2-N3	4.24	119.64	115.17
24	3K	39	PSU	C6-N1-C2	-4.18	118.81	122.69
23	2K	8	4SU	N3-C2-N1	4.15	120.29	114.89
22	1K	54	5MU	C5M-C5-C6	-4.01	117.43	122.85
22	1L	54	5MU	C5M-C5-C6	-3.97	117.48	122.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2L	56	PSU	C4-N3-C2	-3.83	121.10	126.37
23	2L	8	4SU	C5-C4-S4	-3.82	119.95	124.31
22	1L	37	T6A	O10-C10-N6	-3.69	117.08	123.64
22	1K	37	T6A	C6-C5-C4	3.64	121.53	117.68
23	2L	56	PSU	N1-C2-N3	3.64	119.00	115.17
22	1K	37	T6A	O10-C10-N6	-3.63	117.19	123.64
23	2L	56	PSU	C6-N1-C2	-3.61	119.34	122.69
24	3K	39	PSU	C4-N3-C2	-3.61	121.40	126.37
22	1K	55	PSU	O2-C2-N1	-3.60	119.08	122.79
24	3K	39	PSU	O2-C2-N1	-3.54	119.13	122.79
56	3L	39	PSU	C3'-C2'-C1'	3.40	105.70	101.69
22	1L	54	5MU	C6-N1-C2	-3.23	118.09	121.30
22	1L	39	PSU	O2-C2-N1	-3.19	119.49	122.79
23	2L	56	PSU	O2-C2-N1	-3.18	119.51	122.79
23	2K	56	PSU	C6-N1-C2	-3.14	119.78	122.69
22	1K	55	PSU	C6-N1-C2	-3.06	119.85	122.69
23	2L	33	OMC	O2-C2-N3	-3.06	117.51	122.33
22	1L	54	5MU	N3-C2-N1	2.92	118.70	114.89
23	2K	8	4SU	C1'-N1-C2	2.84	122.70	117.59
22	1L	34	U8U	C5-C4-N3	2.76	119.42	115.21
22	1K	39	PSU	O2-C2-N1	-2.74	119.96	122.79
56	3L	37	T6A	O10-C10-N6	-2.68	118.87	123.64
23	2L	56	PSU	C6-C5-C4	-2.67	116.37	118.17
23	2L	55	5MU	N3-C2-N1	2.61	118.28	114.89
56	3L	37	T6A	N6-C6-N1	-2.61	115.79	118.71
56	3L	37	T6A	C13-C12-N11	-2.57	104.54	110.17
23	2L	55	5MU	C6-N1-C2	-2.56	118.76	121.30
23	2K	47	G7M	C2-N1-C6	-2.55	120.44	125.11
22	1L	55	PSU	C6-N1-C2	-2.55	120.32	122.69
22	1L	37	T6A	C6-C5-C4	2.53	120.36	117.68
22	1L	55	PSU	C6-C5-C4	2.52	119.87	118.17
23	2L	47	G7M	C2-N1-C6	-2.51	120.52	125.11
22	1K	54	5MU	N3-C2-N1	2.44	118.07	114.89
22	1L	55	PSU	O2-C2-N1	-2.43	120.28	122.79
23	2K	56	PSU	O2-C2-N1	-2.39	120.32	122.79
22	1K	34	U8U	C5-C4-N3	2.37	118.82	115.21
56	3L	37	T6A	C14-C12-N11	2.37	117.99	111.70
56	3L	37	T6A	C6-C5-C4	2.33	120.15	117.68
22	1K	54	5MU	C6-N1-C2	-2.32	118.99	121.30
22	1L	34	U8U	C1'-N1-C6	-2.31	117.35	121.15
23	2K	56	PSU	C6-C5-C4	2.30	119.73	118.17
22	1K	37	T6A	ODB-C13-ODA	-2.29	118.89	124.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1L	37	T6A	C14-C12-N11	2.25	117.68	111.70
23	2L	55	5MU	O4-C4-N3	-2.24	115.91	120.11
22	1L	37	T6A	C15-C14-C12	-2.20	107.95	112.29
22	1K	54	5MU	O2-C2-N1	-2.19	119.94	122.80
23	2L	8	4SU	O2-C2-N1	-2.19	119.95	122.80
56	3L	39	PSU	O2-C2-N1	-2.18	120.54	122.79
22	1L	34	U8U	S2-C2-N3	-2.17	114.02	119.44
23	2L	55	5MU	C1'-N1-C2	2.16	121.47	117.59
22	1K	39	PSU	C5-C4-N3	2.15	121.29	116.55
56	3L	39	PSU	O4'-C1'-C2'	2.14	108.11	105.15
22	1K	39	PSU	C6-N1-C2	-2.13	120.72	122.69
56	3L	37	T6A	C4-C5-N7	-2.12	107.09	109.34
56	3L	37	T6A	C12-N11-C10	2.08	125.44	121.99
22	1K	37	T6A	ODB-C13-C12	2.07	121.33	114.15
56	3L	37	T6A	ODB-C13-ODA	-2.04	119.45	124.08
23	2L	55	5MU	C5M-C5-C4	2.04	120.95	118.78
22	1K	54	5MU	O4-C4-N3	-2.03	116.29	120.11
56	3L	39	PSU	C5-C6-N1	-2.02	119.33	122.14
22	1L	54	5MU	O4-C4-N3	-2.01	116.34	120.11

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	37	T6A	C14-C12-N11-C10
22	1L	34	U8U	N-C-C5-C4
22	1L	34	U8U	N-C-C5-C6
22	1L	34	U8U	C5-C-N-CA
22	1L	37	T6A	C5-C6-N6-C10
22	1L	37	T6A	N1-C6-N6-C10
22	1L	37	T6A	C14-C12-N11-C10
22	1L	37	T6A	C13-C12-C14-O14
22	1L	37	T6A	C13-C12-C14-C15
22	1L	39	PSU	O4'-C4'-C5'-O5'
56	3L	37	T6A	C5-C6-N6-C10
56	3L	37	T6A	N11-C12-C14-O14
56	3L	37	T6A	N11-C12-C14-C15
56	3L	37	T6A	C13-C12-C14-O14
56	3L	37	T6A	C13-C12-C14-C15
23	2L	47	G7M	O4'-C4'-C5'-O5'
24	3K	39	PSU	C3'-C4'-C5'-O5'
22	1L	39	PSU	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	1L	55	PSU	C3'-C4'-C5'-O5'
56	3L	37	T6A	O4'-C4'-C5'-O5'
22	1L	55	PSU	O4'-C4'-C5'-O5'
56	3L	37	T6A	C3'-C4'-C5'-O5'
23	2L	47	G7M	C3'-C4'-C5'-O5'
56	3L	37	T6A	C13-C12-N11-C10
22	1L	37	T6A	N11-C12-C14-O14
22	1K	37	T6A	C14-C12-C13-ODB
56	3L	37	T6A	C14-C12-C13-ODA
24	3K	39	PSU	O4'-C4'-C5'-O5'
56	3L	39	PSU	O4'-C4'-C5'-O5'
22	1K	37	T6A	C13-C12-C14-C15
22	1K	37	T6A	C14-C12-C13-ODA
22	1L	37	T6A	N11-C12-C14-C15
56	3L	37	T6A	C14-C12-C13-ODB
23	2L	55	5MU	C4'-C5'-O5'-P
22	1K	39	PSU	O4'-C1'-C5-C4
22	1L	55	PSU	O4'-C1'-C5-C4
22	1K	34	U8U	C3'-C4'-C5'-O5'
24	3K	39	PSU	C4'-C5'-O5'-P
23	2K	47	G7M	C4'-C5'-O5'-P
22	1K	39	PSU	O4'-C1'-C5-C6
22	1K	37	T6A	N11-C12-C14-C15
56	3L	37	T6A	C14-C12-N11-C10
56	3L	39	PSU	C4'-C5'-O5'-P
23	2L	33	OMC	C2'-C1'-N1-C2
22	1K	34	U8U	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 1269 ligands modelled in this entry, 1265 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	$\# Z > 2$
59	SF4	32	301	-	0,12,12	-	-	-		
58	PAR	13	1749	-	44,45,45	0.85	0	63,67,67	2.04	16 (25%)
58	PAR	1G	1691	-	44,45,45	0.69	0	63,67,67	1.71	17 (26%)
59	SF4	3E	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
59	SF4	32	301	-	-	-	0/6/5/5
58	PAR	13	1749	-	-	3/18/94/94	0/4/4/4
58	PAR	1G	1691	-	-	5/18/94/94	0/4/4/4
59	SF4	3E	301	4	-	-	0/6/5/5

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	13	1749	PAR	C22-C12-C62	-4.93	102.69	110.08
58	13	1749	PAR	C14-O33-C33	-4.92	106.32	117.98
58	13	1749	PAR	C32-C22-C12	-4.82	102.76	111.02
58	1G	1691	PAR	O11-C11-C21	-4.75	100.30	108.08
58	13	1749	PAR	C11-O51-C51	4.54	122.58	113.72
58	13	1749	PAR	O52-C13-O43	-4.44	106.83	111.37
58	13	1749	PAR	C14-O54-C54	4.32	122.17	113.72
58	1G	1691	PAR	C14-O54-C54	4.16	121.85	113.72
58	13	1749	PAR	O51-C51-C41	4.08	117.06	109.70
58	1G	1691	PAR	O11-C42-C32	-3.72	100.31	109.18
58	1G	1691	PAR	O54-C54-C64	3.71	113.19	106.07
58	1G	1691	PAR	C13-O52-C52	-3.47	109.76	117.98
58	13	1749	PAR	O11-C42-C32	-3.22	101.49	109.18
58	1G	1691	PAR	C14-O33-C33	-3.22	110.36	117.98
58	13	1749	PAR	C41-C31-C21	-2.91	106.16	110.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	13	1749	PAR	O11-C11-C21	-2.89	103.34	108.08
58	13	1749	PAR	O54-C14-C24	2.75	116.17	110.08
58	1G	1691	PAR	O51-C11-C21	2.74	116.14	110.08
58	13	1749	PAR	O54-C54-C44	2.70	114.56	109.70
58	1G	1691	PAR	O62-C62-C12	-2.67	104.91	109.90
58	1G	1691	PAR	C62-C12-N12	-2.67	105.68	110.94
58	13	1749	PAR	O51-C11-C21	2.55	115.72	110.08
58	1G	1691	PAR	C31-C21-N21	-2.45	106.04	111.05
58	13	1749	PAR	O52-C52-C42	2.41	113.54	107.42
58	1G	1691	PAR	C32-C22-C12	-2.32	107.04	111.02
58	1G	1691	PAR	O62-C62-C52	2.32	115.87	109.94
58	13	1749	PAR	O11-C42-C52	2.31	113.28	107.42
58	1G	1691	PAR	O11-C42-C52	2.25	113.14	107.42
58	1G	1691	PAR	C11-C21-N21	-2.18	106.27	110.20
58	1G	1691	PAR	C41-C31-C21	-2.09	107.52	110.99
58	13	1749	PAR	C13-O52-C52	-2.02	113.18	117.98
58	1G	1691	PAR	C11-O51-C51	2.02	117.67	113.72
58	1G	1691	PAR	O52-C13-O43	-2.00	109.32	111.37

There are no chirality outliers.

All (8) torsion outliers are listed below:

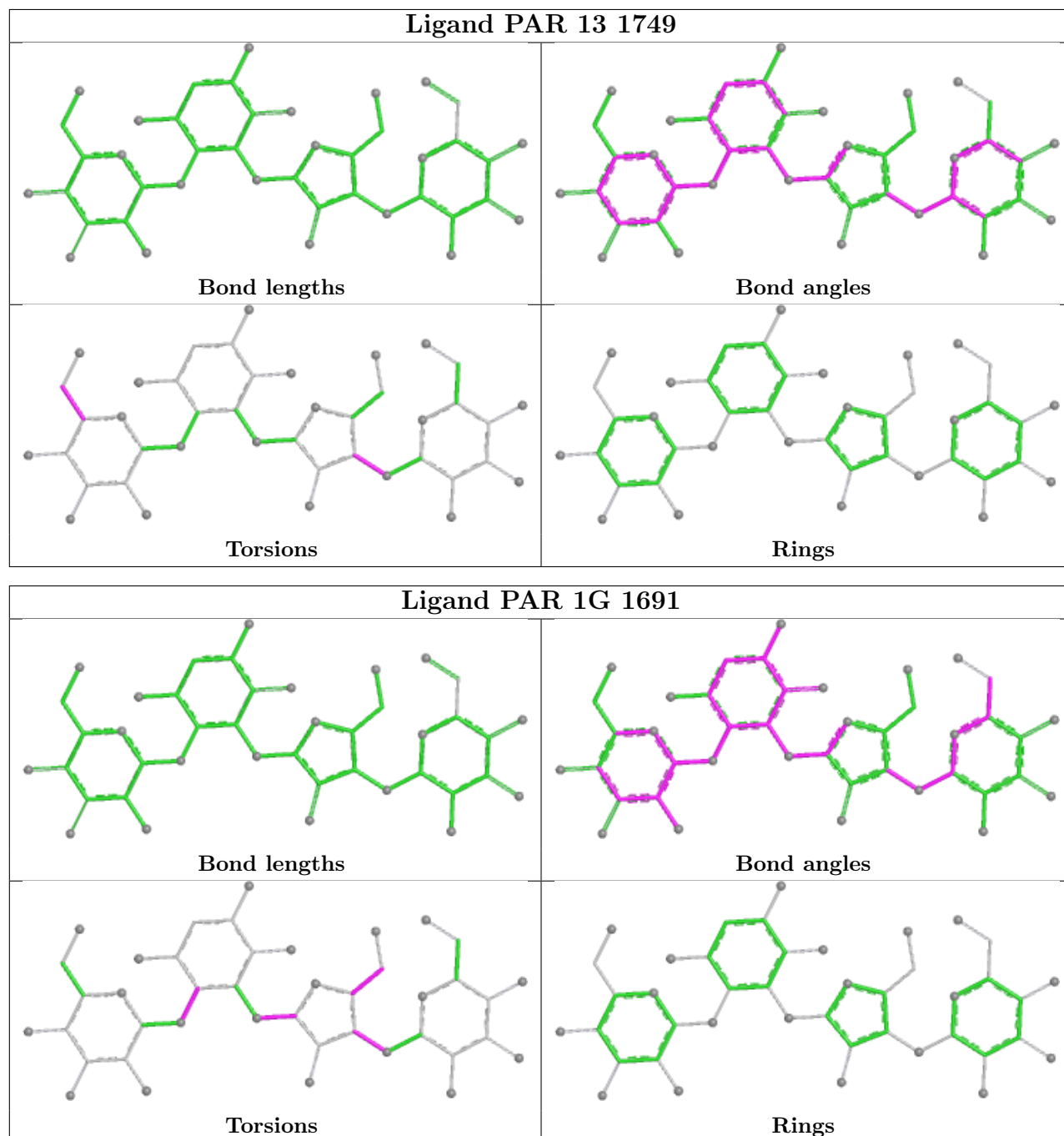
Mol	Chain	Res	Type	Atoms
58	13	1749	PAR	C41-C51-C61-O61
58	1G	1691	PAR	C33-C43-C53-O53
58	1G	1691	PAR	O43-C43-C53-O53
58	13	1749	PAR	O51-C51-C61-O61
58	1G	1691	PAR	C52-C42-O11-C11
58	13	1749	PAR	C43-C33-O33-C14
58	1G	1691	PAR	C43-C33-O33-C14
58	1G	1691	PAR	O43-C13-O52-C52

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 ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	3E	1
34	69	1
10	1A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3E	36:ARG	C	37:PRO	N	1.17
1	69	79:ILE	C	80:PRO	N	1.16
1	1A	76:ASN	C	77:PRO	N	1.12

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	13	1496/1522 (98%)	-0.63	2 (0%) 92 90	58, 99, 162, 246	0
1	1G	1506/1522 (98%)	-0.56	4 (0%) 90 83	73, 114, 168, 253	0
2	12	210/256 (82%)	0.00	1 (0%) 87 77	127, 152, 169, 182	0
2	1E	231/256 (90%)	-0.16	4 (1%) 69 53	105, 136, 157, 168	0
3	22	196/239 (82%)	-0.14	0 100 100	122, 138, 165, 170	0
3	2E	205/239 (85%)	-0.48	1 (0%) 87 77	81, 103, 128, 138	0
4	32	208/209 (99%)	0.10	4 (1%) 66 50	98, 118, 136, 144	0
4	3E	207/209 (99%)	-0.17	1 (0%) 87 77	80, 101, 121, 129	0
5	42	148/162 (91%)	-0.08	0 100 100	104, 121, 137, 147	0
5	4E	149/162 (91%)	-0.33	0 100 100	79, 96, 112, 121	0
6	52	101/101 (100%)	-0.64	0 100 100	83, 101, 118, 131	0
6	5E	100/101 (99%)	-0.28	2 (2%) 64 49	83, 100, 115, 121	0
7	62	139/156 (89%)	-0.37	1 (0%) 84 72	111, 124, 135, 141	0
7	6E	154/156 (98%)	-0.29	2 (1%) 74 59	101, 115, 132, 141	0
8	72	137/138 (99%)	-0.13	1 (0%) 84 72	104, 124, 136, 142	0
8	7E	138/138 (100%)	-0.29	3 (2%) 62 46	91, 106, 118, 127	0
9	82	121/128 (94%)	0.55	9 (7%) 22 15	110, 151, 165, 175	0
9	8E	126/128 (98%)	0.03	1 (0%) 82 69	89, 128, 147, 153	0
10	1A	80/105 (76%)	0.65	7 (8%) 17 11	116, 145, 154, 156	0
10	1I	91/105 (86%)	-0.06	1 (1%) 77 62	80, 121, 156, 161	0
11	2A	113/129 (87%)	-0.35	1 (0%) 81 67	86, 110, 123, 130	0
11	2I	111/129 (86%)	-0.41	0 100 100	77, 102, 118, 125	0
12	3A	122/132 (92%)	-0.06	4 (3%) 49 34	84, 102, 126, 145	0
12	3I	122/132 (92%)	-0.55	0 100 100	67, 77, 99, 122	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	111/126 (88%)	-0.03	3 (2%) 56 40	109, 138, 154, 162	0
13	4I	119/126 (94%)	0.01	4 (3%) 48 33	84, 113, 128, 142	0
14	5A	59/61 (96%)	0.70	4 (6%) 25 16	122, 135, 145, 150	0
14	5I	60/61 (98%)	-0.18	1 (1%) 69 53	82, 92, 108, 112	0
15	6A	88/89 (98%)	-0.31	1 (1%) 77 62	89, 109, 128, 132	0
15	6I	87/89 (97%)	-0.34	0 100 100	83, 99, 116, 124	0
16	7A	84/88 (95%)	-0.08	1 (1%) 76 60	92, 107, 125, 140	0
16	7I	83/88 (94%)	0.28	1 (1%) 76 60	97, 106, 136, 155	0
17	8A	99/105 (94%)	-0.16	0 100 100	95, 114, 127, 134	0
17	8I	100/105 (95%)	-0.07	3 (3%) 52 37	88, 104, 115, 121	0
18	9A	67/88 (76%)	-0.57	0 100 100	93, 111, 130, 132	0
18	9I	68/88 (77%)	-0.47	0 100 100	87, 102, 124, 127	0
19	AA	62/93 (66%)	0.00	0 100 100	123, 142, 153, 156	0
