



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 19, 2026 – 04:44 PM UTC

PDB ID : 4V9P / pdb_00004v9p
Title : Control of ribosomal subunit rotation by elongation factor G
Authors : Pulk, A.; Cate, J.H.D.
Deposited on : 2013-05-03
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

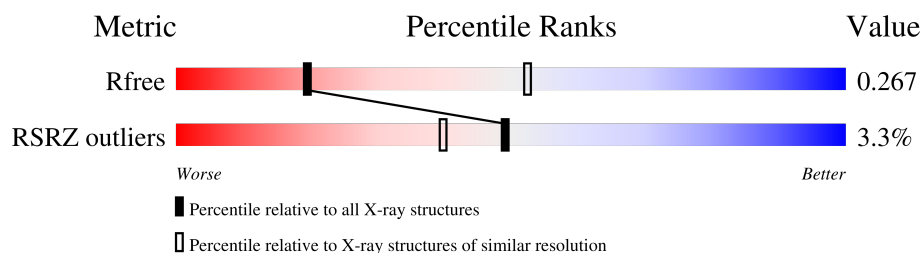
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	KBE	DW	1	-	-	-	X
55	KBE	FW	1	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 590573 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
1	CA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
1	EA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
1	GA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
2	CB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
2	EB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
2	GB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
3	CC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
3	EC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
3	GC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
4	CD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
4	ED	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
4	GD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
5	CE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
5	EE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
5	GE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
6	CF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
6	EF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
6	GF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
7	CG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
7	EG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	GG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	50	Total	C	N	O	S	0	0	0
			384	247	68	68	1			
8	CH	50	Total	C	N	O	S	0	0	0
			384	247	68	68	1			
8	EH	50	Total	C	N	O	S	0	0	0
			384	247	68	68	1			
8	GH	50	Total	C	N	O	S	0	0	0
			384	247	68	68	1			

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
9	CI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
9	EI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
9	GI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
10	CJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
10	EJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
10	GJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
11	CK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
11	EK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
11	GK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
12	CL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
12	EL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
12	GL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
13	CM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
13	EM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
13	GM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
14	CN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
14	EN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	GN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	116	Total	C	N	O		0	0	0
			892	552	178	162				
15	CO	116	Total	C	N	O		0	0	0
			892	552	178	162				
15	EO	116	Total	C	N	O		0	0	0
			892	552	178	162				
15	GO	116	Total	C	N	O		0	0	0
			892	552	178	162				

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
16	CP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
16	EP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
16	GP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	117	Total	C	N	O		0	0	0
			947	604	192	151				
17	CQ	117	Total	C	N	O		0	0	0
			947	604	192	151				
17	EQ	117	Total	C	N	O		0	0	0
			947	604	192	151				
17	GQ	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
18	CR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
18	ER	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
18	GR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
19	CS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
19	ES	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
19	GS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
20	CT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
20	ET	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
20	GT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	102	Total	C	N	O	0	0	0
			779	492	146	141			
21	CU	102	Total	C	N	O	0	0	0
			779	492	146	141			
21	EU	102	Total	C	N	O	0	0	0
			779	492	146	141			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	GU	102	Total	C	N	O	0	0	0
			779	492	146	141			

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
22	CV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
22	EV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
22	GV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
23	CW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
23	EW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
23	GW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
24	CX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
24	EX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
24	GX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
25	CY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
25	EY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
25	GY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	AZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
26	CZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
26	EZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
26	GZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
27	C0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
27	E0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
27	G0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	A1	50	Total	C	N	O	0	0	0
			409	263	75	71			
28	C1	50	Total	C	N	O	0	0	0
			409	263	75	71			
28	E1	50	Total	C	N	O	0	0	0
			409	263	75	71			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	G1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
29	C2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
29	E2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
29	G2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
30	C3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
30	E3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
30	G3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	A4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
31	C4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
31	E4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
31	G4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	A5	148	Total	C	N	O	S	0	0	0
			1117	705	196	209	7			
32	E5	144	Total	C	N	O	S	0	0	0
			1092	691	192	202	7			

- Molecule 33 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			
33	DA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			
33	FA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			
33	HA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
34	DB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
34	FB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
34	HB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
35	DC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
35	FC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
35	HC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
36	DD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
36	FD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
36	HD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
37	DE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
37	FE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
37	HE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
38	DF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
38	FF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
38	HF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
39	DG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
39	FG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	HG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			

- Molecule 40 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
40	DH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
40	FH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
40	HH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
41	DI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
41	FI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
41	HI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
42	DJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
42	FJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
42	HJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
43	DK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
43	FK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
43	HK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
44	DL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
44	FL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
44	HL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
45	DM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
45	FM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
45	HM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			

- Molecule 46 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
46	DN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
46	FN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	HN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- Molecule 47 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
47	DO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
47	FO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
47	HO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 48 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
48	DP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
48	FP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
48	HP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
49	DQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
49	FQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
49	HQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	BR	55	Total	C	N	O	0	0	0
			455	288	86	81			
50	DR	55	Total	C	N	O	0	0	0
			455	288	86	81			
50	FR	55	Total	C	N	O	0	0	0
			455	288	86	81			
50	HR	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
51	DS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
51	FS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
51	HS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
52	DT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
52	FT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
52	HT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 53 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
53	DU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
53	FU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	HU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 54 is a protein called elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BV	689	Total	C	N	O	S	0	0	0
			5319	3345	919	1030	25			
54	DV	689	Total	C	N	O	S	0	0	0
			5319	3345	919	1030	25			
54	FV	689	Total	C	N	O	S	0	0	0
			5319	3345	919	1030	25			
54	HV	689	Total	C	N	O	S	0	0	0
			5319	3345	919	1030	25			

- Molecule 55 is a protein called Viomycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	BW	6	Total	C	N	O	0	0	0
			48	25	13	10			
55	DW	6	Total	C	N	O	0	0	0
			48	25	13	10			
55	FW	6	Total	C	N	O	0	0	0
			48	25	13	10			

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	130	Total	Mg	0	0
			130	130		
56	AB	4	Total	Mg	0	0
			4	4		
56	AC	3	Total	Mg	0	0
			3	3		
56	AD	1	Total	Mg	0	0
			1	1		
56	AE	1	Total	Mg	0	0
			1	1		
56	AT	1	Total	Mg	0	0
			1	1		
56	A3	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BA	40	Total 40	Mg 40	0	0
56	BE	1	Total 1	Mg 1	0	0
56	BL	1	Total 1	Mg 1	0	0
56	BU	1	Total 1	Mg 1	0	0
56	BV	1	Total 1	Mg 1	0	0
56	CA	134	Total 134	Mg 134	0	0
56	CB	4	Total 4	Mg 4	0	0
56	CD	1	Total 1	Mg 1	0	0
56	CE	1	Total 1	Mg 1	0	0
56	C4	1	Total 1	Mg 1	0	0
56	DA	42	Total 42	Mg 42	0	0
56	DU	1	Total 1	Mg 1	0	0
56	DV	1	Total 1	Mg 1	0	0
56	EA	133	Total 133	Mg 133	0	0
56	EB	4	Total 4	Mg 4	0	0
56	EC	1	Total 1	Mg 1	0	0
56	ED	2	Total 2	Mg 2	0	0
56	EQ	1	Total 1	Mg 1	0	0
56	FA	41	Total 41	Mg 41	0	0
56	FE	1	Total 1	Mg 1	0	0
56	FU	1	Total 1	Mg 1	0	0

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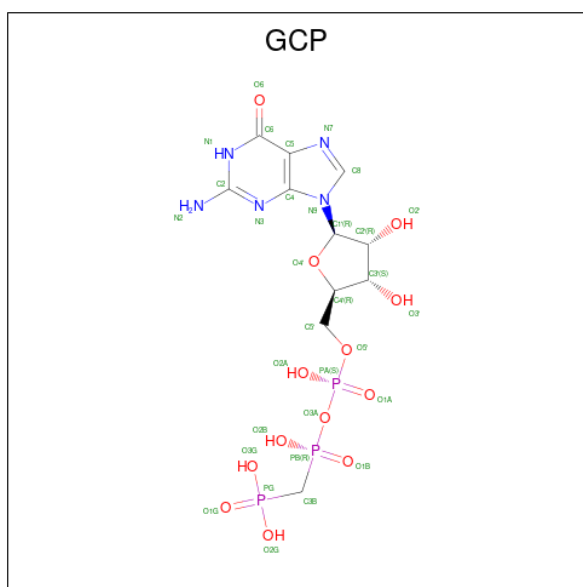
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	FV	1	Total 1	Mg 1	0	0
56	GA	134	Total 134	Mg 134	0	0
56	GB	4	Total 4	Mg 4	0	0
56	GC	1	Total 1	Mg 1	0	0
56	GL	1	Total 1	Mg 1	0	0
56	GS	1	Total 1	Mg 1	0	0
56	HA	40	Total 40	Mg 40	0	0
56	HC	1	Total 1	Mg 1	0	0
56	HE	1	Total 1	Mg 1	0	0
56	HT	1	Total 1	Mg 1	0	0
56	HV	1	Total 1	Mg 1	0	0

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	A4	1	Total 1	Zn 1	0	0
57	C4	1	Total 1	Zn 1	0	0
57	E4	1	Total 1	Zn 1	0	0
57	G4	1	Total 1	Zn 1	0	0

- Molecule 58 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
58	BV	1	Total 32	C 11	N 5	O 13	P 3	0	0
58	DV	1	Total 32	C 11	N 5	O 13	P 3	0	0
58	FV	1	Total 32	C 11	N 5	O 13	P 3	0	0
58	HV	1	Total 32	C 11	N 5	O 13	P 3	0	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AA	608	Total O 608 608	0	0
59	AB	19	Total O 19 19	0	0
59	AC	10	Total O 10 10	0	0
59	AD	3	Total O 3 3	0	0
59	AE	1	Total O 1 1	0	0
59	AJ	1	Total O 1 1	0	0
59	AL	7	Total O 7 7	0	0
59	AN	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AP	1	Total O 1 1	0	0
59	AQ	1	Total O 1 1	0	0
59	AS	1	Total O 1 1	0	0
59	AU	1	Total O 1 1	0	0
59	A0	1	Total O 1 1	0	0
59	A3	1	Total O 1 1	0	0
59	A4	2	Total O 2 2	0	0
59	BA	197	Total O 197 197	0	0
59	BC	1	Total O 1 1	0	0
59	BD	1	Total O 1 1	0	0
59	BI	1	Total O 1 1	0	0
59	BK	1	Total O 1 1	0	0
59	BN	3	Total O 3 3	0	0
59	BT	2	Total O 2 2	0	0
59	BU	1	Total O 1 1	0	0
59	BV	1	Total O 1 1	0	0
59	CA	604	Total O 604 604	0	0
59	CB	20	Total O 20 20	0	0
59	CC	11	Total O 11 11	0	0
59	CD	3	Total O 3 3	0	0
59	CE	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	CF	1	Total 1	O 1	0	0
59	CJ	3	Total 3	O 3	0	0
59	CL	6	Total 6	O 6	0	0
59	CN	4	Total 4	O 4	0	0
59	CS	1	Total 1	O 1	0	0
59	CT	2	Total 2	O 2	0	0
59	C2	1	Total 1	O 1	0	0
59	C3	1	Total 1	O 1	0	0
59	C4	2	Total 2	O 2	0	0
59	DA	193	Total 193	O 193	0	0
59	DC	1	Total 1	O 1	0	0
59	DE	2	Total 2	O 2	0	0
59	DG	1	Total 1	O 1	0	0
59	DK	1	Total 1	O 1	0	0
59	DL	1	Total 1	O 1	0	0
59	DN	6	Total 6	O 6	0	0
59	DQ	1	Total 1	O 1	0	0
59	DT	1	Total 1	O 1	0	0
59	DU	1	Total 1	O 1	0	0
59	DV	1	Total 1	O 1	0	0
59	EA	617	Total 617	O 617	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	EB	20	Total 20	O 20	0	0
59	EC	8	Total 8	O 8	0	0
59	ED	1	Total 1	O 1	0	0
59	EL	4	Total 4	O 4	0	0
59	EN	2	Total 2	O 2	0	0
59	ER	1	Total 1	O 1	0	0
59	ET	1	Total 1	O 1	0	0
59	EU	1	Total 1	O 1	0	0
59	E0	2	Total 2	O 2	0	0
59	E3	2	Total 2	O 2	0	0
59	E4	1	Total 1	O 1	0	0
59	FA	198	Total 198	O 198	0	0
59	FE	1	Total 1	O 1	0	0
59	FK	1	Total 1	O 1	0	0
59	FN	3	Total 3	O 3	0	0
59	FQ	1	Total 1	O 1	0	0
59	FT	4	Total 4	O 4	0	0
59	FV	1	Total 1	O 1	0	0
59	GA	607	Total 607	O 607	0	0
59	GB	19	Total 19	O 19	0	0
59	GC	9	Total 9	O 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	GD	4	Total 4	O 4	0	0
59	GE	2	Total 2	O 2	0	0
59	GL	4	Total 4	O 4	0	0
59	GN	3	Total 3	O 3	0	0
59	GQ	1	Total 1	O 1	0	0
59	GR	2	Total 2	O 2	0	0
59	GS	1	Total 1	O 1	0	0
59	GT	1	Total 1	O 1	0	0
59	GU	2	Total 2	O 2	0	0
59	GV	1	Total 1	O 1	0	0
59	G2	2	Total 2	O 2	0	0
59	G3	1	Total 1	O 1	0	0
59	G4	1	Total 1	O 1	0	0
59	HA	197	Total 197	O 197	0	0
59	HD	1	Total 1	O 1	0	0
59	HE	3	Total 3	O 3	0	0
59	HN	5	Total 5	O 5	0	0
59	HT	1	Total 1	O 1	0	0
59	HU	1	Total 1	O 1	0	0
59	HV	1	Total 1	O 1	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	361.14Å 360.51Å 429.73Å 90.00° 103.22° 90.00°	Depositor
Resolution (Å)	70.00 – 2.90 70.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-2.90) 84.3 (70.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.215 , 0.267 0.217 , 0.267	Depositor DCC
R_{free} test set	3893 reflections (0.13%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	590573	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8072e-03.*

