



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 03:32 PM UTC

PDB ID : 6B4V / pdb_00006b4v
Title : Antibiotic blasticidin S and E. coli release factor 1 bound to the 70S ribosome
Authors : Svidritskiy, E.; Korostelev, A.A.
Deposited on : 2017-09-27
Resolution : 3.40 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 : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

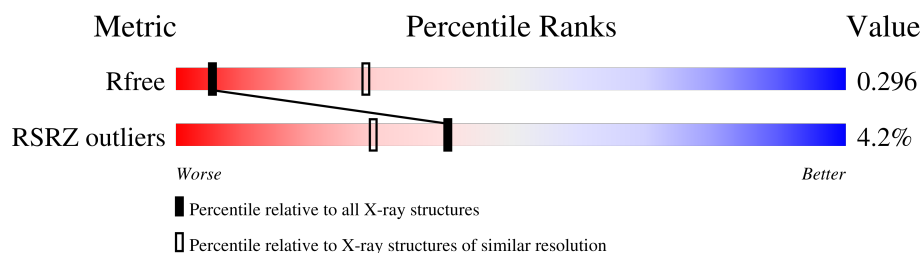
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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
56	MG	A	1604	-	-	-	X
56	MG	A	1620	-	-	-	X
56	MG	A	1628	-	-	-	X
56	MG	A	1696	-	-	-	X
56	MG	A	1721	-	-	-	X
56	MG	B	9134	-	-	-	X
56	MG	B	9140	-	-	-	X
56	MG	C	201	-	-	-	X
56	MG	EB	1603	-	-	-	X
56	MG	EB	1604	-	-	-	X
56	MG	EB	1616	-	-	-	X
56	MG	EB	1619	-	-	-	X
56	MG	EB	1641	-	-	-	X
56	MG	EB	1643	-	-	-	X
56	MG	EB	1791	-	-	-	X
56	MG	EB	1796	-	-	-	X
56	MG	EB	1800	-	-	-	X
56	MG	FB	9006	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	GB	201	-	-	-	X
56	MG	GB	202	-	-	-	X
56	MG	SB	201	-	-	-	X
56	MG	WC	201	-	-	-	X

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 299841 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1507	Total	C	N	O	P	0	0	0
			32394	14424	5998	10465	1507			
1	EB	1507	Total	C	N	O	P	0	0	0
			32394	14424	5998	10465	1507			

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	2880	Total	C	N	O	P	0	0	0
			62031	27612	11589	19950	2880			
2	FB	2880	Total	C	N	O	P	0	0	0
			62031	27612	11589	19950	2880			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	154A	C	UNK	conflict	GB 46197919
FB	154A	C	UNK	conflict	GB 46197919

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			
3	GB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			

- Molecule 4 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	77	Total	C	N	O	P	0	0	0
			1642	734	297	534	76			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	IA	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			
4	HB	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			
4	MC	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			
5	IB	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
6	JB	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			
7	KB	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	181	Total	C	N	O	S	0	0	0
			1471	940	267	260	4			
8	LB	181	Total	C	N	O	S	0	0	0
			1471	940	267	260	4			

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
9	MB	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	146	Total	C	N	O	S	0	0	0
			1137	727	201	208	1			
10	NB	146	Total	C	N	O	S	0	0	0
			1137	727	201	208	1			

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
11	OB	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
12	PB	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
13	QB	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	RB	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
15	SB	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	110	Total	C	N	O	S	0	0	0
			877	553	175	149				
16	TB	110	Total	C	N	O	S	0	0	0
			877	553	175	149				

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			
17	UB	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
18	VB	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
19	WB	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			
20	XB	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
21	YB	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	107	Total	C	N	O	S	0	0	0
			814	523	154	131	6			
22	ZB	107	Total	C	N	O	S	0	0	0
			814	523	154	131	6			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	189	Total	C	N	O	S	0	0	0
			1495	953	266	273	3			
23	AC	189	Total	C	N	O	S	0	0	0
			1495	953	266	273	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
24	BC	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	11	ARG	LYS	conflict	UNP Q72HR3

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Chain	Residue	Modelled	Actual	Comment	Reference
BC	11	ARG	LYS	conflict	UNP Q72HR3

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	97	Total	C	N	O	S	0	0	0
			761	478	151	131	1			
25	CC	97	Total	C	N	O	S	0	0	0
			761	478	151	131	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			
26	DC	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	AA	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			
27	EC	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BA	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			
28	FC	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CA	59	Total	C	N	O	S	0	0	0
			460	290	90	75	5			
29	GC	59	Total	C	N	O	S	0	0	0
			460	290	90	75	5			

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	DA	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
30	HC	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	EA	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
31	IC	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	FA	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
32	JC	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	GA	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
33	KC	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	HA	11	Total	C	N	O	P	0	0	0
			220	98	44	67	11			
34	LC	11	Total	C	N	O	P	0	0	0
			220	98	44	67	11			

- Molecule 35 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	JA	258	Total 2005	C 1227	N 380	O 390	S 8	0	0	0
35	NC	258	Total 2005	C 1227	N 380	O 390	S 8	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
JA	361	LEU	-	expression tag	UNP A7ZKY5
JA	362	GLU	-	expression tag	UNP A7ZKY5
JA	363	HIS	-	expression tag	UNP A7ZKY5
JA	364	HIS	-	expression tag	UNP A7ZKY5
JA	365	HIS	-	expression tag	UNP A7ZKY5
JA	366	HIS	-	expression tag	UNP A7ZKY5
JA	367	HIS	-	expression tag	UNP A7ZKY5
JA	368	HIS	-	expression tag	UNP A7ZKY5
NC	361	LEU	-	expression tag	UNP A7ZKY5
NC	362	GLU	-	expression tag	UNP A7ZKY5
NC	363	HIS	-	expression tag	UNP A7ZKY5
NC	364	HIS	-	expression tag	UNP A7ZKY5
NC	365	HIS	-	expression tag	UNP A7ZKY5
NC	366	HIS	-	expression tag	UNP A7ZKY5
NC	367	HIS	-	expression tag	UNP A7ZKY5
NC	368	HIS	-	expression tag	UNP A7ZKY5

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	KA	234	Total 1900	C 1213	N 341	O 341	S 5	0	0	0
36	OC	234	Total 1900	C 1213	N 341	O 341	S 5	0	0	0

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	LA	206	Total 1612	C 1016	N 314	O 281	S 1	0	0	0
37	PC	206	Total 1612	C 1016	N 314	O 281	S 1	0	0	0

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	MA	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
38	QC	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	NA	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
39	RC	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	OA	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
40	SC	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	PA	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
41	TC	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	QA	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
42	UC	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RA	127	Total	C	N	O		0	0	0
			1011	639	198	174				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	VC	127	Total	C	N	O			
			1011	639	198	174	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	SA	98	Total	C	N	O	S			
			794	499	156	138	1	0	0	0
44	WC	98	Total	C	N	O	S			
			794	499	156	138	1	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	TA	116	Total	C	N	O	S			
			864	537	164	160	3	0	0	0
45	XC	116	Total	C	N	O	S			
			864	537	164	160	3	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	UA	122	Total	C	N	O	S			
			958	604	193	159	2	0	0	0
46	YC	122	Total	C	N	O	S			
			958	604	193	159	2	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	VA	117	Total	C	N	O	S			
			933	577	192	162	2	0	0	0
47	ZC	117	Total	C	N	O	S			
			933	577	192	162	2	0	0	0

- Molecule 48 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	WA	60	Total	C	N	O	S			
			492	312	104	72	4	0	0	0
48	AD	60	Total	C	N	O	S			
			492	312	104	72	4	0	0	0

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	XA	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
49	BD	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	YA	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
50	CD	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	ZA	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			
51	DD	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	AB	70	Total	C	N	O	0	0	0
			574	367	112	95			
52	ED	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BB	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
53	FD	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	CB	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
54	GD	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 55 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	DB	24	Total	C	N	O	0	0	0
			208	128	50	30			
55	HD	24	Total	C	N	O	0	0	0
			208	128	50	30			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	A	214	Total	Mg	0	0
			214	214		
56	B	562	Total	Mg	0	0
			562	562		
56	C	21	Total	Mg	0	0
			21	21		
56	D	5	Total	Mg	0	0
			5	5		
56	E	1	Total	Mg	0	0
			1	1		
56	F	2	Total	Mg	0	0
			2	2		
56	G	2	Total	Mg	0	0
			2	2		
56	H	1	Total	Mg	0	0
			1	1		
56	I	3	Total	Mg	0	0
			3	3		
56	J	2	Total	Mg	0	0
			2	2		
56	K	4	Total	Mg	0	0
			4	4		
56	L	2	Total	Mg	0	0
			2	2		
56	M	5	Total	Mg	0	0
			5	5		
56	O	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	Q	2	Total 2	Mg 2	0	0
56	S	2	Total 2	Mg 2	0	0
56	T	3	Total 3	Mg 3	0	0
56	U	2	Total 2	Mg 2	0	0
56	V	2	Total 2	Mg 2	0	0
56	W	2	Total 2	Mg 2	0	0
56	X	1	Total 1	Mg 1	0	0
56	Y	1	Total 1	Mg 1	0	0
56	Z	4	Total 4	Mg 4	0	0
56	AA	2	Total 2	Mg 2	0	0
56	BA	1	Total 1	Mg 1	0	0
56	CA	1	Total 1	Mg 1	0	0
56	DA	2	Total 2	Mg 2	0	0
56	EA	1	Total 1	Mg 1	0	0
56	HA	3	Total 3	Mg 3	0	0
56	IA	6	Total 6	Mg 6	0	0
56	JA	6	Total 6	Mg 6	0	0
56	KA	1	Total 1	Mg 1	0	0
56	LA	2	Total 2	Mg 2	0	0
56	MA	2	Total 2	Mg 2	0	0
56	NA	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	2	Total 2	Mg 2	0	0
56	SA	3	Total 3	Mg 3	0	0
56	TA	3	Total 3	Mg 3	0	0
56	UA	4	Total 4	Mg 4	0	0
56	XA	6	Total 6	Mg 6	0	0
56	ZA	1	Total 1	Mg 1	0	0
56	AB	2	Total 2	Mg 2	0	0
56	CB	1	Total 1	Mg 1	0	0
56	EB	206	Total 206	Mg 206	0	0
56	FB	475	Total 475	Mg 475	0	0
56	GB	15	Total 15	Mg 15	0	0
56	HB	9	Total 9	Mg 9	0	0
56	IB	4	Total 4	Mg 4	0	0
56	JB	2	Total 2	Mg 2	0	0
56	KB	4	Total 4	Mg 4	0	0
56	MB	2	Total 2	Mg 2	0	0
56	NB	3	Total 3	Mg 3	0	0
56	OB	3	Total 3	Mg 3	0	0
56	PB	1	Total 1	Mg 1	0	0
56	RB	1	Total 1	Mg 1	0	0
56	SB	2	Total 2	Mg 2	0	0

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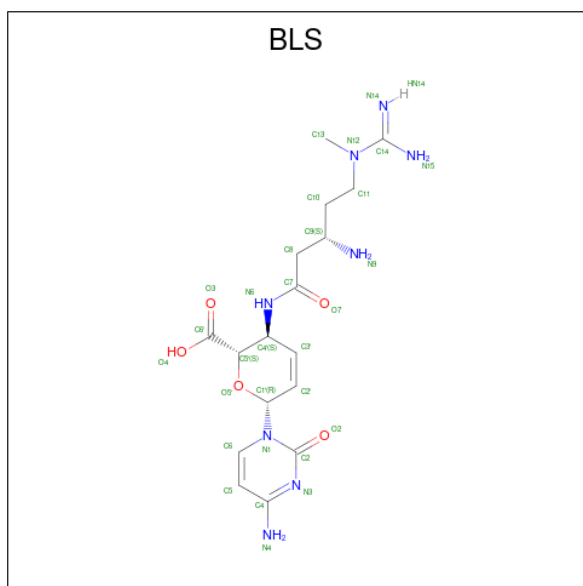
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	TB	1	Total 1	Mg 1	0	0
56	UB	3	Total 3	Mg 3	0	0
56	VB	1	Total 1	Mg 1	0	0
56	WB	1	Total 1	Mg 1	0	0
56	ZB	2	Total 2	Mg 2	0	0
56	BC	1	Total 1	Mg 1	0	0
56	CC	7	Total 7	Mg 7	0	0
56	DC	1	Total 1	Mg 1	0	0
56	EC	1	Total 1	Mg 1	0	0
56	FC	1	Total 1	Mg 1	0	0
56	JC	1	Total 1	Mg 1	0	0
56	LC	1	Total 1	Mg 1	0	0
56	MC	5	Total 5	Mg 5	0	0
56	NC	5	Total 5	Mg 5	0	0
56	OC	5	Total 5	Mg 5	0	0
56	PC	1	Total 1	Mg 1	0	0
56	QC	4	Total 4	Mg 4	0	0
56	RC	3	Total 3	Mg 3	0	0
56	SC	1	Total 1	Mg 1	0	0
56	TC	1	Total 1	Mg 1	0	0
56	UC	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	VC	1	Total	Mg	0	0
			1	1		
56	WC	1	Total	Mg	0	0
			1	1		
56	XC	1	Total	Mg	0	0
			1	1		
56	YC	5	Total	Mg	0	0
			5	5		
56	AD	2	Total	Mg	0	0
			2	2		
56	BD	1	Total	Mg	0	0
			1	1		
56	CD	1	Total	Mg	0	0
			1	1		

- Molecule 57 is BLASTICIDIN S (CCD ID: BLS) (formula: $C_{17}H_{26}N_8O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	B	1	Total	C	N	O	0	0
			30	17	8	5		
57	FB	1	Total	C	N	O	0	0
			30	17	8	5		

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	V	1	Total 1	Zn 1	0	0
58	BA	1	Total 1	Zn 1	0	0
58	CA	1	Total 1	Zn 1	0	0
58	DA	1	Total 1	Zn 1	0	0
58	GA	1	Total 1	Zn 1	0	0
58	ZB	1	Total 1	Zn 1	0	0
58	FC	1	Total 1	Zn 1	0	0
58	GC	1	Total 1	Zn 1	0	0
58	HC	1	Total 1	Zn 1	0	0
58	KC	1	Total 1	Zn 1	0	0

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

3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.85Å 452.54Å 624.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.40 50.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.40) 99.9 (50.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.41Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	(Not available) , (Not available) 0.260 , 0.296	Depositor DCC
R_{free} test set	16277 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	100.4	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	299841	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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](#)