19	AI	81/93 (87%)	-0.29	0 100 100	91, 110, 132, 138	0
20	BA	99/106 (93%)	-0.22	1 (1%) 79 65	90, 110, 133, 142	0
20	BI	97/106 (91%)	0.14	4 (4%) 42 28	104, 121, 147, 152	0
21	1B	22/27 (81%)	1.48	6 (27%) 2 1	119, 130, 141, 145	0
21	1F	23/27 (85%)	0.06	0 100 100	89, 102, 110, 112	0
22	1K	64/76 (84%)	-0.11	4 (6%) 27 17	84, 173, 191, 198	0
22	1L	68/76 (89%)	0.04	3 (4%) 39 26	115, 198, 216, 220	0
23	2K	72/77 (93%)	-0.61	0 100 100	74, 96, 123, 139	0
23	2L	72/77 (93%)	-0.50	0 100 100	81, 109, 138, 153	0
24	3K	75/76 (98%)	-0.19	1 (1%) 74 59	76, 207, 224, 234	0
25	4K	20/27 (74%)	0.13	0 100 100	73, 133, 219, 222	0
25	4L	19/27 (70%)	0.30	1 (5%) 33 21	92, 146, 215, 217	0
26	14	2861/2917 (98%)	-0.79	2 (0%) 92 90	54, 86, 192, 250	0
26	1H	2833/2917 (97%)	-0.86	6 (0%) 92 87	44, 76, 171, 250	0
27	16	122/122 (100%)	-0.85	0 100 100	69, 93, 114, 188	0
27	1J	122/122 (100%)	-0.47	1 (0%) 82 69	87, 113, 134, 182	0
28	71	133/229 (58%)	0.39	8 (6%) 29 18	135, 198, 223, 231	0
28	79	57/229 (24%)	0.23	3 (5%) 33 21	141, 174, 199, 206	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	11	273/276 (98%)	-0.35	3 (1%) 77 62	43, 68, 86, 96	0
29	19	274/276 (99%)	-0.28	3 (1%) 77 62	52, 75, 91, 115	0
30	21	203/206 (98%)	0.06	9 (4%) 39 26	55, 93, 129, 137	0
30	29	204/206 (99%)	-0.08	3 (1%) 71 57	63, 94, 125, 142	0
31	31	202/210 (96%)	-0.43	0 100 100	49, 80, 114, 128	0
31	39	204/210 (97%)	-0.34	0 100 100	60, 101, 144, 170	0
32	41	179/182 (98%)	-0.20	4 (2%) 62 46	80, 101, 132, 143	0
32	49	179/182 (98%)	-0.23	2 (1%) 77 62	107, 123, 144, 167	0
33	51	171/180 (95%)	-0.23	0 100 100	84, 103, 118, 126	0
33	59	74/180 (41%)	0.53	6 (8%) 19 13	127, 155, 176, 191	0
34	61	146/148 (98%)	-0.30	1 (0%) 84 72	80, 125, 142, 155	0
34	69	145/148 (97%)	-0.17	3 (2%) 63 48	86, 121, 142, 152	0
35	15	138/140 (98%)	-0.07	2 (1%) 73 58	80, 104, 132, 141	0
35	58	138/140 (98%)	-0.16	2 (1%) 73 58	67, 94, 126, 137	0
36	25	122/122 (100%)	-0.33	3 (2%) 58 42	69, 87, 103, 112	0
36	68	122/122 (100%)	-0.27	0 100 100	61, 79, 95, 103	0
37	35	147/150 (98%)	0.06	3 (2%) 64 49	60, 102, 129, 139	0
37	78	147/150 (98%)	-0.18	1 (0%) 84 72	50, 84, 111, 117	0
38	45	138/141 (97%)	0.24	6 (4%) 40 27	74, 100, 118, 130	0
38	88	141/141 (100%)	-0.38	1 (0%) 84 72	61, 80, 100, 123	0
39	55	118/118 (100%)	-0.48	0 100 100	64, 80, 96, 107	0
39	98	118/118 (100%)	-0.29	0 100 100	66, 89, 106, 118	0
40	65	110/112 (98%)	-0.00	4 (3%) 46 31	84, 106, 121, 127	0
40	A8	111/112 (99%)	-0.37	1 (0%) 81 67	76, 88, 107, 116	0
41	75	133/146 (91%)	0.01	6 (4%) 39 25	76, 95, 122, 143	0
41	B8	133/146 (91%)	-0.07	3 (2%) 61 45	71, 94, 126, 141	0
42	85	116/118 (98%)	-0.22	0 100 100	67, 90, 121, 132	0
42	C8	115/118 (97%)	0.01	1 (0%) 81 67	60, 84, 111, 120	0
43	95	100/101 (99%)	-0.00	5 (5%) 35 23	68, 117, 131, 142	0
43	D8	100/101 (99%)	0.01	2 (2%) 64 49	62, 103, 123, 129	0
44	A5	113/113 (100%)	-0.35	0 100 100	61, 75, 104, 155	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	E8	112/113 (99%)	-0.46	0 100 100	60, 76, 104, 136	0
45	B5	94/96 (97%)	-0.38	1 (1%) 77 62	72, 83, 104, 119	0
45	F8	95/96 (98%)	-0.58	0 100 100	59, 74, 97, 107	0
46	C5	104/110 (94%)	0.19	1 (0%) 79 65	89, 114, 147, 154	0
46	G8	105/110 (95%)	0.11	6 (5%) 30 19	72, 94, 124, 135	0
47	D5	132/206 (64%)	-0.19	1 (0%) 82 69	104, 132, 155, 163	0
47	H8	171/206 (83%)	-0.31	1 (0%) 85 75	87, 118, 188, 193	0
48	E5	77/85 (90%)	0.09	1 (1%) 74 59	69, 87, 102, 123	0
48	I8	76/85 (89%)	-0.18	2 (2%) 57 41	59, 72, 85, 100	0
49	F5	94/98 (95%)	0.09	5 (5%) 33 21	66, 84, 115, 128	0
49	J8	94/98 (95%)	-0.24	1 (1%) 77 62	54, 77, 114, 120	0
50	G5	66/72 (91%)	-0.20	1 (1%) 71 57	81, 101, 121, 132	0
50	K8	68/72 (94%)	-0.16	1 (1%) 71 57	67, 84, 98, 115	0
51	H5	58/60 (96%)	-0.27	1 (1%) 69 53	77, 98, 128, 136	0
51	L8	58/60 (96%)	-0.57	0 100 100	65, 83, 107, 123	0
52	M8	47/71 (66%)	-0.02	1 (2%) 63 48	102, 135, 150, 157	0
53	J5	56/60 (93%)	-0.23	1 (1%) 67 52	59, 87, 127, 134	0
53	N8	48/60 (80%)	-0.22	0 100 100	55, 86, 128, 132	0
54	L5	47/49 (95%)	-0.38	2 (4%) 40 27	54, 62, 83, 88	0
54	P8	47/49 (95%)	-0.42	1 (2%) 63 48	49, 55, 72, 81	0
55	M5	64/65 (98%)	0.06	2 (3%) 51 36	68, 78, 93, 111	0
55	Q8	64/65 (98%)	-0.27	0 100 100	62, 70, 84, 97	0
56	3L	73/76 (96%)	0.10	3 (4%) 42 28	84, 205, 228, 235	0
All	All	20602/21967 (93%)	-0.41	213 (1%) 79 65	43, 99, 165, 253	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
41	B8	1	MET	7.9
41	75	1	MET	6.9
41	B8	104	ASN	5.9
22	1L	76	A	5.2
21	1B	2	GLY	5.0
14	5I	2	ALA	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	BI	70	SER	4.5
40	65	20	ARG	4.5
26	1H	2476	A	4.4
9	82	125	TYR	4.3
41	75	6	LEU	4.1
22	1K	76	A	4.1
41	75	2	ASN	4.0
33	59	171	LEU	3.9
34	69	20	ASP	3.9
41	75	104	ASN	3.8
41	75	106	SER	3.8
27	1J	88	C	3.7
9	82	75	ASP	3.6
33	59	169	VAL	3.5
21	1B	23	PRO	3.5
21	1B	3	LYS	3.5
20	BI	18	GLN	3.4
36	25	80	ASP	3.4
28	71	196	LEU	3.4
7	6E	5	ARG	3.4
49	F5	85	LEU	3.3
30	21	78	LEU	3.3
43	95	83	ARG	3.3
7	6E	8	GLU	3.3
13	4I	120	LYS	3.3
26	1H	2477	C	3.2
34	69	1	MET	3.2
8	7E	91	ARG	3.2
29	19	27	THR	3.2
32	41	26	GLN	3.2
33	59	4	ILE	3.2
38	45	2	LEU	3.2
54	L5	1	MET	3.2
29	11	247	ALA	3.2
10	1A	58	ASP	3.2
28	71	197	GLU	3.2
38	45	91	GLU	3.2
4	3E	209	ARG	3.1
13	4I	2	ALA	3.1
46	C5	105	ALA	3.1
48	I8	9	SER	3.1
16	7I	66	PRO	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	1A	74	ILE	3.1
14	5A	6	LEU	3.1
38	45	90	VAL	3.1
45	B5	69	TYR	3.1
9	8E	126	SER	3.0
42	C8	116	ALA	3.0
6	5E	56	PRO	3.0
40	65	5	THR	3.0
21	1B	6	ARG	3.0
10	1A	85	LEU	3.0
40	65	3	ARG	2.9
53	J5	26	THR	2.9
43	95	81	TYR	2.9
47	D5	138	GLU	2.9
21	1B	14	TRP	2.9
32	49	82	LEU	2.8
29	19	55	GLY	2.8
55	M5	34	TRP	2.8
30	29	76	ARG	2.8
26	1H	1106	G	2.8
37	35	52	GLU	2.8
43	95	93	GLU	2.8
55	M5	40	GLU	2.8
37	35	35	HIS	2.8
6	5E	55	ASP	2.8
29	11	273	ARG	2.7
43	95	80	GLN	2.7
32	41	3	LEU	2.7
30	21	63	LEU	2.7
9	82	44	VAL	2.7
26	14	530	G	2.7
29	11	262	ARG	2.7
4	32	5	ILE	2.7
28	71	192	PHE	2.7
49	F5	77	ALA	2.7
8	7E	1	MET	2.7
9	82	12	GLU	2.7
49	J8	92	LYS	2.7
40	A8	48	LEU	2.7
38	88	140	ALA	2.6
48	E5	7	LEU	2.6
38	45	102	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	5A	39	LEU	2.6
35	58	73	THR	2.6
50	K8	69	ARG	2.6
28	79	209	LEU	2.6
38	45	103	MET	2.6
13	4A	102	ARG	2.6
40	65	17	ARG	2.6
46	G8	2	ARG	2.6
2	1E	11	LEU	2.6
13	4I	6	GLY	2.6
22	1L	75	C	2.5
30	21	75	VAL	2.5
34	61	20	ASP	2.5
9	82	50	LEU	2.5
20	BI	23	ARG	2.5
30	21	90	THR	2.5
32	41	82	LEU	2.5
9	82	115	GLY	2.5
46	G8	98	VAL	2.5
9	82	71	SER	2.5
20	BA	9	ASN	2.5
30	21	50	GLY	2.5
49	F5	36	GLY	2.5
37	78	36	LYS	2.5
28	71	175	VAL	2.5
28	71	49	ILE	2.5
33	59	148	ILE	2.5
30	21	76	ARG	2.5
25	4L	24	A	2.5
26	1H	2117	A	2.5
13	4A	100	GLY	2.5
51	H5	17	LYS	2.5
30	29	7	VAL	2.5
1	1G	963	G	2.4
10	1A	59	SER	2.4
10	1A	46	ARG	2.4
2	1E	14	GLY	2.4
1	1G	1286	A	2.4
11	2A	126	ARG	2.4
33	59	55	PRO	2.3
8	7E	132	GLU	2.3
2	12	43	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	82	43	ALA	2.3
34	69	3	VAL	2.3
35	15	46	VAL	2.3
29	19	30	GLU	2.3
3	2E	2	GLY	2.3
35	58	93	THR	2.3
13	4A	10	PRO	2.3
30	21	51	PHE	2.3
35	15	92	ALA	2.3
47	H8	165	VAL	2.3
8	72	112	LEU	2.3
36	25	81	ASP	2.3
22	1L	74	C	2.3
46	G8	106	LEU	2.3
46	G8	89	PHE	2.2
43	D8	80	GLN	2.2
17	8I	33	GLY	2.2
28	79	47	LEU	2.2
46	G8	105	ALA	2.2
32	41	75	LYS	2.2
22	1K	73	A	2.2
26	1H	1032	A	2.2
26	1H	2119	A	2.2
1	13	76	G	2.2
12	3A	28	LYS	2.2
13	4I	7	VAL	2.2
28	71	29	VAL	2.2
56	3L	34	U	2.2
14	5A	38	GLY	2.2
50	G5	66	GLU	2.2
49	F5	86	SER	2.2
54	L5	47	ARG	2.2
43	95	76	LYS	2.2
16	7A	64	ALA	2.2
48	I8	42	GLY	2.2
1	1G	974	A	2.2
10	1A	65	LEU	2.2
20	BI	20	LEU	2.2
22	1K	74	C	2.1
30	29	159	HIS	2.1
4	32	135	LEU	2.1
33	59	141	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
43	D8	81	TYR	2.1
10	1A	57	LYS	2.1
52	M8	34	GLU	2.1
15	6A	31	LEU	2.1
56	3L	17	U	2.1
4	32	134	ASP	2.1
46	G8	94	LYS	2.1
17	8I	29	HIS	2.1
38	45	83	MET	2.1
12	3A	18	VAL	2.1
22	1K	75	C	2.1
12	3A	91	LYS	2.1
30	21	151	TYR	2.1
30	21	186	GLY	2.1
54	P8	47	ARG	2.1
14	5A	37	PHE	2.1
1	1G	630	G	2.1
2	1E	10	LEU	2.1
36	25	117	LEU	2.1
9	82	76	ALA	2.1
41	B8	106	SER	2.1
7	62	37	ASN	2.1
28	71	208	PHE	2.1
37	35	47	ASP	2.1
41	75	105	LEU	2.1
2	1E	137	ARG	2.0
1	13	933	G	2.0
12	3A	27	LEU	2.0
28	79	222	VAL	2.0
56	3L	7	U	2.0
4	32	122	ARG	2.0
17	8I	24	GLU	2.0
49	F5	78	LYS	2.0
32	49	138	GLN	2.0
28	71	28	LEU	2.0
10	1I	55	LYS	2.0
21	1B	13	ILE	2.0
24	3K	65	C	2.0
26	14	2145	C	2.0

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
56	PSU	3L	39	20/21	0.77	0.11	118,132,140,141	0
22	PSU	1L	55	20/21	0.82	0.08	126,149,158,158	0
23	5MU	2L	55	21/22	0.85	0.09	105,114,119,125	0
24	PSU	3K	39	20/21	0.86	0.07	109,116,128,137	0
23	PSU	2L	56	20/21	0.87	0.06	106,110,116,120	0
22	5MU	1K	54	21/22	0.88	0.07	118,126,140,143	0
22	PSU	1K	55	20/21	0.88	0.07	107,132,143,147	0
56	T6A	3L	37	32/33	0.88	0.10	121,132,147,147	0
23	G7M	2L	47	24/25	0.89	0.08	114,121,128,132	0
22	5MU	1L	54	21/22	0.90	0.07	131,141,157,158	0
23	5MU	2K	55	21/22	0.91	0.07	90,103,110,112	0
23	4SU	2L	8	20/21	0.91	0.07	100,111,114,121	0
23	PSU	2K	56	20/21	0.91	0.07	95,100,104,111	0
22	T6A	1L	37	32/33	0.91	0.15	104,115,143,144	0
23	G7M	2K	47	24/25	0.92	0.06	90,101,110,116	0
22	T6A	1K	37	32/33	0.93	0.18	66,85,127,129	0
22	U8U	1L	34	23/24	0.93	0.13	115,123,131,134	0
23	4SU	2K	8	20/21	0.94	0.07	87,92,97,98	0
22	U8U	1K	34	23/24	0.94	0.09	81,89,100,107	0
22	PSU	1K	39	20/21	0.95	0.07	79,97,103,106	0
22	PSU	1L	39	20/21	0.95	0.07	104,123,128,130	0
23	OMC	2L	33	21/22	0.95	0.09	96,100,104,113	0
23	OMC	2K	33	21/22	0.96	0.08	73,80,83,87	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($\text{\AA}^2$)	Q<0.9