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](#)

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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](#)

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4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

12 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	$\# Z > 2$
55	KBE	BW	1	55	8,8,9	0.90	0	6,8,10	1.09	1 (16%)
55	KBE	FW	1	55	8,8,9	0.96	0	6,8,10	1.91	1 (16%)
55	5OH	BW	6	55	7,12,13	1.66	2 (28%)	4,16,18	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	DPP	DW	2	55	4,5,6	0.83	0	1,5,7	0.29	0
55	UAL	BW	5	55	6,8,9	2.90	3 (50%)	4,9,11	4.66	1 (25%)
55	UAL	DW	5	55	6,8,9	2.69	3 (50%)	4,9,11	4.44	1 (25%)
55	5OH	DW	6	55	7,12,13	1.85	2 (28%)	4,16,18	1.41	1 (25%)
55	DPP	BW	2	55	4,5,6	1.07	0	1,5,7	0.71	0
55	5OH	FW	6	55	7,12,13	1.98	2 (28%)	4,16,18	1.25	0
55	DPP	FW	2	55	4,5,6	0.83	0	1,5,7	0.01	0
55	UAL	FW	5	55	6,8,9	2.41	3 (50%)	4,9,11	2.80	2 (50%)
55	KBE	DW	1	55	8,8,9	0.91	0	6,8,10	1.14	1 (16%)

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
55	KBE	BW	1	55	-	3/7/7/8	-
55	KBE	FW	1	55	-	3/7/7/8	-
55	5OH	BW	6	55	-	2/2/18/20	0/1/1/1
55	DPP	DW	2	55	-	0/2/4/6	-
55	UAL	BW	5	55	-	1/3/7/9	-
55	UAL	DW	5	55	-	1/3/7/9	-
55	5OH	DW	6	55	-	1/2/18/20	0/1/1/1
55	DPP	BW	2	55	-	0/2/4/6	-
55	5OH	FW	6	55	-	0/2/18/20	0/1/1/1
55	DPP	FW	2	55	-	0/2/4/6	-
55	UAL	FW	5	55	-	0/3/7/9	-
55	KBE	DW	1	55	-	4/7/7/8	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	BW	5	UAL	CB-N1	4.25	1.46	1.35
55	DW	5	UAL	CB-N1	4.07	1.46	1.35
55	BW	5	UAL	C-CA	4.05	1.51	1.45
55	DW	5	UAL	C1-N1	3.84	1.46	1.40
55	FW	5	UAL	CB-N1	3.84	1.45	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BW	5	UAL	O-C-CA	-9.02	114.08	125.39
55	DW	5	UAL	O-C-CA	-8.62	114.58	125.39
55	FW	5	UAL	O-C-CA	-5.01	119.11	125.39
55	FW	1	KBE	CB-CA-C	4.19	118.93	112.17
55	BW	1	KBE	O-C-CA	-2.37	118.47	125.38

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	BW	1	KBE	O-C-CA-CB
55	BW	1	KBE	C-CA-CB-N
55	BW	1	KBE	C-CA-CB-CG
55	BW	6	5OH	C-CA-CB-CR
55	DW	1	KBE	N-CB-CG-CD

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 748 ligands modelled in this entry, 744 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	GCP	BV	801	56	32,34,34	1.71	7 (21%)	49,54,54	1.91	14 (28%)
58	GCP	DV	801	56	32,34,34	1.71	6 (18%)	49,54,54	1.90	14 (28%)
58	GCP	HV	801	56	32,34,34	1.67	7 (21%)	49,54,54	1.87	10 (20%)
58	GCP	FV	801	56	32,34,34	1.47	7 (21%)	49,54,54	1.82	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GCP	BV	801	56	-	3/19/38/38	0/3/3/3
58	GCP	DV	801	56	-	2/19/38/38	0/3/3/3
58	GCP	HV	801	56	-	3/19/38/38	0/3/3/3
58	GCP	FV	801	56	-	3/19/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	DV	801	GCP	C2-N2	4.86	1.45	1.34
58	HV	801	GCP	C2-N2	4.69	1.45	1.34
58	BV	801	GCP	C2-N2	4.67	1.45	1.34
58	BV	801	GCP	C2'-C3'	-4.12	1.42	1.53
58	DV	801	GCP	C2'-C3'	-4.07	1.42	1.53

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	FV	801	GCP	C5-C4-N3	-6.18	118.55	128.39
58	DV	801	GCP	C2-N3-C4	5.41	121.61	112.30
58	FV	801	GCP	C2-N3-C4	5.05	121.00	112.30
58	HV	801	GCP	C5-C4-N3	-5.03	120.39	128.39
58	BV	801	GCP	C2-N3-C4	4.93	120.79	112.30

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

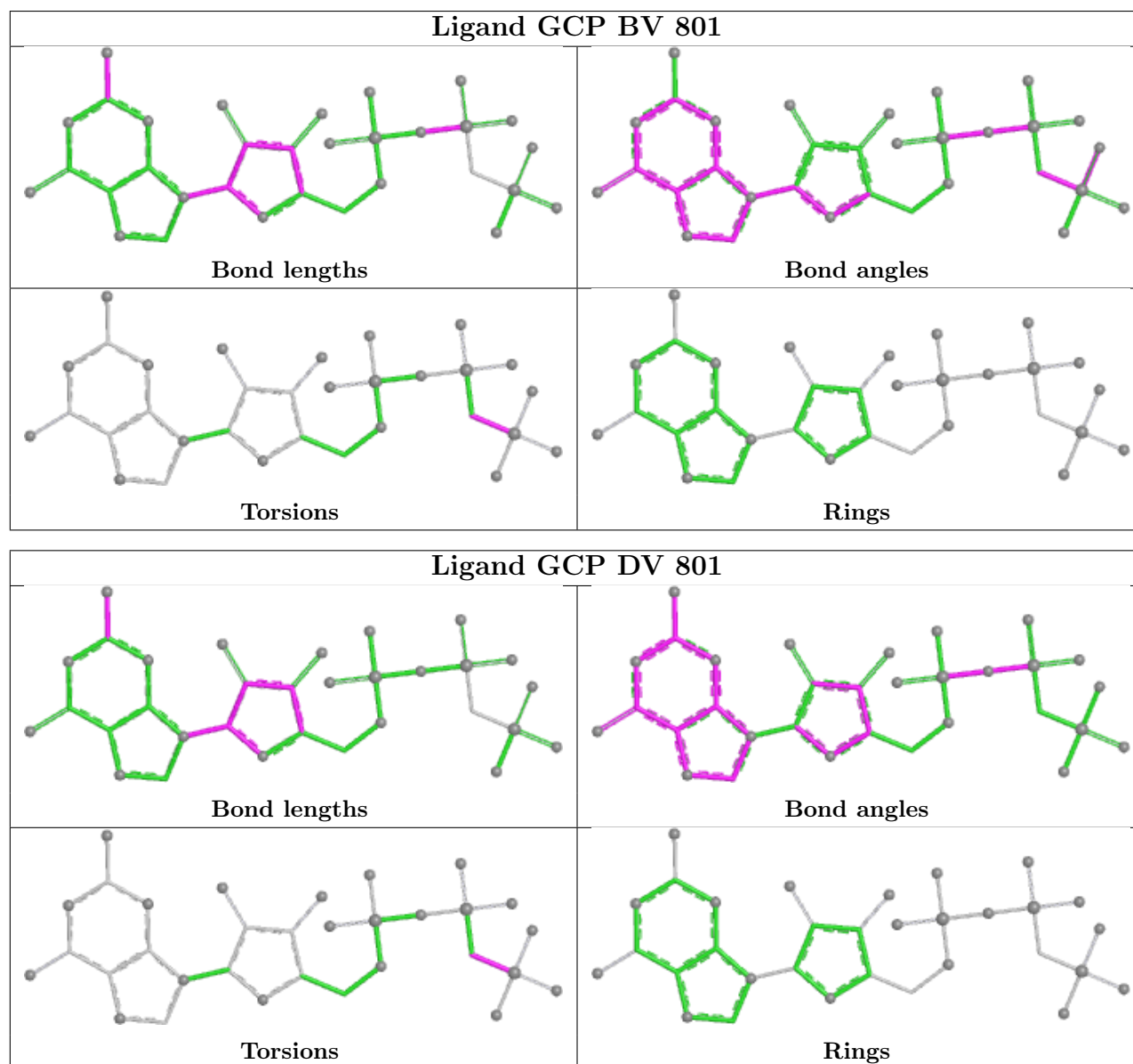
Mol	Chain	Res	Type	Atoms
58	BV	801	GCP	PB-C3B-PG-O1G
58	BV	801	GCP	PB-C3B-PG-O2G
58	BV	801	GCP	PB-C3B-PG-O3G
58	HV	801	GCP	PB-C3B-PG-O1G
58	HV	801	GCP	PB-C3B-PG-O3G