64 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	$\# Z > 2$
1	PSU	A	516	1	18,21,22	1.79	3 (16%)	21,30,33	1.58	5 (23%)
1	2MG	A	1207	1	23,26,27	2.23	4 (17%)	33,38,41	2.25	10 (30%)
2	4OC	FB	1920	2	19,22,24	1.10	1 (5%)	25,31,35	1.24	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MA6	A	1518	1	23,26,27	1.59	4 (17%)	33,38,41	2.39	13 (39%)
1	5MC	EB	1407	1	19,22,23	2.52	4 (21%)	26,32,35	1.34	2 (7%)
1	5MC	EB	1400	1	19,22,23	2.70	4 (21%)	26,32,35	1.05	2 (7%)
1	MA6	A	1519	1	23,26,27	1.67	5 (21%)	33,38,41	1.93	9 (27%)
1	MA6	EB	1518	1	23,26,27	1.70	4 (17%)	33,38,41	2.38	13 (39%)
2	PSU	FB	1917	2	18,21,22	1.81	3 (16%)	21,30,33	1.91	6 (28%)
2	OMG	B	2251	2	23,26,27	2.06	4 (17%)	32,38,41	2.01	9 (28%)
2	PSU	B	1917	2	18,21,22	1.47	3 (16%)	21,30,33	1.90	6 (28%)
1	5MC	A	1400	1	19,22,23	2.64	5 (26%)	26,32,35	1.11	4 (15%)
1	5MC	A	967	1	19,22,23	2.67	4 (21%)	26,32,35	1.11	2 (7%)
2	5MC	B	1962	2	19,22,23	2.77	4 (21%)	26,32,35	1.50	4 (15%)
4	5MC	HB	32	4	19,22,23	2.57	5 (26%)	26,32,35	1.01	2 (7%)
4	5MC	MC	32	4	19,22,23	2.79	4 (21%)	26,32,35	1.30	3 (11%)
1	4OC	A	1402	1	20,23,24	0.96	1 (5%)	25,32,35	1.16	2 (8%)
46	0TD	YC	92	46	8,9,10	2.11	3 (37%)	6,11,13	2.02	2 (33%)
4	5MU	HB	54	4	19,22,23	2.05	3 (15%)	27,32,35	2.12	8 (29%)
1	UR3	EB	1498	1	19,22,23	1.76	2 (10%)	26,32,35	1.69	5 (19%)
2	5MU	B	1939	2	19,22,23	2.16	4 (21%)	27,32,35	2.49	9 (33%)
4	4SU	IA	8	4	18,21,22	5.95	1 (5%)	25,30,33	0.65	0
4	5MC	D	32	4	19,22,23	2.67	5 (26%)	26,32,35	0.98	2 (7%)
2	PSU	B	1911	2	18,21,22	1.69	3 (16%)	21,30,33	1.36	3 (14%)
4	5MC	IA	32	4	19,22,23	2.86	5 (26%)	26,32,35	1.20	3 (11%)
4	PSU	MC	55	4	18,21,22	1.65	3 (16%)	21,30,33	1.65	4 (19%)
2	2MU	FB	2552	2	19,22,24	2.50	5 (26%)	25,31,36	2.08	8 (32%)
2	5MC	FB	1962	2	19,22,23	2.81	5 (26%)	26,32,35	1.20	1 (3%)
1	PSU	EB	516	1	18,21,22	1.73	4 (22%)	21,30,33	1.51	4 (19%)
4	5MU	MC	54	4	19,22,23	2.14	3 (15%)	27,32,35	2.00	8 (29%)
2	2MU	B	2552	2	19,22,24	2.60	5 (26%)	25,31,36	2.36	7 (28%)
2	PSU	FB	1911	2	18,21,22	1.75	3 (16%)	21,30,33	1.89	4 (19%)
1	2MG	EB	1207	1,56	23,26,27	2.27	4 (17%)	33,38,41	2.23	12 (36%)
2	5MU	FB	1915	2	19,22,23	2.13	3 (15%)	27,32,35	2.01	7 (25%)
2	PSU	B	2605	2	18,21,22	1.80	4 (22%)	21,30,33	1.82	4 (19%)
1	M2G	EB	966	1	24,27,28	2.26	4 (16%)	33,40,43	1.86	7 (21%)
46	0TD	UA	92	46	8,9,10	3.14	2 (25%)	6,11,13	2.01	3 (50%)
1	5MC	A	1407	1	19,22,23	2.64	4 (21%)	26,32,35	1.35	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MA6	EB	1519	1	23,26,27	1.57	4 (17%)	33,38,41	1.96	10 (30%)
2	2MA	B	2503	2	22,25,26	1.68	5 (22%)	32,37,40	2.06	8 (25%)
1	5MC	A	1404	1	19,22,23	2.24	4 (21%)	26,32,35	1.38	3 (11%)
1	M2G	A	966	1	24,27,28	2.24	3 (12%)	33,40,43	1.94	8 (24%)
4	4SU	MC	8	4	18,21,22	5.96	1 (5%)	25,30,33	0.69	0
2	5MC	FB	1942	2,56	19,22,23	2.98	4 (21%)	26,32,35	1.21	1 (3%)
2	5MC	B	1942	2	19,22,23	2.74	4 (21%)	26,32,35	1.46	3 (11%)
2	OMG	FB	2251	2,4	23,26,27	2.04	3 (13%)	32,38,41	1.97	9 (28%)
4	PSU	D	55	4	18,21,22	1.78	2 (11%)	21,30,33	1.60	4 (19%)
2	PSU	FB	2605	2	18,21,22	1.63	3 (16%)	21,30,33	1.93	5 (23%)
4	4SU	D	8	4	18,21,22	5.94	1 (5%)	25,30,33	0.64	0
2	2MA	FB	2503	2,56	22,25,26	1.73	5 (22%)	32,37,40	2.06	7 (21%)
2	5MU	FB	1939	2	19,22,23	2.13	3 (15%)	27,32,35	2.68	9 (33%)
4	4SU	HB	8	4	18,21,22	5.94	1 (5%)	25,30,33	0.63	0
4	PSU	HB	55	4	18,21,22	1.82	2 (11%)	21,30,33	1.67	4 (19%)
4	PSU	IA	55	4	18,21,22	1.70	2 (11%)	21,30,33	1.66	4 (19%)
1	7MG	A	527	1	23,26,27	3.04	7 (30%)	27,39,42	2.24	7 (25%)
1	7MG	EB	527	1	23,26,27	3.16	7 (30%)	27,39,42	2.35	7 (25%)
2	5MU	B	1915	2,56	19,22,23	2.06	3 (15%)	27,32,35	2.41	8 (29%)
2	4OC	B	1920	2	19,22,24	1.12	1 (5%)	25,31,35	1.15	2 (8%)
1	5MC	EB	1404	1	19,22,23	2.62	4 (21%)	26,32,35	1.38	4 (15%)
4	5MU	D	54	4	19,22,23	2.10	3 (15%)	27,32,35	2.10	8 (29%)
1	4OC	EB	1402	1	20,23,24	0.96	2 (10%)	25,32,35	1.20	1 (4%)
1	5MC	EB	967	1	19,22,23	2.71	4 (21%)	26,32,35	1.10	3 (11%)
1	UR3	A	1498	1	19,22,23	1.81	2 (10%)	26,32,35	1.84	5 (19%)
4	5MU	IA	54	4	19,22,23	2.09	3 (15%)	27,32,35	2.16	8 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	516	1	-	1/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	3/9/27/28	0/3/3/3
2	4OC	FB	1920	2	-	2/9/27/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	A	1518	1	-	5/11/29/30	0/3/3/3
1	5MC	EB	1407	1	-	0/7/25/26	0/2/2/2
1	5MC	EB	1400	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	6/11/29/30	0/3/3/3
1	MA6	EB	1518	1	-	5/11/29/30	0/3/3/3
2	PSU	FB	1917	2	-	1/7/25/26	0/2/2/2
2	OMG	B	2251	2	-	3/9/27/28	0/3/3/3
2	PSU	B	1917	2	-	2/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
2	5MC	B	1962	2	-	1/7/25/26	0/2/2/2
4	5MC	HB	32	4	-	0/7/25/26	0/2/2/2
4	5MC	MC	32	4	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
46	0TD	YC	92	46	-	4/7/12/14	-
4	5MU	HB	54	4	-	0/7/25/26	0/2/2/2
1	UR3	EB	1498	1	-	2/7/25/26	0/2/2/2
2	5MU	B	1939	2	-	0/7/25/26	0/2/2/2
4	4SU	IA	8	4	-	0/7/25/26	0/2/2/2
4	5MC	D	32	4	-	0/7/25/26	0/2/2/2
2	PSU	B	1911	2	-	2/7/25/26	0/2/2/2
4	5MC	IA	32	4	-	0/7/25/26	0/2/2/2
4	PSU	MC	55	4	-	2/7/25/26	0/2/2/2
2	2MU	FB	2552	2	-	1/9/27/28	0/2/2/2
2	5MC	FB	1962	2	-	1/7/25/26	0/2/2/2
1	PSU	EB	516	1	-	1/7/25/26	0/2/2/2
4	5MU	MC	54	4	-	0/7/25/26	0/2/2/2
2	2MU	B	2552	2	-	1/9/27/28	0/2/2/2
2	PSU	FB	1911	2	-	2/7/25/26	0/2/2/2
1	2MG	EB	1207	1,56	-	4/9/27/28	0/3/3/3
2	5MU	FB	1915	2	-	0/7/25/26	0/2/2/2
2	PSU	B	2605	2	-	0/7/25/26	0/2/2/2
1	M2G	EB	966	1	-	1/11/29/30	0/3/3/3
46	0TD	UA	92	46	-	4/7/12/14	-
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	EB	1519	1	-	6/11/29/30	0/3/3/3
2	2MA	B	2503	2	-	0/7/25/26	0/3/3/3
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	1/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	4SU	MC	8	4	-	0/7/25/26	0/2/2/2
2	5MC	FB	1942	2,56	-	0/7/25/26	0/2/2/2
2	5MC	B	1942	2	-	0/7/25/26	0/2/2/2
2	OMG	FB	2251	2,4	-	3/9/27/28	0/3/3/3
4	PSU	D	55	4	-	1/7/25/26	0/2/2/2
2	PSU	FB	2605	2	-	0/7/25/26	0/2/2/2
4	4SU	D	8	4	-	0/7/25/26	0/2/2/2
2	2MA	FB	2503	2,56	-	0/7/25/26	0/3/3/3
2	5MU	FB	1939	2	-	0/7/25/26	0/2/2/2
4	4SU	HB	8	4	-	0/7/25/26	0/2/2/2
4	PSU	HB	55	4	-	1/7/25/26	0/2/2/2
4	PSU	IA	55	4	-	2/7/25/26	0/2/2/2
1	7MG	A	527	1	-	3/7/37/38	0/3/3/3
1	7MG	EB	527	1	-	3/7/37/38	0/3/3/3
2	5MU	B	1915	2,56	-	0/7/25/26	0/2/2/2
2	4OC	B	1920	2	-	2/9/27/30	0/2/2/2
1	5MC	EB	1404	1	-	0/7/25/26	0/2/2/2
4	5MU	D	54	4	-	0/7/25/26	0/2/2/2
1	4OC	EB	1402	1	-	2/9/29/30	0/2/2/2
1	5MC	EB	967	1	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
4	5MU	IA	54	4	-	0/7/25/26	0/2/2/2

All (220) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	MC	8	4SU	C4-S4	-25.21	1.23	1.68
4	HB	8	4SU	C4-S4	-25.18	1.23	1.68
4	IA	8	4SU	C4-S4	-25.17	1.23	1.68
4	D	8	4SU	C4-S4	-25.16	1.23	1.68
2	FB	1942	5MC	C5-C4	-11.11	1.35	1.44
4	IA	32	5MC	C5-C4	-10.24	1.36	1.44
2	B	1962	5MC	C5-C4	-10.23	1.36	1.44
2	FB	1962	5MC	C5-C4	-10.05	1.36	1.44
1	EB	527	7MG	O6-C6	10.04	1.42	1.23
2	B	1942	5MC	C5-C4	-9.94	1.36	1.44
4	MC	32	5MC	C5-C4	-9.84	1.36	1.44
1	A	527	7MG	O6-C6	9.78	1.42	1.23
1	A	1407	5MC	C5-C4	-9.61	1.36	1.44
1	A	967	5MC	C5-C4	-9.56	1.36	1.44
1	EB	967	5MC	C5-C4	-9.56	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	EB	1400	5MC	C5-C4	-9.41	1.37	1.44
1	EB	1404	5MC	C5-C4	-9.31	1.37	1.44
1	EB	1207	2MG	O6-C6	9.16	1.40	1.23
4	D	32	5MC	C5-C4	-9.04	1.37	1.44
1	A	1400	5MC	C5-C4	-9.03	1.37	1.44