57	MG	14	3232	1/1	0.30	0.25	130,130,130,130	0
57	MG	13	1646	1/1	0.32	0.26	109,109,109,109	0
57	MG	1G	1628	1/1	0.44	0.22	124,124,124,124	0
57	MG	1H	3282	1/1	0.47	0.30	96,96,96,96	0
57	MG	13	1650	1/1	0.49	0.35	100,100,100,100	0
57	MG	13	1642	1/1	0.49	0.36	107,107,107,107	0
57	MG	14	3031	1/1	0.53	0.30	105,105,105,105	0
57	MG	1H	3183	1/1	0.54	0.35	92,92,92,92	0
57	MG	1H	3018	1/1	0.56	0.28	80,80,80,80	0
57	MG	45	202	1/1	0.59	0.28	102,102,102,102	0
57	MG	1G	1621	1/1	0.60	0.31	103,103,103,103	0
57	MG	1H	3178	1/1	0.61	0.25	93,93,93,93	0
57	MG	1G	1692	1/1	0.62	0.31	105,105,105,105	0
57	MG	14	3162	1/1	0.62	0.23	67,67,67,67	0
57	MG	14	3248	1/1	0.63	0.24	75,75,75,75	0
57	MG	14	3241	1/1	0.63	0.35	84,84,84,84	0
57	MG	14	3265	1/1	0.64	0.23	79,79,79,79	0
57	MG	14	3266	1/1	0.64	0.29	84,84,84,84	0
57	MG	1G	1631	1/1	0.64	0.29	107,107,107,107	0
57	MG	14	3157	1/1	0.65	0.28	99,99,99,99	0
57	MG	13	1668	1/1	0.65	0.23	95,95,95,95	0
57	MG	1G	1645	1/1	0.65	0.31	88,88,88,88	0
57	MG	14	3120	1/1	0.65	0.24	67,67,67,67	0
57	MG	1G	1647	1/1	0.66	0.26	115,115,115,115	0
57	MG	1H	3272	1/1	0.66	0.37	95,95,95,95	0
57	MG	14	3170	1/1	0.66	0.45	86,86,86,86	0
57	MG	1H	3277	1/1	0.67	0.25	77,77,77,77	0
57	MG	14	3116	1/1	0.67	0.31	87,87,87,87	0
57	MG	16	207	1/1	0.67	0.26	77,77,77,77	0
57	MG	1H	3080	1/1	0.68	0.27	82,82,82,82	0
57	MG	1G	1694	1/1	0.68	0.27	98,98,98,98	0
57	MG	14	3260	1/1	0.68	0.15	117,117,117,117	0
57	MG	14	3016	1/1	0.68	0.27	73,73,73,73	0
57	MG	13	1625	1/1	0.68	0.57	96,96,96,96	0
57	MG	16	205	1/1	0.68	0.20	81,81,81,81	0
57	MG	2L	104	1/1	0.69	0.20	72,72,72,72	0
57	MG	14	3142	1/1	0.69	0.26	82,82,82,82	0
57	MG	1J	203	1/1	0.69	0.32	93,93,93,93	0
57	MG	1H	3210	1/1	0.69	0.21	74,74,74,74	0
57	MG	13	1662	1/1	0.70	0.18	119,119,119,119	0
57	MG	13	1661	1/1	0.70	0.30	102,102,102,102	0
57	MG	14	3257	1/1	0.70	0.36	87,87,87,87	0
57	MG	1H	3015	1/1	0.70	0.17	72,72,72,72	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	14	3237	1/1	0.71	0.28	72,72,72,72	0
57	MG	13	1667	1/1	0.71	0.24	97,97,97,97	0
57	MG	14	3242	1/1	0.71	0.16	95,95,95,95	0
57	MG	14	3186	1/1	0.71	0.29	84,84,84,84	0
57	MG	2L	103	1/1	0.71	0.31	80,80,80,80	0
57	MG	1J	202	1/1	0.72	0.25	94,94,94,94	0
57	MG	14	3183	1/1	0.73	0.26	74,74,74,74	0
57	MG	1H	3177	1/1	0.73	0.27	81,81,81,81	0
57	MG	13	1636	1/1	0.73	0.28	75,75,75,75	0
57	MG	14	3144	1/1	0.73	0.31	80,80,80,80	0
57	MG	14	3035	1/1	0.73	0.41	83,83,83,83	0
57	MG	14	3102	1/1	0.73	0.21	86,86,86,86	0
57	MG	13	1648	1/1	0.73	0.39	90,90,90,90	0
57	MG	1H	3140	1/1	0.74	0.21	62,62,62,62	0
57	MG	14	3269	1/1	0.74	0.26	102,102,102,102	0
57	MG	1H	3014	1/1	0.74	0.26	75,75,75,75	0
57	MG	2K	101	1/1	0.74	0.23	95,95,95,95	0
57	MG	1H	3110	1/1	0.74	0.25	84,84,84,84	0
57	MG	14	3224	1/1	0.75	0.16	80,80,80,80	0
57	MG	14	3075	1/1	0.75	0.34	70,70,70,70	0
57	MG	1H	3115	1/1	0.75	0.23	82,82,82,82	0
57	MG	1H	3275	1/1	0.75	0.26	95,95,95,95	0
57	MG	13	1643	1/1	0.75	0.23	89,89,89,89	0
57	MG	13	1669	1/1	0.75	0.23	74,74,74,74	0
57	MG	14	3254	1/1	0.75	0.26	81,81,81,81	0
57	MG	14	3004	1/1	0.75	0.37	77,77,77,77	0
57	MG	1G	1640	1/1	0.75	0.22	100,100,100,100	0
57	MG	16	203	1/1	0.75	0.16	79,79,79,79	0
57	MG	1H	3247	1/1	0.75	0.36	77,77,77,77	0
57	MG	14	3036	1/1	0.75	0.32	76,76,76,76	0
57	MG	14	3063	1/1	0.75	0.24	76,76,76,76	0
57	MG	14	3206	1/1	0.75	0.26	95,95,95,95	0
57	MG	14	3211	1/1	0.75	0.25	78,78,78,78	0
57	MG	14	3104	1/1	0.76	0.29	81,81,81,81	0
57	MG	14	3259	1/1	0.76	0.19	97,97,97,97	0
57	MG	1I	201	1/1	0.76	0.21	100,100,100,100	0
57	MG	41	202	1/1	0.76	0.23	82,82,82,82	0
57	MG	14	3239	1/1	0.76	0.36	87,87,87,87	0
57	MG	1H	3493	1/1	0.76	0.20	94,94,94,94	0
57	MG	14	3198	1/1	0.76	0.18	81,81,81,81	0
57	MG	1H	3245	1/1	0.76	0.35	69,69,69,69	0
57	MG	13	1659	1/1	0.76	0.40	75,75,75,75	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	1H	3108	1/1	0.77	0.36	82,82,82,82	0
57	MG	1H	3218	1/1	0.77	0.33	70,70,70,70	0
57	MG	1H	3139	1/1	0.77	0.32	71,71,71,71	0
57	MG	2L	102	1/1	0.77	0.26	96,96,96,96	0
57	MG	14	3267	1/1	0.77	0.26	83,83,83,83	0
57	MG	1G	1637	1/1	0.77	0.19	77,77,77,77	0
57	MG	1H	3279	1/1	0.77	0.32	71,71,71,71	0
57	MG	14	3215	1/1	0.77	0.31	64,64,64,64	0
57	MG	35	202	1/1	0.77	0.20	75,75,75,75	0
57	MG	13	1666	1/1	0.77	0.29	77,77,77,77	0
57	MG	14	3175	1/1	0.78	0.20	90,90,90,90	0
57	MG	1G	1623	1/1	0.78	0.32	77,77,77,77	0
57	MG	14	3106	1/1	0.78	0.38	82,82,82,82	0
57	MG	14	3108	1/1	0.78	0.16	90,90,90,90	0
57	MG	14	3199	1/1	0.78	0.30	84,84,84,84	0
57	MG	14	3202	1/1	0.78	0.21	90,90,90,90	0
57	MG	14	3017	1/1	0.78	0.22	97,97,97,97	0
57	MG	1H	3185	1/1	0.78	0.32	90,90,90,90	0
57	MG	1H	3199	1/1	0.78	0.37	75,75,75,75	0
57	MG	1H	3288	1/1	0.78	0.23	80,80,80,80	0
57	MG	1G	1638	1/1	0.78	0.30	88,88,88,88	0
57	MG	1H	3126	1/1	0.78	0.22	70,70,70,70	0
57	MG	14	3168	1/1	0.78	0.23	89,89,89,89	0
57	MG	16	201	1/1	0.78	0.22	87,87,87,87	0
57	MG	1H	3122	1/1	0.79	0.20	73,73,73,73	0
57	MG	1H	3027	1/1	0.79	0.31	63,63,63,63	0
57	MG	1H	3197	1/1	0.79	0.18	67,67,67,67	0
57	MG	1H	3128	1/1	0.79	0.21	64,64,64,64	0
57	MG	1H	3208	1/1	0.79	0.21	76,76,76,76	0
57	MG	14	3110	1/1	0.79	0.23	86,86,86,86	0
57	MG	13	1629	1/1	0.79	0.19	98,98,98,98	0
57	MG	1H	3211	1/1	0.79	0.53	80,80,80,80	0
57	MG	1H	3213	1/1	0.79	0.20	92,92,92,92	0
57	MG	1H	3214	1/1	0.79	0.30	92,92,92,92	0
57	MG	13	1673	1/1	0.79	0.28	90,90,90,90	0
57	MG	1H	3230	1/1	0.79	0.26	78,78,78,78	0
57	MG	14	3163	1/1	0.79	0.31	72,72,72,72	0
57	MG	1H	3236	1/1	0.79	0.37	75,75,75,75	0
57	MG	14	3264	1/1	0.79	0.36	90,90,90,90	0
57	MG	13	1676	1/1	0.79	0.30	101,101,101,101	0
57	MG	1G	1626	1/1	0.79	0.32	73,73,73,73	0
57	MG	14	3033	1/1	0.79	0.23	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3185	1/1	0.79	0.22	89,89,89,89	0
57	MG	13	1652	1/1	0.79	0.40	89,89,89,89	0
57	MG	1H	3180	1/1	0.79	0.27	76,76,76,76	0
57	MG	29	301	1/1	0.79	0.24	80,80,80,80	0
57	MG	14	3039	1/1	0.79	0.24	73,73,73,73	0
57	MG	1G	1633	1/1	0.79	0.27	100,100,100,100	0
57	MG	1H	3091	1/1	0.80	0.18	57,57,57,57	0
57	MG	14	3048	1/1	0.80	0.35	75,75,75,75	0
57	MG	1H	3276	1/1	0.80	0.22	98,98,98,98	0
57	MG	11	303	1/1	0.80	0.27	65,65,65,65	0
57	MG	1H	3196	1/1	0.80	0.34	88,88,88,88	0
57	MG	1G	1609	1/1	0.80	0.23	108,108,108,108	0
57	MG	1G	1611	1/1	0.80	0.25	74,74,74,74	0
57	MG	1H	3154	1/1	0.80	0.18	75,75,75,75	0
57	MG	13	1633	1/1	0.80	0.16	85,85,85,85	0
57	MG	1H	3287	1/1	0.80	0.26	80,80,80,80	0
57	MG	14	3210	1/1	0.80	0.27	80,80,80,80	0
57	MG	1G	1627	1/1	0.80	0.21	86,86,86,86	0
57	MG	13	1647	1/1	0.80	0.23	104,104,104,104	0
57	MG	1H	3291	1/1	0.80	0.40	88,88,88,88	0
57	MG	1H	3135	1/1	0.80	0.18	81,81,81,81	0
57	MG	29	304	1/1	0.80	0.11	71,71,71,71	0
57	MG	13	1603	1/1	0.80	0.21	76,76,76,76	0
57	MG	1H	3212	1/1	0.80	0.30	77,77,77,77	0
57	MG	14	3044	1/1	0.81	0.27	76,76,76,76	0
57	MG	13	1604	1/1	0.81	0.31	112,112,112,112	0
57	MG	1G	1622	1/1	0.81	0.30	76,76,76,76	0
57	MG	1H	3010	1/1	0.81	0.26	59,59,59,59	0
57	MG	14	3180	1/1	0.81	0.14	69,69,69,69	0
57	MG	13	1679	1/1	0.81	0.25	86,86,86,86	0
57	MG	1H	3168	1/1	0.81	0.34	80,80,80,80	0
57	MG	14	3105	1/1	0.81	0.27	55,55,55,55	0
57	MG	13	1682	1/1	0.81	0.32	90,90,90,90	0
57	MG	1H	3284	1/1	0.81	0.22	75,75,75,75	0
57	MG	1G	1632	1/1	0.81	0.20	132,132,132,132	0
57	MG	14	3203	1/1	0.81	0.16	89,89,89,89	0
57	MG	1H	3251	1/1	0.81	0.21	78,78,78,78	0
57	MG	1G	1636	1/1	0.81	0.29	89,89,89,89	0
57	MG	14	3129	1/1	0.81	0.20	69,69,69,69	0
57	MG	1G	1604	1/1	0.81	0.28	87,87,87,87	0
57	MG	1H	3258	1/1	0.81	0.13	79,79,79,79	0
57	MG	13	1635	1/1	0.81	0.09	85,85,85,85	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	1G	1618	1/1	0.81	0.20	86,86,86,86	0
57	MG	1H	3193	1/1	0.82	0.50	84,84,84,84	0
57	MG	14	3213	1/1	0.82	0.26	87,87,87,87	0
57	MG	13	1688	1/1	0.82	0.30	90,90,90,90	0
57	MG	14	3220	1/1	0.82	0.31	88,88,88,88	0
57	MG	13	1656	1/1	0.82	0.33	62,62,62,62	0
57	MG	14	3190	1/1	0.82	0.42	82,82,82,82	0
57	MG	14	3192	1/1	0.82	0.27	100,100,100,100	0
57	MG	14	3270	1/1	0.82	0.25	83,83,83,83	0
57	MG	14	3107	1/1	0.82	0.31	81,81,81,81	0
57	MG	13	1641	1/1	0.82	0.25	69,69,69,69	0
57	MG	88	201	1/1	0.82	0.44	82,82,82,82	0
57	MG	1H	3156	1/1	0.82	0.22	61,61,61,61	0
57	MG	35	201	1/1	0.82	0.26	71,71,71,71	0
57	MG	14	3094	1/1	0.82	0.30	85,85,85,85	0
57	MG	1H	3087	1/1	0.82	0.25	68,68,68,68	0
57	MG	1G	1619	1/1	0.83	0.24	92,92,92,92	0
57	MG	1H	3252	1/1	0.83	0.32	80,80,80,80	0
57	MG	1H	3191	1/1	0.83	0.12	95,95,95,95	0
57	MG	13	1644	1/1	0.83	0.17	80,80,80,80	0
57	MG	5I	101	1/1	0.83	0.19	88,88,88,88	0
57	MG	14	3226	1/1	0.83	0.24	78,78,78,78	0
57	MG	14	3143	1/1	0.83	0.20	73,73,73,73	0
57	MG	13	1618	1/1	0.83	0.28	64,64,64,64	0
57	MG	14	3155	1/1	0.83	0.17	66,66,66,66	0
57	MG	14	3021	1/1	0.83	0.27	53,53,53,53	0
57	MG	16	206	1/1	0.83	0.27	81,81,81,81	0
57	MG	1G	1629	1/1	0.83	0.29	83,83,83,83	0
57	MG	1G	1630	1/1	0.83	0.23	113,113,113,113	0
57	MG	1H	3066	1/1	0.83	0.20	57,57,57,57	0
57	MG	13	1665	1/1	0.83	0.32	82,82,82,82	0
57	MG	14	3179	1/1	0.83	0.28	74,74,74,74	0
57	MG	21	303	1/1	0.83	0.25	69,69,69,69	0
57	MG	1G	1635	1/1	0.83	0.28	97,97,97,97	0
57	MG	14	3058	1/1	0.83	0.19	66,66,66,66	0
57	MG	1H	3280	1/1	0.83	0.19	80,80,80,80	0
57	MG	14	3188	1/1	0.83	0.24	66,66,66,66	0
57	MG	1H	3242	1/1	0.83	0.31	80,80,80,80	0
57	MG	1H	3209	1/1	0.83	0.20	78,78,78,78	0
57	MG	1G	1639	1/1	0.83	0.22	97,97,97,97	0
57	MG	13	1689	1/1	0.83	0.27	99,99,99,99	0
57	MG	1H	3186	1/1	0.83	0.10	57,57,57,57	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	1G	1614	1/1	0.83	0.19	99,99,99,99	0