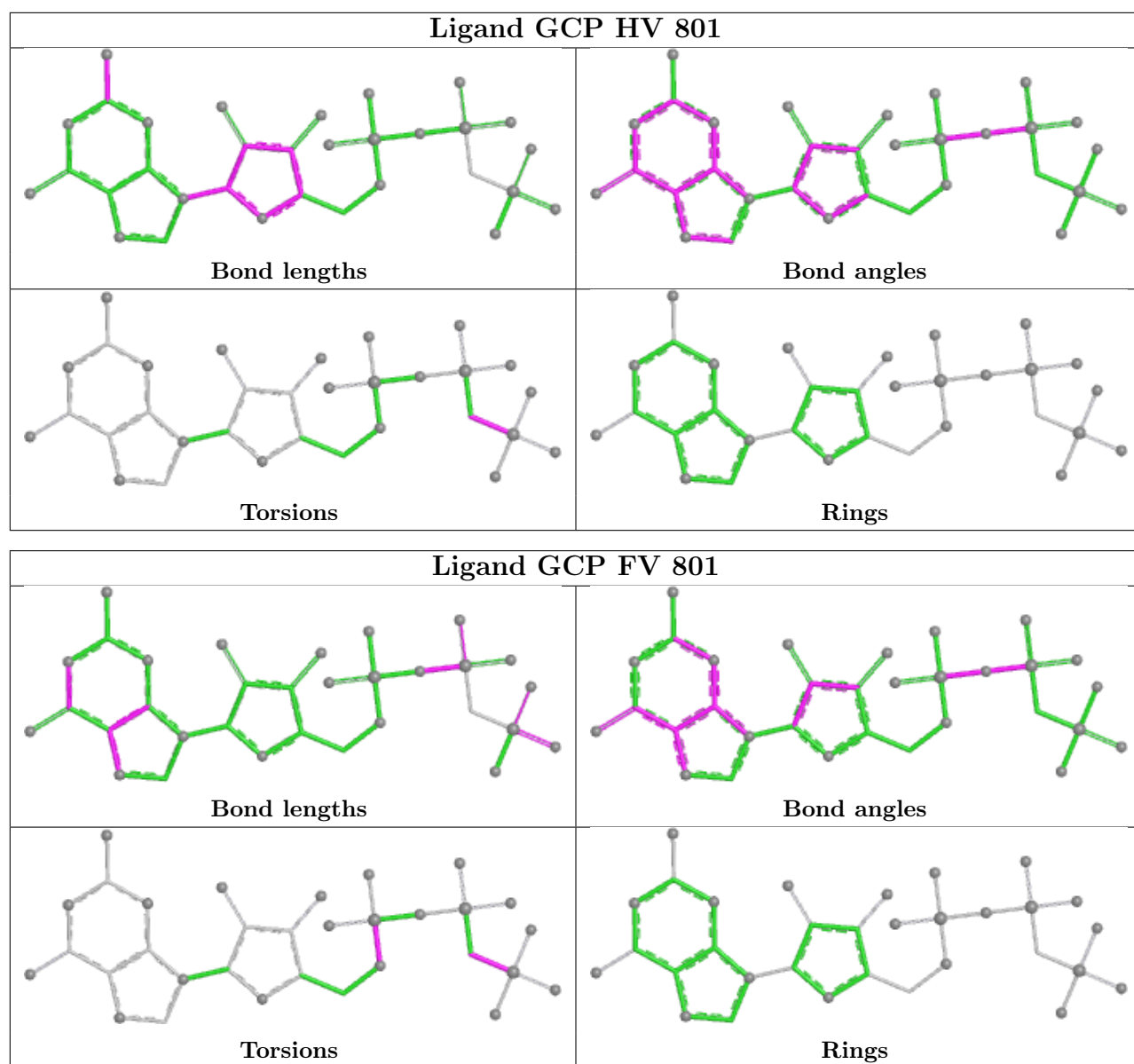
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	2854/2904 (98%)	-0.65	52 (1%) 67 59	4, 28, 65, 87	0
1	CA	2854/2904 (98%)	-0.76	47 (1%) 70 62	3, 25, 63, 88	0
1	EA	2854/2904 (98%)	-0.87	27 (0%) 81 75	1, 14, 60, 92	0
1	GA	2854/2904 (98%)	-0.65	34 (1%) 76 69	5, 29, 68, 89	0
2	AB	118/120 (98%)	-0.38	0 100 100	18, 48, 62, 72	0
2	CB	118/120 (98%)	-0.76	0 100 100	18, 41, 54, 72	0
2	EB	118/120 (98%)	-0.95	0 100 100	3, 25, 45, 56	0
2	GB	118/120 (98%)	-0.60	0 100 100	23, 44, 61, 78	0
3	AC	271/273 (99%)	-0.23	5 (1%) 67 59	5, 26, 40, 60	0
3	CC	271/273 (99%)	-0.32	4 (1%) 72 64	2, 18, 34, 44	0
3	EC	271/273 (99%)	-0.35	3 (1%) 78 71	1, 15, 32, 57	0
3	GC	271/273 (99%)	-0.37	3 (1%) 78 71	3, 17, 30, 42	0
4	AD	209/209 (100%)	-0.19	5 (2%) 59 50	6, 27, 47, 60	0
4	CD	209/209 (100%)	-0.02	5 (2%) 59 50	3, 31, 52, 61	0
4	ED	209/209 (100%)	-0.23	5 (2%) 59 50	1, 20, 43, 56	0
4	GD	209/209 (100%)	0.04	5 (2%) 59 50	4, 36, 54, 62	0
5	AE	201/201 (100%)	-0.12	2 (0%) 79 73	7, 33, 55, 63	0
5	CE	201/201 (100%)	-0.21	2 (0%) 79 73	4, 33, 54, 60	0
5	EE	201/201 (100%)	-0.44	0 100 100	2, 19, 45, 69	0
5	GE	201/201 (100%)	-0.09	4 (1%) 65 56	7, 41, 56, 67	0
6	AF	177/179 (98%)	1.42	50 (28%) 1 1	45, 61, 71, 79	0
6	CF	177/179 (98%)	0.12	2 (1%) 78 71	32, 49, 63, 67	0
6	EF	177/179 (98%)	-0.05	0 100 100	19, 42, 61, 68	0
6	GF	177/179 (98%)	0.92	22 (12%) 8 7	36, 61, 72, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
7	AG	176/177 (99%)	0.20	3 (1%) 69 61	20, 42, 60, 69	0
7	CG	176/177 (99%)	0.26	5 (2%) 55 46	23, 46, 61, 69	0
7	EG	176/177 (99%)	0.04	3 (1%) 69 61	19, 37, 55, 63	0
7	GG	176/177 (99%)	0.47	4 (2%) 61 52	32, 48, 63, 68	0
8	AH	50/50 (100%)	0.47	4 (8%) 18 15	28, 51, 67, 77	0
8	CH	50/50 (100%)	0.65	3 (6%) 27 21	39, 56, 68, 74	0
8	EH	50/50 (100%)	0.28	2 (4%) 42 34	24, 49, 69, 79	0
8	GH	50/50 (100%)	0.43	0 100 100	26, 46, 64, 69	0
9	AI	141/142 (99%)	1.10	26 (18%) 3 3	44, 64, 75, 82	0
9	CI	141/142 (99%)	1.05	19 (13%) 7 5	49, 63, 73, 76	0
9	EI	141/142 (99%)	1.15	28 (19%) 3 2	48, 65, 77, 82	0
9	GI	141/142 (99%)	1.65	44 (31%) 1 1	49, 68, 77, 81	0
10	AJ	142/142 (100%)	-0.10	2 (1%) 73 65	12, 29, 41, 60	0
10	CJ	142/142 (100%)	-0.08	3 (2%) 63 54	13, 29, 42, 58	0
10	EJ	142/142 (100%)	-0.33	3 (2%) 63 54	3, 13, 30, 47	0
10	GJ	142/142 (100%)	0.00	6 (4%) 40 32	15, 32, 47, 61	0
11	AK	122/123 (99%)	-0.27	1 (0%) 82 77	5, 19, 34, 54	0
11	CK	122/123 (99%)	-0.19	4 (3%) 49 40	9, 22, 39, 56	0
11	EK	122/123 (99%)	-0.30	2 (1%) 70 62	4, 18, 37, 49	0
11	GK	122/123 (99%)	-0.11	2 (1%) 70 62	13, 27, 42, 59	0
12	AL	143/144 (99%)	-0.07	0 100 100	10, 30, 48, 58	0
12	CL	143/144 (99%)	-0.22	1 (0%) 84 79	3, 29, 47, 62	0
12	EL	143/144 (99%)	-0.28	0 100 100	1, 18, 39, 54	0
12	GL	143/144 (99%)	0.02	1 (0%) 84 79	10, 35, 53, 67	0
13	AM	136/136 (100%)	-0.37	0 100 100	8, 19, 37, 55	0
13	CM	136/136 (100%)	-0.39	1 (0%) 84 79	8, 21, 38, 56	0
13	EM	136/136 (100%)	-0.55	1 (0%) 84 79	1, 11, 29, 60	0
13	GM	136/136 (100%)	-0.25	0 100 100	11, 28, 45, 58	0
14	AN	120/127 (94%)	-0.09	0 100 100	14, 29, 41, 62	0
14	CN	120/127 (94%)	-0.16	0 100 100	18, 31, 43, 62	0
14	EN	120/127 (94%)	-0.48	0 100 100	6, 18, 32, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	GN	120/127 (94%)	-0.15	1 (0%) 82 77	19, 31, 43, 72	0
15	AO	116/117 (99%)	0.28	3 (2%) 57 48	28, 47, 56, 62	0
15	CO	116/117 (99%)	-0.00	2 (1%) 69 61	28, 42, 55, 61	0
15	EO	116/117 (99%)	-0.28	0 100 100	16, 30, 43, 55	0
15	GO	116/117 (99%)	-0.09	1 (0%) 81 75	28, 40, 58, 63	0
16	AP	114/115 (99%)	-0.05	2 (1%) 67 59	13, 31, 47, 62	0
16	CP	114/115 (99%)	-0.09	3 (2%) 57 48	17, 35, 49, 62	0
16	EP	114/115 (99%)	-0.37	1 (0%) 81 75	6, 24, 43, 66	0
16	GP	114/115 (99%)	-0.08	1 (0%) 81 75	14, 35, 50, 59	0
17	AQ	117/118 (99%)	-0.03	3 (2%) 57 48	10, 26, 43, 56	0
17	CQ	117/118 (99%)	-0.05	3 (2%) 57 48	6, 24, 39, 60	0
17	EQ	117/118 (99%)	-0.40	3 (2%) 57 48	2, 9, 25, 46	0
17	GQ	117/118 (99%)	0.03	4 (3%) 48 39	19, 29, 42, 56	0
18	AR	103/103 (100%)	-0.08	2 (1%) 66 58	10, 37, 52, 60	0
18	CR	103/103 (100%)	-0.09	1 (0%) 79 73	9, 34, 49, 63	0
18	ER	103/103 (100%)	-0.32	1 (0%) 79 73	2, 21, 41, 52	0
18	GR	103/103 (100%)	0.17	3 (2%) 53 45	13, 40, 53, 63	0
19	AS	110/110 (100%)	-0.12	1 (0%) 81 75	13, 28, 45, 62	0
19	CS	110/110 (100%)	-0.26	0 100 100	7, 27, 45, 65	0
19	ES	110/110 (100%)	-0.43	0 100 100	2, 12, 36, 49	0
19	GS	110/110 (100%)	-0.15	1 (0%) 81 75	12, 31, 50, 69	0
20	AT	93/100 (93%)	0.28	6 (6%) 25 20	18, 37, 58, 63	0
20	CT	93/100 (93%)	0.11	3 (3%) 50 41	14, 37, 57, 67	0
20	ET	93/100 (93%)	0.04	3 (3%) 50 41	6, 24, 53, 61	0
20	GT	93/100 (93%)	0.21	2 (2%) 62 53	19, 36, 57, 62	0
21	AU	102/104 (98%)	0.31	2 (1%) 65 56	24, 40, 56, 64	0
21	CU	102/104 (98%)	0.20	3 (2%) 53 45	24, 41, 61, 73	0
21	EU	102/104 (98%)	0.03	3 (2%) 53 45	13, 28, 51, 65	0
21	GU	102/104 (98%)	0.57	8 (7%) 19 16	32, 46, 63, 75	0
22	AV	94/94 (100%)	-0.15	0 100 100	23, 38, 48, 57	0
22	CV	94/94 (100%)	-0.17	1 (1%) 78 71	25, 39, 52, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
22	EV	94/94 (100%)	-0.51	0 100 100	9, 22, 40, 45	0
22	GV	94/94 (100%)	-0.10	0 100 100	29, 42, 55, 60	0
23	AW	79/85 (92%)	0.81	10 (12%) 8 6	17, 35, 52, 61	0
23	CW	79/85 (92%)	0.57	6 (7%) 20 16	15, 29, 51, 65	0
23	EW	79/85 (92%)	0.58	11 (13%) 6 5	5, 17, 44, 50	0
23	GW	79/85 (92%)	0.88	10 (12%) 8 6	15, 33, 55, 63	0
24	AX	77/78 (98%)	0.11	3 (3%) 43 35	16, 31, 47, 57	0
24	CX	77/78 (98%)	-0.25	0 100 100	8, 22, 46, 49	0
24	EX	77/78 (98%)	-0.44	1 (1%) 75 67	4, 18, 40, 50	0
24	GX	77/78 (98%)	-0.14	1 (1%) 75 67	14, 25, 46, 56	0
25	AY	63/63 (100%)	0.23	2 (3%) 50 41	30, 47, 61, 65	0
25	CY	63/63 (100%)	0.29	3 (4%) 35 28	27, 44, 58, 67	0
25	EY	63/63 (100%)	0.10	2 (3%) 50 41	13, 33, 51, 70	0
25	GY	63/63 (100%)	0.22	2 (3%) 50 41	29, 45, 60, 68	0
26	AZ	58/59 (98%)	-0.07	1 (1%) 69 61	15, 31, 55, 71	0
26	CZ	58/59 (98%)	-0.10	1 (1%) 69 61	17, 30, 53, 65	0
26	EZ	58/59 (98%)	-0.33	1 (1%) 69 61	2, 10, 35, 59	0
26	GZ	58/59 (98%)	-0.05	0 100 100	20, 32, 51, 53	0
27	A0	56/57 (98%)	0.00	1 (1%) 67 59	11, 33, 54, 62	0
27	C0	56/57 (98%)	-0.13	0 100 100	8, 35, 50, 60	0
27	E0	56/57 (98%)	-0.12	0 100 100	3, 25, 48, 56	0
27	G0	56/57 (98%)	-0.07	1 (1%) 67 59	15, 35, 58, 67	0
28	A1	50/55 (90%)	0.04	1 (2%) 65 56	27, 38, 51, 61	0