1	A	1207	2MG	O6-C6	8.91	1.40	1.23
1	EB	1407	5MC	C5-C4	-8.70	1.37	1.44
1	EB	966	M2G	O6-C6	8.66	1.40	1.23
1	A	966	M2G	O6-C6	8.58	1.39	1.23
4	HB	32	5MC	C5-C4	-8.39	1.37	1.44
2	B	2552	2MU	O4-C4	8.24	1.40	1.24
2	B	2251	OMG	O6-C6	8.02	1.38	1.23
2	FB	2251	OMG	O6-C6	7.82	1.38	1.23
2	FB	2552	2MU	O4-C4	7.73	1.39	1.24
1	EB	527	7MG	C5-N7	7.16	1.44	1.35
1	A	1404	5MC	C5-C4	-7.01	1.38	1.44
1	A	1498	UR3	O4-C4	6.92	1.38	1.23
1	EB	1498	UR3	O4-C4	6.82	1.38	1.23
1	A	527	7MG	C5-N7	6.70	1.44	1.35
46	UA	92	0TD	CB-CA	-6.47	1.52	1.54
2	FB	1939	5MU	C4-C5	-6.38	1.34	1.44
4	MC	54	5MU	O4-C4	6.33	1.35	1.23
4	D	54	5MU	O4-C4	6.32	1.35	1.23
2	B	1939	5MU	O4-C4	6.25	1.35	1.23
4	IA	54	5MU	O4-C4	6.14	1.35	1.23
2	FB	1915	5MU	C4-C5	-6.01	1.35	1.44
4	HB	54	5MU	O4-C4	6.01	1.35	1.23
2	FB	1915	5MU	O4-C4	5.98	1.34	1.23
4	HB	55	PSU	C6-C5	5.87	1.41	1.35
2	B	1915	5MU	C4-C5	-5.86	1.35	1.44
4	IA	54	5MU	C4-C5	-5.78	1.35	1.44
4	MC	54	5MU	C4-C5	-5.77	1.35	1.44
2	FB	1911	PSU	C6-C5	5.76	1.41	1.35
2	FB	1917	PSU	C6-C5	5.70	1.41	1.35
4	D	55	PSU	C6-C5	5.70	1.41	1.35
2	B	1915	5MU	O4-C4	5.69	1.34	1.23
2	B	1939	5MU	C4-C5	-5.64	1.35	1.44
2	FB	1939	5MU	O4-C4	5.64	1.34	1.23
4	IA	55	PSU	C6-C5	5.57	1.41	1.35
2	B	2605	PSU	C6-C5	5.51	1.41	1.35
4	D	54	5MU	C4-C5	-5.47	1.35	1.44
2	B	2503	2MA	C8-N7	5.45	1.42	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	HB	54	5MU	C4-C5	-5.45	1.36	1.44
2	FB	2503	2MA	C8-N7	5.43	1.42	1.31
4	MC	55	PSU	C6-C5	5.42	1.41	1.35
1	A	516	PSU	C6-C5	5.42	1.41	1.35
1	EB	966	M2G	C2-N2	5.32	1.44	1.35
2	FB	2605	PSU	C6-C5	5.30	1.41	1.35
1	EB	516	PSU	C6-C5	5.26	1.41	1.35
2	B	1911	PSU	C6-C5	5.24	1.41	1.35
46	UA	92	0TD	CB-SB	-5.16	1.77	1.82
1	A	966	M2G	C2-N2	5.05	1.44	1.35
2	B	2552	2MU	C3'-C2'	-4.85	1.42	1.53
1	EB	527	7MG	C8-N9	-4.84	1.42	1.45
2	FB	2552	2MU	C3'-C2'	-4.62	1.42	1.53
1	A	527	7MG	C4-N9	4.61	1.43	1.37
2	B	1917	PSU	C6-C5	4.54	1.40	1.35
4	HB	32	5MC	C6-C5	4.51	1.42	1.34
1	EB	1518	MA6	C6-N6	4.49	1.49	1.36
1	A	1518	MA6	C4-N3	4.43	1.42	1.34
1	EB	527	7MG	C4-N9	4.38	1.43	1.37
1	EB	1518	MA6	C4-N3	4.38	1.42	1.34
1	A	1400	5MC	C4-N4	4.29	1.45	1.34
4	IA	32	5MC	C6-C5	4.27	1.41	1.34
4	D	32	5MC	C6-C5	4.26	1.41	1.34
2	FB	1962	5MC	C4-N4	4.23	1.44	1.34
4	MC	32	5MC	C6-C5	4.22	1.41	1.34
4	HB	32	5MC	C4-N4	4.21	1.44	1.34
1	A	1519	MA6	C4-N3	4.18	1.42	1.34
1	A	1519	MA6	C6-N6	4.18	1.48	1.36
4	D	32	5MC	C4-N4	4.18	1.44	1.34
1	A	527	7MG	C8-N9	-4.15	1.43	1.45
4	MC	32	5MC	C4-N4	4.13	1.44	1.34
1	A	1404	5MC	C4-N4	4.11	1.44	1.34
1	A	1518	MA6	C6-N6	4.10	1.48	1.36
1	EB	1400	5MC	C6-C5	4.08	1.41	1.34
1	EB	1519	MA6	C4-N3	4.08	1.42	1.34
4	IA	32	5MC	C4-N4	4.07	1.44	1.34
1	EB	967	5MC	C4-N4	4.05	1.44	1.34
1	EB	1407	5MC	C4-N4	4.04	1.44	1.34
2	FB	1942	5MC	C4-N4	4.03	1.44	1.34
1	A	967	5MC	C4-N4	4.02	1.44	1.34
1	EB	1400	5MC	C4-N4	3.99	1.44	1.34
1	EB	1407	5MC	C6-N1	-3.82	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1942	5MC	C6-N1	-3.80	1.31	1.38
46	YC	92	0TD	CB-SB	-3.80	1.78	1.82
1	A	967	5MC	C6-N1	-3.71	1.31	1.38
2	FB	1942	5MC	C6-N1	-3.70	1.31	1.38
1	A	1407	5MC	C6-N1	-3.70	1.31	1.38
1	EB	1404	5MC	C6-N1	-3.67	1.31	1.38
2	B	1942	5MC	C4-N4	3.65	1.43	1.34
1	A	1400	5MC	C6-C5	3.65	1.40	1.34
1	EB	1404	5MC	C4-N4	3.65	1.43	1.34
1	EB	1519	MA6	C6-N6	3.63	1.46	1.36
46	YC	92	0TD	CB-CA	-3.62	1.53	1.54
1	A	1207	2MG	C2-N2	3.60	1.40	1.33
1	EB	967	5MC	C6-C5	3.58	1.40	1.34
1	EB	1207	2MG	C2-N2	3.56	1.40	1.33
2	B	1962	5MC	C4-N4	3.56	1.43	1.34
1	EB	967	5MC	C6-N1	-3.56	1.32	1.38
1	A	1404	5MC	C6-C5	3.55	1.40	1.34
2	B	1962	5MC	C6-C5	3.55	1.40	1.34
1	A	1407	5MC	C4-N4	3.55	1.43	1.34
2	FB	2251	OMG	C2-N2	3.55	1.42	1.34
2	FB	1920	4OC	C4-N4	3.55	1.42	1.33
2	B	1942	5MC	C6-C5	3.53	1.40	1.34
2	FB	1962	5MC	C6-N1	-3.52	1.32	1.38
2	B	1920	4OC	C4-N4	3.49	1.42	1.33
1	A	527	7MG	C6-N1	-3.48	1.32	1.38
2	B	1962	5MC	C6-N1	-3.41	1.32	1.38
2	B	2251	OMG	C2-N2	3.40	1.42	1.34
1	EB	1404	5MC	C6-C5	3.38	1.40	1.34
1	EB	1518	MA6	C2-N1	3.34	1.39	1.33
2	FB	1962	5MC	C6-C5	3.32	1.40	1.34
1	A	1400	5MC	C6-N1	-3.30	1.32	1.38
2	FB	2503	2MA	C2-N1	3.29	1.39	1.34
1	A	1519	MA6	C2-N1	3.28	1.39	1.33
1	A	516	PSU	C6-N1	3.24	1.41	1.36
1	EB	527	7MG	C6-N1	-3.23	1.32	1.38
1	EB	527	7MG	C2-N2	3.22	1.41	1.34
2	B	2605	PSU	C6-N1	3.21	1.41	1.36
4	MC	32	5MC	C6-N1	-3.18	1.32	1.38
1	A	1407	5MC	C6-C5	3.17	1.39	1.34
1	EB	1400	5MC	C6-N1	-3.17	1.32	1.38
1	A	1404	5MC	C6-N1	-3.15	1.32	1.38
1	EB	516	PSU	C6-N1	3.12	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	967	5MC	C6-C5	3.11	1.39	1.34
2	FB	1915	5MU	C6-C5	3.11	1.39	1.34
2	FB	1942	5MC	C6-C5	3.11	1.39	1.34
1	A	527	7MG	C2-N2	3.04	1.41	1.34
1	EB	1519	MA6	C2-N1	3.03	1.39	1.33
4	D	32	5MC	C6-N1	-3.00	1.32	1.38
1	EB	1407	5MC	C6-C5	2.98	1.39	1.34
2	FB	1917	PSU	C6-N1	2.97	1.41	1.36
4	D	55	PSU	C6-N1	2.95	1.41	1.36
1	EB	527	7MG	C2-N3	2.93	1.40	1.33
1	A	1518	MA6	C2-N1	2.88	1.39	1.33
4	IA	32	5MC	C6-N1	-2.86	1.33	1.38
4	HB	55	PSU	C6-N1	2.85	1.41	1.36
1	A	1207	2MG	C2-N3	2.85	1.37	1.32
2	FB	2552	2MU	C4-N3	-2.78	1.33	1.38
4	HB	32	5MC	C6-N1	-2.77	1.33	1.38
1	A	966	M2G	C4-N3	2.76	1.40	1.34
2	FB	1939	5MU	C6-C5	2.75	1.39	1.34
2	B	1911	PSU	C6-N1	2.72	1.40	1.36
4	HB	54	5MU	C6-C5	2.72	1.39	1.34
2	FB	2503	2MA	C5-C4	2.70	1.43	1.39
2	FB	1911	PSU	C6-N1	2.69	1.40	1.36
1	EB	1207	2MG	C2-N3	2.69	1.37	1.32
2	FB	2251	OMG	C6-N1	-2.68	1.33	1.38
1	A	527	7MG	C2-N3	2.67	1.39	1.33
2	FB	2605	PSU	C6-N1	2.67	1.40	1.36
2	B	2503	2MA	C2-N3	-2.62	1.29	1.34
1	A	1402	4OC	C4-N4	2.57	1.41	1.36
4	IA	55	PSU	C6-N1	2.56	1.40	1.36
4	MC	55	PSU	C6-N1	2.56	1.40	1.36
4	D	54	5MU	C6-C5	2.52	1.38	1.34
2	B	1915	5MU	C6-C5	2.51	1.38	1.34
2	B	2605	PSU	C1'-C5	2.51	1.55	1.50
2	B	2503	2MA	C4-N9	2.47	1.42	1.37
4	MC	54	5MU	C6-C5	2.46	1.38	1.34
2	B	2552	2MU	O3'-C3'	-2.46	1.36	1.43
2	B	2552	2MU	C2'-C1'	-2.46	1.47	1.53
2	B	2552	2MU	C4-N3	-2.44	1.34	1.38
1	EB	1402	4OC	C4-N4	2.44	1.41	1.36
1	A	1519	MA6	C6-N1	2.39	1.38	1.34
1	EB	1518	MA6	C6-N1	2.36	1.38	1.34
1	EB	966	M2G	C4-N3	2.34	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2503	2MA	C2-N1	2.33	1.38	1.34
2	FB	1911	PSU	C1'-C5	2.29	1.55	1.50
1	A	1207	2MG	C2-N1	-2.28	1.33	1.36
2	FB	2503	2MA	C4-N9	2.25	1.42	1.37
2	B	1917	PSU	C6-N1	2.25	1.40	1.36
2	B	1939	5MU	C6-C5	2.23	1.38	1.34
1	A	516	PSU	C1'-C5	2.22	1.55	1.50
4	IA	32	5MC	C4-N3	2.22	1.37	1.34
4	IA	54	5MU	C6-C5	2.21	1.38	1.34
2	B	1939	5MU	C2-N3	-2.20	1.34	1.38
2	B	2251	OMG	C4-N3	2.19	1.39	1.34
1	EB	516	PSU	C1'-C5	2.19	1.55	1.50
4	HB	32	5MC	C4-N3	2.18	1.37	1.34
1	EB	1402	4OC	C4-N3	2.18	1.36	1.32
1	A	1400	5MC	C4-N3	2.17	1.37	1.34
1	EB	1498	UR3	C4-N3	-2.16	1.36	1.40
2	B	2503	2MA	C5-C4	2.15	1.42	1.39
2	FB	2552	2MU	C5-C4	-2.15	1.39	1.43
2	FB	1917	PSU	C2-N1	2.13	1.39	1.36
2	FB	2605	PSU	C1'-C5	2.12	1.55	1.50
2	B	1917	PSU	O4'-C1'	-2.12	1.40	1.43
2	B	1911	PSU	C1'-C5	2.11	1.55	1.50
1	EB	966	M2G	C6-N1	-2.11	1.34	1.38
4	MC	55	PSU	C1'-C5	2.10	1.55	1.50
1	A	1498	UR3	C4-N3	-2.07	1.36	1.40
1	A	1518	MA6	C6-N1	2.06	1.38	1.34
1	EB	1207	2MG	C2-N1	-2.05	1.33	1.36
2	B	2605	PSU	C2-N1	2.05	1.39	1.36
2	B	2251	OMG	C6-N1	-2.05	1.35	1.38
2	FB	1962	5MC	C4-N3	2.05	1.37	1.34
4	D	32	5MC	C4-N3	2.05	1.37	1.34
1	EB	1519	MA6	C5-C4	2.04	1.42	1.39
1	A	1519	MA6	C5-C4	2.03	1.42	1.39
46	YC	92	0TD	OD1-CG	2.03	1.28	1.22
2	FB	2552	2MU	C3'-C4'	-2.01	1.47	1.53
1	EB	516	PSU	O4'-C1'	-2.01	1.41	1.43
2	FB	2503	2MA	C2-N3	-2.01	1.30	1.34