57	MG	1G	1616	1/1	0.83	0.26	86,86,86,86	0
57	MG	1H	3289	1/1	0.83	0.29	82,82,82,82	0
57	MG	1H	3233	1/1	0.84	0.26	70,70,70,70	0
57	MG	13	1674	1/1	0.84	0.23	78,78,78,78	0
57	MG	1H	3278	1/1	0.84	0.30	82,82,82,82	0
57	MG	13	1621	1/1	0.84	0.17	67,67,67,67	0
57	MG	1H	3036	1/1	0.84	0.15	78,78,78,78	0
57	MG	1G	1601	1/1	0.84	0.19	86,86,86,86	0
57	MG	14	3189	1/1	0.84	0.22	69,69,69,69	0
57	MG	1H	3246	1/1	0.84	0.28	85,85,85,85	0
57	MG	1H	3047	1/1	0.84	0.19	61,61,61,61	0
57	MG	1H	3120	1/1	0.84	0.14	63,63,63,63	0
57	MG	14	3261	1/1	0.84	0.21	102,102,102,102	0
57	MG	1G	1613	1/1	0.84	0.29	73,73,73,73	0
57	MG	1H	3159	1/1	0.84	0.17	56,56,56,56	0
57	MG	1H	3254	1/1	0.84	0.26	82,82,82,82	0
57	MG	1H	3255	1/1	0.84	0.12	88,88,88,88	0
57	MG	1H	3257	1/1	0.84	0.28	84,84,84,84	0
57	MG	1H	3011	1/1	0.84	0.35	72,72,72,72	0
57	MG	1J	201	1/1	0.84	0.20	85,85,85,85	0
57	MG	1H	3263	1/1	0.84	0.46	93,93,93,93	0
57	MG	14	3077	1/1	0.84	0.34	80,80,80,80	0
57	MG	14	3219	1/1	0.84	0.27	64,64,64,64	0
57	MG	13	1637	1/1	0.84	0.26	86,86,86,86	0
57	MG	14	3221	1/1	0.84	0.22	73,73,73,73	0
57	MG	13	1645	1/1	0.84	0.23	93,93,93,93	0
57	MG	14	3176	1/1	0.84	0.10	88,88,88,88	0
57	MG	55	201	1/1	0.84	0.35	83,83,83,83	0
57	MG	14	3233	1/1	0.85	0.31	79,79,79,79	0
57	MG	1H	3117	1/1	0.85	0.31	72,72,72,72	0
57	MG	1H	3283	1/1	0.85	0.34	82,82,82,82	0
57	MG	1H	3059	1/1	0.85	0.23	66,66,66,66	0
57	MG	13	1622	1/1	0.85	0.24	81,81,81,81	0
57	MG	1G	1608	1/1	0.85	0.21	91,91,91,91	0
57	MG	13	1602	1/1	0.85	0.28	88,88,88,88	0
57	MG	14	3109	1/1	0.85	0.20	60,60,60,60	0
57	MG	14	3026	1/1	0.85	0.27	72,72,72,72	0
57	MG	14	3113	1/1	0.85	0.27	73,73,73,73	0
57	MG	1H	3082	1/1	0.85	0.17	49,49,49,49	0
57	MG	14	3263	1/1	0.85	0.30	80,80,80,80	0
57	MG	13	1672	1/1	0.85	0.26	96,96,96,96	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	14	3034	1/1	0.85	0.25	57,57,57,57	0
57	MG	14	3131	1/1	0.85	0.19	78,78,78,78	0
57	MG	1H	3090	1/1	0.85	0.24	57,57,57,57	0
57	MG	1H	3007	1/1	0.85	0.19	68,68,68,68	0
57	MG	1H	3151	1/1	0.85	0.20	91,91,91,91	0
57	MG	14	3357	1/1	0.85	0.08	84,84,84,84	0
57	MG	14	3212	1/1	0.85	0.34	80,80,80,80	0
57	MG	16	204	1/1	0.85	0.23	90,90,90,90	0
57	MG	14	3046	1/1	0.85	0.19	58,58,58,58	0
57	MG	1G	1642	1/1	0.85	0.42	82,82,82,82	0
57	MG	1H	3240	1/1	0.85	0.17	72,72,72,72	0
57	MG	1H	3033	1/1	0.85	0.18	62,62,62,62	0
57	MG	13	1640	1/1	0.85	0.16	71,71,71,71	0
57	MG	1H	3111	1/1	0.85	0.20	80,80,80,80	0
57	MG	13	1628	1/1	0.85	0.44	96,96,96,96	0
57	MG	1H	3051	1/1	0.86	0.16	93,93,93,93	0
57	MG	1H	3025	1/1	0.86	0.20	56,56,56,56	0
57	MG	1H	3187	1/1	0.86	0.11	88,88,88,88	0
57	MG	14	3243	1/1	0.86	0.21	86,86,86,86	0
57	MG	1H	3114	1/1	0.86	0.21	78,78,78,78	0
57	MG	14	3191	1/1	0.86	0.30	73,73,73,73	0
57	MG	14	3255	1/1	0.86	0.18	87,87,87,87	0
57	MG	14	3062	1/1	0.86	0.18	85,85,85,85	0
57	MG	14	3134	1/1	0.86	0.17	98,98,98,98	0
57	MG	1H	3152	1/1	0.86	0.15	87,87,87,87	0
57	MG	14	3013	1/1	0.86	0.21	74,74,74,74	0
57	MG	1H	3008	1/1	0.86	0.20	57,57,57,57	0
57	MG	14	3205	1/1	0.86	0.39	77,77,77,77	0
57	MG	14	3146	1/1	0.86	0.30	76,76,76,76	0
57	MG	14	3147	1/1	0.86	0.16	72,72,72,72	0
57	MG	14	3088	1/1	0.86	0.23	65,65,65,65	0
57	MG	13	1660	1/1	0.86	0.28	83,83,83,83	0
57	MG	14	3097	1/1	0.86	0.27	65,65,65,65	0
57	MG	1H	3034	1/1	0.86	0.16	54,54,54,54	0
57	MG	14	3443	1/1	0.86	0.10	108,108,108,108	0
57	MG	1H	3035	1/1	0.86	0.24	57,57,57,57	0
57	MG	13	1678	1/1	0.86	0.25	83,83,83,83	0
57	MG	1H	3041	1/1	0.86	0.23	72,72,72,72	0
57	MG	1H	3129	1/1	0.86	0.26	76,76,76,76	0
57	MG	14	3225	1/1	0.86	0.35	80,80,80,80	0
57	MG	1H	3181	1/1	0.86	0.35	77,77,77,77	0
57	MG	1H	3285	1/1	0.86	0.28	87,87,87,87	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	1H	3021	1/1	0.86	0.17	90,90,90,90	0
57	MG	14	3111	1/1	0.86	0.20	79,79,79,79	0
57	MG	14	3240	1/1	0.87	0.21	85,85,85,85	0
57	MG	14	3043	1/1	0.87	0.17	75,75,75,75	0
57	MG	1H	3044	1/1	0.87	0.21	62,62,62,62	0
57	MG	1H	3205	1/1	0.87	0.20	77,77,77,77	0
57	MG	14	3244	1/1	0.87	0.25	77,77,77,77	0
57	MG	13	1605	1/1	0.87	0.20	68,68,68,68	0
57	MG	14	3053	1/1	0.87	0.30	77,77,77,77	0
57	MG	14	3195	1/1	0.87	0.13	105,105,105,105	0
57	MG	1G	1625	1/1	0.87	0.21	89,89,89,89	0
57	MG	14	3140	1/1	0.87	0.19	81,81,81,81	0
57	MG	1H	3105	1/1	0.87	0.27	79,79,79,79	0
57	MG	1H	3106	1/1	0.87	0.31	74,74,74,74	0
57	MG	1H	3248	1/1	0.87	0.19	79,79,79,79	0
57	MG	13	1653	1/1	0.87	0.18	66,66,66,66	0
57	MG	14	3078	1/1	0.87	0.16	86,86,86,86	0
57	MG	14	3150	1/1	0.87	0.19	68,68,68,68	0
57	MG	14	3082	1/1	0.87	0.24	55,55,55,55	0
57	MG	14	3268	1/1	0.87	0.19	60,60,60,60	0
57	MG	13	1655	1/1	0.87	0.31	71,71,71,71	0
57	MG	13	1681	1/1	0.87	0.33	86,86,86,86	0
57	MG	14	3271	1/1	0.87	0.24	80,80,80,80	0
57	MG	14	3272	1/1	0.87	0.31	77,77,77,77	0
57	MG	1G	1605	1/1	0.87	0.17	92,92,92,92	0
57	MG	1H	3076	1/1	0.87	0.18	76,76,76,76	0
57	MG	14	3022	1/1	0.87	0.29	60,60,60,60	0
57	MG	13	1611	1/1	0.87	0.29	79,79,79,79	0
57	MG	13	1675	1/1	0.87	0.23	79,79,79,79	0
57	MG	1H	3259	1/1	0.87	0.37	74,74,74,74	0
57	MG	14	3229	1/1	0.87	0.24	74,74,74,74	0
57	MG	1H	3083	1/1	0.87	0.17	74,74,74,74	0
57	MG	1H	3265	1/1	0.87	0.12	89,89,89,89	0
57	MG	1H	3023	1/1	0.87	0.29	81,81,81,81	0
57	MG	1H	3238	1/1	0.87	0.12	78,78,78,78	0
57	MG	14	3059	1/1	0.88	0.23	69,69,69,69	0
57	MG	14	3061	1/1	0.88	0.20	61,61,61,61	0
57	MG	1H	3157	1/1	0.88	0.23	64,64,64,64	0
57	MG	13	1626	1/1	0.88	0.15	87,87,87,87	0
57	MG	1H	3162	1/1	0.88	0.18	61,61,61,61	0
57	MG	14	3238	1/1	0.88	0.29	69,69,69,69	0
57	MG	14	3167	1/1	0.88	0.17	65,65,65,65	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	1H	3164	1/1	0.88	0.13	47,47,47,47	0
57	MG	1H	3286	1/1	0.88	0.18	82,82,82,82	0
57	MG	14	3171	1/1	0.88	0.25	73,73,73,73	0
57	MG	14	3081	1/1	0.88	0.41	74,74,74,74	0
57	MG	13	1684	1/1	0.88	0.18	85,85,85,85	0
57	MG	14	3245	1/1	0.88	0.19	79,79,79,79	0
57	MG	14	3085	1/1	0.88	0.23	65,65,65,65	0
57	MG	1H	3200	1/1	0.88	0.22	73,73,73,73	0
57	MG	1H	3202	1/1	0.88	0.22	58,58,58,58	0
57	MG	1H	3204	1/1	0.88	0.23	86,86,86,86	0
57	MG	1H	3169	1/1	0.88	0.13	85,85,85,85	0
57	MG	1H	3498	1/1	0.88	0.06	85,85,85,85	0
57	MG	1H	3171	1/1	0.88	0.23	68,68,68,68	0
57	MG	1H	3174	1/1	0.88	0.26	59,59,59,59	0
57	MG	1H	3112	1/1	0.88	0.26	66,66,66,66	0
57	MG	13	1631	1/1	0.88	0.14	73,73,73,73	0
57	MG	14	3027	1/1	0.88	0.21	83,83,83,83	0
57	MG	1H	3061	1/1	0.88	0.25	68,68,68,68	0
57	MG	1H	3142	1/1	0.88	0.26	85,85,85,85	0
57	MG	14	3200	1/1	0.88	0.15	69,69,69,69	0
57	MG	1H	3062	1/1	0.88	0.26	66,66,66,66	0
57	MG	13	1658	1/1	0.88	0.21	88,88,88,88	0
57	MG	13	1624	1/1	0.88	0.13	81,81,81,81	0
57	MG	1G	1634	1/1	0.88	0.19	93,93,93,93	0
57	MG	14	3040	1/1	0.88	0.18	64,64,64,64	0
57	MG	78	201	1/1	0.88	0.23	75,75,75,75	0
57	MG	1H	3232	1/1	0.88	0.24	65,65,65,65	0
57	MG	13	1654	1/1	0.88	0.31	75,75,75,75	0
57	MG	1G	1602	1/1	0.88	0.16	72,72,72,72	0
57	MG	14	3050	1/1	0.88	0.22	59,59,59,59	0
57	MG	14	3145	1/1	0.88	0.30	74,74,74,74	0
57	MG	1H	3188	1/1	0.88	0.34	74,74,74,74	0
57	MG	1H	3190	1/1	0.88	0.31	74,74,74,74	0
57	MG	14	3149	1/1	0.88	0.14	96,96,96,96	0
57	MG	1H	3144	1/1	0.89	0.30	75,75,75,75	0
57	MG	1H	3182	1/1	0.89	0.26	72,72,72,72	0
57	MG	1H	3147	1/1	0.89	0.14	51,51,51,51	0
57	MG	1H	3060	1/1	0.89	0.21	55,55,55,55	0
57	MG	14	3055	1/1	0.89	0.27	57,57,57,57	0
57	MG	13	1634	1/1	0.89	0.29	71,71,71,71	0
57	MG	1H	3267	1/1	0.89	0.09	67,67,67,67	0
57	MG	1H	3013	1/1	0.89	0.23	60,60,60,60	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	1H	3063	1/1	0.89	0.17	52,52,52,52	0
57	MG	14	3156	1/1	0.89	0.24	75,75,75,75	0
57	MG	1H	3220	1/1	0.89	0.26	73,73,73,73	0
57	MG	14	3069	1/1	0.89	0.32	67,67,67,67	0
57	MG	14	3072	1/1	0.89	0.23	69,69,69,69	0
57	MG	1G	1657	1/1	0.89	0.10	105,105,105,105	0
57	MG	14	3076	1/1	0.89	0.20	77,77,77,77	0
57	MG	1H	3221	1/1	0.89	0.12	60,60,60,60	0
57	MG	1H	3229	1/1	0.89	0.21	73,73,73,73	0
57	MG	1G	1610	1/1	0.89	0.15	114,114,114,114	0
57	MG	1H	3092	1/1	0.89	0.21	57,57,57,57	0
57	MG	14	3178	1/1	0.89	0.11	71,71,71,71	0
57	MG	1H	3231	1/1	0.89	0.26	65,65,65,65	0
57	MG	1H	3121	1/1	0.89	0.24	79,79,79,79	0
57	MG	14	3182	1/1	0.89	0.31	67,67,67,67	0
57	MG	1H	3099	1/1	0.89	0.13	60,60,60,60	0
57	MG	1H	3234	1/1	0.89	0.10	72,72,72,72	0
57	MG	1H	3235	1/1	0.89	0.10	65,65,65,65	0
57	MG	1H	3194	1/1	0.89	0.30	66,66,66,66	0
57	MG	1H	3101	1/1	0.89	0.15	58,58,58,58	0
57	MG	1H	3065	1/1	0.89	0.13	56,56,56,56	0
57	MG	1H	3241	1/1	0.89	0.34	71,71,71,71	0
57	MG	1H	3198	1/1	0.89	0.23	76,76,76,76	0
57	MG	1H	3006	1/1	0.89	0.15	86,86,86,86	0
57	MG	1H	3132	1/1	0.89	0.23	75,75,75,75	0
57	MG	1H	3201	1/1	0.89	0.20	65,65,65,65	0
57	MG	1H	3107	1/1	0.89	0.15	64,64,64,64	0
57	MG	14	3037	1/1	0.89	0.25	63,63,63,63	0
57	MG	14	3118	1/1	0.89	0.18	66,66,66,66	0
57	MG	13	1615	1/1	0.89	0.18	91,91,91,91	0
57	MG	14	3127	1/1	0.89	0.18	48,48,48,48	0
57	MG	13	1630	1/1	0.89	0.18	92,92,92,92	0
57	MG	14	3130	1/1	0.89	0.21	71,71,71,71	0
57	MG	14	3042	1/1	0.89	0.27	58,58,58,58	0
57	MG	1H	3206	1/1	0.89	0.24	56,56,56,56	0
57	MG	13	1687	1/1	0.89	0.18	70,70,70,70	0
57	MG	14	3216	1/1	0.89	0.30	74,74,74,74	0
57	MG	14	3217	1/1	0.89	0.23	76,76,76,76	0
57	MG	1G	1615	1/1	0.90	0.18	92,92,92,92	0
57	MG	13	1750	1/1	0.90	0.18	76,76,76,76	0
57	MG	1H	3476	1/1	0.90	0.07	93,93,93,93	0
57	MG	14	3064	1/1	0.90	0.18	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	14	3222	1/1	0.90	0.23	64,64,64,64	0
57	MG	14	3223	1/1	0.90	0.32	75,75,75,75	0
57	MG	1H	3134	1/1	0.90	0.28	76,76,76,76	0
57	MG	14	3071	1/1	0.90	0.12	73,73,73,73	0
57	MG	1H	3005	1/1	0.90	0.34	74,74,74,74	0