28	C1	50/55 (90%)	0.05	2 (4%) 42 34	21, 35, 48, 59	0
28	E1	50/55 (90%)	-0.24	1 (2%) 65 56	11, 26, 44, 47	0
28	G1	50/55 (90%)	0.09	2 (4%) 42 34	25, 38, 55, 61	0
29	A2	46/46 (100%)	-0.06	2 (4%) 40 31	9, 22, 34, 55	0
29	C2	46/46 (100%)	-0.09	2 (4%) 40 31	7, 14, 30, 54	0
29	E2	46/46 (100%)	-0.49	1 (2%) 62 53	2, 7, 15, 53	0
29	G2	46/46 (100%)	0.03	3 (6%) 25 20	8, 17, 28, 51	0
30	A3	64/65 (98%)	-0.00	1 (1%) 70 62	12, 22, 37, 40	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
30	C3	64/65 (98%)	-0.17	1 (1%) 70 62	10, 18, 27, 35	0
30	E3	64/65 (98%)	-0.38	1 (1%) 70 62	2, 8, 14, 27	0
30	G3	64/65 (98%)	-0.08	2 (3%) 51 42	13, 22, 37, 48	0
31	A4	38/38 (100%)	-0.14	0 100 100	13, 22, 36, 38	0
31	C4	38/38 (100%)	0.02	1 (2%) 57 48	14, 27, 39, 46	0
31	E4	38/38 (100%)	-0.23	0 100 100	5, 16, 35, 38	0
31	G4	38/38 (100%)	0.08	0 100 100	22, 33, 44, 49	0
32	A5	148/165 (89%)	1.50	45 (30%) 1 1	36, 54, 65, 74	0
32	E5	144/165 (87%)	1.55	43 (29%) 1 1	35, 61, 72, 82	0
33	BA	1533/1542 (99%)	-0.47	13 (0%) 82 77	11, 42, 70, 91	0
33	DA	1533/1542 (99%)	-0.45	17 (1%) 78 71	12, 43, 69, 85	0
33	FA	1533/1542 (99%)	-0.69	8 (0%) 87 83	8, 33, 61, 85	0
33	HA	1533/1542 (99%)	-0.55	16 (1%) 79 73	15, 41, 72, 90	0
34	BB	218/241 (90%)	0.45	6 (2%) 55 46	41, 58, 69, 79	0
34	DB	218/241 (90%)	0.42	10 (4%) 37 29	40, 57, 69, 79	0
34	FB	218/241 (90%)	0.07	2 (0%) 81 75	26, 49, 63, 69	0
34	HB	218/241 (90%)	0.26	14 (6%) 25 20	33, 51, 67, 73	0
35	BC	206/233 (88%)	0.18	8 (3%) 43 35	30, 50, 60, 69	0
35	DC	206/233 (88%)	0.05	2 (0%) 79 73	35, 50, 60, 67	0
35	FC	206/233 (88%)	-0.33	0 100 100	13, 30, 46, 58	0
35	HC	206/233 (88%)	-0.17	3 (1%) 72 64	21, 40, 56, 66	0
36	BD	205/206 (99%)	0.02	6 (2%) 53 45	23, 39, 57, 64	0
36	DD	205/206 (99%)	0.31	6 (2%) 53 45	26, 47, 60, 65	0
36	FD	205/206 (99%)	0.01	4 (1%) 65 56	27, 44, 60, 73	0
36	HD	205/206 (99%)	0.43	11 (5%) 31 24	25, 47, 61, 79	0
37	BE	150/167 (89%)	0.10	3 (2%) 65 56	17, 48, 63, 76	0
37	DE	150/167 (89%)	0.21	8 (5%) 32 25	25, 45, 62, 71	0
37	FE	150/167 (89%)	-0.12	1 (0%) 84 79	18, 34, 50, 65	0
37	HE	150/167 (89%)	-0.04	0 100 100	21, 37, 54, 67	0
38	BF	100/135 (74%)	1.09	12 (12%) 9 7	50, 62, 70, 74	0
38	DF	100/135 (74%)	0.24	3 (3%) 52 43	32, 49, 62, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
38	FF	100/135 (74%)	0.38	2 (2%) 65 56	32, 51, 63, 66	0
38	HF	100/135 (74%)	0.16	3 (3%) 52 43	31, 51, 64, 71	0
39	BG	151/179 (84%)	0.20	1 (0%) 84 79	28, 49, 60, 66	0
39	DG	151/179 (84%)	-0.02	2 (1%) 75 67	32, 46, 58, 63	0
39	FG	151/179 (84%)	0.04	2 (1%) 75 67	23, 39, 55, 63	0
39	HG	151/179 (84%)	0.30	9 (5%) 27 21	32, 48, 62, 68	0
40	BH	129/130 (99%)	0.19	2 (1%) 70 62	40, 51, 62, 70	0
40	DH	129/130 (99%)	0.16	2 (1%) 70 62	28, 47, 59, 73	0
40	FH	129/130 (99%)	-0.17	1 (0%) 82 77	20, 32, 47, 66	0
40	HH	129/130 (99%)	-0.32	0 100 100	23, 35, 51, 69	0
41	BI	127/130 (97%)	0.60	7 (5%) 30 24	24, 52, 65, 70	0
41	DI	127/130 (97%)	0.46	5 (3%) 43 35	31, 52, 64, 74	0
41	FI	127/130 (97%)	0.15	5 (3%) 43 35	14, 43, 60, 69	0
41	HI	127/130 (97%)	0.82	10 (7%) 18 15	29, 55, 70, 75	0
42	BJ	98/103 (95%)	0.79	13 (13%) 7 6	30, 55, 68, 72	0
42	DJ	98/103 (95%)	0.75	5 (5%) 33 26	35, 57, 70, 74	0
42	FJ	98/103 (95%)	0.30	6 (6%) 27 21	14, 32, 59, 65	0
42	HJ	98/103 (95%)	0.75	10 (10%) 12 10	30, 51, 69, 78	0
43	BK	117/129 (90%)	1.04	16 (13%) 6 5	33, 56, 66, 80	0
43	DK	117/129 (90%)	0.22	5 (4%) 40 31	26, 41, 56, 60	0
43	FK	117/129 (90%)	0.10	2 (1%) 69 61	18, 42, 59, 64	0
43	HK	117/129 (90%)	1.17	28 (23%) 2 2	23, 50, 70, 74	0
44	BL	123/124 (99%)	-0.12	5 (4%) 41 33	15, 24, 43, 74	0
44	DL	123/124 (99%)	0.14	3 (2%) 59 50	20, 34, 48, 61	0
44	FL	123/124 (99%)	-0.10	5 (4%) 41 33	9, 28, 44, 67	0
44	HL	123/124 (99%)	0.13	2 (1%) 70 62	21, 37, 55, 63	0
45	BM	114/118 (96%)	0.11	3 (2%) 57 48	28, 49, 64, 74	0
45	DM	114/118 (96%)	0.11	1 (0%) 81 75	36, 50, 63, 67	0
45	FM	114/118 (96%)	0.09	3 (2%) 57 48	19, 45, 63, 68	0
45	HM	114/118 (96%)	1.27	24 (21%) 2 2	42, 63, 72, 75	0
46	BN	96/101 (95%)	0.45	5 (5%) 33 26	32, 46, 60, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
46	DN	96/101 (95%)	0.52	7 (7%) 21 17	30, 49, 62, 65	0
46	FN	96/101 (95%)	0.16	8 (8%) 17 14	11, 24, 53, 60	0
46	HN	96/101 (95%)	0.56	9 (9%) 14 12	27, 47, 64, 70	0
47	BO	88/89 (98%)	0.21	0 100 100	35, 50, 61, 64	0
47	DO	88/89 (98%)	0.04	1 (1%) 78 71	31, 45, 56, 61	0
47	FO	88/89 (98%)	-0.41	0 100 100	23, 37, 49, 56	0
47	HO	88/89 (98%)	-0.10	2 (2%) 61 52	22, 39, 53, 70	0
48	BP	82/82 (100%)	0.10	4 (4%) 35 27	24, 35, 61, 68	0
48	DP	82/82 (100%)	0.52	4 (4%) 35 27	28, 43, 62, 79	0
48	FP	82/82 (100%)	-0.08	2 (2%) 59 50	21, 34, 62, 77	0
48	HP	82/82 (100%)	0.30	3 (3%) 45 37	22, 39, 62, 71	0
49	BQ	80/84 (95%)	0.20	2 (2%) 58 48	30, 45, 55, 63	0
49	DQ	80/84 (95%)	0.14	3 (3%) 44 36	29, 44, 57, 68	0
49	FQ	80/84 (95%)	-0.01	2 (2%) 58 48	22, 38, 54, 63	0
49	HQ	80/84 (95%)	0.28	0 100 100	27, 41, 51, 57	0
50	BR	55/75 (73%)	0.77	4 (7%) 21 17	46, 55, 66, 69	0
50	DR	55/75 (73%)	0.03	2 (3%) 46 38	35, 44, 60, 66	0
50	FR	55/75 (73%)	0.01	1 (1%) 67 59	35, 44, 53, 61	0
50	HR	55/75 (73%)	-0.05	3 (5%) 30 24	26, 40, 55, 64	0
51	BS	79/92 (85%)	-0.01	1 (1%) 75 67	30, 44, 59, 64	0
51	DS	79/92 (85%)	0.35	4 (5%) 33 26	36, 49, 63, 67	0
51	FS	79/92 (85%)	-0.07	3 (3%) 44 36	22, 32, 52, 63	0
51	HS	79/92 (85%)	1.23	13 (16%) 4 3	43, 58, 70, 74	0
52	BT	85/87 (97%)	0.28	2 (2%) 59 50	25, 40, 50, 59	0
52	DT	85/87 (97%)	0.36	7 (8%) 17 14	30, 40, 55, 73	0
52	FT	85/87 (97%)	-0.07	5 (5%) 28 22	24, 36, 50, 63	0
52	HT	85/87 (97%)	0.09	5 (5%) 28 22	23, 38, 53, 56	0
53	BU	51/71 (71%)	1.67	19 (37%) 1 0	53, 62, 71, 82	0
53	DU	51/71 (71%)	1.06	9 (17%) 4 3	40, 54, 69, 74	0
53	FU	51/71 (71%)	1.17	8 (15%) 5 4	40, 53, 65, 69	0
53	HU	51/71 (71%)	1.40	15 (29%) 1 1	40, 57, 67, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
54	BV	689/704 (97%)	0.10	25 (3%) 46 38	18, 46, 66, 76	0
54	DV	689/704 (97%)	0.14	26 (3%) 44 36	27, 50, 68, 77	0
54	FV	689/704 (97%)	1.40	184 (26%) 1 1	33, 66, 76, 82	0
54	HV	689/704 (97%)	0.53	42 (6%) 27 21	32, 56, 70, 80	0
55	BW	2/6 (33%)	2.58	1 (50%) 0 0	25, 25, 25, 26	2 (100%)
55	DW	2/6 (33%)	2.72	1 (50%) 0 0	27, 27, 27, 30	2 (100%)
55	FW	2/6 (33%)	1.70	0 100 100	23, 23, 23, 23	2 (100%)
All	All	43562/44972 (96%)	-0.17	1443 (3%) 49 40	1, 37, 66, 92	6 (0%)