All (328) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2503	2MA	C5-C4-N3	-7.76	119.01	127.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	FB	2503	2MA	C5-C4-N3	-7.60	119.17	127.18
1	A	1207	2MG	C5-C4-N3	-6.41	118.20	128.39
1	A	966	M2G	C5-C4-N3	-6.34	118.29	128.39
1	A	1207	2MG	C2-N3-C4	6.30	119.88	112.00
2	B	1915	5MU	C5-C4-N3	6.24	120.75	115.32
2	FB	1939	5MU	C4-N3-C2	-6.17	119.25	127.34
2	B	1939	5MU	C4-N3-C2	-6.13	119.30	127.34
1	EB	966	M2G	C5-C4-N3	-6.13	118.63	128.39
2	B	2552	2MU	C4-N3-C2	-6.11	119.03	126.61
1	EB	1207	2MG	C5-C4-N3	-6.10	118.69	128.39
2	B	2251	OMG	C5-C4-N3	-6.09	118.69	128.39
2	FB	2251	OMG	C5-C4-N3	-6.09	118.70	128.39
1	EB	1207	2MG	C2-N3-C4	6.03	119.54	112.00
1	A	1518	MA6	C5-C4-N3	-5.97	118.50	126.72
2	B	1939	5MU	N3-C2-N1	5.86	122.52	114.89
2	FB	1939	5MU	N3-C2-N1	5.75	122.38	114.89
2	B	1915	5MU	C4-N3-C2	-5.74	119.81	127.34
1	EB	527	7MG	N9-C4-N3	5.59	133.65	125.46
1	EB	1518	MA6	C5-C4-N3	-5.57	119.04	126.72
2	B	1939	5MU	C5-C4-N3	5.49	120.09	115.32
1	A	1498	UR3	C4-N3-C2	-5.42	120.22	124.58
1	EB	527	7MG	C5-C6-N1	5.38	120.41	110.94
1	EB	527	7MG	C2-N3-C4	5.37	121.55	112.30
2	FB	1939	5MU	C6-C5-C4	5.32	122.40	118.02
4	IA	54	5MU	C5-C4-N3	5.24	119.88	115.32
1	A	527	7MG	C5-C6-N1	5.18	120.06	110.94
2	B	2552	2MU	N3-C2-N1	5.13	121.57	114.89
1	A	527	7MG	N9-C4-N3	5.11	132.95	125.46
4	HB	54	5MU	C4-N3-C2	-5.06	120.71	127.34
2	FB	2605	PSU	C4-N3-C2	-5.04	119.43	126.37
4	D	54	5MU	C4-N3-C2	-5.01	120.78	127.34
4	IA	54	5MU	C4-N3-C2	-4.99	120.80	127.34
2	FB	2552	2MU	C4-N3-C2	-4.99	120.42	126.61
4	HB	54	5MU	C5-C4-N3	4.97	119.65	115.32
1	EB	1519	MA6	C5-C4-N3	-4.96	119.89	126.72
2	B	2605	PSU	C4-N3-C2	-4.95	119.55	126.37
1	A	527	7MG	C2-N3-C4	4.95	120.83	112.30
2	B	1915	5MU	O4-C4-C5	-4.94	119.26	124.92
2	B	1942	5MC	C5-C6-N1	-4.92	117.97	123.31
1	A	1519	MA6	C5-C4-N3	-4.88	119.99	126.72
1	A	1518	MA6	N3-C4-N9	4.82	135.37	127.17
2	B	1915	5MU	N3-C2-N1	4.79	121.13	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EB	1498	UR3	C4-N3-C2	-4.78	120.73	124.58
1	EB	527	7MG	C5-C4-N3	-4.74	119.23	128.13
2	FB	1915	5MU	O4-C4-C5	-4.70	119.55	124.92
1	A	527	7MG	C5-C4-N3	-4.67	119.36	128.13
2	B	2251	OMG	N9-C4-N3	4.67	135.29	125.95
4	D	54	5MU	C5-C4-N3	4.65	119.36	115.32
2	FB	2605	PSU	N1-C2-N3	4.57	119.99	115.17
2	B	1917	PSU	N1-C2-N3	4.54	119.96	115.17
4	MC	54	5MU	C4-N3-C2	-4.54	121.39	127.34
2	B	2503	2MA	N3-C4-N9	4.54	132.75	126.99
2	FB	2251	OMG	N9-C4-N3	4.53	135.01	125.95
4	IA	54	5MU	O4-C4-C5	-4.53	119.73	124.92
2	FB	1911	PSU	O2-C2-N1	-4.52	118.13	122.79
1	A	966	M2G	N9-C4-N3	4.52	134.98	125.95
1	A	1407	5MC	C5-C6-N1	-4.51	118.41	123.31
2	FB	1939	5MU	C5-C6-N1	-4.51	118.42	123.31
4	MC	54	5MU	O4-C4-C5	-4.48	119.80	124.92
4	MC	54	5MU	C5-C4-N3	4.47	119.21	115.32
1	EB	1518	MA6	C4-C5-C6	4.45	120.51	115.91
2	FB	2503	2MA	N3-C4-N9	4.43	132.61	126.99
1	EB	1518	MA6	N3-C4-N9	4.43	134.70	127.17
2	FB	1939	5MU	C5-C4-N3	4.39	119.14	115.32
2	FB	1917	PSU	C4-N3-C2	-4.39	120.32	126.37
2	B	1917	PSU	C4-N3-C2	-4.38	120.34	126.37
2	FB	1917	PSU	N1-C2-N3	4.36	119.77	115.17
1	EB	966	M2G	N9-C4-N3	4.32	134.59	125.95
2	FB	1915	5MU	C4-N3-C2	-4.31	121.68	127.34
1	EB	1404	5MC	C5-C6-N1	-4.31	118.63	123.31
1	A	1498	UR3	C6-N1-C2	-4.30	118.28	121.80
1	EB	1518	MA6	N1-C6-N6	4.30	122.10	116.86
2	FB	1911	PSU	N1-C2-N3	4.30	119.70	115.17
1	EB	1518	MA6	N1-C2-N3	-4.28	122.10	128.58
4	HB	54	5MU	N3-C2-N1	4.28	120.46	114.89
1	A	1518	MA6	N1-C2-N3	-4.27	122.11	128.58
2	FB	1915	5MU	C5-C4-N3	4.27	119.03	115.32
2	FB	1939	5MU	O4-C4-C5	-4.27	120.04	124.92
4	D	54	5MU	N3-C2-N1	4.23	120.40	114.89
1	A	1404	5MC	C5-C6-N1	-4.23	118.72	123.31
2	B	2251	OMG	C2-N3-C4	4.21	119.55	112.30
1	A	1519	MA6	N1-C2-N3	-4.15	122.30	128.58
1	EB	1407	5MC	C5-C6-N1	-4.11	118.85	123.31
4	IA	54	5MU	N3-C2-N1	4.08	120.20	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1962	5MC	C5-C6-N1	-4.05	118.92	123.31
4	HB	55	PSU	N1-C2-N3	4.05	119.44	115.17
2	B	2552	2MU	C2'-C1'-N1	-4.04	106.57	114.24
1	A	1207	2MG	C2-N1-C6	-4.01	119.70	124.55
1	A	516	PSU	C4-N3-C2	-3.99	120.88	126.37
1	A	1518	MA6	C4-C5-C6	3.98	120.03	115.91
4	IA	55	PSU	N1-C2-N3	3.98	119.37	115.17
2	FB	2552	2MU	C5-C4-N3	3.98	120.37	114.80
2	B	2552	2MU	C5-C4-N3	3.94	120.32	114.80
2	FB	2251	OMG	C2-N3-C4	3.92	119.06	112.30
1	A	1207	2MG	N9-C4-N3	3.91	133.78	125.95
1	A	966	M2G	C2-N3-C4	3.90	119.72	112.51
4	MC	54	5MU	N3-C2-N1	3.89	119.96	114.89
1	EB	1518	MA6	C2-N1-C6	3.89	121.33	111.83
4	D	55	PSU	N1-C2-N3	3.86	119.24	115.17
2	FB	1939	5MU	O2-C2-N1	-3.86	117.78	122.80
4	MC	55	PSU	N1-C2-N3	3.85	119.23	115.17
4	D	54	5MU	O4-C4-C5	-3.85	120.51	124.92
2	FB	1942	5MC	C5-C6-N1	-3.84	119.14	123.31
1	EB	1498	UR3	C6-N1-C2	-3.82	118.68	121.80
2	FB	1911	PSU	C4-N3-C2	-3.78	121.16	126.37
1	EB	1519	MA6	N1-C2-N3	-3.78	122.86	128.58
1	EB	1207	2MG	N9-C4-N3	3.77	133.50	125.95
1	A	1498	UR3	C1'-N1-C2	3.77	123.21	117.04
4	MC	55	PSU	C4-N3-C2	-3.77	121.18	126.37
46	YC	92	0TD	OD2-CG-CB	3.74	121.22	113.15
1	A	1519	MA6	C2-N1-C6	3.72	120.91	111.83
4	HB	54	5MU	O4-C4-C5	-3.72	120.67	124.92
2	FB	1915	5MU	N3-C2-N1	3.70	119.71	114.89
2	B	1939	5MU	C5-C6-N1	-3.70	119.30	123.31
1	EB	966	M2G	C2-N3-C4	3.67	119.29	112.51
1	EB	516	PSU	C4-N3-C2	-3.66	121.33	126.37
1	A	1518	MA6	C2-N1-C6	3.62	120.68	111.83
1	EB	1519	MA6	C2-N1-C6	3.62	120.66	111.83
2	FB	2552	2MU	C2'-C1'-N1	-3.61	107.40	114.24
1	A	1518	MA6	N1-C6-N6	3.60	121.24	116.86
4	D	55	PSU	C4-N3-C2	-3.58	121.44	126.37
4	IA	55	PSU	C4-N3-C2	-3.58	121.44	126.37
2	B	2605	PSU	N1-C2-N3	3.54	118.90	115.17
1	EB	967	5MC	C5-C6-N1	-3.48	119.53	123.31
4	HB	55	PSU	C4-N3-C2	-3.47	121.59	126.37
1	A	967	5MC	C5-C6-N1	-3.46	119.56	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	HB	55	PSU	O2-C2-N1	-3.42	119.26	122.79
1	A	1518	MA6	C5-C6-N6	-3.42	119.92	125.33
2	FB	2552	2MU	N3-C2-N1	3.42	119.34	114.89
1	A	1404	5MC	CM5-C5-C6	-3.41	118.24	122.85
1	EB	1498	UR3	C1'-N1-C2	3.40	122.60	117.04
1	EB	1207	2MG	C2-N1-C6	-3.39	120.45	124.55
2	FB	2503	2MA	C4-C5-N7	-3.39	106.71	110.58
46	UA	92	0TD	OD2-CG-CB	3.39	120.46	113.15
1	EB	1519	MA6	C4-C5-N7	-3.38	106.71	110.58
4	D	54	5MU	C5-C6-N1	-3.34	119.68	123.31
1	A	1519	MA6	N3-C4-N9	3.34	132.85	127.17
1	EB	1519	MA6	N3-C4-N9	3.32	132.81	127.17
1	EB	1407	5MC	CM5-C5-C6	-3.31	118.37	122.85
1	A	1518	MA6	C2-N3-C4	3.28	119.85	111.83
1	A	516	PSU	N1-C2-N3	3.27	118.61	115.17
1	EB	1518	MA6	C5-C6-N6	-3.26	120.17	125.33
1	EB	1402	4OC	CM4-N4-C4	-3.25	116.10	122.45
1	EB	1519	MA6	C5-N7-C8	3.23	108.53	103.45
2	FB	1962	5MC	C5-C6-N1	-3.21	119.83	123.31
2	FB	1915	5MU	C6-C5-C4	3.21	120.67	118.02
1	A	1518	MA6	N9-C8-N7	-3.20	109.39	113.94
4	HB	54	5MU	C5-C6-N1	-3.17	119.87	123.31
1	EB	1519	MA6	N9-C8-N7	-3.16	109.45	113.94
1	A	1518	MA6	C5-N7-C8	3.16	108.41	103.45
2	B	1911	PSU	C4-N3-C2	-3.15	122.03	126.37
4	IA	32	5MC	C5-C6-N1	-3.15	119.89	123.31
2	FB	1917	PSU	C6-C5-C4	3.13	120.28	118.17
4	IA	55	PSU	O2-C2-N1	-3.12	119.57	122.79
2	FB	1915	5MU	C5-C6-N1	-3.09	119.95	123.31
4	MC	32	5MC	C5-C6-N1	-3.09	119.96	123.31
2	B	1915	5MU	C5-C6-N1	-3.08	119.97	123.31
1	EB	1404	5MC	CM5-C5-C6	-3.08	118.68	122.85
1	EB	1518	MA6	N9-C8-N7	-3.07	109.59	113.94
1	A	1519	MA6	C4-C5-N7	-3.06	107.08	110.58
1	EB	1518	MA6	C2-N3-C4	3.06	119.30	111.83
1	EB	1518	MA6	C5-N7-C8	3.06	108.25	103.45
2	B	2605	PSU	C5-C6-N1	-3.03	117.93	122.14
2	FB	2552	2MU	O2'-C2'-C1'	3.03	114.75	108.99
1	A	1519	MA6	C2-N3-C4	3.02	119.21	111.83
1	EB	1207	2MG	C8-N7-C5	3.02	109.63	104.26
1	EB	1207	2MG	C4-C5-N7	-3.01	105.89	110.67
2	FB	1911	PSU	C6-N1-C2	-3.00	119.91	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EB	527	7MG	O6-C6-C5	-3.00	120.26	127.62
2	B	1917	PSU	O2-C2-N1	-3.00	119.70	122.79
2	B	2552	2MU	C6'-O2'-C2'	2.98	122.13	114.47
1	EB	1498	UR3	C3U-N3-C2	2.97	122.51	117.33
2	B	1939	5MU	C6-N1-C2	-2.97	118.35	121.30
1	EB	966	M2G	N9-C8-N7	-2.97	107.90	113.40
2	B	1939	5MU	C6-C5-C4	2.94	120.44	118.02
4	MC	55	PSU	O2-C2-N1	-2.93	119.76	122.79
1	EB	1207	2MG	N9-C8-N7	-2.93	107.97	113.40
1	A	1519	MA6	C4-C5-C6	2.93	118.94	115.91
1	A	1407	5MC	CM5-C5-C6	-2.92	118.89	122.85
4	D	55	PSU	O2-C2-N1	-2.92	119.78	122.79
1	EB	516	PSU	N1-C2-N3	2.92	118.25	115.17
2	B	1920	4OC	CM2-O2'-C2'	2.91	121.94	114.47
2	FB	1939	5MU	C6-N1-C2	-2.91	118.41	121.30
1	A	1519	MA6	C5-N7-C8	2.90	108.01	103.45
1	EB	1519	MA6	C4-C5-C6	2.89	118.89	115.91
1	A	527	7MG	O6-C6-C5	-2.88	120.55	127.62
4	MC	32	5MC	C5-C4-N3	-2.87	118.81	121.75
1	A	1402	4OC	C6-C5-C4	2.87	120.45	117.00
2	B	1915	5MU	C6-N1-C2	-2.87	118.45	121.30
1	A	966	M2G	N9-C8-N7	-2.85	108.12	113.40
2	B	1962	5MC	C5-C4-N4	-2.84	117.39	121.39
1	EB	1519	MA6	C2-N3-C4	2.83	118.75	111.83
4	D	54	5MU	C6-C5-C4	2.81	120.33	118.02
2	B	2251	OMG	CM2-O2'-C2'	2.80	121.65	114.47
2	FB	1917	PSU	C5-C6-N1	-2.79	118.26	122.14
2	B	1962	5MC	C4-N3-C2	-2.78	116.95	120.81
4	D	32	5MC	C5-C6-N1	-2.77	120.30	123.31
1	EB	1400	5MC	C5-C4-N3	-2.77	118.91	121.75
1	A	1519	MA6	N9-C8-N7	-2.77	110.01	113.94
2	FB	1920	4OC	O2-C2-N3	-2.76	117.97	122.33
2	FB	2503	2MA	N9-C8-N7	-2.74	110.05	113.94
4	IA	54	5MU	C5-C6-N1	-2.74	120.34	123.31
2	FB	2503	2MA	C5-N7-C8	2.73	107.74	103.45
46	YC	92	0TD	OD2-CG-OD1	-2.73	117.89	124.08
1	A	1402	4OC	CM4-N4-C4	-2.71	117.16	122.45
2	FB	2251	OMG	N9-C8-N7	-2.70	108.39	113.40
2	B	1911	PSU	O2-C2-N1	-2.69	120.01	122.79
1	A	1207	2MG	C4-C5-N7	-2.68	106.42	110.67
2	FB	2251	OMG	CM2-O2'-C2'	2.68	121.36	114.47
4	MC	32	5MC	O2-C2-N3	-2.65	118.16	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	FB	2552	2MU	O2-C2-N1	-2.64	119.36	122.80
2	FB	2251	OMG	C2-N1-C6	-2.64	120.32	125.11
2	B	2503	2MA	N3-C2-N1	-2.64	121.11	125.77
2	FB	1920	4OC	CM2-O2'-C2'	2.63	121.23	114.47
1	A	1518	MA6	C4-C5-N7	-2.63	107.57	110.58
4	HB	32	5MC	C5-C6-N1	-2.63	120.46	123.31
2	B	1939	5MU	C5M-C5-C6	-2.63	119.30	122.85
4	HB	32	5MC	C5-C4-N3	-2.62	119.06	121.75
1	A	1518	MA6	C4-N9-C8	2.62	108.49	105.74
2	B	1911	PSU	N1-C2-N3	2.62	117.93	115.17
1	EB	527	7MG	C6-C5-C4	-2.62	117.80	122.40
2	B	2251	OMG	C2-N1-C6	-2.62	120.37	125.11
46	UA	92	0TD	OD2-CG-OD1	-2.61	118.16	124.08
1	EB	516	PSU	O2-C2-N1	-2.61	120.10	122.79
4	HB	55	PSU	C6-N1-C2	-2.61	120.27	122.69
2	FB	1920	4OC	C1'-N1-C2	2.60	124.19	118.44
1	EB	1518	MA6	C4-C5-N7	-2.59	107.62	110.58
2	B	2503	2MA	C4-C5-N7	-2.59	107.62	110.58
2	B	1939	5MU	O2-C2-N3	-2.58	116.73	121.49
2	FB	2552	2MU	O4-C4-C5	-2.58	120.71	125.16
1	A	966	M2G	C5-C6-N1	2.58	119.81	113.25
1	A	1498	UR3	C3U-N3-C2	2.57	121.81	117.33
2	B	2251	OMG	N9-C8-N7	-2.57	108.64	113.40
2	FB	2503	2MA	N6-C6-N1	2.57	120.49	117.03
1	A	1518	MA6	C1'-N9-C8	-2.55	121.43	127.09
1	EB	1518	MA6	C1'-N9-C8	-2.55	121.45	127.09
4	D	32	5MC	C5-C4-N3	-2.54	119.15	121.75
1	A	1400	5MC	C5-C4-N3	-2.53	119.16	121.75
2	B	2605	PSU	C5-C4-N3	2.52	122.10	116.55
4	HB	54	5MU	C6-C5-C4	2.51	120.09	118.02
2	B	1939	5MU	O4-C4-C5	-2.49	122.07	124.92
2	B	2552	2MU	O2-C2-N1	-2.49	119.56	122.80
1	A	527	7MG	C6-C5-C4	-2.46	118.07	122.40
4	IA	55	PSU	C6-N1-C2	-2.46	120.41	122.69
1	EB	966	M2G	C8-N7-C5	2.44	108.61	104.26
4	MC	54	5MU	C5-C6-N1	-2.43	120.67	123.31
1	A	1207	2MG	C8-N7-C5	2.43	108.59	104.26
1	A	967	5MC	CM5-C5-C6	-2.43	119.56	122.85
1	EB	1518	MA6	C4-N9-C8	2.42	108.28	105.74
2	FB	2605	PSU	C5-C4-N3	2.41	121.86	116.55
2	B	1917	PSU	C6-C5-C4	2.41	119.80	118.17
2	FB	2605	PSU	C5-C6-N1	-2.41	118.80	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EB	516	PSU	O4'-C1'-C2'	2.39	108.46	105.15
1	EB	1404	5MC	C1'-N1-C6	-2.39	117.21	121.15
1	A	527	7MG	C2-N1-C6	-2.39	120.77	125.11
1	EB	527	7MG	C2-N1-C6	-2.38	120.80	125.11
4	IA	32	5MC	C5-C4-N4	-2.37	118.06	121.39
2	FB	1915	5MU	C6-N1-C2	-2.36	118.95	121.30
4	D	54	5MU	C5M-C5-C6	-2.36	119.66	122.85
2	B	2251	OMG	C5-C6-N1	2.36	119.26	113.25
2	FB	2251	OMG	O6-C6-C5	-2.35	120.33	126.53
1	A	1207	2MG	N9-C8-N7	-2.35	109.05	113.40
1	A	1207	2MG	C5-C6-N1	2.35	119.22	113.25
4	MC	54	5MU	C6-N1-C2	-2.34	118.97	121.30
2	B	2503	2MA	N6-C6-N1	2.34	120.18	117.03
4	IA	54	5MU	C6-N1-C2	-2.33	118.98	121.30
4	HB	54	5MU	C5M-C5-C6	-2.33	119.70	122.85
2	B	1942	5MC	O2-C2-N3	-2.32	118.67	122.33
1	A	966	M2G	C8-N7-C5	2.32	108.39	104.26
1	A	1404	5MC	O2-C2-N3	-2.32	118.68	122.33
2	B	2503	2MA	N9-C8-N7	-2.29	110.68	113.94
2	B	1915	5MU	C6-C5-C4	2.27	119.89	118.02
1	EB	1207	2MG	C1'-N9-C8	-2.26	120.31	126.73
2	B	1942	5MC	CM5-C5-C6	-2.25	119.81	122.85
2	FB	1917	PSU	O2-C2-N1	-2.25	120.47	122.79
1	A	1400	5MC	O2-C2-N3	-2.24	118.80	122.33
2	B	2503	2MA	C5-C4-N9	2.24	108.25	105.81
1	A	516	PSU	O4'-C1'-C2'	2.23	108.24	105.15
1	A	1400	5MC	CM5-C5-C6	-2.23	119.83	122.85
2	B	2503	2MA	C5-N7-C8	2.23	106.95	103.45
4	D	55	PSU	C6-N1-C2	-2.22	120.63	122.69
1	A	1498	UR3	C5-C4-N3	2.21	117.95	115.04
2	FB	2552	2MU	C6'-O2'-C2'	2.21	120.15	114.47
2	FB	2503	2MA	C5-C4-N9	2.20	108.21	105.81
2	B	2251	OMG	O6-C6-C5	-2.19	120.74	126.53
2	B	1917	PSU	C5-C6-N1	-2.19	119.10	122.14
2	FB	1939	5MU	C5M-C5-C6	-2.18	119.90	122.85
4	IA	54	5MU	C5M-C5-C6	-2.18	119.91	122.85
2	FB	2251	OMG	C8-N7-C5	2.17	108.12	104.26
4	MC	54	5MU	C6-C5-C4	2.16	119.80	118.02
2	FB	2251	OMG	C5-C6-N1	2.16	118.74	113.25
1	EB	1519	MA6	C4-N9-C8	2.16	108.00	105.74
2	FB	1917	PSU	O4'-C1'-C2'	2.15	108.13	105.15
2	B	1915	5MU	O2-C2-N3	-2.15	117.52	121.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	IA	54	5MU	C6-C5-C4	2.15	119.79	118.02
1	EB	967	5MC	C5-C4-N3	-2.15	119.55	121.75
2	B	1962	5MC	CM5-C5-C6	-2.14	119.95	122.85
46	UA	92	0TD	CSB-SB-CB	2.14	106.21	102.36
1	EB	1498	UR3	C5-C4-N3	2.14	117.86	115.04
4	MC	55	PSU	C6-N1-C2	-2.14	120.70	122.69
1	EB	1207	2MG	N1-C2-N2	2.14	118.74	116.56
1	EB	966	M2G	C5-C6-N1	2.13	118.68	113.25
1	EB	1404	5MC	O2-C2-N3	-2.13	118.98	122.33
1	A	516	PSU	O2-C2-N1	-2.13	120.60	122.79
1	A	1207	2MG	O6-C6-C5	-2.13	120.92	126.53
1	EB	1207	2MG	CM2-N2-C2	-2.12	119.08	123.65
1	EB	967	5MC	CM5-C5-C6	-2.12	119.98	122.85
1	A	966	M2G	O6-C6-C5	-2.12	120.93	126.53
2	FB	2605	PSU	O4-C4-C5	-2.11	118.76	124.01
2	B	1920	4OC	C1'-N1-C6	-2.10	116.30	120.78
4	HB	54	5MU	C6-N1-C2	-2.09	119.22	121.30
2	B	2552	2MU	O2'-C2'-C1'	2.09	112.95	108.99
1	EB	1207	2MG	C5-C6-N1	2.09	118.56	113.25
2	B	2251	OMG	C8-N7-C5	2.08	107.97	104.26
1	A	1400	5MC	C5-C6-N1	-2.08	121.06	123.31
4	MC	54	5MU	O2-C2-N1	-2.07	120.10	122.80
1	A	1207	2MG	C1'-N9-C8	-2.07	120.86	126.73
1	A	1407	5MC	C4-N3-C2	-2.06	117.95	120.81
1	EB	1207	2MG	C6-C5-N7	2.06	134.03	130.29
2	FB	1920	4OC	C1'-N1-C6	-2.05	116.39	120.78
1	EB	966	M2G	C4-C5-N7	-2.05	107.42	110.67
1	A	966	M2G	C4-C5-N7	-2.04	107.43	110.67
1	EB	1400	5MC	CM5-C5-C6	-2.04	120.09	122.85
1	A	516	PSU	O4-C4-C5	-2.03	118.95	124.01
4	D	54	5MU	O2-C2-N1	-2.03	120.16	122.80
4	IA	32	5MC	CM5-C5-C4	-2.02	117.18	120.51
2	B	1917	PSU	O4'-C1'-C2'	2.01	107.93	105.15