57	MG	14	3006	1/1	0.90	0.21	66,66,66,66	0
57	MG	14	3230	1/1	0.90	0.21	70,70,70,70	0
57	MG	14	3009	1/1	0.90	0.22	68,68,68,68	0
57	MG	1H	3499	1/1	0.90	0.21	67,67,67,67	0
57	MG	14	3236	1/1	0.90	0.19	88,88,88,88	0
57	MG	1H	3138	1/1	0.90	0.22	55,55,55,55	0
57	MG	16	202	1/1	0.90	0.15	73,73,73,73	0
57	MG	1H	3176	1/1	0.90	0.34	67,67,67,67	0
57	MG	1H	3054	1/1	0.90	0.19	59,59,59,59	0
57	MG	14	3023	1/1	0.90	0.15	54,54,54,54	0
57	MG	14	3091	1/1	0.90	0.18	85,85,85,85	0
57	MG	14	3024	1/1	0.90	0.13	58,58,58,58	0
57	MG	1H	3113	1/1	0.90	0.39	82,82,82,82	0
57	MG	14	3099	1/1	0.90	0.16	57,57,57,57	0
57	MG	1H	3269	1/1	0.90	0.23	73,73,73,73	0
57	MG	1H	3067	1/1	0.90	0.18	52,52,52,52	0
57	MG	1H	3070	1/1	0.90	0.14	45,45,45,45	0
57	MG	1H	3100	1/1	0.90	0.15	44,44,44,44	0
57	MG	1H	3207	1/1	0.90	0.09	56,56,56,56	0
57	MG	1H	3119	1/1	0.90	0.14	71,71,71,71	0
57	MG	13	1670	1/1	0.90	0.30	78,78,78,78	0
57	MG	1H	3243	1/1	0.90	0.30	62,62,62,62	0
57	MG	1H	3281	1/1	0.90	0.38	69,69,69,69	0
57	MG	14	3112	1/1	0.90	0.31	88,88,88,88	0
57	MG	1H	3103	1/1	0.90	0.31	82,82,82,82	0
57	MG	14	3194	1/1	0.90	0.17	68,68,68,68	0
57	MG	1H	3077	1/1	0.90	0.25	74,74,74,74	0
57	MG	1H	3125	1/1	0.90	0.31	61,61,61,61	0
57	MG	1H	3158	1/1	0.90	0.38	68,68,68,68	0
57	MG	14	3123	1/1	0.90	0.37	70,70,70,70	0
57	MG	1H	3250	1/1	0.90	0.15	67,67,67,67	0
57	MG	14	3128	1/1	0.90	0.13	60,60,60,60	0
57	MG	14	3421	1/1	0.90	0.09	75,75,75,75	0
57	MG	1G	1646	1/1	0.90	0.30	84,84,84,84	0
57	MG	14	3052	1/1	0.90	0.18	62,62,62,62	0
57	MG	14	3207	1/1	0.90	0.09	71,71,71,71	0
57	MG	14	3208	1/1	0.90	0.22	75,75,75,75	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	1H	3031	1/1	0.90	0.16	53,53,53,53	0
57	MG	14	3133	1/1	0.90	0.19	71,71,71,71	0
57	MG	1G	1648	1/1	0.90	0.16	86,86,86,86	0
57	MG	14	3136	1/1	0.90	0.26	59,59,59,59	0
57	MG	45	201	1/1	0.90	0.21	72,72,72,72	0
57	MG	13	1614	1/1	0.90	0.27	64,64,64,64	0
57	MG	1H	3045	1/1	0.90	0.16	54,54,54,54	0
57	MG	14	3067	1/1	0.91	0.10	68,68,68,68	0
57	MG	1H	3086	1/1	0.91	0.19	71,71,71,71	0
57	MG	1H	3244	1/1	0.91	0.36	84,84,84,84	0
57	MG	41	201	1/1	0.91	0.18	75,75,75,75	0
57	MG	1H	3160	1/1	0.91	0.29	67,67,67,67	0
57	MG	1H	3189	1/1	0.91	0.23	87,87,87,87	0
57	MG	14	3148	1/1	0.91	0.20	69,69,69,69	0
57	MG	1H	3161	1/1	0.91	0.20	72,72,72,72	0
57	MG	13	1609	1/1	0.91	0.24	58,58,58,58	0
57	MG	14	3153	1/1	0.91	0.10	79,79,79,79	0
57	MG	14	3154	1/1	0.91	0.39	74,74,74,74	0
57	MG	14	3025	1/1	0.91	0.13	58,58,58,58	0
57	MG	14	3231	1/1	0.91	0.48	76,76,76,76	0
57	MG	1H	3215	1/1	0.91	0.22	65,65,65,65	0
57	MG	14	3083	1/1	0.91	0.17	61,61,61,61	0
57	MG	14	3084	1/1	0.91	0.20	56,56,56,56	0
57	MG	13	1651	1/1	0.91	0.19	68,68,68,68	0
57	MG	14	3165	1/1	0.91	0.11	78,78,78,78	0
57	MG	14	3166	1/1	0.91	0.15	61,61,61,61	0
57	MG	14	3030	1/1	0.91	0.15	68,68,68,68	0
57	MG	1H	3037	1/1	0.91	0.24	55,55,55,55	0
57	MG	14	3093	1/1	0.91	0.18	51,51,51,51	0
57	MG	1H	3004	1/1	0.91	0.19	54,54,54,54	0
57	MG	14	3173	1/1	0.91	0.20	69,69,69,69	0
57	MG	14	3095	1/1	0.91	0.12	85,85,85,85	0
57	MG	13	1607	1/1	0.91	0.18	74,74,74,74	0
57	MG	14	3098	1/1	0.91	0.12	67,67,67,67	0
57	MG	13	1686	1/1	0.91	0.17	96,96,96,96	0
57	MG	1H	3175	1/1	0.91	0.32	65,65,65,65	0
57	MG	14	3258	1/1	0.91	0.45	83,83,83,83	0
57	MG	1H	3471	1/1	0.91	0.06	82,82,82,82	0
57	MG	13	1639	1/1	0.91	0.12	84,84,84,84	0
57	MG	13	1612	1/1	0.91	0.29	85,85,85,85	0
57	MG	14	3041	1/1	0.91	0.20	64,64,64,64	0
57	MG	1H	3148	1/1	0.91	0.20	65,65,65,65	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	1H	3266	1/1	0.91	0.13	75,75,75,75	0
57	MG	13	1677	1/1	0.91	0.26	76,76,76,76	0
57	MG	1H	3055	1/1	0.91	0.20	72,72,72,72	0
57	MG	7A	101	1/1	0.91	0.42	89,89,89,89	0
57	MG	2L	101	1/1	0.91	0.20	70,70,70,70	0
57	MG	14	3051	1/1	0.91	0.17	62,62,62,62	0
57	MG	1H	3271	1/1	0.91	0.22	74,74,74,74	0
57	MG	13	1649	1/1	0.91	0.34	78,78,78,78	0
57	MG	14	3121	1/1	0.91	0.33	77,77,77,77	0
57	MG	14	3054	1/1	0.91	0.34	67,67,67,67	0
57	MG	1G	1624	1/1	0.91	0.16	87,87,87,87	0
57	MG	14	3003	1/1	0.91	0.20	65,65,65,65	0
57	MG	13	1671	1/1	0.91	0.18	71,71,71,71	0
57	MG	14	3060	1/1	0.91	0.20	74,74,74,74	0
57	MG	1H	3085	1/1	0.91	0.28	71,71,71,71	0
57	MG	14	3209	1/1	0.91	0.31	64,64,64,64	0
57	MG	14	3007	1/1	0.91	0.14	50,50,50,50	0
57	MG	1H	3131	1/1	0.91	0.24	67,67,67,67	0
57	MG	14	3010	1/1	0.91	0.23	69,69,69,69	0
57	MG	14	3139	1/1	0.91	0.22	58,58,58,58	0
57	MG	14	3066	1/1	0.91	0.10	53,53,53,53	0
57	MG	1H	3150	1/1	0.92	0.05	50,50,50,50	0
57	MG	14	3045	1/1	0.92	0.14	64,64,64,64	0
57	MG	14	3164	1/1	0.92	0.24	65,65,65,65	0
57	MG	1G	1612	1/1	0.92	0.21	67,67,67,67	0
57	MG	14	3227	1/1	0.92	0.35	83,83,83,83	0
57	MG	14	3228	1/1	0.92	0.22	81,81,81,81	0
57	MG	14	3103	1/1	0.92	0.32	68,68,68,68	0
57	MG	1H	3050	1/1	0.92	0.21	66,66,66,66	0
57	MG	13	1657	1/1	0.92	0.34	73,73,73,73	0
57	MG	14	3169	1/1	0.92	0.10	65,65,65,65	0
57	MG	1H	3411	1/1	0.92	0.07	81,81,81,81	0
57	MG	1H	3093	1/1	0.92	0.32	71,71,71,71	0
57	MG	1H	3069	1/1	0.92	0.36	65,65,65,65	0
57	MG	1H	3124	1/1	0.92	0.15	74,74,74,74	0
57	MG	1G	1620	1/1	0.92	0.21	79,79,79,79	0
57	MG	1H	3019	1/1	0.92	0.25	78,78,78,78	0
57	MG	1H	3261	1/1	0.92	0.16	67,67,67,67	0
57	MG	1H	3228	1/1	0.92	0.34	69,69,69,69	0
57	MG	1H	3071	1/1	0.92	0.24	54,54,54,54	0
57	MG	1H	3192	1/1	0.92	0.36	82,82,82,82	0
57	MG	1H	3074	1/1	0.92	0.16	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3246	1/1	0.92	0.14	76,76,76,76	0
57	MG	14	3247	1/1	0.92	0.13	67,67,67,67	0
57	MG	1H	3075	1/1	0.92	0.12	60,60,60,60	0
57	MG	1H	3020	1/1	0.92	0.17	107,107,107,107	0
57	MG	14	3126	1/1	0.92	0.30	64,64,64,64	0
57	MG	14	3256	1/1	0.92	0.12	91,91,91,91	0
57	MG	1H	3056	1/1	0.92	0.14	52,52,52,52	0
57	MG	14	3068	1/1	0.92	0.15	67,67,67,67	0
57	MG	1H	3166	1/1	0.92	0.12	70,70,70,70	0
57	MG	1H	3078	1/1	0.92	0.18	60,60,60,60	0
57	MG	1H	3109	1/1	0.92	0.27	65,65,65,65	0
57	MG	1H	3058	1/1	0.92	0.13	53,53,53,53	0
57	MG	1H	3172	1/1	0.92	0.13	73,73,73,73	0
57	MG	13	1616	1/1	0.92	0.15	48,48,48,48	0
57	MG	L8	101	1/1	0.92	0.25	72,72,72,72	0
57	MG	1H	3022	1/1	0.92	0.16	81,81,81,81	0
57	MG	14	3204	1/1	0.92	0.18	90,90,90,90	0
57	MG	13	1601	1/1	0.92	0.12	68,68,68,68	0
57	MG	1H	3143	1/1	0.92	0.33	89,89,89,89	0
57	MG	13	1685	1/1	0.92	0.15	101,101,101,101	0
57	MG	1G	1641	1/1	0.92	0.45	78,78,78,78	0
57	MG	14	3087	1/1	0.92	0.15	97,97,97,97	0
57	MG	1G	1606	1/1	0.92	0.21	67,67,67,67	0
57	MG	14	3089	1/1	0.92	0.17	56,56,56,56	0
57	MG	14	3090	1/1	0.92	0.08	60,60,60,60	0
57	MG	1G	1643	1/1	0.92	0.39	67,67,67,67	0
57	MG	14	3214	1/1	0.92	0.36	73,73,73,73	0
57	MG	14	3151	1/1	0.92	0.08	72,72,72,72	0
57	MG	1G	1607	1/1	0.92	0.12	91,91,91,91	0
57	MG	39	301	1/1	0.92	0.05	95,95,95,95	0
57	MG	13	1751	1/1	0.92	0.17	87,87,87,87	0
57	MG	13	1680	1/1	0.92	0.21	75,75,75,75	0
57	MG	14	3096	1/1	0.92	0.17	65,65,65,65	0
57	MG	1H	3149	1/1	0.92	0.10	61,61,61,61	0
57	MG	14	3158	1/1	0.92	0.09	70,70,70,70	0
57	MG	1H	3167	1/1	0.93	0.14	63,63,63,63	0
57	MG	1H	3095	1/1	0.93	0.29	65,65,65,65	0
57	MG	1H	3096	1/1	0.93	0.18	67,67,67,67	0
57	MG	1H	3097	1/1	0.93	0.12	51,51,51,51	0
57	MG	14	3172	1/1	0.93	0.18	63,63,63,63	0
57	MG	1H	3274	1/1	0.93	0.09	70,70,70,70	0
57	MG	14	3174	1/1	0.93	0.20	71,71,71,71	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	14	3234	1/1	0.93	0.08	64,64,64,64	0
57	MG	14	3119	1/1	0.93	0.34	63,63,63,63	0
57	MG	21	301	1/1	0.93	0.24	66,66,66,66	0
57	MG	1H	3118	1/1	0.93	0.07	60,60,60,60	0
57	MG	14	3122	1/1	0.93	0.08	104,104,104,104	0
57	MG	1H	3016	1/1	0.93	0.21	49,49,49,49	0
57	MG	14	3181	1/1	0.93	0.18	63,63,63,63	0
57	MG	14	3125	1/1	0.93	0.13	54,54,54,54	0
57	MG	1H	3146	1/1	0.93	0.33	51,51,51,51	0
57	MG	1H	3203	1/1	0.93	0.15	64,64,64,64	0
57	MG	1H	3038	1/1	0.93	0.18	53,53,53,53	0
57	MG	14	3187	1/1	0.93	0.13	80,80,80,80	0
57	MG	13	1663	1/1	0.93	0.42	71,71,71,71	0
57	MG	P8	101	1/1	0.93	0.27	66,66,66,66	0
57	MG	14	3251	1/1	0.93	0.20	82,82,82,82	0
57	MG	1H	3068	1/1	0.93	0.28	69,69,69,69	0
57	MG	1H	3123	1/1	0.93	0.18	71,71,71,71	0
57	MG	1H	3104	1/1	0.93	0.20	62,62,62,62	0
57	MG	14	3135	1/1	0.93	0.30	71,71,71,71	0
57	MG	1H	3084	1/1	0.93	0.13	82,82,82,82	0
57	MG	14	3138	1/1	0.93	0.13	68,68,68,68	0
57	MG	1H	3057	1/1	0.93	0.27	53,53,53,53	0
57	MG	1H	3249	1/1	0.93	0.23	61,61,61,61	0
57	MG	14	3141	1/1	0.93	0.17	50,50,50,50	0
57	MG	14	3038	1/1	0.93	0.12	76,76,76,76	0
57	MG	1H	3184	1/1	0.93	0.22	67,67,67,67	0
57	MG	1H	3043	1/1	0.93	0.17	70,70,70,70	0
57	MG	13	1613	1/1	0.93	0.14	65,65,65,65	0
57	MG	1H	3130	1/1	0.93	0.26	67,67,67,67	0
57	MG	1G	1649	1/1	0.93	0.09	115,115,115,115	0
57	MG	1H	3088	1/1	0.93	0.18	53,53,53,53	0
57	MG	1H	3452	1/1	0.93	0.07	89,89,89,89	0
57	MG	1H	3465	1/1	0.93	0.15	53,53,53,53	0
57	MG	14	3047	1/1	0.93	0.17	42,42,42,42	0
57	MG	1H	3012	1/1	0.93	0.24	42,42,42,42	0
57	MG	1H	3133	1/1	0.93	0.41	80,80,80,80	0
57	MG	14	3100	1/1	0.93	0.12	43,43,43,43	0
57	MG	13	1619	1/1	0.93	0.18	90,90,90,90	0
57	MG	1H	3496	1/1	0.93	0.07	94,94,94,94	0
57	MG	1H	3260	1/1	0.93	0.19	65,65,65,65	0
57	MG	29	303	1/1	0.93	0.20	67,67,67,67	0
57	MG	14	3159	1/1	0.93	0.12	71,71,71,71	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	13	1627	1/1	0.93	0.20	64,64,64,64	0
57	MG	39	302	1/1	0.93	0.07	63,63,63,63	0
57	MG	1H	3165	1/1	0.93	0.31	72,72,72,72	0
57	MG	14	3056	1/1	0.93	0.45	82,82,82,82	0
57	MG	14	3005	1/1	0.93	0.14	70,70,70,70	0
57	MG	13	1620	1/1	0.93	0.20	58,58,58,58	0
57	MG	1H	3195	1/1	0.93	0.21	73,73,73,73	0
60	ZN	G8	201	1/1	0.93	0.16	146,146,146,146	0
60	ZN	C5	202	1/1	0.93	0.08	169,169,169,169	0