The worst 5 of 1443 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	EA	2133	G	7.8
33	BA	78	A	7.6
1	EA	2157	G	7.5
26	AZ	1	ALA	7.3
18	CR	50	GLY	7.0

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
55	KBE	DW	1	9/10	0.52	0.45	32,33,40,41	9
55	5OH	FW	6	12/13	0.52	0.27	37,42,45,46	12
55	KBE	FW	1	9/10	0.56	0.64	28,36,40,42	9
55	UAL	FW	5	9/10	0.59	0.23	35,37,39,41	9
55	UAL	BW	5	9/10	0.66	0.23	32,40,42,42	9
55	5OH	BW	6	12/13	0.69	0.27	36,37,41,43	12
55	KBE	BW	1	9/10	0.71	0.39	37,39,42,44	9
55	DPP	FW	2	6/7	0.75	0.35	37,42,43,43	6
55	UAL	DW	5	9/10	0.76	0.15	35,39,42,46	9
55	5OH	DW	6	12/13	0.81	0.19	33,41,43,48	12
55	DPP	BW	2	6/7	0.84	0.17	34,36,39,40	6
55	DPP	DW	2	6/7	0.88	0.22	32,34,37,44	6

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
56	MG	DA	1629	1/1	0.72	0.18	54,54,54,54	0
56	MG	AA	3068	1/1	0.73	0.19	59,59,59,59	0
56	MG	HA	1626	1/1	0.81	0.23	32,32,32,32	0
56	MG	CA	3091	1/1	0.82	0.19	40,40,40,40	0
56	MG	AA	3011	1/1	0.83	0.13	18,18,18,18	0
56	MG	FA	1636	1/1	0.84	0.11	38,38,38,38	0
56	MG	AA	3078	1/1	0.85	0.26	29,29,29,29	0
56	MG	EA	3087	1/1	0.85	0.26	30,30,30,30	0
56	MG	CA	3114	1/1	0.85	0.18	25,25,25,25	0
56	MG	GA	3011	1/1	0.85	0.16	46,46,46,46	0
56	MG	CA	3118	1/1	0.85	0.08	29,29,29,29	0
56	MG	GA	3018	1/1	0.86	0.07	36,36,36,36	0
56	MG	AA	3115	1/1	0.86	0.08	32,32,32,32	0
56	MG	HA	1617	1/1	0.87	0.17	62,62,62,62	0
56	MG	FA	1610	1/1	0.87	0.06	35,35,35,35	0
56	MG	GA	3069	1/1	0.88	0.16	63,63,63,63	0
56	MG	CA	3011	1/1	0.88	0.19	23,23,23,23	0
56	MG	DA	1627	1/1	0.88	0.07	21,21,21,21	0
56	MG	HE	201	1/1	0.88	0.09	39,39,39,39	0
56	MG	BA	1614	1/1	0.89	0.11	26,26,26,26	0
56	MG	EA	3108	1/1	0.89	0.14	31,31,31,31	0
56	MG	ED	301	1/1	0.89	0.09	7,7,7,7	0
56	MG	GB	1201	1/1	0.89	0.16	38,38,38,38	0
56	MG	EQ	201	1/1	0.89	0.15	31,31,31,31	0
56	MG	BE	201	1/1	0.89	0.16	43,43,43,43	0
56	MG	EA	3068	1/1	0.89	0.17	35,35,35,35	0
58	GCP	FV	801	32/32	0.89	0.10	43,58,69,87	0
56	MG	AA	3019	1/1	0.90	0.16	33,33,33,33	0
56	MG	GA	3077	1/1	0.90	0.17	33,33,33,33	0
56	MG	GA	3078	1/1	0.90	0.24	40,40,40,40	0
56	MG	BA	1629	1/1	0.90	0.18	41,41,41,41	0
56	MG	HA	1601	1/1	0.90	0.24	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AC	301	1/1	0.90	0.22	10,10,10,10	0
56	MG	EA	3133	1/1	0.90	0.14	32,32,32,32	0
56	MG	DA	1639	1/1	0.90	0.13	40,40,40,40	0
56	MG	GA	3063	1/1	0.90	0.27	3,3,3,3	0
56	MG	GA	3047	1/1	0.91	0.20	27,27,27,27	0
56	MG	GA	3060	1/1	0.91	0.11	23,23,23,23	0
56	MG	BL	201	1/1	0.91	0.13	51,51,51,51	0
56	MG	HT	101	1/1	0.91	0.10	41,41,41,41	0
56	MG	AB	1202	1/1	0.91	0.15	44,44,44,44	0
56	MG	DU	101	1/1	0.92	0.05	36,36,36,36	0
56	MG	AA	3093	1/1	0.92	0.09	34,34,34,34	0
56	MG	FA	1638	1/1	0.92	0.10	33,33,33,33	0
56	MG	BA	1621	1/1	0.92	0.10	52,52,52,52	0
56	MG	CB	1201	1/1	0.92	0.13	41,41,41,41	0
56	MG	HA	1603	1/1	0.92	0.05	38,38,38,38	0
56	MG	GA	3046	1/1	0.92	0.08	35,35,35,35	0
56	MG	HA	1619	1/1	0.92	0.21	34,34,34,34	0
56	MG	AB	1201	1/1	0.92	0.15	38,38,38,38	0
56	MG	GA	3055	1/1	0.92	0.15	12,12,12,12	0
56	MG	BA	1631	1/1	0.92	0.06	28,28,28,28	0
56	MG	CA	3094	1/1	0.92	0.20	34,34,34,34	0
56	MG	EA	3010	1/1	0.93	0.17	11,11,11,11	0
56	MG	EA	3057	1/1	0.93	0.08	15,15,15,15	0
56	MG	GA	3134	1/1	0.93	0.04	16,16,16,16	0
56	MG	CA	3005	1/1	0.93	0.23	31,31,31,31	0
56	MG	BA	1613	1/1	0.93	0.10	38,38,38,38	0
56	MG	CA	3055	1/1	0.93	0.10	20,20,20,20	0
56	MG	EA	3121	1/1	0.93	0.17	1,1,1,1	0
56	MG	DA	1628	1/1	0.93	0.22	37,37,37,37	0
56	MG	AA	3028	1/1	0.93	0.20	2,2,2,2	0
56	MG	BA	1620	1/1	0.93	0.10	20,20,20,20	0
56	MG	AC	303	1/1	0.93	0.35	34,34,34,34	0
56	MG	GA	3073	1/1	0.93	0.12	20,20,20,20	0
56	MG	BA	1612	1/1	0.94	0.16	5,5,5,5	0
56	MG	GA	3033	1/1	0.94	0.07	12,12,12,12	0
56	MG	CA	3122	1/1	0.94	0.08	7,7,7,7	0
56	MG	CA	3047	1/1	0.94	0.12	31,31,31,31	0
56	MG	CE	301	1/1	0.94	0.20	16,16,16,16	0
56	MG	GA	3059	1/1	0.94	0.32	44,44,44,44	0
56	MG	DA	1618	1/1	0.94	0.09	33,33,33,33	0
56	MG	EA	3130	1/1	0.94	0.12	29,29,29,29	0
56	MG	DA	1622	1/1	0.94	0.15	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	EB	1201	1/1	0.94	0.07	26,26,26,26	0
56	MG	BA	1637	1/1	0.94	0.27	29,29,29,29	0
56	MG	AA	3098	1/1	0.94	0.18	5,5,5,5	0
56	MG	GA	3094	1/1	0.94	0.12	22,22,22,22	0
56	MG	GA	3108	1/1	0.94	0.13	16,16,16,16	0
56	MG	FA	1602	1/1	0.94	0.08	23,23,23,23	0
56	MG	CA	3093	1/1	0.94	0.16	25,25,25,25	0
56	MG	GB	1202	1/1	0.94	0.19	36,36,36,36	0
56	MG	FA	1627	1/1	0.94	0.22	23,23,23,23	0
56	MG	FA	1630	1/1	0.94	0.08	16,16,16,16	0
56	MG	HA	1609	1/1	0.94	0.07	29,29,29,29	0
56	MG	BA	1624	1/1	0.94	0.10	28,28,28,28	0
56	MG	CA	3097	1/1	0.94	0.60	22,22,22,22	0
56	MG	HA	1625	1/1	0.94	0.22	22,22,22,22	0
56	MG	FU	101	1/1	0.94	0.18	24,24,24,24	0
56	MG	HA	1633	1/1	0.94	0.12	52,52,52,52	0
56	MG	HA	1634	1/1	0.94	0.08	24,24,24,24	0
56	MG	HC	401	1/1	0.94	0.08	49,49,49,49	0
56	MG	FV	802	1/1	0.94	0.06	48,48,48,48	0
56	MG	GA	3010	1/1	0.94	0.17	15,15,15,15	0
56	MG	AA	3089	1/1	0.94	0.07	26,26,26,26	0
56	MG	DA	1602	1/1	0.95	0.07	31,31,31,31	0
56	MG	EA	3127	1/1	0.95	0.06	0,0,0,0	0
56	MG	DA	1604	1/1	0.95	0.12	23,23,23,23	0
56	MG	GA	3068	1/1	0.95	0.16	15,15,15,15	0
56	MG	AT	201	1/1	0.95	0.14	36,36,36,36	0
56	MG	CA	3092	1/1	0.95	0.13	30,30,30,30	0
56	MG	BA	1603	1/1	0.95	0.13	21,21,21,21	0
56	MG	BA	1623	1/1	0.95	0.06	24,24,24,24	0
56	MG	GA	3083	1/1	0.95	0.18	33,33,33,33	0
56	MG	GA	3093	1/1	0.95	0.06	28,28,28,28	0
56	MG	AA	3111	1/1	0.95	0.13	21,21,21,21	0
56	MG	DA	1637	1/1	0.95	0.16	23,23,23,23	0
56	MG	CA	3110	1/1	0.95	0.19	20,20,20,20	0
56	MG	DA	1642	1/1	0.95	0.10	29,29,29,29	0
56	MG	CA	3111	1/1	0.95	0.09	13,13,13,13	0
56	MG	AA	3007	1/1	0.95	0.04	44,44,44,44	0
56	MG	EA	3015	1/1	0.95	0.30	1,1,1,1	0
56	MG	HA	1608	1/1	0.95	0.08	14,14,14,14	0
56	MG	EA	3055	1/1	0.95	0.17	14,14,14,14	0
56	MG	HA	1610	1/1	0.95	0.20	13,13,13,13	0
56	MG	HA	1613	1/1	0.95	0.14	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	HA	1615	1/1	0.95	0.22	38,38,38,38	0
56	MG	GA	3009	1/1	0.95	0.16	20,20,20,20	0
56	MG	HA	1618	1/1	0.95	0.04	19,19,19,19	0
56	MG	CA	3020	1/1	0.95	0.07	19,19,19,19	0
56	MG	AA	3069	1/1	0.95	0.12	6,6,6,6	0
56	MG	EA	3082	1/1	0.95	0.05	13,13,13,13	0
56	MG	HA	1629	1/1	0.95	0.12	17,17,17,17	0
56	MG	GA	3029	1/1	0.95	0.12	5,5,5,5	0
56	MG	BA	1636	1/1	0.95	0.17	40,40,40,40	0
56	MG	HA	1637	1/1	0.95	0.09	47,47,47,47	0
56	MG	EA	3090	1/1	0.95	0.12	29,29,29,29	0
56	MG	CA	3069	1/1	0.95	0.10	45,45,45,45	0
56	MG	EA	3109	1/1	0.95	0.14	8,8,8,8	0
56	MG	GA	3057	1/1	0.95	0.15	22,22,22,22	0
58	GCP	HV	801	32/32	0.95	0.06	24,48,54,56	0
56	MG	DA	1606	1/1	0.96	0.07	26,26,26,26	0
56	MG	EA	3099	1/1	0.96	0.20	2,2,2,2	0
56	MG	DA	1609	1/1	0.96	0.11	16,16,16,16	0
56	MG	DA	1611	1/1	0.96	0.07	15,15,15,15	0
56	MG	GA	3061	1/1	0.96	0.13	10,10,10,10	0
56	MG	DA	1612	1/1	0.96	0.14	11,11,11,11	0
56	MG	AA	3004	1/1	0.96	0.14	34,34,34,34	0
56	MG	AA	3082	1/1	0.96	0.08	29,29,29,29	0
56	MG	BU	101	1/1	0.96	0.14	39,39,39,39	0
56	MG	AA	3087	1/1	0.96	0.10	31,31,31,31	0
56	MG	AA	3018	1/1	0.96	0.19	12,12,12,12	0
56	MG	GA	3082	1/1	0.96	0.11	35,35,35,35	0
56	MG	DA	1635	1/1	0.96	0.05	38,38,38,38	0
56	MG	FA	1601	1/1	0.96	0.17	28,28,28,28	0
56	MG	CA	3015	1/1	0.96	0.14	14,14,14,14	0
56	MG	FA	1604	1/1	0.96	0.10	33,33,33,33	0
56	MG	GA	3115	1/1	0.96	0.20	23,23,23,23	0
56	MG	GA	3129	1/1	0.96	0.17	19,19,19,19	0
56	MG	GA	3131	1/1	0.96	0.16	41,41,41,41	0
56	MG	FA	1605	1/1	0.96	0.14	36,36,36,36	0
56	MG	BA	1632	1/1	0.96	0.07	40,40,40,40	0
56	MG	CA	3045	1/1	0.96	0.11	21,21,21,21	0
56	MG	GS	201	1/1	0.96	0.10	33,33,33,33	0
56	MG	CA	3120	1/1	0.96	0.07	3,3,3,3	0
56	MG	FA	1631	1/1	0.96	0.06	21,21,21,21	0
56	MG	BA	1635	1/1	0.96	0.07	29,29,29,29	0
56	MG	AE	301	1/1	0.96	0.10	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FA	1639	1/1	0.96	0.25	25,25,25,25	0
56	MG	EA	3031	1/1	0.96	0.15	2,2,2,2	0
56	MG	HA	1614	1/1	0.96	0.10	37,37,37,37	0
56	MG	CB	1204	1/1	0.96	0.09	16,16,16,16	0
56	MG	GA	3004	1/1	0.96	0.16	19,19,19,19	0
56	MG	GA	3005	1/1	0.96	0.17	15,15,15,15	0
56	MG	GA	3008	1/1	0.96	0.16	12,12,12,12	0
56	MG	HA	1621	1/1	0.96	0.10	29,29,29,29	0
56	MG	AA	3120	1/1	0.96	0.10	6,6,6,6	0
56	MG	EA	3066	1/1	0.96	0.15	0,0,0,0	0
56	MG	DA	1601	1/1	0.96	0.09	37,37,37,37	0