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1207	2MG	O4'-C4'-C5'-O5'
1	A	1207	2MG	N3-C2-N2-CM2
1	A	1518	MA6	O4'-C4'-C5'-O5'
1	A	1518	MA6	C5-C6-N6-C9

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Mol	Chain	Res	Type	Atoms
1	A	1519	MA6	O4'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C9
2	B	2251	OMG	C1'-C2'-O2'-CM2
2	B	2552	2MU	C1'-C2'-O2'-C6'
1	EB	1207	2MG	O4'-C4'-C5'-O5'
1	EB	1207	2MG	N1-C2-N2-CM2
1	EB	1207	2MG	N3-C2-N2-CM2
1	EB	1518	MA6	O4'-C4'-C5'-O5'
1	EB	1518	MA6	C5-C6-N6-C9
1	EB	1519	MA6	O4'-C4'-C5'-O5'
1	EB	1519	MA6	C5-C6-N6-C9
2	FB	2251	OMG	C1'-C2'-O2'-CM2
2	FB	2552	2MU	C1'-C2'-O2'-C6'
46	YC	92	0TD	CA-CB-CG-OD1
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1207	2MG	C3'-C4'-C5'-O5'
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	1518	MA6	C3'-C4'-C5'-O5'
1	EB	527	7MG	C3'-C4'-C5'-O5'
1	EB	1207	2MG	C3'-C4'-C5'-O5'
1	EB	1498	UR3	O4'-C4'-C5'-O5'
1	EB	1518	MA6	C3'-C4'-C5'-O5'
1	EB	1402	4OC	O4'-C4'-C5'-O5'
1	A	1518	MA6	N1-C6-N6-C9
1	A	1519	MA6	N1-C6-N6-C9
1	EB	1518	MA6	N1-C6-N6-C9
1	EB	1519	MA6	N1-C6-N6-C9
1	A	1519	MA6	C3'-C4'-C5'-O5'
1	EB	1519	MA6	C3'-C4'-C5'-O5'
1	A	527	7MG	O4'-C4'-C5'-O5'
1	EB	527	7MG	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1498	UR3	C3'-C4'-C5'-O5'
1	EB	1498	UR3	C3'-C4'-C5'-O5'
1	EB	1402	4OC	C3'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1518	MA6	C5-C6-N6-C10
46	YC	92	0TD	CA-CB-CG-OD2
2	B	1917	PSU	O4'-C4'-C5'-O5'
1	A	1519	MA6	C4'-C5'-O5'-P
1	EB	1519	MA6	C4'-C5'-O5'-P
1	A	516	PSU	O4'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
2	B	1911	PSU	O4'-C1'-C5-C4
1	EB	516	PSU	O4'-C1'-C5-C4
2	FB	1911	PSU	O4'-C1'-C5-C4
4	IA	55	PSU	O4'-C1'-C5-C4
4	MC	55	PSU	O4'-C1'-C5-C4
1	A	527	7MG	C4'-C5'-O5'-P
1	EB	527	7MG	C4'-C5'-O5'-P
2	B	2251	OMG	O4'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C10
1	EB	1518	MA6	C5-C6-N6-C10
1	EB	1519	MA6	C5-C6-N6-C10
2	B	1962	5MC	O4'-C4'-C5'-O5'
2	FB	1917	PSU	O4'-C4'-C5'-O5'
1	A	966	M2G	C4'-C5'-O5'-P
1	EB	966	M2G	C4'-C5'-O5'-P
2	B	2251	OMG	C3'-C4'-C5'-O5'
46	UA	92	0TD	SB-CB-CG-OD2
46	YC	92	0TD	SB-CB-CG-OD2
2	FB	1920	4OC	C2'-C1'-N1-C6
2	B	1911	PSU	O4'-C1'-C5-C6
2	FB	1911	PSU	O4'-C1'-C5-C6
4	IA	55	PSU	O4'-C1'-C5-C6
4	MC	55	PSU	O4'-C1'-C5-C6
2	FB	1920	4OC	C2'-C1'-N1-C2
2	FB	1962	5MC	O4'-C4'-C5'-O5'
2	B	1920	4OC	C2'-C1'-N1-C6
46	UA	92	0TD	CA-CB-CG-OD2
46	UA	92	0TD	CA-CB-CG-OD1
2	B	1920	4OC	C2'-C1'-N1-C2
46	UA	92	0TD	CG-CB-SB-CSB
46	YC	92	0TD	CG-CB-SB-CSB
4	D	55	PSU	C3'-C4'-C5'-O5'
2	B	1917	PSU	C3'-C4'-C5'-O5'
2	FB	2251	OMG	O4'-C4'-C5'-O5'
4	HB	55	PSU	C3'-C4'-C5'-O5'
2	FB	2251	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 1695 ligands modelled in this entry, 1693 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
57	BLS	FB	9001	-	30,31,31	3.11	11 (36%)	30,43,43	1.87	10 (33%)
57	BLS	B	9001	-	30,31,31	3.10	12 (40%)	30,43,43	1.80	9 (30%)

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
57	BLS	FB	9001	-	-	4/25/38/38	0/2/2/2
57	BLS	B	9001	-	-	5/25/38/38	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	FB	9001	BLS	C14-N12	8.93	1.54	1.35
57	B	9001	BLS	C14-N12	8.56	1.53	1.35
57	FB	9001	BLS	C7-N6	7.29	1.49	1.34
57	B	9001	BLS	C7-N6	7.10	1.49	1.34
57	B	9001	BLS	C4-N4	5.71	1.47	1.33
57	FB	9001	BLS	C4-N4	5.28	1.46	1.33
57	B	9001	BLS	C3'-C2'	5.00	1.48	1.33
57	FB	9001	BLS	C11-N12	4.84	1.56	1.47
57	FB	9001	BLS	C3'-C2'	4.77	1.47	1.33
57	B	9001	BLS	C11-N12	4.68	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	FB	9001	BLS	C13-N12	4.56	1.61	1.45
57	B	9001	BLS	C13-N12	4.31	1.60	1.45
57	B	9001	BLS	O5'-C5'	4.14	1.51	1.43
57	FB	9001	BLS	O5'-C5'	3.93	1.51	1.43
57	FB	9001	BLS	C4'-C5'	-2.72	1.47	1.53
57	B	9001	BLS	C4'-C5'	-2.57	1.47	1.53
57	B	9001	BLS	C4'-N6	2.47	1.49	1.46
57	B	9001	BLS	C2-N1	-2.47	1.34	1.40
57	B	9001	BLS	C5'-C6'	-2.34	1.48	1.53
57	FB	9001	BLS	C5'-C6'	-2.22	1.48	1.53
57	B	9001	BLS	C1'-N1	-2.15	1.45	1.48
57	FB	9001	BLS	C4'-N6	2.10	1.49	1.46
57	FB	9001	BLS	C1'-N1	-2.10	1.45	1.48

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	FB	9001	BLS	C1'-C2'-C3'	-4.87	116.46	122.45
57	B	9001	BLS	C1'-C2'-C3'	-4.31	117.15	122.45
57	FB	9001	BLS	O3-C6'-C5'	-3.69	107.50	120.81
57	B	9001	BLS	O3-C6'-C5'	-3.57	107.91	120.81
57	B	9001	BLS	C13-N12-C11	3.49	122.85	115.90
57	FB	9001	BLS	O4-C6'-O3	3.10	131.12	124.08
57	FB	9001	BLS	C13-N12-C11	2.97	121.80	115.90
57	B	9001	BLS	O4-C6'-O3	2.59	129.95	124.08
57	B	9001	BLS	C11-C10-C9	2.51	119.13	113.96
57	FB	9001	BLS	C3'-C4'-N6	-2.47	105.89	110.44
57	FB	9001	BLS	C8-C7-N6	2.42	119.56	116.25
57	B	9001	BLS	C3'-C4'-N6	-2.39	106.05	110.44
57	FB	9001	BLS	C5-C6-N1	-2.36	118.00	121.84
57	B	9001	BLS	O4-C6'-C5'	2.35	122.14	113.64
57	B	9001	BLS	C8-C7-N6	2.28	119.36	116.25
57	B	9001	BLS	O5'-C5'-C6'	2.20	113.02	106.14
57	FB	9001	BLS	O4-C6'-C5'	2.14	121.38	113.64
57	FB	9001	BLS	C11-C10-C9	2.10	118.29	113.96
57	FB	9001	BLS	O5'-C5'-C6'	2.03	112.50	106.14

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	B	9001	BLS	N6-C7-C8-C9

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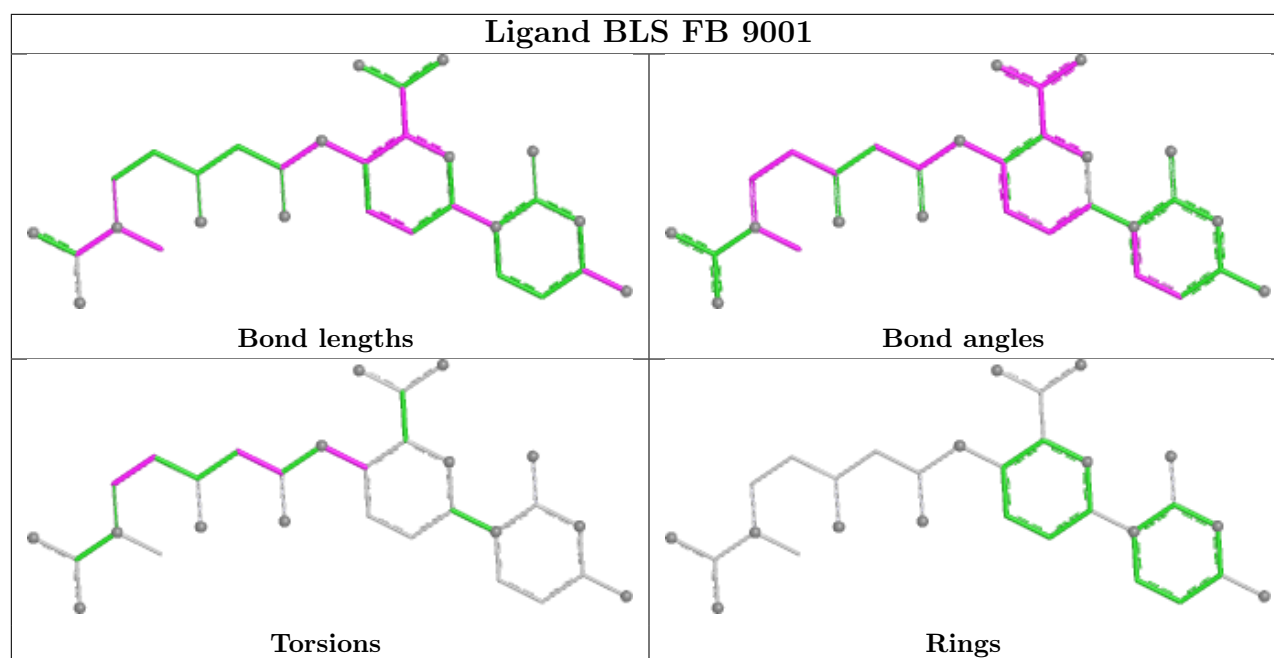
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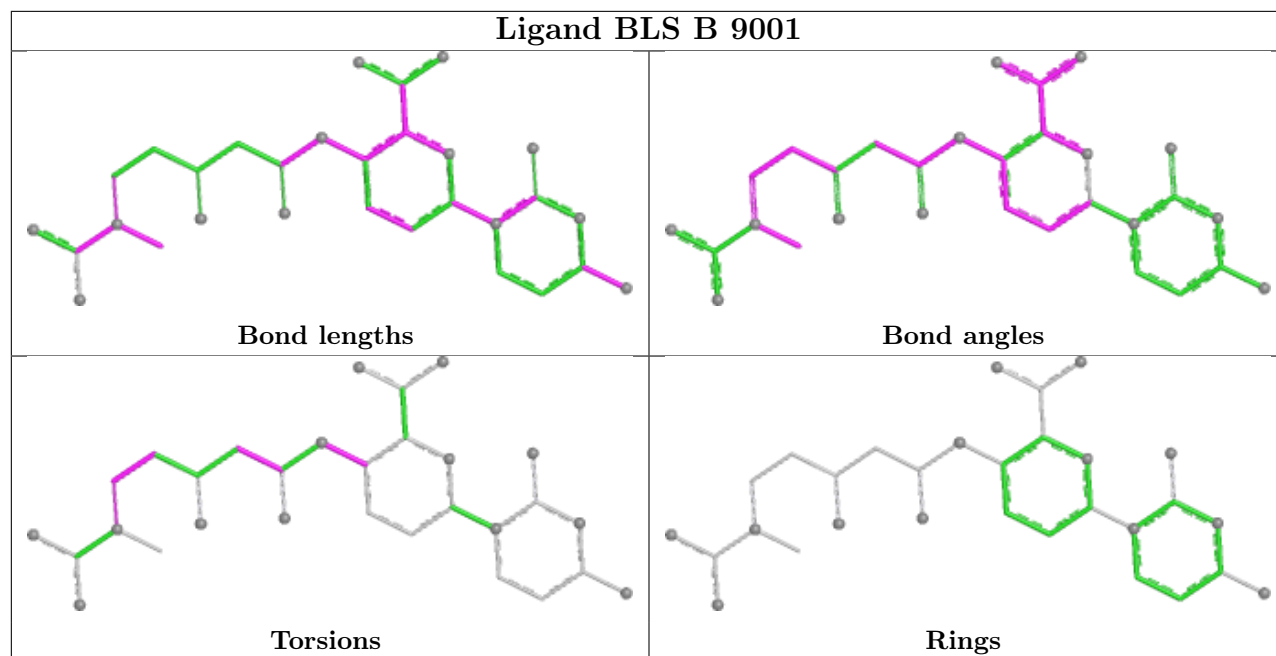
Mol	Chain	Res	Type	Atoms
57	B	9001	BLS	O7-C7-C8-C9
57	B	9001	BLS	C9-C10-C11-N12
57	FB	9001	BLS	N6-C7-C8-C9
57	FB	9001	BLS	O7-C7-C8-C9
57	FB	9001	BLS	C9-C10-C11-N12
57	B	9001	BLS	C10-C11-N12-C13
57	B	9001	BLS	C5'-C4'-N6-C7
57	FB	9001	BLS	C5'-C4'-N6-C7