57	MG	14	3193	1/1	0.94	0.10	70,70,70,70	0
57	MG	1H	3145	1/1	0.94	0.17	46,46,46,46	0
57	MG	1H	3049	1/1	0.94	0.15	68,68,68,68	0
57	MG	14	3101	1/1	0.94	0.27	64,64,64,64	0
57	MG	21	302	1/1	0.94	0.26	50,50,50,50	0
57	MG	1H	3028	1/1	0.94	0.13	51,51,51,51	0
57	MG	1H	3072	1/1	0.94	0.32	73,73,73,73	0
57	MG	14	3250	1/1	0.94	0.12	65,65,65,65	0
57	MG	14	3057	1/1	0.94	0.23	41,41,41,41	0
57	MG	1H	3029	1/1	0.94	0.17	49,49,49,49	0
57	MG	14	3015	1/1	0.94	0.18	77,77,77,77	0
57	MG	1H	3098	1/1	0.94	0.37	63,63,63,63	0
57	MG	13	1742	1/1	0.94	0.06	100,100,100,100	0
57	MG	14	3019	1/1	0.94	0.23	58,58,58,58	0
57	MG	13	1744	1/1	0.94	0.10	94,94,94,94	0
57	MG	14	3161	1/1	0.94	0.13	73,73,73,73	0
57	MG	13	1748	1/1	0.94	0.12	115,115,115,115	0
57	MG	13	1623	1/1	0.94	0.20	61,61,61,61	0
57	MG	14	3115	1/1	0.94	0.28	71,71,71,71	0
57	MG	1H	3127	1/1	0.94	0.15	56,56,56,56	0
57	MG	1H	3079	1/1	0.94	0.15	47,47,47,47	0
57	MG	13	1617	1/1	0.94	0.11	53,53,53,53	0
57	MG	13	1608	1/1	0.94	0.12	75,75,75,75	0
57	MG	1H	3403	1/1	0.94	0.09	89,89,89,89	0
57	MG	14	3073	1/1	0.94	0.11	57,57,57,57	0
57	MG	3I	201	1/1	0.94	0.11	57,57,57,57	0
57	MG	1H	3428	1/1	0.94	0.06	87,87,87,87	0
57	MG	1G	1644	1/1	0.94	0.22	67,67,67,67	0
57	MG	1H	3039	1/1	0.94	0.10	90,90,90,90	0
57	MG	1H	3226	1/1	0.94	0.07	64,64,64,64	0
57	MG	14	3448	1/1	0.94	0.06	92,92,92,92	0
57	MG	14	3452	1/1	0.94	0.11	113,113,113,113	0
57	MG	1H	3040	1/1	0.94	0.15	60,60,60,60	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	13	1664	1/1	0.94	0.46	81,81,81,81	0
57	MG	1H	3024	1/1	0.94	0.24	45,45,45,45	0
57	MG	13	1729	1/1	0.94	0.06	91,91,91,91	0
57	MG	29	302	1/1	0.94	0.17	40,40,40,40	0
57	MG	1G	1684	1/1	0.94	0.10	121,121,121,121	0
57	MG	1H	3089	1/1	0.94	0.19	51,51,51,51	0
57	MG	1H	3026	1/1	0.94	0.23	40,40,40,40	0
57	MG	1H	3170	1/1	0.94	0.38	72,72,72,72	0
57	MG	1H	3046	1/1	0.94	0.35	73,73,73,73	0
57	MG	1H	3116	1/1	0.94	0.19	63,63,63,63	0
57	MG	1H	3273	1/1	0.94	0.09	57,57,57,57	0
57	MG	1H	3237	1/1	0.94	0.12	61,61,61,61	0
57	MG	45	203	1/1	0.94	0.25	71,71,71,71	0
57	MG	14	3049	1/1	0.94	0.19	63,63,63,63	0
57	MG	1H	3173	1/1	0.94	0.15	63,63,63,63	0
57	MG	2K	102	1/1	0.94	0.07	92,92,92,92	0
57	MG	1H	3290	1/1	0.95	0.24	62,62,62,62	0
57	MG	1H	3225	1/1	0.95	0.22	67,67,67,67	0
57	MG	5E	201	1/1	0.95	0.12	81,81,81,81	0
57	MG	1H	3081	1/1	0.95	0.10	47,47,47,47	0
57	MG	13	1610	1/1	0.95	0.11	79,79,79,79	0
57	MG	1H	3433	1/1	0.95	0.06	86,86,86,86	0
57	MG	1H	3136	1/1	0.95	0.51	73,73,73,73	0
57	MG	14	3029	1/1	0.95	0.15	59,59,59,59	0
57	MG	1H	3137	1/1	0.95	0.14	72,72,72,72	0
57	MG	1H	3163	1/1	0.95	0.19	59,59,59,59	0
57	MG	14	3032	1/1	0.95	0.08	47,47,47,47	0
57	MG	14	3086	1/1	0.95	0.14	61,61,61,61	0
57	MG	14	3423	1/1	0.95	0.07	144,144,144,144	0
57	MG	14	3428	1/1	0.95	0.08	104,104,104,104	0
57	MG	14	3431	1/1	0.95	0.06	90,90,90,90	0
57	MG	1H	3009	1/1	0.95	0.14	54,54,54,54	0
57	MG	14	3446	1/1	0.95	0.05	109,109,109,109	0
57	MG	1H	3487	1/1	0.95	0.06	91,91,91,91	0
57	MG	1H	3264	1/1	0.95	0.19	74,74,74,74	0
57	MG	14	3117	1/1	0.95	0.19	66,66,66,66	0
57	MG	1H	3053	1/1	0.95	0.30	56,56,56,56	0
57	MG	1H	3102	1/1	0.95	0.28	70,70,70,70	0
57	MG	14	3092	1/1	0.95	0.14	56,56,56,56	0
57	MG	2K	103	1/1	0.95	0.20	61,61,61,61	0
57	MG	14	3152	1/1	0.95	0.19	67,67,67,67	0
57	MG	14	3012	1/1	0.95	0.12	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3252	1/1	0.95	0.12	67,67,67,67	0
57	MG	14	3253	1/1	0.95	0.10	63,63,63,63	0
57	MG	1H	3268	1/1	0.95	0.15	81,81,81,81	0
57	MG	14	3124	1/1	0.95	0.30	64,64,64,64	0
57	MG	1H	3042	1/1	0.95	0.13	79,79,79,79	0
57	MG	1H	3270	1/1	0.95	0.11	71,71,71,71	0
57	MG	1H	3048	1/1	0.95	0.07	80,80,80,80	0
57	MG	1H	3253	1/1	0.95	0.25	76,76,76,76	0
57	MG	E5	101	1/1	0.95	0.28	72,72,72,72	0
58	PAR	13	1749	42/42	0.95	0.09	64,70,78,81	0
57	MG	14	3160	1/1	0.95	0.17	51,51,51,51	0
57	MG	14	3020	1/1	0.95	0.19	51,51,51,51	0
57	MG	16	212	1/1	0.96	0.05	88,88,88,88	0
57	MG	14	3070	1/1	0.96	0.27	52,52,52,52	0
57	MG	14	3114	1/1	0.96	0.29	63,63,63,63	0
57	MG	1G	1674	1/1	0.96	0.04	107,107,107,107	0
57	MG	1G	1679	1/1	0.96	0.07	91,91,91,91	0
57	MG	1G	1683	1/1	0.96	0.05	96,96,96,96	0
57	MG	14	3074	1/1	0.96	0.15	62,62,62,62	0
57	MG	13	1727	1/1	0.96	0.09	110,110,110,110	0
57	MG	14	3262	1/1	0.96	0.05	72,72,72,72	0
57	MG	1H	3153	1/1	0.96	0.13	59,59,59,59	0
57	MG	1G	1693	1/1	0.96	0.09	92,92,92,92	0
57	MG	1H	3224	1/1	0.96	0.18	63,63,63,63	0
57	MG	14	3080	1/1	0.96	0.27	46,46,46,46	0
57	MG	1H	3435	1/1	0.96	0.05	94,94,94,94	0
57	MG	13	1606	1/1	0.96	0.19	52,52,52,52	0
57	MG	1H	3455	1/1	0.96	0.05	103,103,103,103	0
57	MG	13	1739	1/1	0.96	0.06	104,104,104,104	0
57	MG	1H	3470	1/1	0.96	0.05	100,100,100,100	0
57	MG	1H	3003	1/1	0.96	0.18	57,57,57,57	0
57	MG	14	3308	1/1	0.96	0.06	96,96,96,96	0
57	MG	14	3324	1/1	0.96	0.05	107,107,107,107	0
57	MG	14	3340	1/1	0.96	0.09	73,73,73,73	0
57	MG	1H	3256	1/1	0.96	0.26	71,71,71,71	0
57	MG	14	3365	1/1	0.96	0.04	88,88,88,88	0
57	MG	14	3406	1/1	0.96	0.10	76,76,76,76	0
57	MG	14	3417	1/1	0.96	0.04	87,87,87,87	0
57	MG	Q8	101	1/1	0.96	0.09	73,73,73,73	0
57	MG	1H	3478	1/1	0.96	0.04	85,85,85,85	0
57	MG	14	3427	1/1	0.96	0.09	102,102,102,102	0
57	MG	1H	3480	1/1	0.96	0.06	78,78,78,78	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	14	3008	1/1	0.96	0.05	72,72,72,72	0
57	MG	1H	3481	1/1	0.96	0.04	92,92,92,92	0
57	MG	14	3444	1/1	0.96	0.06	87,87,87,87	0
57	MG	14	3137	1/1	0.96	0.15	72,72,72,72	0
57	MG	1H	3064	1/1	0.96	0.10	54,54,54,54	0
57	MG	14	3011	1/1	0.96	0.34	72,72,72,72	0
57	MG	1H	3491	1/1	0.96	0.12	75,75,75,75	0
57	MG	14	3235	1/1	0.96	0.25	69,69,69,69	0
57	MG	1H	3179	1/1	0.96	0.10	49,49,49,49	0
57	MG	1J	206	1/1	0.96	0.06	94,94,94,94	0
57	MG	13	1638	1/1	0.96	0.26	58,58,58,58	0
57	MG	13	1710	1/1	0.96	0.09	108,108,108,108	0
57	MG	1H	3141	1/1	0.96	0.08	67,67,67,67	0
57	MG	1H	3501	1/1	0.96	0.11	72,72,72,72	0
57	MG	1H	3216	1/1	0.96	0.08	57,57,57,57	0
57	MG	1H	3369	1/1	0.96	0.09	74,74,74,74	0
57	MG	1H	3381	1/1	0.96	0.10	95,95,95,95	0
57	MG	1H	3387	1/1	0.96	0.05	64,64,64,64	0
57	MG	14	3197	1/1	0.96	0.06	56,56,56,56	0
57	MG	13	1724	1/1	0.96	0.06	114,114,114,114	0
57	MG	1G	1617	1/1	0.96	0.24	61,61,61,61	0
57	MG	1H	3406	1/1	0.96	0.07	87,87,87,87	0
57	MG	14	3065	1/1	0.96	0.12	54,54,54,54	0
57	MG	M5	101	1/1	0.96	0.12	77,77,77,77	0
57	MG	1H	3409	1/1	0.96	0.04	69,69,69,69	0
58	PAR	1G	1691	42/42	0.96	0.08	70,82,88,95	0
57	MG	14	3028	1/1	0.96	0.15	60,60,60,60	0
57	MG	1G	1655	1/1	0.96	0.04	120,120,120,120	0
57	MG	1H	3017	1/1	0.97	0.06	55,55,55,55	0
57	MG	1H	3458	1/1	0.97	0.06	87,87,87,87	0
57	MG	13	1734	1/1	0.97	0.04	86,86,86,86	0
57	MG	1H	3467	1/1	0.97	0.07	77,77,77,77	0
57	MG	14	3079	1/1	0.97	0.11	64,64,64,64	0
57	MG	1H	3468	1/1	0.97	0.04	71,71,71,71	0
57	MG	1H	3227	1/1	0.97	0.07	70,70,70,70	0
57	MG	1H	3094	1/1	0.97	0.04	52,52,52,52	0
57	MG	1H	3473	1/1	0.97	0.06	85,85,85,85	0
57	MG	1H	3475	1/1	0.97	0.04	88,88,88,88	0
57	MG	14	3201	1/1	0.97	0.17	58,58,58,58	0
57	MG	13	1737	1/1	0.97	0.09	147,147,147,147	0
57	MG	13	1738	1/1	0.97	0.04	97,97,97,97	0
57	MG	13	1708	1/1	0.97	0.04	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1G	1653	1/1	0.97	0.04	110,110,110,110	0
57	MG	13	1741	1/1	0.97	0.05	79,79,79,79	0
57	MG	1H	3482	1/1	0.97	0.05	72,72,72,72	0
57	MG	1G	1665	1/1	0.97	0.09	97,97,97,97	0
57	MG	1G	1666	1/1	0.97	0.04	106,106,106,106	0
57	MG	1G	1667	1/1	0.97	0.08	100,100,100,100	0
57	MG	1G	1669	1/1	0.97	0.05	114,114,114,114	0
57	MG	14	3280	1/1	0.97	0.05	54,54,54,54	0
57	MG	14	3303	1/1	0.97	0.05	63,63,63,63	0
57	MG	1G	1672	1/1	0.97	0.04	91,91,91,91	0
57	MG	14	3318	1/1	0.97	0.07	67,67,67,67	0
57	MG	1H	3485	1/1	0.97	0.04	76,76,76,76	0
57	MG	14	3329	1/1	0.97	0.06	90,90,90,90	0
57	MG	14	3330	1/1	0.97	0.06	113,113,113,113	0
57	MG	1G	1676	1/1	0.97	0.08	86,86,86,86	0
57	MG	14	3342	1/1	0.97	0.05	58,58,58,58	0
57	MG	14	3351	1/1	0.97	0.05	72,72,72,72	0
57	MG	1H	3334	1/1	0.97	0.06	82,82,82,82	0
57	MG	1G	1682	1/1	0.97	0.13	127,127,127,127	0
57	MG	14	3366	1/1	0.97	0.06	76,76,76,76	0
57	MG	14	3372	1/1	0.97	0.04	73,73,73,73	0
57	MG	14	3374	1/1	0.97	0.05	96,96,96,96	0
57	MG	14	3377	1/1	0.97	0.10	67,67,67,67	0
57	MG	14	3383	1/1	0.97	0.04	101,101,101,101	0
57	MG	14	3384	1/1	0.97	0.05	95,95,95,95	0
57	MG	14	3388	1/1	0.97	0.09	82,82,82,82	0
57	MG	1H	3488	1/1	0.97	0.09	113,113,113,113	0
57	MG	14	3410	1/1	0.97	0.04	85,85,85,85	0
57	MG	14	3414	1/1	0.97	0.05	85,85,85,85	0
57	MG	1H	3489	1/1	0.97	0.07	125,125,125,125	0
57	MG	1G	1685	1/1	0.97	0.05	109,109,109,109	0
57	MG	14	3422	1/1	0.97	0.05	84,84,84,84	0
57	MG	1G	1686	1/1	0.97	0.05	92,92,92,92	0
57	MG	14	3425	1/1	0.97	0.07	122,122,122,122	0
57	MG	1G	1687	1/1	0.97	0.04	95,95,95,95	0
57	MG	1G	1690	1/1	0.97	0.04	118,118,118,118	0
57	MG	14	3430	1/1	0.97	0.04	90,90,90,90	0
57	MG	1H	3364	1/1	0.97	0.04	106,106,106,106	0
57	MG	14	3435	1/1	0.97	0.04	103,103,103,103	0
57	MG	14	3438	1/1	0.97	0.05	93,93,93,93	0
57	MG	14	3442	1/1	0.97	0.04	95,95,95,95	0
57	MG	1H	3492	1/1	0.97	0.08	105,105,105,105	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	1H	3052	1/1	0.97	0.19	57,57,57,57	0
57	MG	1H	3495	1/1	0.97	0.03	98,98,98,98	0
57	MG	1H	3376	1/1	0.97	0.04	88,88,88,88	0
57	MG	14	3449	1/1	0.97	0.10	95,95,95,95	0
57	MG	1H	3378	1/1	0.97	0.08	84,84,84,84	0
57	MG	14	3453	1/1	0.97	0.07	88,88,88,88	0
57	MG	14	3454	1/1	0.97	0.06	79,79,79,79	0
57	MG	13	1726	1/1	0.97	0.09	85,85,85,85	0
57	MG	1H	3383	1/1	0.97	0.05	78,78,78,78	0
57	MG	1H	3386	1/1	0.97	0.04	84,84,84,84	0
57	MG	13	1632	1/1	0.97	0.10	77,77,77,77	0