56	MG	HA	1630	1/1	0.96	0.11	40,40,40,40	0
56	MG	EA	3069	1/1	0.96	0.17	4,4,4,4	0
56	MG	GA	3023	1/1	0.96	0.10	7,7,7,7	0
56	MG	EA	3076	1/1	0.96	0.13	18,18,18,18	0
56	MG	GA	3030	1/1	0.96	0.18	11,11,11,11	0
56	MG	CA	3077	1/1	0.96	0.04	35,35,35,35	0
56	MG	GA	3040	1/1	0.96	0.16	16,16,16,16	0
56	MG	EA	3086	1/1	0.96	0.09	34,34,34,34	0
56	MG	BA	1640	1/1	0.96	0.04	33,33,33,33	0
56	MG	GA	3044	1/1	0.97	0.17	23,23,23,23	0
56	MG	CA	3083	1/1	0.97	0.06	22,22,22,22	0
56	MG	EA	3093	1/1	0.97	0.10	21,21,21,21	0
56	MG	GA	3050	1/1	0.97	0.12	9,9,9,9	0
56	MG	GA	3051	1/1	0.97	0.16	4,4,4,4	0
56	MG	CA	3087	1/1	0.97	0.03	29,29,29,29	0
56	MG	DA	1614	1/1	0.97	0.16	44,44,44,44	0
56	MG	CA	3088	1/1	0.97	0.09	28,28,28,28	0
56	MG	EA	3110	1/1	0.97	0.08	24,24,24,24	0
56	MG	EA	3114	1/1	0.97	0.15	1,1,1,1	0
56	MG	AA	3090	1/1	0.97	0.06	23,23,23,23	0
56	MG	EA	3125	1/1	0.97	0.05	3,3,3,3	0
56	MG	DA	1624	1/1	0.97	0.12	48,48,48,48	0
56	MG	GA	3070	1/1	0.97	0.17	13,13,13,13	0
56	MG	AA	3091	1/1	0.97	0.17	16,16,16,16	0
56	MG	BA	1601	1/1	0.97	0.07	33,33,33,33	0
56	MG	AA	3042	1/1	0.97	0.15	11,11,11,11	0
56	MG	EB	1204	1/1	0.97	0.04	12,12,12,12	0
56	MG	DA	1632	1/1	0.97	0.11	28,28,28,28	0
56	MG	GA	3084	1/1	0.97	0.14	25,25,25,25	0
56	MG	GA	3087	1/1	0.97	0.04	19,19,19,19	0
56	MG	GA	3090	1/1	0.97	0.07	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	1606	1/1	0.97	0.10	39,39,39,39	0
56	MG	DA	1636	1/1	0.97	0.07	41,41,41,41	0
56	MG	GA	3100	1/1	0.97	0.15	19,19,19,19	0
56	MG	GA	3102	1/1	0.97	0.08	40,40,40,40	0
56	MG	GA	3103	1/1	0.97	0.16	12,12,12,12	0
56	MG	GA	3107	1/1	0.97	0.06	27,27,27,27	0
56	MG	BA	1607	1/1	0.97	0.16	8,8,8,8	0
56	MG	GA	3114	1/1	0.97	0.12	10,10,10,10	0
56	MG	FA	1603	1/1	0.97	0.07	30,30,30,30	0
56	MG	GA	3128	1/1	0.97	0.04	20,20,20,20	0
56	MG	BA	1609	1/1	0.97	0.10	38,38,38,38	0
56	MG	AA	3047	1/1	0.97	0.13	30,30,30,30	0
56	MG	GA	3133	1/1	0.97	0.14	4,4,4,4	0
56	MG	CA	3002	1/1	0.97	0.10	17,17,17,17	0
56	MG	FA	1620	1/1	0.97	0.11	6,6,6,6	0
56	MG	FA	1621	1/1	0.97	0.16	10,10,10,10	0
56	MG	GB	1204	1/1	0.97	0.10	21,21,21,21	0
56	MG	GL	201	1/1	0.97	0.13	7,7,7,7	0
56	MG	DV	802	1/1	0.97	0.06	34,34,34,34	0
56	MG	EA	3009	1/1	0.97	0.16	0,0,0,0	0
56	MG	AA	3100	1/1	0.97	0.07	6,6,6,6	0
56	MG	FA	1632	1/1	0.97	0.09	28,28,28,28	0
56	MG	AA	3005	1/1	0.97	0.25	23,23,23,23	0
56	MG	FA	1637	1/1	0.97	0.13	34,34,34,34	0
56	MG	EA	3020	1/1	0.97	0.16	4,4,4,4	0
56	MG	BA	1619	1/1	0.97	0.14	28,28,28,28	0
56	MG	FE	201	1/1	0.97	0.13	52,52,52,52	0
56	MG	EA	3042	1/1	0.97	0.16	2,2,2,2	0
56	MG	EA	3044	1/1	0.97	0.11	11,11,11,11	0
56	MG	AA	3006	1/1	0.97	0.07	38,38,38,38	0
56	MG	AA	3024	1/1	0.97	0.13	20,20,20,20	0
56	MG	HA	1622	1/1	0.97	0.06	36,36,36,36	0
56	MG	GA	3007	1/1	0.97	0.15	28,28,28,28	0
56	MG	EA	3060	1/1	0.97	0.12	3,3,3,3	0
56	MG	HA	1627	1/1	0.97	0.15	24,24,24,24	0
56	MG	C4	101	1/1	0.97	0.05	22,22,22,22	0
56	MG	EA	3067	1/1	0.97	0.14	4,4,4,4	0
56	MG	AA	3016	1/1	0.97	0.07	10,10,10,10	0
56	MG	AA	3084	1/1	0.97	0.11	12,12,12,12	0
56	MG	AA	3029	1/1	0.97	0.05	21,21,21,21	0
56	MG	HA	1638	1/1	0.97	0.09	26,26,26,26	0
56	MG	GA	3025	1/1	0.97	0.08	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	EA	3078	1/1	0.97	0.11	3,3,3,3	0
56	MG	CA	3076	1/1	0.97	0.04	25,25,25,25	0
58	GCP	DV	801	32/32	0.97	0.06	20,38,49,52	0
56	MG	AA	3037	1/1	0.97	0.15	9,9,9,9	0
56	MG	DA	1610	1/1	0.97	0.04	48,48,48,48	0
56	MG	CA	3107	1/1	0.98	0.12	6,6,6,6	0
56	MG	ED	302	1/1	0.98	0.08	2,2,2,2	0
56	MG	CA	3109	1/1	0.98	0.11	26,26,26,26	0
56	MG	AA	3048	1/1	0.98	0.04	2,2,2,2	0
56	MG	AA	3050	1/1	0.98	0.06	7,7,7,7	0
56	MG	CA	3113	1/1	0.98	0.08	14,14,14,14	0
56	MG	BA	1615	1/1	0.98	0.12	22,22,22,22	0
56	MG	BA	1616	1/1	0.98	0.10	35,35,35,35	0
56	MG	FA	1607	1/1	0.98	0.09	18,18,18,18	0
56	MG	FA	1608	1/1	0.98	0.07	14,14,14,14	0
56	MG	FA	1609	1/1	0.98	0.14	16,16,16,16	0
56	MG	BA	1617	1/1	0.98	0.10	25,25,25,25	0
56	MG	FA	1611	1/1	0.98	0.14	0,0,0,0	0
56	MG	FA	1617	1/1	0.98	0.06	9,9,9,9	0
56	MG	FA	1618	1/1	0.98	0.09	28,28,28,28	0
56	MG	FA	1619	1/1	0.98	0.07	25,25,25,25	0
56	MG	AA	3096	1/1	0.98	0.10	33,33,33,33	0
56	MG	CA	3128	1/1	0.98	0.11	6,6,6,6	0
56	MG	FA	1622	1/1	0.98	0.11	15,15,15,15	0
56	MG	FA	1626	1/1	0.98	0.05	15,15,15,15	0
56	MG	CA	3134	1/1	0.98	0.15	23,23,23,23	0
56	MG	FA	1628	1/1	0.98	0.20	19,19,19,19	0
56	MG	AA	3056	1/1	0.98	0.17	24,24,24,24	0
56	MG	CB	1202	1/1	0.98	0.09	55,55,55,55	0
56	MG	AA	3099	1/1	0.98	0.06	15,15,15,15	0
56	MG	FA	1633	1/1	0.98	0.05	28,28,28,28	0
56	MG	BA	1622	1/1	0.98	0.18	32,32,32,32	0
56	MG	AA	3058	1/1	0.98	0.12	9,9,9,9	0
56	MG	AA	3102	1/1	0.98	0.18	0,0,0,0	0
56	MG	AA	3103	1/1	0.98	0.11	10,10,10,10	0
56	MG	FA	1640	1/1	0.98	0.04	23,23,23,23	0
56	MG	FA	1641	1/1	0.98	0.09	18,18,18,18	0
56	MG	AA	3107	1/1	0.98	0.15	18,18,18,18	0
56	MG	AA	3108	1/1	0.98	0.08	21,21,21,21	0
56	MG	DA	1607	1/1	0.98	0.08	16,16,16,16	0
56	MG	GA	3001	1/1	0.98	0.05	32,32,32,32	0
56	MG	DA	1608	1/1	0.98	0.05	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	1633	1/1	0.98	0.08	35,35,35,35	0
56	MG	AA	3110	1/1	0.98	0.15	4,4,4,4	0
56	MG	AA	3059	1/1	0.98	0.25	12,12,12,12	0
56	MG	AA	3112	1/1	0.98	0.04	7,7,7,7	0
56	MG	BA	1639	1/1	0.98	0.07	19,19,19,19	0
56	MG	DA	1617	1/1	0.98	0.06	45,45,45,45	0
56	MG	GA	3014	1/1	0.98	0.23	8,8,8,8	0
56	MG	GA	3017	1/1	0.98	0.07	24,24,24,24	0
56	MG	AA	3065	1/1	0.98	0.10	2,2,2,2	0
56	MG	GA	3020	1/1	0.98	0.10	3,3,3,3	0
56	MG	AA	3116	1/1	0.98	0.15	3,3,3,3	0
56	MG	GA	3024	1/1	0.98	0.12	8,8,8,8	0
56	MG	AA	3119	1/1	0.98	0.08	13,13,13,13	0
56	MG	AA	3014	1/1	0.98	0.10	4,4,4,4	0
56	MG	CA	3001	1/1	0.98	0.07	10,10,10,10	0
56	MG	AA	3123	1/1	0.98	0.12	14,14,14,14	0
56	MG	GA	3034	1/1	0.98	0.12	16,16,16,16	0
56	MG	GA	3036	1/1	0.98	0.10	35,35,35,35	0
56	MG	GA	3037	1/1	0.98	0.13	19,19,19,19	0
56	MG	GA	3038	1/1	0.98	0.04	11,11,11,11	0
56	MG	DA	1631	1/1	0.98	0.12	25,25,25,25	0
56	MG	GA	3041	1/1	0.98	0.07	10,10,10,10	0
56	MG	GA	3042	1/1	0.98	0.12	24,24,24,24	0
56	MG	AA	3124	1/1	0.98	0.13	9,9,9,9	0
56	MG	CA	3007	1/1	0.98	0.03	15,15,15,15	0
56	MG	CA	3008	1/1	0.98	0.11	15,15,15,15	0
56	MG	GA	3048	1/1	0.98	0.12	6,6,6,6	0
56	MG	AA	3125	1/1	0.98	0.08	23,23,23,23	0
56	MG	DA	1638	1/1	0.98	0.06	40,40,40,40	0
56	MG	GA	3052	1/1	0.98	0.11	8,8,8,8	0
56	MG	GA	3053	1/1	0.98	0.10	4,4,4,4	0
56	MG	AA	3129	1/1	0.98	0.06	20,20,20,20	0
56	MG	DA	1640	1/1	0.98	0.11	21,21,21,21	0
56	MG	GA	3058	1/1	0.98	0.10	17,17,17,17	0
56	MG	CA	3016	1/1	0.98	0.08	8,8,8,8	0
56	MG	CA	3017	1/1	0.98	0.12	2,2,2,2	0
56	MG	CA	3018	1/1	0.98	0.09	26,26,26,26	0
56	MG	EA	3004	1/1	0.98	0.06	13,13,13,13	0
56	MG	GA	3067	1/1	0.98	0.12	16,16,16,16	0
56	MG	EA	3008	1/1	0.98	0.16	1,1,1,1	0
56	MG	AA	3030	1/1	0.98	0.06	13,13,13,13	0
56	MG	CA	3021	1/1	0.98	0.04	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	GA	3071	1/1	0.98	0.12	20,20,20,20	0
56	MG	GA	3072	1/1	0.98	0.08	13,13,13,13	0
56	MG	EA	3011	1/1	0.98	0.49	17,17,17,17	0
56	MG	GA	3076	1/1	0.98	0.10	23,23,23,23	0
56	MG	CA	3030	1/1	0.98	0.10	11,11,11,11	0
56	MG	EA	3018	1/1	0.98	0.11	8,8,8,8	0
56	MG	GA	3079	1/1	0.98	0.04	18,18,18,18	0
56	MG	GA	3081	1/1	0.98	0.10	16,16,16,16	0
56	MG	EA	3019	1/1	0.98	0.04	13,13,13,13	0
56	MG	CA	3034	1/1	0.98	0.09	18,18,18,18	0
56	MG	EA	3025	1/1	0.98	0.11	0,0,0,0	0
56	MG	GA	3086	1/1	0.98	0.07	26,26,26,26	0
56	MG	EA	3029	1/1	0.98	0.06	0,0,0,0	0
56	MG	CA	3041	1/1	0.98	0.11	13,13,13,13	0
56	MG	GA	3091	1/1	0.98	0.12	11,11,11,11	0
56	MG	EA	3040	1/1	0.98	0.09	1,1,1,1	0
56	MG	EA	3041	1/1	0.98	0.09	2,2,2,2	0
56	MG	GA	3097	1/1	0.98	0.09	26,26,26,26	0
56	MG	GA	3098	1/1	0.98	0.12	25,25,25,25	0
56	MG	GA	3099	1/1	0.98	0.07	12,12,12,12	0
56	MG	CA	3042	1/1	0.98	0.11	8,8,8,8	0
56	MG	CA	3044	1/1	0.98	0.09	22,22,22,22	0
56	MG	EA	3048	1/1	0.98	0.04	11,11,11,11	0
56	MG	EA	3049	1/1	0.98	0.18	8,8,8,8	0
56	MG	EA	3050	1/1	0.98	0.08	13,13,13,13	0
56	MG	GA	3109	1/1	0.98	0.06	9,9,9,9	0
56	MG	GA	3113	1/1	0.98	0.05	26,26,26,26	0
56	MG	AA	3076	1/1	0.98	0.10	21,21,21,21	0
56	MG	EA	3056	1/1	0.98	0.09	2,2,2,2	0
56	MG	GA	3118	1/1	0.98	0.13	9,9,9,9	0
56	MG	GA	3123	1/1	0.98	0.11	11,11,11,11	0
56	MG	GA	3126	1/1	0.98	0.06	18,18,18,18	0
56	MG	GA	3127	1/1	0.98	0.05	1,1,1,1	0
56	MG	AB	1203	1/1	0.98	0.11	14,14,14,14	0