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	A	1495/1507 (99%)	-0.14	11 (0%) 84 73	75, 127, 186, 250	0
1	EB	1495/1507 (99%)	-0.07	16 (1%) 78 65	80, 106, 179, 236	0
2	B	2869/2880 (99%)	-0.29	22 (0%) 82 71	56, 77, 167, 223	0
2	FB	2869/2880 (99%)	-0.09	35 (1%) 76 63	69, 92, 191, 294	0
3	C	120/120 (100%)	-0.25	0 100 100	92, 118, 133, 146	0
3	GB	120/120 (100%)	0.03	1 (0%) 82 71	102, 127, 142, 153	0
4	D	73/77 (94%)	-0.04	1 (1%) 73 59	98, 185, 199, 203	0
4	HB	73/77 (94%)	-0.02	0 100 100	103, 189, 204, 209	0
4	IA	73/77 (94%)	-0.02	0 100 100	111, 153, 173, 175	0
4	MC	73/77 (94%)	0.02	1 (1%) 73 59	110, 162, 186, 192	0
5	E	275/275 (100%)	0.20	5 (1%) 67 53	57, 66, 77, 83	0
5	IB	275/275 (100%)	0.35	8 (2%) 53 39	66, 76, 86, 95	0
6	F	204/206 (99%)	0.07	6 (2%) 53 39	59, 76, 92, 100	0
6	JB	204/206 (99%)	0.46	10 (4%) 35 26	70, 91, 114, 124	0
7	G	202/205 (98%)	0.02	1 (0%) 87 78	59, 78, 92, 99	0
7	KB	202/205 (98%)	0.10	1 (0%) 87 78	63, 92, 105, 110	0
8	H	181/182 (99%)	0.67	15 (8%) 17 15	116, 138, 152, 155	0
8	LB	181/182 (99%)	0.42	8 (4%) 39 28	131, 148, 162, 167	0
9	I	174/180 (96%)	0.30	6 (3%) 48 35	90, 96, 102, 117	0
9	MB	174/180 (96%)	1.00	26 (14%) 5 7	130, 166, 175, 183	0
10	J	146/148 (98%)	0.42	6 (4%) 41 29	84, 113, 127, 128	0
10	NB	146/148 (98%)	0.82	18 (12%) 8 9	98, 132, 139, 141	0
11	K	140/140 (100%)	0.11	3 (2%) 63 48	61, 75, 94, 99	0
11	OB	140/140 (100%)	0.43	3 (2%) 63 48	82, 101, 118, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
12	L	122/122 (100%)	0.11	0 100 100	63, 74, 82, 85	0
12	PB	122/122 (100%)	0.31	6 (4%) 35 26	76, 86, 93, 95	0
13	M	150/150 (100%)	0.46	5 (3%) 49 36	55, 86, 107, 109	0
13	QB	150/150 (100%)	0.69	11 (7%) 21 18	70, 106, 125, 127	0
14	N	141/141 (100%)	0.58	10 (7%) 22 18	73, 85, 98, 102	0
14	RB	141/141 (100%)	0.69	11 (7%) 19 16	85, 100, 113, 122	0
15	O	118/118 (100%)	0.24	5 (4%) 40 29	61, 72, 85, 92	0
15	SB	118/118 (100%)	0.67	3 (2%) 58 43	75, 89, 97, 102	0
16	P	110/112 (98%)	0.65	10 (9%) 15 14	105, 112, 116, 117	0
16	TB	110/112 (98%)	1.00	16 (14%) 6 7	111, 124, 130, 132	0
17	Q	137/146 (93%)	0.19	3 (2%) 62 47	74, 82, 128, 151	0
17	UB	137/146 (93%)	0.32	4 (2%) 53 39	86, 95, 119, 129	0
18	R	117/118 (99%)	0.16	2 (1%) 69 54	56, 72, 84, 87	0
18	VB	117/118 (99%)	0.56	5 (4%) 40 29	73, 97, 115, 119	0
19	S	101/101 (100%)	0.09	3 (2%) 52 39	56, 82, 90, 94	0
19	WB	101/101 (100%)	0.49	6 (5%) 28 22	72, 103, 114, 120	0
20	T	112/113 (99%)	-0.01	1 (0%) 81 68	52, 63, 79, 87	0
20	XB	112/113 (99%)	0.30	3 (2%) 56 42	67, 80, 94, 102	0
21	U	95/96 (98%)	0.15	4 (4%) 40 29	62, 70, 80, 86	0
21	YB	95/96 (98%)	0.68	3 (3%) 50 37	85, 93, 101, 103	0
22	V	107/110 (97%)	0.29	1 (0%) 81 68	77, 83, 91, 96	0
22	ZB	107/110 (97%)	0.83	10 (9%) 14 14	93, 102, 112, 117	0
23	AC	189/206 (91%)	0.28	5 (2%) 57 42	107, 122, 132, 134	0
23	W	189/206 (91%)	0.30	4 (2%) 63 48	92, 106, 119, 124	0
24	BC	84/85 (98%)	1.15	18 (21%) 2 4	94, 98, 126, 134	0
24	X	84/85 (98%)	0.86	12 (14%) 6 8	85, 88, 111, 118	0
25	CC	97/98 (98%)	0.60	5 (5%) 33 24	73, 92, 119, 127	0
25	Y	97/98 (98%)	0.50	5 (5%) 33 24	62, 82, 107, 115	0
26	DC	70/72 (97%)	0.22	1 (1%) 73 59	97, 103, 110, 111	0
26	Z	70/72 (97%)	0.11	1 (1%) 73 59	72, 78, 84, 89	0
27	AA	60/60 (100%)	0.33	1 (1%) 69 54	70, 82, 99, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	EC	60/60 (100%)	0.46	0 100 100	85, 93, 105, 109	0
28	BA	69/71 (97%)	0.44	2 (2%) 53 39	156, 160, 166, 169	0
28	FC	69/71 (97%)	0.47	0 100 100	165, 174, 188, 191	0
29	CA	59/60 (98%)	-0.02	0 100 100	55, 79, 85, 86	0
29	GC	59/60 (98%)	0.14	1 (1%) 69 54	69, 93, 102, 106	0
30	DA	53/54 (98%)	1.25	9 (16%) 4 5	158, 159, 159, 159	0
30	HC	53/54 (98%)	1.13	8 (15%) 5 7	164, 168, 172, 173	0
31	EA	48/49 (97%)	0.44	3 (6%) 26 20	56, 60, 64, 65	0
31	IC	48/49 (97%)	0.32	2 (4%) 40 29	67, 71, 80, 84	0
32	FA	64/65 (98%)	0.61	4 (6%) 26 20	63, 75, 95, 103	0
32	JC	64/65 (98%)	0.95	7 (10%) 10 11	75, 85, 102, 110	0
33	GA	37/37 (100%)	1.28	6 (16%) 4 6	96, 97, 98, 98	0
33	KC	37/37 (100%)	1.64	13 (35%) 1 1	111, 119, 128, 132	0
34	HA	11/23 (47%)	0.78	1 (9%) 15 14	110, 111, 126, 127	0
34	LC	11/23 (47%)	0.65	0 100 100	108, 109, 126, 128	0
35	JA	258/368 (70%)	0.42	17 (6%) 24 19	90, 116, 133, 137	0
35	NC	258/368 (70%)	0.46	14 (5%) 31 24	105, 119, 136, 146	0
36	KA	234/256 (91%)	0.51	16 (6%) 23 19	138, 150, 162, 167	0
36	OC	234/256 (91%)	0.42	14 (5%) 27 21	115, 136, 149, 169	0
37	LA	206/239 (86%)	0.35	14 (6%) 23 19	126, 146, 163, 166	0
37	PC	206/239 (86%)	0.50	8 (3%) 43 31	117, 129, 142, 148	0
38	MA	208/209 (99%)	1.02	30 (14%) 6 7	115, 130, 140, 145	0
38	QC	208/209 (99%)	0.49	10 (4%) 35 26	92, 99, 108, 113	0
39	NA	151/162 (93%)	0.49	10 (6%) 24 19	110, 121, 128, 139	0
39	RC	151/162 (93%)	0.34	6 (3%) 42 30	91, 102, 110, 117	0
40	OA	101/101 (100%)	0.30	3 (2%) 52 39	98, 102, 112, 123	0
40	SC	101/101 (100%)	0.36	1 (0%) 79 66	105, 112, 120, 123	0
41	PA	155/156 (99%)	0.63	19 (12%) 8 9	126, 145, 154, 156	0
41	TC	155/156 (99%)	0.62	12 (7%) 19 16	128, 147, 155, 160	0
42	QA	138/138 (100%)	0.61	6 (4%) 40 29	109, 124, 132, 138	0
42	UC	138/138 (100%)	0.48	7 (5%) 33 25	93, 108, 116, 118	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	RA	127/128 (99%)	1.18	26 (20%) 2 4	127, 168, 173, 175	0
43	VC	127/128 (99%)	1.39	33 (25%) 1 3	128, 166, 174, 176	0
44	SA	98/105 (93%)	1.12	17 (17%) 4 5	142, 167, 173, 176	0
44	WC	98/105 (93%)	1.07	11 (11%) 10 11	128, 159, 165, 166	0
45	TA	116/129 (89%)	0.45	5 (4%) 40 29	87, 107, 115, 118	0
45	XC	116/129 (89%)	0.21	4 (3%) 48 35	93, 111, 118, 121	0
46	UA	121/132 (91%)	0.66	13 (10%) 11 11	97, 101, 110, 117	0
46	YC	121/132 (91%)	0.37	5 (4%) 41 29	84, 89, 94, 98	0
47	VA	117/126 (92%)	0.50	6 (5%) 33 25	136, 160, 164, 166	0
47	ZC	117/126 (92%)	0.98	15 (12%) 7 9	140, 168, 172, 172	0
48	AD	60/61 (98%)	1.25	10 (16%) 4 6	128, 138, 154, 154	0
48	WA	60/61 (98%)	1.31	9 (15%) 5 7	141, 149, 154, 155	0
49	BD	88/89 (98%)	0.21	1 (1%) 78 65	91, 101, 109, 111	0
49	XA	88/89 (98%)	0.48	4 (4%) 38 28	94, 106, 116, 117	0
50	CD	83/88 (94%)	0.68	7 (8%) 17 15	92, 100, 115, 126	0
50	YA	83/88 (94%)	1.18	15 (18%) 3 5	122, 134, 146, 157	0
51	DD	99/105 (94%)	0.37	2 (2%) 65 49	87, 92, 96, 97	0
51	ZA	99/105 (94%)	0.57	5 (5%) 33 25	95, 107, 112, 118	0
52	AB	70/88 (79%)	0.20	2 (2%) 53 39	101, 110, 118, 119	0
52	ED	70/88 (79%)	0.22	0 100 100	103, 109, 113, 120	0
53	BB	83/93 (89%)	1.20	15 (18%) 3 5	138, 159, 162, 164	0
53	FD	83/93 (89%)	1.07	15 (18%) 3 5	146, 162, 168, 169	0
54	CB	99/106 (93%)	1.29	26 (26%) 1 3	118, 128, 139, 140	0
54	GD	99/106 (93%)	1.06	21 (21%) 2 4	95, 108, 122, 124	0
55	DB	24/27 (88%)	2.38	15 (62%) 0 0	152, 157, 160, 164	0
55	HD	24/27 (88%)	1.92	8 (33%) 1 1	156, 161, 165, 167	0
All	All	21478/22220 (96%)	0.23	910 (4%) 40 29	52, 102, 169, 294	0

All (910) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	DA	5	VAL	9.5
25	Y	2	SER	9.0

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Mol	Chain	Res	Type	RSRZ
24	X	8	GLY	8.1
24	BC	4	LYS	7.4
54	GD	26	ASN	6.4
2	FB	1094	U	6.3
35	NC	242	SER	6.2
36	OC	214	ILE	6.2
24	X	4	LYS	6.1
55	HD	14	TRP	6.1
24	BC	2	ALA	6.0
47	ZC	102	ARG	6.0
24	X	9	SER	6.0
43	RA	110	GLU	5.9
50	CD	68	ASP	5.8
53	BB	59	PRO	5.7
24	BC	5	LYS	5.7
24	X	2	ALA	5.6
54	CB	29	LYS	5.4
43	RA	121	ARG	5.4
54	CB	70	SER	5.4
44	SA	66	ARG	5.2
46	UA	95	GLY	5.1
24	BC	3	HIS	5.0
24	X	3	HIS	5.0
44	SA	55	LYS	5.0
43	RA	14	VAL	4.9
24	BC	9	SER	4.8
38	MA	9	CYS	4.8
38	QC	9	CYS	4.8
18	VB	56	ASP	4.8
2	FB	1095	A	4.7
46	YC	91	LYS	4.7
1	EB	723	U	4.7
43	RA	13	ALA	4.7
2	FB	2798	C	4.7
16	TB	52	SER	4.6
44	SA	47	PHE	4.6
44	SA	58	ASP	4.6
55	HD	6	ARG	4.6
47	ZC	87	TYR	4.6
36	KA	88	ALA	4.5
18	VB	37	GLU	4.5
54	GD	24	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
10	NB	92	VAL	4.5
24	BC	41	ARG	4.4
33	KC	21	GLY	4.4
41	PA	35	LYS	4.4
55	HD	17	THR	4.3
43	VC	119	ALA	4.3
54	CB	11	SER	4.3
23	AC	97	GLU	4.3
42	UC	2	LEU	4.3
1	EB	1398	A	4.2
48	WA	7	ILE	4.2
24	X	7	LEU	4.2
37	LA	197	GLY	4.2
2	FB	1064	C	4.2
9	MB	169	VAL	4.2
38	MA	135	LEU	4.2
48	WA	25	VAL	4.2
33	KC	13	LYS	4.1
22	ZB	1	MET	4.1
35	JA	199	SER	4.1
39	RC	24	ARG	4.1
16	P	45	GLY	4.1
2	FB	1762	A	4.0
38	MA	4	TYR	4.0
19	WB	82	ARG	4.0
24	X	74	ARG	4.0
55	DB	14	TRP	4.0
2	B	2334	G	4.0
35	NC	240	THR	4.0
2	FB	1096	A	4.0
36	OC	240	GLN	4.0
47	ZC	60	VAL	4.0
53	BB	56	GLN	4.0
24	BC	8	GLY	4.0
38	MA	2	GLY	4.0
41	PA	82	GLY	3.9
16	P	12	PHE	3.9
38	MA	21	LEU	3.9
50	YA	29	ASP	3.9
2	B	271(D)	U	3.9
43	RA	109	VAL	3.9
55	DB	17	THR	3.9

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Mol	Chain	Res	Type	RSRZ
41	PA	38	LEU	3.9
39	NA	24	ARG	3.9
35	NC	132	PHE	3.9
46	UA	32	PHE	3.9
48	AD	19	ARG	3.8
37	PC	10	PHE	3.8
32	JC	36	LYS	3.8
44	SA	64	GLU	3.8
54	GD	28	ALA	3.8
43	RA	106	ALA	3.8
43	VC	64	THR	3.8
54	GD	23	ARG	3.8
54	CB	71	THR	3.8
8	H	159	VAL	3.7
46	UA	91	LYS	3.7
55	DB	16	GLY	3.7
43	VC	61	ALA	3.7
9	MB	170	ARG	3.7
18	VB	55	ARG	3.7
38	MA	31	CYS	3.7
35	NC	234	GLY	3.7
44	WC	55	LYS	3.7
50	YA	30	GLY	3.7
14	RB	38	GLU	3.6
30	DA	2	ALA	3.6
55	DB	13	ILE	3.6
55	DB	18	TYR	3.6
10	NB	38	LEU	3.6
14	RB	37	LEU	3.6
43	VC	32	ASP	3.6
25	Y	26	ARG	3.6
54	CB	25	ARG	3.6
9	MB	141	VAL	3.6
14	N	130	LYS	3.6
43	VC	117	HIS	3.5
41	PA	120	ILE	3.5
1	EB	84	U	3.5
35	NC	235	GLN	3.5
43	VC	28	VAL	3.5
16	TB	56	LEU	3.5
45	TA	126	ARG	3.5
15	SB	14	SER	3.5

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Mol	Chain	Res	Type	RSRZ
30	DA	24	GLU	3.5
2	FB	1083	U	3.5
42	QA	1	MET	3.5
35	JA	123	GLU	3.5
24	X	10	THR	3.5
53	BB	48	THR	3.5
10	NB	84	GLY	3.5
43	RA	117	HIS	3.5
10	NB	111	PRO	3.5
2	FB	1093	G	3.5
22	ZB	46	LYS	3.4
33	KC	37	GLY	3.4
43	RA	127	LYS	3.4
14	RB	104	PHE	3.4
2	FB	2121	G	3.4
54	CB	10	LEU	3.4
38	MA	26	CYS	3.4
38	MA	24	GLU	3.4
53	FD	52	TYR	3.4
5	IB	51	VAL	3.4
53	BB	76	PRO	3.4
54	GD	74	LYS	3.4
25	CC	2	SER	3.4
15	O	72	ASP	3.4
55	DB	8	THR	3.4
43	RA	66	ARG	3.4
38	MA	32	ALA	3.4
50	CD	7	ALA	3.4
47	ZC	97	PRO	3.4
24	BC	74	ARG	3.3
38	MA	56	VAL	3.3
53	BB	49	ILE	3.3
55	DB	15	ARG	3.3
24	BC	75	LEU	3.3
41	PA	156	TRP	3.3
33	KC	7	VAL	3.3
1	EB	1286	A	3.3
10	NB	1	MET	3.3
24	BC	18	ALA	3.3
2	FB	34	C	3.3
2	FB	1100	C	3.3
36	OC	152	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
38	MA	151	LYS	3.3
43	VC	74	ILE	3.3
16	P	88	ASP	3.3
51	DD	30	PRO	3.3
50	YA	8	ARG	3.3
54	GD	18	GLN	3.3
44	SA	63	PHE	3.3
53	FD	71	LEU	3.3
45	XC	11	LYS	3.3
54	GD	19	SER	3.3
5	E	230	ASP	3.3
43	RA	116	LYS	3.3
55	DB	3	LYS	3.3
10	NB	39	ALA	3.3
43	RA	74	ILE	3.3
54	CB	22	ARG	3.2
36	KA	163	PHE	3.2
36	OC	71	VAL	3.2
2	FB	2799	A	3.2
45	XC	126	ARG	3.2
48	AD	23	ARG	3.2
37	LA	87	LEU	3.2
46	YC	93	LEU	3.2
36	OC	239	VAL	3.2
43	RA	43	ALA	3.2
9	MB	93	GLY	3.2
53	BB	81	ARG	3.2
43	VC	125	TYR	3.2
35	NC	239	THR	3.2
13	QB	150	ALA	3.2
41	PA	2	ALA	3.2
37	LA	175	LEU	3.2
16	P	87	PHE	3.2
22	ZB	37	VAL	3.2
38	MA	137	SER	3.2
37	PC	166	GLU	3.2
54	CB	18	GLN	3.2
54	GD	25	ARG	3.2
47	ZC	105	THR	3.2
25	Y	48	LYS	3.1
38	QC	4	TYR	3.1
2	B	615	G	3.1