57	MG	13	1745	1/1	0.97	0.04	117,117,117,117	0
57	MG	1H	3001	1/1	0.97	0.06	53,53,53,53	0
57	MG	1H	3002	1/1	0.97	0.13	39,39,39,39	0
57	MG	1H	3219	1/1	0.97	0.09	62,62,62,62	0
57	MG	14	3177	1/1	0.97	0.28	79,79,79,79	0
57	MG	1H	3420	1/1	0.97	0.04	64,64,64,64	0
57	MG	13	1715	1/1	0.97	0.07	110,110,110,110	0
57	MG	1H	3431	1/1	0.97	0.04	52,52,52,52	0
57	MG	13	1730	1/1	0.97	0.06	82,82,82,82	0
57	MG	1H	3222	1/1	0.97	0.05	68,68,68,68	0
57	MG	14	3014	1/1	0.97	0.10	72,72,72,72	0
57	MG	14	3184	1/1	0.97	0.10	60,60,60,60	0
57	MG	85	201	1/1	0.97	0.18	72,72,72,72	0
57	MG	1H	3442	1/1	0.97	0.06	86,86,86,86	0
57	MG	31	301	1/1	0.97	0.08	61,61,61,61	0
57	MG	1H	3451	1/1	0.97	0.04	95,95,95,95	0
57	MG	14	3249	1/1	0.97	0.16	60,60,60,60	0
57	MG	14	3018	1/1	0.97	0.12	49,49,49,49	0
57	MG	1H	3030	1/1	0.97	0.15	45,45,45,45	0
57	MG	13	1720	1/1	0.98	0.04	86,86,86,86	0
57	MG	1H	3262	1/1	0.98	0.07	68,68,68,68	0
57	MG	1H	3413	1/1	0.98	0.03	78,78,78,78	0
57	MG	1H	3032	1/1	0.98	0.08	61,61,61,61	0
57	MG	16	209	1/1	0.98	0.07	73,73,73,73	0
57	MG	16	210	1/1	0.98	0.11	88,88,88,88	0
57	MG	1G	1654	1/1	0.98	0.04	93,93,93,93	0
57	MG	16	211	1/1	0.98	0.04	84,84,84,84	0
57	MG	1G	1656	1/1	0.98	0.11	105,105,105,105	0
57	MG	1H	3422	1/1	0.98	0.05	79,79,79,79	0
57	MG	1H	3424	1/1	0.98	0.04	68,68,68,68	0
57	MG	14	3196	1/1	0.98	0.07	90,90,90,90	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	14	3282	1/1	0.98	0.06	58,58,58,58	0
57	MG	1H	3425	1/1	0.98	0.05	83,83,83,83	0
57	MG	14	3306	1/1	0.98	0.07	55,55,55,55	0
57	MG	1H	3426	1/1	0.98	0.03	57,57,57,57	0
57	MG	14	3312	1/1	0.98	0.04	77,77,77,77	0
57	MG	14	3315	1/1	0.98	0.08	81,81,81,81	0
57	MG	14	3316	1/1	0.98	0.06	102,102,102,102	0
57	MG	14	3317	1/1	0.98	0.04	59,59,59,59	0
57	MG	1G	1668	1/1	0.98	0.06	111,111,111,111	0
57	MG	14	3319	1/1	0.98	0.07	91,91,91,91	0
57	MG	14	3320	1/1	0.98	0.08	83,83,83,83	0
57	MG	14	3323	1/1	0.98	0.05	72,72,72,72	0
57	MG	1H	3223	1/1	0.98	0.14	64,64,64,64	0
57	MG	14	3325	1/1	0.98	0.04	78,78,78,78	0
57	MG	14	3326	1/1	0.98	0.04	74,74,74,74	0
57	MG	14	3328	1/1	0.98	0.06	93,93,93,93	0
57	MG	1G	1670	1/1	0.98	0.05	108,108,108,108	0
57	MG	13	1705	1/1	0.98	0.07	76,76,76,76	0
57	MG	14	3336	1/1	0.98	0.04	83,83,83,83	0
57	MG	14	3338	1/1	0.98	0.03	72,72,72,72	0
57	MG	1H	3432	1/1	0.98	0.05	75,75,75,75	0
57	MG	1G	1675	1/1	0.98	0.04	88,88,88,88	0
57	MG	14	3345	1/1	0.98	0.05	68,68,68,68	0
57	MG	13	1707	1/1	0.98	0.09	90,90,90,90	0
57	MG	14	3354	1/1	0.98	0.06	78,78,78,78	0
57	MG	1G	1678	1/1	0.98	0.03	115,115,115,115	0
57	MG	14	3364	1/1	0.98	0.07	73,73,73,73	0
57	MG	1H	3434	1/1	0.98	0.08	73,73,73,73	0
57	MG	14	3132	1/1	0.98	0.08	58,58,58,58	0
57	MG	14	3369	1/1	0.98	0.08	56,56,56,56	0
57	MG	14	3370	1/1	0.98	0.04	81,81,81,81	0
57	MG	1G	1680	1/1	0.98	0.04	103,103,103,103	0
57	MG	14	3373	1/1	0.98	0.04	93,93,93,93	0
57	MG	13	1683	1/1	0.98	0.10	67,67,67,67	0
57	MG	1H	3439	1/1	0.98	0.06	81,81,81,81	0
57	MG	14	3378	1/1	0.98	0.04	93,93,93,93	0
57	MG	14	3380	1/1	0.98	0.03	93,93,93,93	0
57	MG	1H	3441	1/1	0.98	0.07	94,94,94,94	0
57	MG	13	1709	1/1	0.98	0.04	75,75,75,75	0
57	MG	1H	3444	1/1	0.98	0.03	77,77,77,77	0
57	MG	14	3389	1/1	0.98	0.05	81,81,81,81	0
57	MG	14	3399	1/1	0.98	0.07	78,78,78,78	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	14	3400	1/1	0.98	0.04	86,86,86,86	0
57	MG	14	3405	1/1	0.98	0.03	83,83,83,83	0
57	MG	1H	3449	1/1	0.98	0.05	69,69,69,69	0
57	MG	14	3407	1/1	0.98	0.05	74,74,74,74	0
57	MG	1G	1688	1/1	0.98	0.06	100,100,100,100	0
57	MG	14	3412	1/1	0.98	0.04	120,120,120,120	0
57	MG	1G	1689	1/1	0.98	0.04	126,126,126,126	0
57	MG	14	3415	1/1	0.98	0.03	77,77,77,77	0
57	MG	14	3416	1/1	0.98	0.07	66,66,66,66	0
57	MG	1G	1603	1/1	0.98	0.09	81,81,81,81	0
57	MG	1H	3450	1/1	0.98	0.03	87,87,87,87	0
57	MG	13	1702	1/1	0.98	0.06	76,76,76,76	0
57	MG	1H	3155	1/1	0.98	0.05	75,75,75,75	0
57	MG	1H	3292	1/1	0.98	0.04	50,50,50,50	0
57	MG	14	3426	1/1	0.98	0.04	80,80,80,80	0
57	MG	1H	3457	1/1	0.98	0.04	82,82,82,82	0
57	MG	1H	3299	1/1	0.98	0.09	50,50,50,50	0
57	MG	14	3429	1/1	0.98	0.06	98,98,98,98	0
57	MG	1H	3463	1/1	0.98	0.05	82,82,82,82	0
57	MG	1H	3303	1/1	0.98	0.04	63,63,63,63	0
57	MG	14	3432	1/1	0.98	0.07	83,83,83,83	0
57	MG	14	3434	1/1	0.98	0.04	82,82,82,82	0
57	MG	14	3001	1/1	0.98	0.05	103,103,103,103	0
57	MG	1H	3466	1/1	0.98	0.04	83,83,83,83	0
57	MG	14	3439	1/1	0.98	0.04	96,96,96,96	0
57	MG	14	3440	1/1	0.98	0.04	94,94,94,94	0
57	MG	1H	3311	1/1	0.98	0.05	53,53,53,53	0
57	MG	1H	3316	1/1	0.98	0.04	63,63,63,63	0
57	MG	1H	3469	1/1	0.98	0.04	100,100,100,100	0
57	MG	1H	3319	1/1	0.98	0.08	67,67,67,67	0
57	MG	14	3447	1/1	0.98	0.04	101,101,101,101	0
57	MG	1H	3325	1/1	0.98	0.06	69,69,69,69	0
57	MG	1H	3472	1/1	0.98	0.10	93,93,93,93	0
57	MG	14	3451	1/1	0.98	0.12	77,77,77,77	0
57	MG	1H	3326	1/1	0.98	0.10	49,49,49,49	0
57	MG	1H	3327	1/1	0.98	0.10	55,55,55,55	0
57	MG	13	1731	1/1	0.98	0.04	86,86,86,86	0
57	MG	1H	3337	1/1	0.98	0.06	73,73,73,73	0
57	MG	1H	3359	1/1	0.98	0.04	52,52,52,52	0
57	MG	1H	3363	1/1	0.98	0.04	61,61,61,61	0
57	MG	1J	205	1/1	0.98	0.06	95,95,95,95	0
57	MG	13	1732	1/1	0.98	0.10	108,108,108,108	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	1H	3483	1/1	0.98	0.04	106,106,106,106	0
57	MG	1H	3366	1/1	0.98	0.04	65,65,65,65	0
57	MG	1H	3486	1/1	0.98	0.06	61,61,61,61	0
57	MG	13	1711	1/1	0.98	0.05	99,99,99,99	0
57	MG	1H	3372	1/1	0.98	0.04	89,89,89,89	0
57	MG	1H	3073	1/1	0.98	0.10	36,36,36,36	0
57	MG	13	1735	1/1	0.98	0.06	118,118,118,118	0
57	MG	1H	3380	1/1	0.98	0.07	55,55,55,55	0
57	MG	13	1736	1/1	0.98	0.07	95,95,95,95	0
57	MG	1H	3494	1/1	0.98	0.05	126,126,126,126	0
57	MG	BI	201	1/1	0.98	0.04	103,103,103,103	0
57	MG	1H	3384	1/1	0.98	0.06	73,73,73,73	0
57	MG	13	1712	1/1	0.98	0.04	75,75,75,75	0
57	MG	13	1713	1/1	0.98	0.05	89,89,89,89	0
57	MG	1H	3399	1/1	0.98	0.04	61,61,61,61	0
57	MG	1H	3502	1/1	0.98	0.06	59,59,59,59	0
57	MG	1H	3402	1/1	0.98	0.04	73,73,73,73	0
59	SF4	3E	301	8/8	0.98	0.06	71,78,87,91	0
57	MG	1H	3239	1/1	0.98	0.07	67,67,67,67	0
57	MG	13	1704	1/1	0.98	0.04	105,105,105,105	0
57	MG	1H	3298	1/1	0.99	0.05	61,61,61,61	0
57	MG	1H	3423	1/1	0.99	0.03	55,55,55,55	0
57	MG	13	1703	1/1	0.99	0.06	95,95,95,95	0
57	MG	1H	3300	1/1	0.99	0.04	54,54,54,54	0
57	MG	1H	3301	1/1	0.99	0.07	49,49,49,49	0
57	MG	1H	3427	1/1	0.99	0.03	88,88,88,88	0
57	MG	1H	3302	1/1	0.99	0.09	47,47,47,47	0
57	MG	1H	3429	1/1	0.99	0.04	75,75,75,75	0
57	MG	1H	3430	1/1	0.99	0.03	85,85,85,85	0
57	MG	13	1725	1/1	0.99	0.10	71,71,71,71	0
57	MG	1H	3305	1/1	0.99	0.05	53,53,53,53	0
57	MG	1H	3306	1/1	0.99	0.03	60,60,60,60	0
57	MG	1H	3307	1/1	0.99	0.05	57,57,57,57	0
57	MG	1H	3308	1/1	0.99	0.05	61,61,61,61	0
57	MG	1H	3436	1/1	0.99	0.03	65,65,65,65	0
57	MG	1H	3437	1/1	0.99	0.03	57,57,57,57	0
57	MG	1H	3438	1/1	0.99	0.04	75,75,75,75	0
57	MG	1H	3310	1/1	0.99	0.03	58,58,58,58	0
57	MG	1H	3440	1/1	0.99	0.03	87,87,87,87	0
57	MG	13	1691	1/1	0.99	0.02	79,79,79,79	0
57	MG	1H	3313	1/1	0.99	0.05	72,72,72,72	0
57	MG	1G	1650	1/1	0.99	0.09	87,87,87,87	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	1G	1651	1/1	0.99	0.04	81,81,81,81	0
57	MG	1G	1652	1/1	0.99	0.03	82,82,82,82	0
57	MG	1H	3314	1/1	0.99	0.04	75,75,75,75	0
57	MG	1H	3445	1/1	0.99	0.03	97,97,97,97	0
57	MG	1H	3446	1/1	0.99	0.02	93,93,93,93	0
57	MG	1H	3447	1/1	0.99	0.07	97,97,97,97	0
57	MG	1H	3448	1/1	0.99	0.05	62,62,62,62	0
57	MG	1G	1658	1/1	0.99	0.04	94,94,94,94	0
57	MG	1G	1659	1/1	0.99	0.06	79,79,79,79	0
57	MG	1G	1660	1/1	0.99	0.03	96,96,96,96	0
57	MG	1G	1661	1/1	0.99	0.07	111,111,111,111	0
57	MG	1G	1662	1/1	0.99	0.04	76,76,76,76	0
57	MG	1G	1663	1/1	0.99	0.03	87,87,87,87	0
57	MG	1G	1664	1/1	0.99	0.07	91,91,91,91	0
57	MG	1H	3315	1/1	0.99	0.03	73,73,73,73	0
57	MG	13	1692	1/1	0.99	0.05	81,81,81,81	0
57	MG	1H	3318	1/1	0.99	0.05	54,54,54,54	0
57	MG	13	1728	1/1	0.99	0.04	91,91,91,91	0
57	MG	1H	3453	1/1	0.99	0.04	83,83,83,83	0
57	MG	1H	3454	1/1	0.99	0.03	62,62,62,62	0
57	MG	1G	1671	1/1	0.99	0.04	117,117,117,117	0
57	MG	1H	3320	1/1	0.99	0.03	67,67,67,67	0
57	MG	14	3273	1/1	0.99	0.04	58,58,58,58	0
57	MG	14	3275	1/1	0.99	0.03	61,61,61,61	0
57	MG	14	3276	1/1	0.99	0.03	62,62,62,62	0
57	MG	14	3278	1/1	0.99	0.04	65,65,65,65	0
57	MG	1G	1673	1/1	0.99	0.06	84,84,84,84	0
57	MG	14	3281	1/1	0.99	0.03	66,66,66,66	0
57	MG	1H	3456	1/1	0.99	0.02	72,72,72,72	0
57	MG	14	3283	1/1	0.99	0.04	74,74,74,74	0
57	MG	14	3285	1/1	0.99	0.07	59,59,59,59	0
57	MG	14	3290	1/1	0.99	0.03	64,64,64,64	0
57	MG	14	3291	1/1	0.99	0.03	66,66,66,66	0
57	MG	14	3295	1/1	0.99	0.02	58,58,58,58	0
57	MG	14	3296	1/1	0.99	0.05	59,59,59,59	0
57	MG	14	3298	1/1	0.99	0.03	79,79,79,79	0
57	MG	14	3299	1/1	0.99	0.05	60,60,60,60	0
57	MG	14	3300	1/1	0.99	0.03	57,57,57,57	0
57	MG	14	3302	1/1	0.99	0.03	68,68,68,68	0
57	MG	1H	3321	1/1	0.99	0.04	77,77,77,77	0
57	MG	14	3304	1/1	0.99	0.11	59,59,59,59	0
57	MG	1H	3322	1/1	0.99	0.03	82,82,82,82	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	14	3307	1/1	0.99	0.05	79,79,79,79	0
57	MG	1G	1677	1/1	0.99	0.03	105,105,105,105	0
57	MG	14	3309	1/1	0.99	0.09	73,73,73,73	0
57	MG	14	3310	1/1	0.99	0.04	68,68,68,68	0
57	MG	14	3311	1/1	0.99	0.04	66,66,66,66	0
57	MG	1H	3459	1/1	0.99	0.05	91,91,91,91	0
57	MG	14	3313	1/1	0.99	0.03	72,72,72,72	0
57	MG	14	3314	1/1	0.99	0.06	75,75,75,75	0
57	MG	1H	3460	1/1	0.99	0.06	62,62,62,62	0
57	MG	1H	3461	1/1	0.99	0.02	85,85,85,85	0
57	MG	1G	1681	1/1	0.99	0.03	85,85,85,85	0
57	MG	1H	3462	1/1	0.99	0.10	54,54,54,54	0
57	MG	1H	3323	1/1	0.99	0.03	61,61,61,61	0