56	MG	CA	3049	1/1	0.98	0.13	9,9,9,9	0
56	MG	CA	3051	1/1	0.98	0.12	7,7,7,7	0
56	MG	CA	3054	1/1	0.98	0.11	6,6,6,6	0
56	MG	AA	3077	1/1	0.98	0.07	36,36,36,36	0
56	MG	CA	3061	1/1	0.98	0.11	3,3,3,3	0
56	MG	CA	3063	1/1	0.98	0.12	2,2,2,2	0
56	MG	AC	302	1/1	0.98	0.11	19,19,19,19	0
56	MG	AA	3036	1/1	0.98	0.08	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	3079	1/1	0.98	0.04	11,11,11,11	0
56	MG	CA	3078	1/1	0.98	0.10	25,25,25,25	0
56	MG	HA	1602	1/1	0.98	0.09	48,48,48,48	0
56	MG	AA	3025	1/1	0.98	0.10	8,8,8,8	0
56	MG	HA	1605	1/1	0.98	0.08	39,39,39,39	0
56	MG	EA	3091	1/1	0.98	0.11	11,11,11,11	0
56	MG	CA	3084	1/1	0.98	0.14	4,4,4,4	0
56	MG	EA	3094	1/1	0.98	0.14	15,15,15,15	0
56	MG	HA	1612	1/1	0.98	0.17	8,8,8,8	0
56	MG	EA	3095	1/1	0.98	0.07	5,5,5,5	0
56	MG	AA	3026	1/1	0.98	0.03	10,10,10,10	0
56	MG	EA	3101	1/1	0.98	0.09	26,26,26,26	0
56	MG	HA	1616	1/1	0.98	0.05	33,33,33,33	0
56	MG	EA	3102	1/1	0.98	0.15	0,0,0,0	0
56	MG	AA	3085	1/1	0.98	0.03	30,30,30,30	0
56	MG	CA	3089	1/1	0.98	0.10	2,2,2,2	0
56	MG	HA	1620	1/1	0.98	0.10	14,14,14,14	0
56	MG	BA	1604	1/1	0.98	0.07	20,20,20,20	0
56	MG	EA	3111	1/1	0.98	0.14	2,2,2,2	0
56	MG	HA	1623	1/1	0.98	0.09	18,18,18,18	0
56	MG	EA	3112	1/1	0.98	0.10	5,5,5,5	0
56	MG	EA	3113	1/1	0.98	0.13	0,0,0,0	0
56	MG	AA	3086	1/1	0.98	0.04	35,35,35,35	0
56	MG	EA	3117	1/1	0.98	0.07	11,11,11,11	0
56	MG	EA	3119	1/1	0.98	0.18	0,0,0,0	0
56	MG	HA	1632	1/1	0.98	0.10	25,25,25,25	0
56	MG	AA	3044	1/1	0.98	0.07	17,17,17,17	0
56	MG	EA	3123	1/1	0.98	0.18	2,2,2,2	0
56	MG	AA	3045	1/1	0.98	0.06	18,18,18,18	0
56	MG	CA	3096	1/1	0.98	0.12	10,10,10,10	0
56	MG	EA	3129	1/1	0.98	0.17	0,0,0,0	0
56	MG	AA	3012	1/1	0.98	0.13	7,7,7,7	0
56	MG	EA	3131	1/1	0.98	0.12	5,5,5,5	0
57	ZN	C4	102	1/1	0.98	0.04	76,76,76,76	0
57	ZN	E4	101	1/1	0.98	0.05	54,54,54,54	0
58	GCP	BV	801	32/32	0.98	0.05	17,36,43,49	0
56	MG	CA	3100	1/1	0.98	0.11	1,1,1,1	0
56	MG	CA	3103	1/1	0.98	0.09	0,0,0,0	0
56	MG	CA	3104	1/1	0.98	0.07	4,4,4,4	0
56	MG	EA	3098	1/1	0.99	0.07	6,6,6,6	0
56	MG	CA	3081	1/1	0.99	0.05	10,10,10,10	0
56	MG	CA	3082	1/1	0.99	0.05	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	3046	1/1	0.99	0.06	7,7,7,7	0
56	MG	EA	3103	1/1	0.99	0.04	10,10,10,10	0
56	MG	EA	3104	1/1	0.99	0.07	1,1,1,1	0
56	MG	EA	3105	1/1	0.99	0.09	4,4,4,4	0
56	MG	EA	3107	1/1	0.99	0.10	0,0,0,0	0
56	MG	AA	3003	1/1	0.99	0.06	26,26,26,26	0
56	MG	CA	3085	1/1	0.99	0.13	28,28,28,28	0
56	MG	CA	3086	1/1	0.99	0.07	20,20,20,20	0
56	MG	AA	3092	1/1	0.99	0.04	31,31,31,31	0
56	MG	AA	3008	1/1	0.99	0.07	15,15,15,15	0
56	MG	AA	3094	1/1	0.99	0.04	20,20,20,20	0
56	MG	AA	3049	1/1	0.99	0.10	3,3,3,3	0
56	MG	EA	3116	1/1	0.99	0.12	0,0,0,0	0
56	MG	BA	1618	1/1	0.99	0.14	3,3,3,3	0
56	MG	AA	3015	1/1	0.99	0.15	22,22,22,22	0
56	MG	AA	3052	1/1	0.99	0.03	2,2,2,2	0
56	MG	EA	3122	1/1	0.99	0.09	0,0,0,0	0
56	MG	CA	3095	1/1	0.99	0.11	21,21,21,21	0
56	MG	AA	3027	1/1	0.99	0.08	8,8,8,8	0
56	MG	EA	3126	1/1	0.99	0.11	2,2,2,2	0
56	MG	AA	3101	1/1	0.99	0.08	7,7,7,7	0
56	MG	EA	3128	1/1	0.99	0.07	4,4,4,4	0
56	MG	CA	3098	1/1	0.99	0.06	10,10,10,10	0
56	MG	AA	3057	1/1	0.99	0.07	18,18,18,18	0
56	MG	CA	3101	1/1	0.99	0.06	10,10,10,10	0
56	MG	EA	3132	1/1	0.99	0.15	6,6,6,6	0
56	MG	CA	3102	1/1	0.99	0.03	32,32,32,32	0
56	MG	AA	3009	1/1	0.99	0.17	12,12,12,12	0
56	MG	EB	1202	1/1	0.99	0.06	19,19,19,19	0
56	MG	EB	1203	1/1	0.99	0.10	3,3,3,3	0
56	MG	BA	1625	1/1	0.99	0.08	21,21,21,21	0
56	MG	CA	3105	1/1	0.99	0.10	6,6,6,6	0
56	MG	BA	1626	1/1	0.99	0.04	36,36,36,36	0
56	MG	CA	3108	1/1	0.99	0.06	3,3,3,3	0
56	MG	BA	1627	1/1	0.99	0.04	25,25,25,25	0
56	MG	BA	1628	1/1	0.99	0.05	26,26,26,26	0
56	MG	AA	3104	1/1	0.99	0.08	12,12,12,12	0
56	MG	CA	3112	1/1	0.99	0.09	4,4,4,4	0
56	MG	AA	3105	1/1	0.99	0.09	12,12,12,12	0
56	MG	FA	1606	1/1	0.99	0.04	13,13,13,13	0
56	MG	AA	3017	1/1	0.99	0.13	1,1,1,1	0
56	MG	CA	3115	1/1	0.99	0.09	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3116	1/1	0.99	0.04	13,13,13,13	0
56	MG	AA	3060	1/1	0.99	0.12	25,25,25,25	0
56	MG	CA	3119	1/1	0.99	0.12	3,3,3,3	0
56	MG	FA	1612	1/1	0.99	0.25	17,17,17,17	0
56	MG	FA	1613	1/1	0.99	0.06	9,9,9,9	0
56	MG	FA	1614	1/1	0.99	0.04	5,5,5,5	0
56	MG	FA	1615	1/1	0.99	0.11	16,16,16,16	0
56	MG	FA	1616	1/1	0.99	0.12	16,16,16,16	0
56	MG	BA	1634	1/1	0.99	0.04	14,14,14,14	0
56	MG	CA	3121	1/1	0.99	0.10	3,3,3,3	0
56	MG	AA	3062	1/1	0.99	0.14	2,2,2,2	0
56	MG	CA	3123	1/1	0.99	0.11	8,8,8,8	0
56	MG	CA	3125	1/1	0.99	0.09	9,9,9,9	0
56	MG	CA	3126	1/1	0.99	0.08	7,7,7,7	0
56	MG	FA	1623	1/1	0.99	0.11	7,7,7,7	0
56	MG	FA	1624	1/1	0.99	0.12	18,18,18,18	0
56	MG	FA	1625	1/1	0.99	0.04	18,18,18,18	0
56	MG	CA	3127	1/1	0.99	0.05	11,11,11,11	0
56	MG	AA	3064	1/1	0.99	0.08	20,20,20,20	0
56	MG	CA	3129	1/1	0.99	0.11	9,9,9,9	0
56	MG	FA	1629	1/1	0.99	0.04	16,16,16,16	0
56	MG	CA	3130	1/1	0.99	0.08	1,1,1,1	0
56	MG	CA	3133	1/1	0.99	0.04	13,13,13,13	0
56	MG	AA	3010	1/1	0.99	0.11	13,13,13,13	0
56	MG	BA	1638	1/1	0.99	0.06	31,31,31,31	0
56	MG	FA	1634	1/1	0.99	0.04	19,19,19,19	0
56	MG	FA	1635	1/1	0.99	0.09	8,8,8,8	0
56	MG	AA	3066	1/1	0.99	0.10	6,6,6,6	0
56	MG	CB	1203	1/1	0.99	0.10	6,6,6,6	0
56	MG	AA	3067	1/1	0.99	0.03	29,29,29,29	0
56	MG	AA	3117	1/1	0.99	0.07	7,7,7,7	0
56	MG	AA	3031	1/1	0.99	0.08	8,8,8,8	0
56	MG	AA	3033	1/1	0.99	0.08	8,8,8,8	0
56	MG	BV	802	1/1	0.99	0.10	27,27,27,27	0
56	MG	DA	1603	1/1	0.99	0.06	22,22,22,22	0
56	MG	AA	3121	1/1	0.99	0.03	20,20,20,20	0
56	MG	DA	1605	1/1	0.99	0.07	28,28,28,28	0
56	MG	GA	3002	1/1	0.99	0.11	14,14,14,14	0
56	MG	GA	3003	1/1	0.99	0.12	15,15,15,15	0
56	MG	AA	3122	1/1	0.99	0.05	2,2,2,2	0
56	MG	CA	3003	1/1	0.99	0.08	12,12,12,12	0
56	MG	GA	3006	1/1	0.99	0.04	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	3070	1/1	0.99	0.05	11,11,11,11	0
56	MG	CA	3006	1/1	0.99	0.05	15,15,15,15	0
56	MG	AA	3071	1/1	0.99	0.06	3,3,3,3	0
56	MG	AA	3073	1/1	0.99	0.10	8,8,8,8	0
56	MG	CA	3009	1/1	0.99	0.08	18,18,18,18	0
56	MG	GA	3012	1/1	0.99	0.12	2,2,2,2	0
56	MG	GA	3013	1/1	0.99	0.07	1,1,1,1	0
56	MG	CA	3010	1/1	0.99	0.10	10,10,10,10	0
56	MG	GA	3015	1/1	0.99	0.07	18,18,18,18	0
56	MG	DA	1615	1/1	0.99	0.10	24,24,24,24	0
56	MG	DA	1616	1/1	0.99	0.16	26,26,26,26	0
56	MG	GA	3019	1/1	0.99	0.05	5,5,5,5	0
56	MG	AA	3127	1/1	0.99	0.08	16,16,16,16	0
56	MG	GA	3021	1/1	0.99	0.09	9,9,9,9	0
56	MG	CA	3012	1/1	0.99	0.02	3,3,3,3	0
56	MG	DA	1619	1/1	0.99	0.07	33,33,33,33	0
56	MG	DA	1620	1/1	0.99	0.08	22,22,22,22	0
56	MG	GA	3026	1/1	0.99	0.10	6,6,6,6	0
56	MG	GA	3027	1/1	0.99	0.13	6,6,6,6	0
56	MG	GA	3028	1/1	0.99	0.04	10,10,10,10	0
56	MG	DA	1621	1/1	0.99	0.08	22,22,22,22	0
56	MG	CA	3014	1/1	0.99	0.05	9,9,9,9	0
56	MG	GA	3032	1/1	0.99	0.04	8,8,8,8	0
56	MG	DA	1623	1/1	0.99	0.04	12,12,12,12	0
56	MG	AA	3074	1/1	0.99	0.06	9,9,9,9	0
56	MG	GA	3035	1/1	0.99	0.08	15,15,15,15	0
56	MG	DA	1625	1/1	0.99	0.04	23,23,23,23	0
56	MG	DA	1626	1/1	0.99	0.06	24,24,24,24	0
56	MG	AA	3130	1/1	0.99	0.04	27,27,27,27	0
56	MG	AA	3075	1/1	0.99	0.04	15,15,15,15	0
56	MG	AA	3034	1/1	0.99	0.05	14,14,14,14	0
56	MG	DA	1630	1/1	0.99	0.05	34,34,34,34	0
56	MG	GA	3043	1/1	0.99	0.05	8,8,8,8	0
56	MG	CA	3019	1/1	0.99	0.03	22,22,22,22	0
56	MG	AA	3035	1/1	0.99	0.12	3,3,3,3	0
56	MG	DA	1633	1/1	0.99	0.04	45,45,45,45	0
56	MG	DA	1634	1/1	0.99	0.04	33,33,33,33	0
56	MG	AB	1204	1/1	0.99	0.03	8,8,8,8	0
56	MG	CA	3022	1/1	0.99	0.07	0,0,0,0	0
56	MG	CA	3023	1/1	0.99	0.11	5,5,5,5	0
56	MG	CA	3025	1/1	0.99	0.03	7,7,7,7	0
56	MG	GA	3054	1/1	0.99	0.07	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3026	1/1	0.99	0.05	5,5,5,5	0
56	MG	GA	3056	1/1	0.99	0.10	4,4,4,4	0
56	MG	CA	3029	1/1	0.99	0.04	8,8,8,8	0
56	MG	DA	1641	1/1	0.99	0.03	30,30,30,30	0
56	MG	AA	3002	1/1	0.99	0.04	20,20,20,20	0
56	MG	CA	3032	1/1	0.99	0.09	3,3,3,3	0
56	MG	CA	3033	1/1	0.99	0.10	9,9,9,9	0
56	MG	GA	3062	1/1	0.99	0.05	18,18,18,18	0
56	MG	EA	3001	1/1	0.99	0.05	9,9,9,9	0
56	MG	GA	3066	1/1	0.99	0.10	4,4,4,4	0
56	MG	EA	3002	1/1	0.99	0.10	4,4,4,4	0
56	MG	EA	3003	1/1	0.99	0.06	6,6,6,6	0
56	MG	AA	3020	1/1	0.99	0.07	24,24,24,24	0
56	MG	EA	3005	1/1	0.99	0.22	27,27,27,27	0
56	MG	EA	3006	1/1	0.99	0.09	19,19,19,19	0
56	MG	EA	3007	1/1	0.99	0.07	15,15,15,15	0
56	MG	CA	3035	1/1	0.99	0.07	3,3,3,3	0