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Mol	Chain	Res	Type	RSRZ
9	MB	72	ILE	3.1
33	KC	17	ILE	3.1
10	NB	83	ALA	3.1
23	W	78	LYS	3.1
46	UA	47	LYS	3.1
36	OC	215	LEU	3.1
38	QC	26	CYS	3.1
2	B	1762	A	3.1
2	FB	1084	A	3.1
36	KA	172	ILE	3.1
37	LA	39	ILE	3.1
30	HC	11	LEU	3.1
41	PA	124	LEU	3.1
41	TC	101	LEU	3.1
2	FB	1058	G	3.1
32	JC	28	GLY	3.1
44	WC	58	ASP	3.1
36	OC	136	VAL	3.1
43	RA	120	ARG	3.1
16	TB	91	PRO	3.1
21	YB	72	LYS	3.1
33	KC	33	LYS	3.1
39	NA	17	ALA	3.1
1	A	1251	A	3.1
30	DA	23	THR	3.1
33	GA	8	LYS	3.1
2	FB	1059	G	3.1
9	MB	164	TYR	3.1
47	ZC	19	LEU	3.1
54	CB	62	LEU	3.1
10	NB	91	SER	3.1
53	FD	11	VAL	3.1
10	NB	85	GLU	3.1
48	AD	15	LYS	3.1
43	VC	49	PRO	3.1
10	J	43	ASN	3.0
30	HC	2	ALA	3.0
52	AB	79	LEU	3.0
2	B	1058	G	3.0
38	MA	3	ARG	3.0
38	QC	2	GLY	3.0
30	DA	52	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
54	GD	30	LYS	3.0
32	JC	65	GLU	3.0
54	CB	60	GLU	3.0
43	VC	21	PRO	3.0
35	JA	259	ASP	3.0
16	TB	7	TYR	3.0
43	VC	19	LEU	3.0
46	UA	30	ALA	3.0
54	CB	21	LYS	3.0
41	TC	26	PHE	3.0
16	TB	51	ALA	3.0
50	CD	17	TYR	3.0
46	YC	14	GLY	3.0
38	MA	128	VAL	3.0
43	RA	108	VAL	3.0
44	SA	44	VAL	3.0
50	YA	59	TRP	3.0
41	PA	85	TYR	3.0
24	X	5	LYS	3.0
16	TB	58	LEU	3.0
39	NA	128	PRO	3.0
41	PA	4	ARG	3.0
54	CB	28	ALA	3.0
30	HC	8	LYS	3.0
1	EB	85	U	3.0
15	O	23	ASN	3.0
1	A	1253	G	2.9
9	MB	168	PRO	2.9
6	JB	184	VAL	2.9
54	GD	69	GLY	2.9
17	UB	76	PHE	2.9
43	VC	18	PHE	2.9
43	VC	33	PHE	2.9
1	EB	526	C	2.9
1	A	82	U	2.9
42	QA	36	LEU	2.9
44	WC	100	THR	2.9
48	AD	22	THR	2.9
2	FB	1099	G	2.9
33	KC	26	ILE	2.9
38	QC	21	LEU	2.9
54	GD	10	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	FB	961	C	2.9
1	EB	1364	U	2.9
6	F	195	LEU	2.9
32	JC	46	ARG	2.9
36	OC	132	LYS	2.9
2	B	508	G	2.9
1	EB	974	A	2.9
53	FD	34	TRP	2.9
44	SA	72	VAL	2.9
43	RA	114	TYR	2.9
45	TA	118	GLY	2.9
31	IC	48	LYS	2.9
55	HD	3	LYS	2.9
47	VA	5	ALA	2.9
51	ZA	7	THR	2.9
9	MB	144	VAL	2.9
9	MB	174	GLY	2.9
50	YA	25	ARG	2.9
2	B	988	A	2.9
10	J	89	TYR	2.9
33	KC	9	ARG	2.9
50	YA	39	TYR	2.9
45	TA	21	ILE	2.9
54	CB	16	HIS	2.8
47	VA	118	ALA	2.8
8	LB	164	GLU	2.8
43	RA	128	ARG	2.8
35	JA	160	LYS	2.8
11	OB	60	ILE	2.8
50	CD	6	LEU	2.8
35	JA	156	HIS	2.8
1	A	1531	A	2.8
2	B	945	A	2.8
9	MB	12	PRO	2.8
18	VB	52	ARG	2.8
55	HD	15	ARG	2.8
5	IB	261	LYS	2.8
55	DB	25	LYS	2.8
10	NB	140	LEU	2.8
13	M	82	GLY	2.8
43	VC	43	ALA	2.8
46	UA	22	SER	2.8

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Mol	Chain	Res	Type	RSRZ
13	QB	50	ARG	2.8
6	JB	150	VAL	2.8
24	BC	10	THR	2.8
35	JA	184	VAL	2.8
5	E	276	LYS	2.8
43	VC	127	LYS	2.8
53	FD	33	THR	2.8
14	N	19	GLY	2.8
32	FA	64	TYR	2.8
11	OB	114	ARG	2.8
20	XB	97	LYS	2.8
53	FD	38	SER	2.8
8	H	176	LEU	2.8
9	I	171	LEU	2.8
32	JC	32	LEU	2.8
44	SA	42	THR	2.8
53	FD	73	GLU	2.8
5	IB	49	ILE	2.8
41	TC	120	ILE	2.8
50	YA	33	ILE	2.8
38	QC	161	ASN	2.8
2	B	154(A)	C	2.8
16	P	6	ALA	2.8
19	WB	19	LYS	2.8
43	VC	38	GLN	2.8
22	ZB	61	ILE	2.8
24	BC	22	GLY	2.7
50	YA	26	ARG	2.7
10	J	95	LYS	2.7
16	TB	33	LYS	2.7
40	OA	48	LEU	2.7
48	WA	44	LEU	2.7
8	H	29	TRP	2.7
33	GA	33	LYS	2.7
53	FD	70	LYS	2.7
54	GD	75	ASN	2.7
43	VC	13	ALA	2.7
19	WB	80	GLN	2.7
41	PA	62	PHE	2.7
1	A	87	A	2.7
22	ZB	22	GLY	2.7
37	LA	2	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
47	ZC	63	THR	2.7
54	CB	35	THR	2.7
47	ZC	99	ARG	2.7
46	UA	126	LYS	2.7
1	EB	1509	C	2.7
21	YB	26	TYR	2.7
48	AD	21	TYR	2.7
13	QB	128	HIS	2.7
48	WA	20	ALA	2.7
2	FB	1055	G	2.7
36	KA	214	ILE	2.7
39	NA	76	ILE	2.7
11	K	10	GLU	2.7
55	DB	9	ARG	2.7
41	TC	77	SER	2.7
46	UA	21	LYS	2.7
12	PB	32	TYR	2.7
10	J	92	VAL	2.7
10	NB	72	LEU	2.7
41	PA	153	HIS	2.7
37	LA	10	PHE	2.7
39	NA	45	PHE	2.7
9	MB	175	LYS	2.7
54	CB	68	LYS	2.7
31	EA	45	ALA	2.7
46	UA	108	ALA	2.7
53	FD	51	VAL	2.7
35	NC	238	ASN	2.7
14	RB	103	MET	2.6
14	N	85	LYS	2.6
48	WA	17	LYS	2.6
54	GD	21	LYS	2.6
6	JB	163	GLU	2.6
22	ZB	29	GLU	2.6
24	BC	6	GLY	2.6
38	QC	31	CYS	2.6
8	H	133	LEU	2.6
38	MA	120	LEU	2.6
53	FD	5	LEU	2.6
54	CB	24	LEU	2.6
14	N	138	ASP	2.6
42	QA	25	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
16	P	13	ARG	2.6
16	TB	3	ARG	2.6
1	A	1351	U	2.6
46	UA	16	GLU	2.6
37	LA	207	VAL	2.6
38	MA	112	VAL	2.6
41	TC	2	ALA	2.6
43	VC	99	LEU	2.6
2	B	2136	C	2.6
4	D	17	C	2.6
38	MA	146	ILE	2.6
38	QC	18	LYS	2.6
54	CB	80	ARG	2.6
55	DB	22	ARG	2.6
9	MB	123	PHE	2.6
22	ZB	66	PRO	2.6
30	DA	4	GLU	2.6
10	NB	81	VAL	2.6
15	SB	25	ALA	2.6
43	VC	106	ALA	2.6
43	VC	109	VAL	2.6
8	H	39	ILE	2.6
37	LA	5	ILE	2.6
50	YA	1	MET	2.6
20	T	94	ASP	2.6
37	LA	188	LEU	2.6
16	TB	69	VAL	2.6
40	SC	90	VAL	2.6
53	BB	60	VAL	2.6
35	NC	267	LYS	2.6
44	WC	75	ILE	2.6
41	PA	154	TYR	2.6
1	A	1252	A	2.6
47	ZC	101	GLN	2.6
43	RA	115	GLY	2.6
43	VC	34	ASN	2.6
13	QB	45	LEU	2.6
42	QA	39	LEU	2.6
9	MB	96	ALA	2.6
12	PB	41	ALA	2.6
35	NC	232	ALA	2.6
38	MA	18	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
54	GD	12	ALA	2.6
24	BC	43	THR	2.6
17	UB	102	ILE	2.5
14	N	3	MET	2.5
42	UC	1	MET	2.5
51	ZA	6	LEU	2.5
52	AB	44	LEU	2.5
1	EB	1224	G	2.5
17	Q	98	LYS	2.5
17	Q	112	ARG	2.5
38	MA	154	ASN	2.5
46	UA	19	ARG	2.5
50	YA	5	ARG	2.5
2	B	276	A	2.5
27	AA	1	MET	2.5
2	FB	790	C	2.5
44	WC	54	PHE	2.5
48	WA	37	PHE	2.5
33	GA	30	PRO	2.5
37	PC	196	LEU	2.5
33	KC	8	LYS	2.5
48	WA	11	LYS	2.5
8	H	54	GLU	2.5
54	CB	26	ASN	2.5
31	EA	1	MET	2.5
35	NC	226	THR	2.5
19	WB	75	PHE	2.5
24	BC	7	LEU	2.5
4	MC	75	C	2.5
10	NB	90	GLY	2.5
32	JC	44	LYS	2.5
47	ZC	100	GLY	2.5
51	ZA	100	LYS	2.5
53	FD	9	VAL	2.5
35	JA	232	ALA	2.5
54	CB	76	ALA	2.5
17	UB	50	ILE	2.5
45	XC	36	ASP	2.5
53	FD	49	ILE	2.5
39	NA	26	PHE	2.5
9	MB	138	LYS	2.5
16	P	92	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
18	VB	13	LYS	2.5
2	FB	2170	A	2.5
13	QB	43	GLY	2.5
25	Y	28	GLY	2.5
35	JA	258	GLN	2.5
49	BD	71	GLN	2.5
35	JA	257	CYS	2.5
36	OC	173	ALA	2.5
10	NB	120	ILE	2.5
18	R	37	GLU	2.5
36	KA	211	ILE	2.5
48	AD	7	ILE	2.5
44	SA	100	THR	2.5
36	KA	133	LYS	2.5
47	ZC	94	ARG	2.5
5	E	9	TYR	2.5
6	F	148	GLY	2.5
41	PA	81	GLY	2.5
47	ZC	117	VAL	2.5
35	JA	200	ALA	2.4
43	RA	119	ALA	2.4
2	B	1938	A	2.4
16	TB	13	ARG	2.4
24	BC	20	ARG	2.4
35	JA	267	LYS	2.4
55	HD	10	ARG	2.4
10	NB	40	THR	2.4
1	EB	1325	C	2.4
2	B	2798	C	2.4
24	BC	21	LEU	2.4
42	UC	10	LEU	2.4
18	R	2	PRO	2.4
43	RA	36	TYR	2.4
8	LB	20	ILE	2.4
33	GA	28	GLU	2.4
43	VC	37	PHE	2.4
20	XB	99	ARG	2.4
33	GA	2	LYS	2.4
13	QB	88	LEU	2.4
35	JA	238	ASN	2.4
47	ZC	106	ASN	2.4
2	B	2062	A	2.4

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Mol	Chain	Res	Type	RSRZ
43	VC	75	ASP	2.4
9	I	168	PRO	2.4
6	JB	186	GLY	2.4
7	KB	97	TYR	2.4
8	H	25	TYR	2.4
48	WA	55	GLY	2.4
23	AC	118	GLN	2.4
44	SA	50	ILE	2.4
48	AD	30	ALA	2.4
12	PB	1	MET	2.4
14	N	10	ARG	2.4
43	RA	111	ARG	2.4
44	SA	45	ARG	2.4
45	TA	123	LYS	2.4
48	AD	17	LYS	2.4
44	WC	48	THR	2.4
54	CB	98	PRO	2.4
42	UC	4	ASP	2.4
53	BB	9	VAL	2.4
5	IB	55	GLY	2.4
16	P	7	TYR	2.4
24	X	6	GLY	2.4
35	NC	236	HIS	2.4
50	YA	13	HIS	2.4
35	NC	244	ILE	2.4
36	KA	186	ALA	2.4
33	KC	1	MET	2.4
42	QA	88	LYS	2.4
1	EB	110	C	2.4
1	EB	1354	C	2.4
22	ZB	106	LEU	2.4
44	SA	65	LEU	2.4
6	JB	188	VAL	2.4
8	H	160	VAL	2.4
13	QB	19	VAL	2.4
36	KA	202	PRO	2.4
14	RB	19	GLY	2.4
35	JA	122	ASP	2.4
35	NC	194	GLY	2.4
47	VA	100	GLY	2.4
54	GD	9	ASN	2.4
7	G	146	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
9	MB	136	ILE	2.4
16	TB	37	ALA	2.4
53	FD	75	ALA	2.4
14	RB	60	ARG	2.4
21	U	1	MET	2.4
23	W	81	ARG	2.4
46	YC	12	ARG	2.4
43	VC	73	GLN	2.4
36	OC	163	PHE	2.4
2	B	2799	A	2.4
35	JA	153	GLU	2.4
2	FB	1061	U	2.4
32	FA	63	PRO	2.4
53	BB	82	GLY	2.3
6	JB	13	ARG	2.3
8	LB	12	TYR	2.3
25	CC	21	ARG	2.3
16	TB	87	PHE	2.3
23	W	183	LEU	2.3
30	HC	10	LEU	2.3
35	JA	127	PHE	2.3
49	XA	71	GLN	2.3
16	TB	28	VAL	2.3
31	IC	46	VAL	2.3
41	PA	80	VAL	2.3
2	FB	1054	A	2.3
54	GD	70	SER	2.3
8	H	157	ILE	2.3
25	Y	61	ARG	2.3
43	VC	16	ARG	2.3
44	WC	23	ILE	2.3
53	BB	31	ILE	2.3
35	NC	264	HIS	2.3
2	FB	546	C	2.3
37	PC	188	LEU	2.3
8	H	168	GLU	2.3
2	FB	1062	G	2.3
2	FB	2805	G	2.3
9	MB	26	VAL	2.3
33	KC	16	VAL	2.3
43	VC	41	VAL	2.3
43	RA	118	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
48	AD	31	ARG	2.3
50	CD	18	ARG	2.3
19	WB	101	GLY	2.3
38	MA	5	ILE	2.3
47	ZC	118	ALA	2.3
54	CB	59	ALA	2.3
2	FB	1669	A	2.3
15	O	69	ASP	2.3
15	O	71	GLN	2.3
21	U	90	GLU	2.3
32	FA	65	GLU	2.3
46	UA	73	GLU	2.3
2	FB	267	C	2.3
2	FB	2586	C	2.3
12	PB	66	LYS	2.3
29	GC	8	LYS	2.3
47	ZC	98	VAL	2.3
50	YA	2	VAL	2.3
55	DB	6	ARG	2.3
30	HC	41	PRO	2.3
36	KA	167	PRO	2.3
8	H	177	GLY	2.3
44	SA	6	ILE	2.3
10	NB	115	ALA	2.3
43	RA	71	SER	2.3
13	QB	85	LEU	2.3
30	HC	36	LEU	2.3
53	BB	69	HIS	2.3
54	GD	62	LEU	2.3
1	A	107	G	2.3
2	B	275	G	2.3
14	N	32	PHE	2.3
25	CC	16	ASN	2.3
30	DA	33	LYS	2.3
2	FB	1067	A	2.3
14	N	27	VAL	2.3
10	J	119	PRO	2.3
37	LA	152	ILE	2.3
44	SA	41	PRO	2.3
36	KA	99	GLY	2.3
6	F	117	MET	2.3
21	U	56	THR	2.3