57	MG	1H	3464	1/1	0.99	0.06	62,62,62,62	0
57	MG	14	3321	1/1	0.99	0.03	89,89,89,89	0
57	MG	14	3322	1/1	0.99	0.06	74,74,74,74	0
57	MG	1H	3324	1/1	0.99	0.03	47,47,47,47	0
57	MG	13	1693	1/1	0.99	0.06	72,72,72,72	0
57	MG	13	1694	1/1	0.99	0.05	79,79,79,79	0
57	MG	13	1695	1/1	0.99	0.05	76,76,76,76	0
57	MG	14	3327	1/1	0.99	0.06	67,67,67,67	0
57	MG	1H	3328	1/1	0.99	0.07	52,52,52,52	0
57	MG	1H	3329	1/1	0.99	0.04	55,55,55,55	0
57	MG	1H	3331	1/1	0.99	0.03	66,66,66,66	0
57	MG	14	3333	1/1	0.99	0.04	59,59,59,59	0
57	MG	1H	3333	1/1	0.99	0.07	75,75,75,75	0
57	MG	14	3337	1/1	0.99	0.11	76,76,76,76	0
57	MG	1H	3217	1/1	0.99	0.06	59,59,59,59	0
57	MG	14	3339	1/1	0.99	0.03	86,86,86,86	0
57	MG	1H	3474	1/1	0.99	0.08	89,89,89,89	0
57	MG	14	3341	1/1	0.99	0.06	62,62,62,62	0
57	MG	1H	3335	1/1	0.99	0.03	61,61,61,61	0
57	MG	14	3343	1/1	0.99	0.03	63,63,63,63	0
57	MG	14	3344	1/1	0.99	0.03	72,72,72,72	0
57	MG	13	1696	1/1	0.99	0.06	86,86,86,86	0
57	MG	14	3346	1/1	0.99	0.07	75,75,75,75	0
57	MG	14	3348	1/1	0.99	0.04	88,88,88,88	0
57	MG	14	3349	1/1	0.99	0.04	81,81,81,81	0
57	MG	14	3350	1/1	0.99	0.03	56,56,56,56	0
57	MG	1H	3477	1/1	0.99	0.03	65,65,65,65	0
57	MG	14	3352	1/1	0.99	0.06	65,65,65,65	0
57	MG	1H	3339	1/1	0.99	0.03	50,50,50,50	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	14	3356	1/1	0.99	0.02	61,61,61,61	0
57	MG	1H	3479	1/1	0.99	0.02	89,89,89,89	0
57	MG	14	3358	1/1	0.99	0.03	54,54,54,54	0
57	MG	14	3360	1/1	0.99	0.04	83,83,83,83	0
57	MG	14	3361	1/1	0.99	0.04	69,69,69,69	0
57	MG	14	3363	1/1	0.99	0.03	68,68,68,68	0
57	MG	1H	3341	1/1	0.99	0.03	57,57,57,57	0
57	MG	1H	3342	1/1	0.99	0.03	71,71,71,71	0
57	MG	1H	3344	1/1	0.99	0.05	49,49,49,49	0
57	MG	14	3367	1/1	0.99	0.12	60,60,60,60	0
57	MG	14	3368	1/1	0.99	0.05	72,72,72,72	0
57	MG	1H	3346	1/1	0.99	0.03	58,58,58,58	0
57	MG	1H	3484	1/1	0.99	0.03	90,90,90,90	0
57	MG	14	3371	1/1	0.99	0.03	83,83,83,83	0
57	MG	1H	3347	1/1	0.99	0.03	69,69,69,69	0
57	MG	1H	3349	1/1	0.99	0.04	53,53,53,53	0
57	MG	1H	3350	1/1	0.99	0.05	69,69,69,69	0
57	MG	14	3375	1/1	0.99	0.03	91,91,91,91	0
57	MG	1H	3352	1/1	0.99	0.06	72,72,72,72	0
57	MG	1H	3353	1/1	0.99	0.03	57,57,57,57	0
57	MG	14	3379	1/1	0.99	0.05	94,94,94,94	0
57	MG	1H	3490	1/1	0.99	0.04	83,83,83,83	0
57	MG	14	3381	1/1	0.99	0.06	52,52,52,52	0
57	MG	14	3382	1/1	0.99	0.04	91,91,91,91	0
57	MG	1H	3354	1/1	0.99	0.06	62,62,62,62	0
57	MG	1H	3356	1/1	0.99	0.02	58,58,58,58	0
57	MG	14	3385	1/1	0.99	0.07	70,70,70,70	0
57	MG	14	3387	1/1	0.99	0.02	97,97,97,97	0
57	MG	1H	3357	1/1	0.99	0.03	68,68,68,68	0
57	MG	13	1733	1/1	0.99	0.05	73,73,73,73	0
57	MG	14	3390	1/1	0.99	0.04	82,82,82,82	0
57	MG	14	3391	1/1	0.99	0.03	86,86,86,86	0
57	MG	14	3392	1/1	0.99	0.03	87,87,87,87	0
57	MG	14	3393	1/1	0.99	0.06	79,79,79,79	0
57	MG	14	3395	1/1	0.99	0.06	78,78,78,78	0
57	MG	14	3396	1/1	0.99	0.03	62,62,62,62	0
57	MG	14	3397	1/1	0.99	0.05	64,64,64,64	0
57	MG	14	3398	1/1	0.99	0.06	83,83,83,83	0
57	MG	1H	3360	1/1	0.99	0.03	60,60,60,60	0
57	MG	1H	3361	1/1	0.99	0.04	53,53,53,53	0
57	MG	14	3402	1/1	0.99	0.04	88,88,88,88	0
57	MG	14	3403	1/1	0.99	0.03	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3404	1/1	0.99	0.08	94,94,94,94	0
57	MG	1H	3497	1/1	0.99	0.03	97,97,97,97	0
57	MG	1H	3362	1/1	0.99	0.03	60,60,60,60	0
57	MG	13	1698	1/1	0.99	0.04	93,93,93,93	0
57	MG	14	3408	1/1	0.99	0.03	78,78,78,78	0
57	MG	14	3409	1/1	0.99	0.03	80,80,80,80	0
57	MG	1H	3500	1/1	0.99	0.03	71,71,71,71	0
57	MG	14	3411	1/1	0.99	0.03	74,74,74,74	0
57	MG	13	1699	1/1	0.99	0.05	73,73,73,73	0
57	MG	14	3413	1/1	0.99	0.02	97,97,97,97	0
57	MG	1H	3365	1/1	0.99	0.04	70,70,70,70	0
57	MG	13	1700	1/1	0.99	0.04	93,93,93,93	0
57	MG	1H	3367	1/1	0.99	0.03	54,54,54,54	0
57	MG	1H	3368	1/1	0.99	0.05	60,60,60,60	0
57	MG	14	3419	1/1	0.99	0.06	70,70,70,70	0
57	MG	14	3420	1/1	0.99	0.05	65,65,65,65	0
57	MG	13	1714	1/1	0.99	0.03	93,93,93,93	0
57	MG	1H	3370	1/1	0.99	0.06	70,70,70,70	0
57	MG	1H	3371	1/1	0.99	0.04	85,85,85,85	0
57	MG	14	3424	1/1	0.99	0.03	107,107,107,107	0
57	MG	13	1701	1/1	0.99	0.02	70,70,70,70	0
57	MG	16	208	1/1	0.99	0.04	67,67,67,67	0
57	MG	1H	3373	1/1	0.99	0.08	66,66,66,66	0
57	MG	1H	3374	1/1	0.99	0.04	55,55,55,55	0
57	MG	1H	3375	1/1	0.99	0.07	57,57,57,57	0
57	MG	13	1716	1/1	0.99	0.03	66,66,66,66	0
57	MG	11	302	1/1	0.99	0.03	57,57,57,57	0
57	MG	1H	3377	1/1	0.99	0.06	76,76,76,76	0
57	MG	14	3433	1/1	0.99	0.05	71,71,71,71	0
57	MG	13	1740	1/1	0.99	0.03	92,92,92,92	0
57	MG	1H	3379	1/1	0.99	0.07	86,86,86,86	0
57	MG	14	3436	1/1	0.99	0.02	108,108,108,108	0
57	MG	13	1717	1/1	0.99	0.05	66,66,66,66	0
57	MG	13	1718	1/1	0.99	0.04	78,78,78,78	0
57	MG	1H	3382	1/1	0.99	0.04	70,70,70,70	0
57	MG	14	3441	1/1	0.99	0.07	72,72,72,72	0
57	MG	13	1743	1/1	0.99	0.04	87,87,87,87	0
57	MG	13	1719	1/1	0.99	0.06	72,72,72,72	0
57	MG	1H	3385	1/1	0.99	0.03	57,57,57,57	0
57	MG	14	3445	1/1	0.99	0.03	87,87,87,87	0
57	MG	I8	101	1/1	0.99	0.05	65,65,65,65	0
57	MG	13	1690	1/1	0.99	0.05	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	13	1746	1/1	0.99	0.04	83,83,83,83	0
57	MG	1H	3389	1/1	0.99	0.05	59,59,59,59	0
57	MG	14	3450	1/1	0.99	0.04	63,63,63,63	0
57	MG	1H	3390	1/1	0.99	0.07	57,57,57,57	0
57	MG	1H	3391	1/1	0.99	0.03	49,49,49,49	0
57	MG	1H	3392	1/1	0.99	0.03	69,69,69,69	0
57	MG	1H	3393	1/1	0.99	0.04	56,56,56,56	0
57	MG	1H	3394	1/1	0.99	0.06	70,70,70,70	0
57	MG	1H	3395	1/1	0.99	0.05	59,59,59,59	0
57	MG	1H	3397	1/1	0.99	0.04	85,85,85,85	0
57	MG	1J	204	1/1	0.99	0.03	82,82,82,82	0
57	MG	1H	3398	1/1	0.99	0.03	50,50,50,50	0
57	MG	13	1747	1/1	0.99	0.03	72,72,72,72	0
57	MG	1H	3400	1/1	0.99	0.07	67,67,67,67	0
57	MG	13	1721	1/1	0.99	0.03	70,70,70,70	0
57	MG	13	1722	1/1	0.99	0.03	92,92,92,92	0
57	MG	1H	3404	1/1	0.99	0.04	76,76,76,76	0
57	MG	13	1723	1/1	0.99	0.06	84,84,84,84	0
57	MG	1H	3407	1/1	0.99	0.04	50,50,50,50	0
57	MG	1H	3408	1/1	0.99	0.07	50,50,50,50	0
57	MG	1H	3293	1/1	0.99	0.08	63,63,63,63	0
57	MG	1H	3410	1/1	0.99	0.02	56,56,56,56	0
57	MG	14	3218	1/1	0.99	0.13	54,54,54,54	0
57	MG	1H	3295	1/1	0.99	0.03	52,52,52,52	0
57	MG	1H	3412	1/1	0.99	0.05	66,66,66,66	0
57	MG	1H	3296	1/1	0.99	0.06	49,49,49,49	0
57	MG	C5	201	1/1	0.99	0.03	110,110,110,110	0
57	MG	1H	3414	1/1	0.99	0.03	53,53,53,53	0
57	MG	1H	3415	1/1	0.99	0.07	52,52,52,52	0
57	MG	1H	3416	1/1	0.99	0.06	48,48,48,48	0
57	MG	1H	3417	1/1	0.99	0.02	56,56,56,56	0
57	MG	1H	3418	1/1	0.99	0.03	69,69,69,69	0
59	SF4	32	301	8/8	0.99	0.03	100,111,117,118	0
57	MG	1H	3297	1/1	0.99	0.04	49,49,49,49	0
60	ZN	5A	101	1/1	0.99	0.03	128,128,128,128	0
57	MG	1H	3421	1/1	0.99	0.03	78,78,78,78	0
57	MG	14	3286	1/1	1.00	0.02	63,63,63,63	0
57	MG	14	3376	1/1	1.00	0.03	52,52,52,52	0
57	MG	14	3287	1/1	1.00	0.04	56,56,56,56	0
57	MG	14	3288	1/1	1.00	0.04	50,50,50,50	0
57	MG	14	3289	1/1	1.00	0.03	58,58,58,58	0
57	MG	1H	3332	1/1	1.00	0.04	63,63,63,63	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	14	3331	1/1	1.00	0.02	66,66,66,66	0
57	MG	14	3332	1/1	1.00	0.06	63,63,63,63	0
57	MG	14	3437	1/1	1.00	0.02	93,93,93,93	0
57	MG	1H	3317	1/1	1.00	0.07	45,45,45,45	0
57	MG	14	3334	1/1	1.00	0.03	61,61,61,61	0
57	MG	14	3335	1/1	1.00	0.04	87,87,87,87	0
57	MG	14	3386	1/1	1.00	0.04	56,56,56,56	0
57	MG	14	3292	1/1	1.00	0.02	61,61,61,61	0
57	MG	14	3293	1/1	1.00	0.02	51,51,51,51	0
57	MG	14	3294	1/1	1.00	0.02	54,54,54,54	0
57	MG	1H	3405	1/1	1.00	0.02	69,69,69,69	0
57	MG	1H	3348	1/1	1.00	0.02	65,65,65,65	0
57	MG	14	3297	1/1	1.00	0.03	74,74,74,74	0
57	MG	13	1697	1/1	1.00	0.04	90,90,90,90	0
57	MG	14	3394	1/1	1.00	0.02	78,78,78,78	0
57	MG	1H	3312	1/1	1.00	0.03	76,76,76,76	0
57	MG	14	3002	1/1	1.00	0.02	49,49,49,49	0
57	MG	14	3301	1/1	1.00	0.02	56,56,56,56	0
57	MG	1H	3351	1/1	1.00	0.01	69,69,69,69	0
57	MG	14	3347	1/1	1.00	0.04	67,67,67,67	0
57	MG	1H	3388	1/1	1.00	0.03	57,57,57,57	0
57	MG	14	3401	1/1	1.00	0.02	66,66,66,66	0
57	MG	1H	3336	1/1	1.00	0.03	61,61,61,61	0
57	MG	14	3305	1/1	1.00	0.04	57,57,57,57	0
57	MG	1H	3294	1/1	1.00	0.02	56,56,56,56	0
57	MG	1H	3338	1/1	1.00	0.06	53,53,53,53	0
57	MG	14	3353	1/1	1.00	0.03	67,67,67,67	0
57	MG	1H	3355	1/1	1.00	0.01	68,68,68,68	0
57	MG	14	3355	1/1	1.00	0.02	59,59,59,59	0
57	MG	1H	3304	1/1	1.00	0.02	55,55,55,55	0
57	MG	1H	3340	1/1	1.00	0.02	54,54,54,54	0
57	MG	1H	3358	1/1	1.00	0.02	67,67,67,67	0
57	MG	14	3359	1/1	1.00	0.02	67,67,67,67	0
57	MG	1H	3396	1/1	1.00	0.02	60,60,60,60	0
57	MG	1H	3419	1/1	1.00	0.06	63,63,63,63	0
57	MG	14	3362	1/1	1.00	0.06	62,62,62,62	0
57	MG	14	3274	1/1	1.00	0.02	62,62,62,62	0
57	MG	11	301	1/1	1.00	0.02	46,46,46,46	0
57	MG	14	3418	1/1	1.00	0.05	75,75,75,75	0
57	MG	1H	3443	1/1	1.00	0.02	67,67,67,67	0
57	MG	14	3277	1/1	1.00	0.01	67,67,67,67	0
57	MG	1H	3309	1/1	1.00	0.03	48,48,48,48	0

Continued on next page...

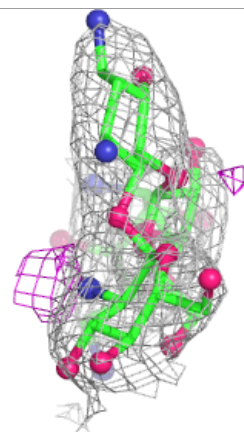
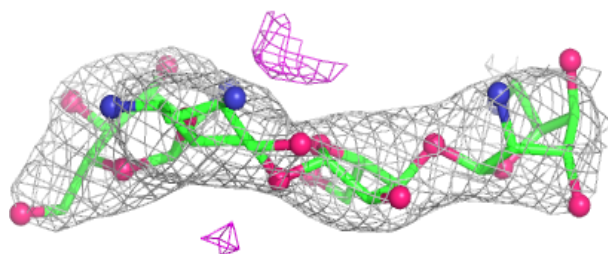
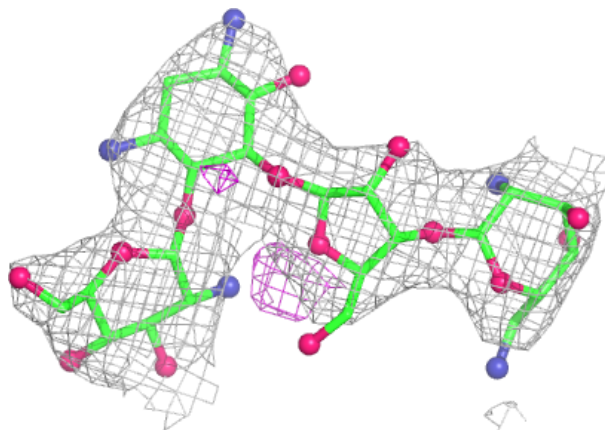
Continued from previous page...

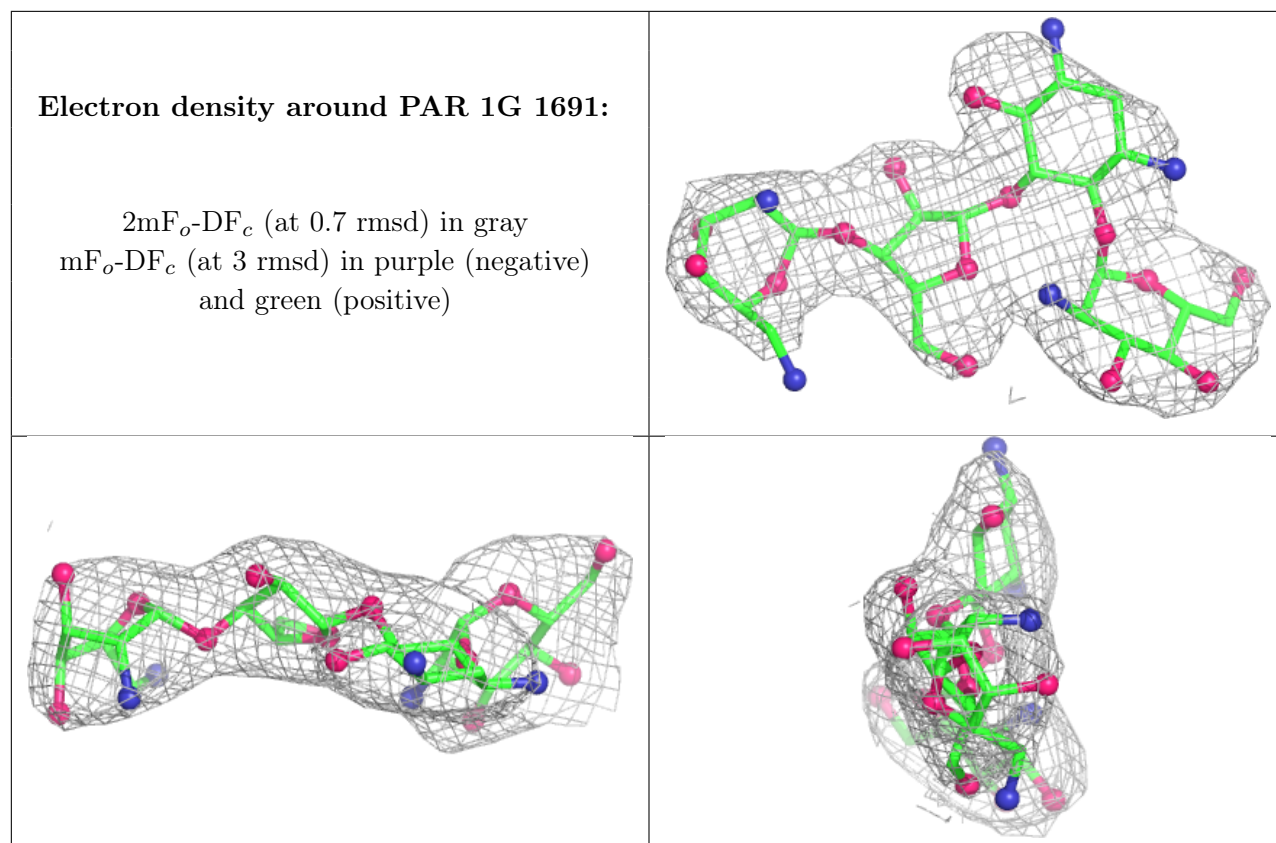
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3279	1/1	1.00	0.04	62,62,62,62	0
57	MG	1H	3330	1/1	1.00	0.03	57,57,57,57	0
57	MG	1H	3343	1/1	1.00	0.04	74,74,74,74	0
57	MG	13	1706	1/1	1.00	0.02	71,71,71,71	0
60	ZN	5I	102	1/1	1.00	0.01	88,88,88,88	0
57	MG	1H	3401	1/1	1.00	0.01	52,52,52,52	0
57	MG	14	3284	1/1	1.00	0.02	57,57,57,57	0
57	MG	1H	3345	1/1	1.00	0.02	56,56,56,56	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 PAR 13 1749:

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 [i](#)

There are no such residues in this entry.