56	MG	GA	3074	1/1	0.99	0.09	2,2,2,2	0
56	MG	CA	3036	1/1	0.99	0.03	19,19,19,19	0
56	MG	CA	3037	1/1	0.99	0.10	1,1,1,1	0
56	MG	CA	3038	1/1	0.99	0.06	7,7,7,7	0
56	MG	EA	3012	1/1	0.99	0.07	1,1,1,1	0
56	MG	GA	3080	1/1	0.99	0.13	5,5,5,5	0
56	MG	EA	3014	1/1	0.99	0.10	0,0,0,0	0
56	MG	AA	3080	1/1	0.99	0.05	7,7,7,7	0
56	MG	EA	3016	1/1	0.99	0.03	6,6,6,6	0
56	MG	EA	3017	1/1	0.99	0.10	3,3,3,3	0
56	MG	AD	301	1/1	0.99	0.06	6,6,6,6	0
56	MG	AA	3039	1/1	0.99	0.08	5,5,5,5	0
56	MG	GA	3088	1/1	0.99	0.10	8,8,8,8	0
56	MG	GA	3089	1/1	0.99	0.09	14,14,14,14	0
56	MG	AA	3083	1/1	0.99	0.18	33,33,33,33	0
56	MG	EA	3022	1/1	0.99	0.12	0,0,0,0	0
56	MG	GA	3092	1/1	0.99	0.04	17,17,17,17	0
56	MG	EA	3023	1/1	0.99	0.07	2,2,2,2	0
56	MG	EA	3024	1/1	0.99	0.08	0,0,0,0	0
56	MG	CA	3046	1/1	0.99	0.09	17,17,17,17	0
56	MG	EA	3026	1/1	0.99	0.13	28,28,28,28	0
56	MG	EA	3027	1/1	0.99	0.13	0,0,0,0	0
56	MG	EA	3028	1/1	0.99	0.07	1,1,1,1	0
56	MG	GA	3101	1/1	0.99	0.04	15,15,15,15	0
56	MG	A3	101	1/1	0.99	0.06	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	EA	3030	1/1	0.99	0.11	0,0,0,0	0
56	MG	GA	3106	1/1	0.99	0.17	3,3,3,3	0
56	MG	AA	3040	1/1	0.99	0.03	24,24,24,24	0
56	MG	EA	3034	1/1	0.99	0.12	0,0,0,0	0
56	MG	EA	3038	1/1	0.99	0.03	2,2,2,2	0
56	MG	GA	3110	1/1	0.99	0.09	12,12,12,12	0
56	MG	GA	3111	1/1	0.99	0.09	11,11,11,11	0
56	MG	GA	3112	1/1	0.99	0.06	15,15,15,15	0
56	MG	EA	3039	1/1	0.99	0.11	0,0,0,0	0
56	MG	CA	3050	1/1	0.99	0.03	12,12,12,12	0
56	MG	BA	1602	1/1	0.99	0.07	15,15,15,15	0
56	MG	GA	3117	1/1	0.99	0.02	22,22,22,22	0
56	MG	AA	3021	1/1	0.99	0.03	11,11,11,11	0
56	MG	GA	3119	1/1	0.99	0.07	5,5,5,5	0
56	MG	GA	3121	1/1	0.99	0.07	4,4,4,4	0
56	MG	GA	3122	1/1	0.99	0.11	14,14,14,14	0
56	MG	EA	3043	1/1	0.99	0.06	4,4,4,4	0
56	MG	GA	3124	1/1	0.99	0.06	16,16,16,16	0
56	MG	GA	3125	1/1	0.99	0.04	5,5,5,5	0
56	MG	AA	3043	1/1	0.99	0.08	21,21,21,21	0
56	MG	EA	3045	1/1	0.99	0.05	1,1,1,1	0
56	MG	EA	3046	1/1	0.99	0.11	9,9,9,9	0
56	MG	EA	3047	1/1	0.99	0.09	6,6,6,6	0
56	MG	CA	3056	1/1	0.99	0.09	7,7,7,7	0
56	MG	CA	3057	1/1	0.99	0.07	1,1,1,1	0
56	MG	CA	3058	1/1	0.99	0.06	5,5,5,5	0
56	MG	EA	3051	1/1	0.99	0.08	0,0,0,0	0
56	MG	EA	3052	1/1	0.99	0.13	2,2,2,2	0
56	MG	GB	1203	1/1	0.99	0.09	16,16,16,16	0
56	MG	EA	3053	1/1	0.99	0.12	1,1,1,1	0
56	MG	EA	3054	1/1	0.99	0.07	5,5,5,5	0
56	MG	CA	3060	1/1	0.99	0.09	13,13,13,13	0
56	MG	BA	1605	1/1	0.99	0.04	21,21,21,21	0
56	MG	CA	3062	1/1	0.99	0.07	5,5,5,5	0
56	MG	EA	3058	1/1	0.99	0.07	6,6,6,6	0
56	MG	HA	1604	1/1	0.99	0.08	27,27,27,27	0
56	MG	AA	3022	1/1	0.99	0.04	8,8,8,8	0
56	MG	HA	1606	1/1	0.99	0.08	17,17,17,17	0
56	MG	HA	1607	1/1	0.99	0.10	11,11,11,11	0
56	MG	EA	3061	1/1	0.99	0.14	0,0,0,0	0
56	MG	EA	3062	1/1	0.99	0.08	0,0,0,0	0
56	MG	EA	3064	1/1	0.99	0.09	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	HA	1611	1/1	0.99	0.14	20,20,20,20	0
56	MG	EA	3065	1/1	0.99	0.04	0,0,0,0	0
56	MG	CA	3066	1/1	0.99	0.11	2,2,2,2	0
56	MG	CA	3068	1/1	0.99	0.07	13,13,13,13	0
56	MG	AA	3088	1/1	0.99	0.03	14,14,14,14	0
56	MG	CA	3070	1/1	0.99	0.13	4,4,4,4	0
56	MG	EA	3070	1/1	0.99	0.08	3,3,3,3	0
56	MG	EA	3071	1/1	0.99	0.06	2,2,2,2	0
56	MG	EA	3072	1/1	0.99	0.06	8,8,8,8	0
56	MG	EA	3073	1/1	0.99	0.11	0,0,0,0	0
56	MG	EA	3075	1/1	0.99	0.06	10,10,10,10	0
56	MG	CA	3071	1/1	0.99	0.11	2,2,2,2	0
56	MG	EA	3077	1/1	0.99	0.13	14,14,14,14	0
56	MG	HA	1624	1/1	0.99	0.07	14,14,14,14	0
56	MG	CA	3072	1/1	0.99	0.07	11,11,11,11	0
56	MG	EA	3079	1/1	0.99	0.09	0,0,0,0	0
56	MG	EA	3080	1/1	0.99	0.11	3,3,3,3	0
56	MG	HA	1628	1/1	0.99	0.06	30,30,30,30	0
56	MG	EA	3081	1/1	0.99	0.08	3,3,3,3	0
56	MG	CA	3073	1/1	0.99	0.12	5,5,5,5	0
56	MG	HA	1631	1/1	0.99	0.08	28,28,28,28	0
56	MG	EA	3083	1/1	0.99	0.05	1,1,1,1	0
56	MG	EA	3085	1/1	0.99	0.07	4,4,4,4	0
56	MG	CA	3074	1/1	0.99	0.04	19,19,19,19	0
56	MG	HA	1635	1/1	0.99	0.07	17,17,17,17	0
56	MG	HA	1636	1/1	0.99	0.03	21,21,21,21	0
56	MG	CA	3075	1/1	0.99	0.08	20,20,20,20	0
56	MG	EA	3088	1/1	0.99	0.09	6,6,6,6	0
56	MG	HA	1639	1/1	0.99	0.09	20,20,20,20	0
56	MG	HA	1640	1/1	0.99	0.04	15,15,15,15	0
56	MG	EA	3089	1/1	0.99	0.04	5,5,5,5	0
56	MG	BA	1608	1/1	0.99	0.03	22,22,22,22	0
56	MG	AA	3023	1/1	0.99	0.10	3,3,3,3	0
56	MG	HV	802	1/1	0.99	0.06	38,38,38,38	0
57	ZN	A4	101	1/1	0.99	0.02	63,63,63,63	0
56	MG	EA	3092	1/1	0.99	0.11	7,7,7,7	0
56	MG	BA	1610	1/1	0.99	0.04	19,19,19,19	0
57	ZN	G4	101	1/1	0.99	0.04	69,69,69,69	0
56	MG	CA	3079	1/1	0.99	0.16	12,12,12,12	0
56	MG	CA	3080	1/1	0.99	0.08	8,8,8,8	0
56	MG	EA	3096	1/1	0.99	0.03	15,15,15,15	0
56	MG	EA	3097	1/1	0.99	0.12	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	3114	1/1	1.00	0.02	1,1,1,1	0
56	MG	AA	3032	1/1	1.00	0.05	14,14,14,14	0
56	MG	DA	1613	1/1	1.00	0.03	12,12,12,12	0
56	MG	CA	3106	1/1	1.00	0.07	13,13,13,13	0
56	MG	GA	3031	1/1	1.00	0.04	4,4,4,4	0
56	MG	EA	3021	1/1	1.00	0.06	5,5,5,5	0
56	MG	CA	3064	1/1	1.00	0.03	1,1,1,1	0
56	MG	CA	3065	1/1	1.00	0.03	1,1,1,1	0
56	MG	GA	3116	1/1	1.00	0.04	3,3,3,3	0
56	MG	CA	3027	1/1	1.00	0.03	2,2,2,2	0
56	MG	EA	3084	1/1	1.00	0.06	2,2,2,2	0
56	MG	CA	3067	1/1	1.00	0.04	4,4,4,4	0
56	MG	GA	3120	1/1	1.00	0.09	5,5,5,5	0
56	MG	CA	3028	1/1	1.00	0.07	7,7,7,7	0
56	MG	GA	3039	1/1	1.00	0.05	15,15,15,15	0
56	MG	AA	3097	1/1	1.00	0.05	8,8,8,8	0
56	MG	AA	3001	1/1	1.00	0.04	11,11,11,11	0
56	MG	CA	3031	1/1	1.00	0.03	11,11,11,11	0
56	MG	AA	3118	1/1	1.00	0.02	11,11,11,11	0
56	MG	AA	3051	1/1	1.00	0.02	4,4,4,4	0
56	MG	GA	3045	1/1	1.00	0.08	7,7,7,7	0
56	MG	EA	3032	1/1	1.00	0.09	0,0,0,0	0
56	MG	GA	3130	1/1	1.00	0.02	9,9,9,9	0
56	MG	EA	3033	1/1	1.00	0.07	1,1,1,1	0
56	MG	GA	3132	1/1	1.00	0.07	7,7,7,7	0
56	MG	CA	3117	1/1	1.00	0.02	7,7,7,7	0
56	MG	GA	3049	1/1	1.00	0.08	8,8,8,8	0
56	MG	EA	3035	1/1	1.00	0.08	0,0,0,0	0
56	MG	EA	3036	1/1	1.00	0.07	1,1,1,1	0
56	MG	EA	3037	1/1	1.00	0.04	2,2,2,2	0
56	MG	CA	3004	1/1	1.00	0.03	6,6,6,6	0
56	MG	GC	301	1/1	1.00	0.07	4,4,4,4	0
56	MG	AA	3072	1/1	1.00	0.08	7,7,7,7	0
56	MG	EA	3100	1/1	1.00	0.04	0,0,0,0	0
56	MG	AA	3061	1/1	1.00	0.07	6,6,6,6	0
56	MG	AA	3041	1/1	1.00	0.11	2,2,2,2	0
56	MG	AA	3063	1/1	1.00	0.02	9,9,9,9	0
56	MG	CA	3039	1/1	1.00	0.08	6,6,6,6	0
56	MG	CA	3124	1/1	1.00	0.09	0,0,0,0	0
56	MG	EA	3106	1/1	1.00	0.06	0,0,0,0	0
56	MG	CA	3040	1/1	1.00	0.05	12,12,12,12	0
56	MG	AA	3053	1/1	1.00	0.03	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	GA	3064	1/1	1.00	0.06	9,9,9,9	0
56	MG	GA	3065	1/1	1.00	0.06	3,3,3,3	0
56	MG	AA	3054	1/1	1.00	0.04	11,11,11,11	0
56	MG	CA	3043	1/1	1.00	0.04	5,5,5,5	0
56	MG	BA	1630	1/1	1.00	0.04	25,25,25,25	0
56	MG	AA	3126	1/1	1.00	0.03	3,3,3,3	0
56	MG	CA	3131	1/1	1.00	0.03	0,0,0,0	0
56	MG	CA	3132	1/1	1.00	0.06	2,2,2,2	0
56	MG	EA	3115	1/1	1.00	0.07	2,2,2,2	0
56	MG	CA	3013	1/1	1.00	0.03	7,7,7,7	0
56	MG	AA	3106	1/1	1.00	0.06	9,9,9,9	0
56	MG	GA	3075	1/1	1.00	0.03	7,7,7,7	0
56	MG	EA	3118	1/1	1.00	0.07	1,1,1,1	0
56	MG	CA	3048	1/1	1.00	0.01	13,13,13,13	0
56	MG	EA	3120	1/1	1.00	0.09	0,0,0,0	0
56	MG	AA	3128	1/1	1.00	0.05	2,2,2,2	0
56	MG	CA	3090	1/1	1.00	0.05	20,20,20,20	0
56	MG	AA	3055	1/1	1.00	0.07	18,18,18,18	0
56	MG	EA	3124	1/1	1.00	0.06	5,5,5,5	0
56	MG	EA	3059	1/1	1.00	0.02	1,1,1,1	0
56	MG	CD	301	1/1	1.00	0.09	3,3,3,3	0
56	MG	GA	3085	1/1	1.00	0.03	16,16,16,16	0
56	MG	BA	1611	1/1	1.00	0.05	15,15,15,15	0
56	MG	CA	3052	1/1	1.00	0.03	10,10,10,10	0
56	MG	EA	3063	1/1	1.00	0.06	1,1,1,1	0
56	MG	CA	3053	1/1	1.00	0.02	5,5,5,5	0
56	MG	AA	3013	1/1	1.00	0.06	5,5,5,5	0
56	MG	AA	3109	1/1	1.00	0.08	6,6,6,6	0
56	MG	AA	3038	1/1	1.00	0.02	6,6,6,6	0
56	MG	GA	3016	1/1	1.00	0.07	9,9,9,9	0
56	MG	AA	3081	1/1	1.00	0.05	16,16,16,16	0
56	MG	GA	3095	1/1	1.00	0.06	2,2,2,2	0
56	MG	GA	3096	1/1	1.00	0.06	4,4,4,4	0
56	MG	CA	3099	1/1	1.00	0.08	17,17,17,17	0
56	MG	AA	3095	1/1	1.00	0.03	9,9,9,9	0
56	MG	EA	3013	1/1	1.00	0.04	0,0,0,0	0
56	MG	EC	301	1/1	1.00	0.08	1,1,1,1	0
56	MG	GA	3022	1/1	1.00	0.06	16,16,16,16	0
56	MG	CA	3059	1/1	1.00	0.06	3,3,3,3	0
56	MG	AA	3113	1/1	1.00	0.04	8,8,8,8	0
56	MG	GA	3104	1/1	1.00	0.08	6,6,6,6	0
56	MG	GA	3105	1/1	1.00	0.09	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	EA	3074	1/1	1.00	0.07	4,4,4,4	0
56	MG	CA	3024	1/1	1.00	0.09	2,2,2,2	0

5.5 Other polymers [i](#)

There are no such residues in this entry.