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Mol	Chain	Res	Type	RSRZ
30	DA	10	LEU	2.3
54	CB	104	LEU	2.3
43	VC	36	TYR	2.3
45	TA	125	PHE	2.3
39	RC	121	LYS	2.3
41	PA	37	ASN	2.3
46	YC	13	LYS	2.3
5	IB	43	ARG	2.3
33	KC	36	GLN	2.3
54	GD	22	ARG	2.3
6	F	127	ASP	2.3
28	BA	56	VAL	2.3
41	TC	80	VAL	2.3
51	DD	58	GLU	2.2
9	MB	148	ILE	2.2
17	UB	110	ILE	2.2
54	CB	69	GLY	2.2
2	B	1095	A	2.2
2	FB	1060	U	2.2
9	MB	67	LEU	2.2
36	OC	28	PHE	2.2
41	TC	62	PHE	2.2
54	CB	74	LYS	2.2
2	FB	271(B)	C	2.2
24	X	11	ARG	2.2
43	RA	93	ARG	2.2
30	HC	43	CYS	2.2
44	WC	24	VAL	2.2
8	LB	168	GLU	2.2
12	PB	68	GLU	2.2
14	RB	42	ILE	2.2
38	MA	67	ILE	2.2
22	ZB	5	MET	2.2
38	MA	101	LEU	2.2
42	QA	2	LEU	2.2
17	Q	113	LYS	2.2
48	WA	4	LYS	2.2
53	BB	63	THR	2.2
54	GD	27	LYS	2.2
54	GD	71	THR	2.2
2	B	614	U	2.2
13	QB	21	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
14	RB	96	VAL	2.2
26	DC	6	VAL	2.2
19	S	53	GLU	2.2
2	B	1537	C	2.2
49	XA	49	ASP	2.2
9	MB	29	PRO	2.2
10	NB	119	PRO	2.2
55	HD	4	GLY	2.2
55	HD	16	GLY	2.2
41	TC	41	ARG	2.2
13	QB	32	THR	2.2
40	OA	50	TYR	2.2
42	UC	53	VAL	2.2
43	VC	108	VAL	2.2
9	I	9	ILE	2.2
39	NA	50	GLU	2.2
49	XA	66	LEU	2.2
39	RC	22	GLY	2.2
53	BB	50	ALA	2.2
8	H	8	LYS	2.2
19	S	6	LYS	2.2
50	YA	12	LYS	2.2
53	BB	78	ARG	2.2
1	A	1397	C	2.2
3	GB	88	C	2.2
6	F	135	HIS	2.2
14	RB	21	THR	2.2
50	CD	69	THR	2.2
9	I	107	VAL	2.2
16	TB	98	VAL	2.2
21	YB	59	VAL	2.2
35	JA	255	VAL	2.2
36	OC	174	VAL	2.2
43	VC	14	VAL	2.2
9	MB	80	SER	2.2
9	MB	151	ILE	2.2
19	S	73	SER	2.2
53	BB	35	SER	2.2
5	IB	147	LEU	2.2
15	O	111	LEU	2.2
36	KA	98	LEU	2.2
47	VA	90	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
36	KA	101	MET	2.2
41	PA	31	MET	2.2
5	E	35	LYS	2.2
16	P	19	LYS	2.2
35	JA	189	ALA	2.2
2	FB	2797	U	2.2
47	VA	94	ARG	2.2
34	HA	15	A	2.2
14	N	21	THR	2.1
37	PC	48	TYR	2.1
44	SA	4	ILE	2.1
47	VA	4	ILE	2.1
39	NA	12	LEU	2.1
43	VC	50	LEU	2.1
23	AC	189	ALA	2.1
43	RA	122	ALA	2.1
21	U	60	ARG	2.1
36	OC	159	PRO	2.1
41	PA	32	ARG	2.1
20	XB	94	ASP	2.1
39	NA	82	VAL	2.1
6	JB	107	THR	2.1
11	OB	78	TYR	2.1
19	WB	70	ILE	2.1
36	KA	185	ILE	2.1
8	LB	75	LYS	2.1
9	MB	71	LEU	2.1
32	FA	36	LYS	2.1
54	GD	29	LYS	2.1
2	B	1099	G	2.1
13	M	38	GLN	2.1
5	IB	209	ALA	2.1
13	M	65	ARG	2.1
38	MA	122	ARG	2.1
38	QC	118	ARG	2.1
39	NA	18	ARG	2.1
39	RC	14	ARG	2.1
41	TC	110	GLN	2.1
51	ZA	93	GLN	2.1
41	PA	83	ALA	2.1
54	CB	17	ARG	2.1
5	E	237	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
38	MA	113	SER	2.1
38	QC	163	GLU	2.1
39	RC	81	GLU	2.1
38	MA	206	PHE	2.1
30	HC	52	VAL	2.1
1	A	1364	U	2.1
13	QB	108	LYS	2.1
23	AC	125	LEU	2.1
33	GA	24	TYR	2.1
37	LA	150	LYS	2.1
41	PA	36	LYS	2.1
43	RA	40	LEU	2.1
43	VC	116	LYS	2.1
46	UA	28	LYS	2.1
51	ZA	32	TYR	2.1
6	F	149	ARG	2.1
31	EA	47	ARG	2.1
8	LB	26	GLN	2.1
44	SA	20	ALA	2.1
1	EB	1092	A	2.1
2	B	1536	A	2.1
9	I	53	GLU	2.1
13	M	11	GLY	2.1
16	P	91	PRO	2.1
2	B	1068	G	2.1
14	N	109	VAL	2.1
22	ZB	15	VAL	2.1
9	MB	85	LYS	2.1
13	M	6	LEU	2.1
23	AC	163	LEU	2.1
32	JC	41	ILE	2.1
38	MA	134	ASP	2.1
50	YA	23	ASP	2.1
54	CB	14	LYS	2.1
28	BA	55	ARG	2.1
37	PC	191	THR	2.1
41	TC	85	TYR	2.1
9	MB	145	ALA	2.1
48	AD	2	ALA	2.1
44	WC	84	GLN	2.1
9	I	159	GLU	2.1
24	X	45	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
42	UC	136	GLU	2.1
43	RA	26	VAL	2.1
2	FB	1069	A	2.1
36	OC	133	LYS	2.1
10	NB	31	LEU	2.1
26	Z	68	ARG	2.1
37	PC	175	LEU	2.1
38	MA	58	LEU	2.1
38	MA	204	ILE	2.1
45	XC	42	TRP	2.1
40	OA	55	ASP	2.1
15	SB	21	TYR	2.1
37	LA	201	TYR	2.1
1	EB	1001	G	2.1
2	FB	1063	G	2.1
5	IB	41	GLY	2.1
8	H	134	GLY	2.1
12	PB	5	GLN	2.1
53	FD	84	GLY	2.1
55	DB	2	GLY	2.1
6	JB	200	GLU	2.1
11	K	100	GLU	2.1
38	MA	179	GLU	2.1
1	A	294	U	2.0
6	JB	155	LYS	2.0
9	MB	140	LYS	2.0
14	RB	72	LYS	2.0
25	CC	32	LYS	2.0
8	H	53	LEU	2.0
10	J	79	ILE	2.0
37	LA	42	LEU	2.0
38	MA	162	LEU	2.0
41	TC	156	TRP	2.0
37	PC	23	TYR	2.0
6	JB	125	GLY	2.0
25	CC	36	GLY	2.0
36	KA	183	PRO	2.0
55	DB	23	PRO	2.0
43	VC	35	GLU	2.0
1	EB	1249	C	2.0
2	FB	2145	C	2.0
16	TB	59	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
9	MB	99	VAL	2.0
36	KA	184	VAL	2.0
44	WC	34	VAL	2.0
44	WC	44	VAL	2.0
8	LB	173	LEU	2.0
37	LA	91	LEU	2.0
39	RC	43	LEU	2.0
41	TC	78	ARG	2.0
42	UC	84	ARG	2.0
43	VC	40	LEU	2.0
50	YA	28	ARG	2.0
55	DB	10	ARG	2.0
49	XA	50	HIS	2.0
8	LB	162	THR	2.0
33	KC	12	ASP	2.0
24	BC	73	GLY	2.0
50	CD	37	GLY	2.0
8	H	36	LYS	2.0
22	V	74	PRO	2.0
30	DA	27	LYS	2.0
53	FD	32	LYS	2.0
14	RB	48	GLU	2.0
23	W	122	ARG	2.0
11	K	112	LEU	2.0
16	TB	32	LEU	2.0
36	KA	200	ILE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PSU	HB	55	20/21	0.58	0.13	204,205,205,206	0
4	PSU	D	55	20/21	0.66	0.08	198,199,201,202	0
4	5MU	D	54	21/22	0.66	0.09	196,198,198,199	0
4	5MC	HB	32	21/22	0.67	0.10	149,150,150,150	0
4	4SU	HB	8	20/21	0.69	0.08	194,196,197,198	0
4	5MU	HB	54	21/22	0.69	0.12	201,202,204,204	0
4	4SU	IA	8	20/21	0.72	0.09	149,150,152,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PSU	MC	55	20/21	0.73	0.11	178,182,187,188	0
4	PSU	IA	55	20/21	0.74	0.09	170,174,179,180	0
4	4SU	MC	8	20/21	0.76	0.09	160,161,164,164	0
4	5MU	MC	54	21/22	0.76	0.14	180,185,189,190	0
4	4SU	D	8	20/21	0.77	0.08	191,192,192,192	0
4	5MC	MC	32	21/22	0.78	0.14	120,120,120,120	0
46	0TD	UA	92	10/11	0.79	0.26	102,103,103,104	0
4	5MC	D	32	21/22	0.81	0.08	164,164,165,165	0
4	5MU	IA	54	21/22	0.81	0.11	171,176,179,181	0
1	2MG	EB	1207	24/25	0.82	0.12	129,130,132,133	0
2	PSU	FB	1917	20/21	0.83	0.09	97,99,101,102	0
2	PSU	FB	1911	20/21	0.84	0.11	99,102,103,104	0
46	0TD	YC	92	10/11	0.85	0.29	93,94,94,94	0
2	5MU	B	1915	21/22	0.85	0.09	96,98,101,101	0
4	5MC	IA	32	21/22	0.86	0.14	119,119,120,120	0
2	PSU	B	1911	20/21	0.87	0.11	93,96,99,99	0
1	PSU	EB	516	20/21	0.87	0.08	98,99,102,102	0
2	5MU	FB	1915	21/22	0.87	0.09	104,105,108,108	0
1	PSU	A	516	20/21	0.88	0.08	112,114,117,117	0
1	4OC	A	1402	22/23	0.89	0.13	99,100,101,102	0
1	2MG	A	1207	24/25	0.89	0.11	134,135,137,138	0
2	5MC	B	1942	21/22	0.90	0.09	67,69,70,71	0
1	UR3	EB	1498	21/22	0.90	0.15	96,96,96,97	0
1	UR3	A	1498	21/22	0.91	0.14	95,95,96,96	0
2	PSU	B	1917	20/21	0.91	0.08	91,92,95,96	0
1	4OC	EB	1402	22/23	0.91	0.12	95,96,97,97	0
1	5MC	EB	967	21/22	0.92	0.09	117,119,122,123	0
2	5MC	FB	1962	21/22	0.93	0.09	78,80,82,82	0
2	PSU	B	2605	20/21	0.93	0.09	59,61,62,62	0
2	5MU	B	1939	21/22	0.93	0.11	63,64,65,66	0
1	5MC	A	967	21/22	0.93	0.10	121,123,125,126	0
1	7MG	EB	527	24/25	0.93	0.16	92,94,95,95	0
1	M2G	EB	966	25/26	0.93	0.12	114,117,120,121	0
2	2MA	B	2503	23/24	0.93	0.12	56,57,57,58	0
2	5MU	FB	1939	21/22	0.93	0.11	73,74,74,75	0
2	5MC	FB	1942	21/22	0.93	0.08	76,78,79,79	0
1	5MC	EB	1400	21/22	0.94	0.10	100,103,105,106	0
1	M2G	A	966	25/26	0.94	0.11	119,121,124,124	0
2	OMG	FB	2251	24/25	0.94	0.11	76,78,80,80	0
1	5MC	EB	1407	21/22	0.94	0.09	89,90,91,91	0
1	5MC	A	1404	21/22	0.94	0.11	91,93,94,94	0
2	5MC	B	1962	21/22	0.94	0.09	70,71,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MC	A	1400	21/22	0.94	0.10	105,107,109,111	0
2	2MU	B	2552	21/23	0.94	0.11	64,66,66,66	0
2	4OC	FB	1920	21/23	0.94	0.11	96,98,99,101	0
2	4OC	B	1920	21/23	0.94	0.09	90,93,94,96	0
1	5MC	EB	1404	21/22	0.95	0.13	87,89,89,90	0
2	2MA	FB	2503	23/24	0.95	0.10	70,71,72,72	0
2	PSU	FB	2605	20/21	0.95	0.09	71,72,73,73	0
1	MA6	EB	1519	24/25	0.95	0.15	84,86,87,87	0
1	5MC	A	1407	21/22	0.95	0.10	87,88,90,91	0
1	MA6	A	1518	24/25	0.96	0.10	84,86,88,88	0
2	2MU	FB	2552	21/23	0.96	0.08	74,76,76,77	0
1	7MG	A	527	24/25	0.96	0.09	102,105,106,107	0
1	MA6	EB	1518	24/25	0.96	0.13	84,86,87,88	0
2	OMG	B	2251	24/25	0.96	0.09	64,66,67,67	0
1	MA6	A	1519	24/25	0.97	0.10	85,87,88,89	0

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FB	9237	1/1	-0.60	0.26	252,252,252,252	0
56	MG	A	1700	1/1	-0.55	0.29	169,169,169,169	0
56	MG	HB	103	1/1	-0.54	0.23	188,188,188,188	0
56	MG	FB	9157	1/1	-0.48	0.17	181,181,181,181	0
56	MG	HB	101	1/1	-0.46	0.32	204,204,204,204	0
56	MG	A	1781	1/1	-0.36	0.18	232,232,232,232	0
56	MG	FB	9396	1/1	-0.28	0.37	245,245,245,245	0
56	MG	EB	1603	1/1	-0.27	0.42	146,146,146,146	0
56	MG	EB	1669	1/1	-0.24	0.35	148,148,148,148	0
56	MG	EB	1706	1/1	-0.21	0.27	181,181,181,181	0
56	MG	A	1670	1/1	-0.21	0.19	168,168,168,168	0
56	MG	B	9177	1/1	-0.17	0.35	188,188,188,188	0
56	MG	A	1611	1/1	-0.15	0.39	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	HB	109	1/1	-0.15	0.24	182,182,182,182	0
56	MG	MC	101	1/1	-0.15	0.28	169,169,169,169	0
56	MG	EB	1709	1/1	-0.13	0.23	181,181,181,181	0
56	MG	AD	101	1/1	-0.13	0.33	137,137,137,137	0
56	MG	A	1631	1/1	-0.12	0.25	180,180,180,180	0
56	MG	A	1778	1/1	-0.11	0.13	243,243,243,243	0
56	MG	B	9522	1/1	-0.09	0.28	137,137,137,137	0
56	MG	A	1789	1/1	-0.07	0.19	183,183,183,183	0
56	MG	EB	1611	1/1	-0.06	0.33	172,172,172,172	0
56	MG	EB	1778	1/1	-0.06	0.16	191,191,191,191	0
56	MG	HB	102	1/1	-0.05	0.24	187,187,187,187	0
56	MG	A	1628	1/1	-0.05	0.45	135,135,135,135	0
56	MG	HB	104	1/1	-0.05	0.17	198,198,198,198	0
56	MG	A	1746	1/1	-0.04	0.33	156,156,156,156	0
56	MG	A	1646	1/1	-0.03	0.22	214,214,214,214	0
56	MG	B	9483	1/1	0.01	0.15	202,202,202,202	0
56	MG	FB	9180	1/1	0.03	0.27	174,174,174,174	0
56	MG	EB	1784	1/1	0.06	0.20	184,184,184,184	0
56	MG	A	1656	1/1	0.06	0.26	162,162,162,162	0
56	MG	B	9219	1/1	0.07	0.21	177,177,177,177	0
56	MG	A	1652	1/1	0.08	0.18	151,151,151,151	0
56	MG	EB	1696	1/1	0.10	0.23	167,167,167,167	0
56	MG	EB	1641	1/1	0.10	0.50	136,136,136,136	0
56	MG	A	1654	1/1	0.12	0.23	169,169,169,169	0
56	MG	B	9414	1/1	0.12	0.23	138,138,138,138	0
56	MG	A	1658	1/1	0.13	0.28	127,127,127,127	0
56	MG	A	1784	1/1	0.13	0.23	152,152,152,152	0
56	MG	EB	1760	1/1	0.14	0.23	153,153,153,153	0
56	MG	EB	1675	1/1	0.15	0.21	164,164,164,164	0
56	MG	A	1620	1/1	0.15	0.47	118,118,118,118	0
56	MG	FB	9383	1/1	0.16	0.23	184,184,184,184	0
56	MG	EB	1758	1/1	0.16	0.25	127,127,127,127	0
56	MG	HB	108	1/1	0.16	0.23	146,146,146,146	0
56	MG	EB	1785	1/1	0.17	0.15	185,185,185,185	0
56	MG	B	9237	1/1	0.17	0.20	149,149,149,149	0
56	MG	A	1675	1/1	0.19	0.32	167,167,167,167	0
56	MG	A	1769	1/1	0.19	0.21	162,162,162,162	0
56	MG	A	1685	1/1	0.21	0.39	142,142,142,142	0
56	MG	EB	1679	1/1	0.22	0.27	137,137,137,137	0
56	MG	A	1727	1/1	0.22	0.22	145,145,145,145	0
56	MG	A	1793	1/1	0.23	0.30	123,123,123,123	0
56	MG	C	206	1/1	0.23	0.35	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	EB	1616	1/1	0.23	0.40	128,128,128,128	0
56	MG	IA	106	1/1	0.23	0.28	144,144,144,144	0
56	MG	SA	201	1/1	0.24	0.20	170,170,170,170	0
56	MG	A	1692	1/1	0.25	0.15	182,182,182,182	0
56	MG	EB	1720	1/1	0.26	0.26	147,147,147,147	0
56	MG	A	1696	1/1	0.27	0.42	141,141,141,141	0
56	MG	HB	107	1/1	0.27	0.23	170,170,170,170	0
56	MG	B	9298	1/1	0.28	0.24	131,131,131,131	0
56	MG	FB	9161	1/1	0.28	0.18	149,149,149,149	0
56	MG	MC	103	1/1	0.28	0.26	151,151,151,151	0
56	MG	SA	203	1/1	0.28	0.16	147,147,147,147	0
56	MG	A	1650	1/1	0.29	0.26	126,126,126,126	0
56	MG	FB	9415	1/1	0.29	0.26	120,120,120,120	0
56	MG	A	1710	1/1	0.29	0.23	138,138,138,138	0
56	MG	B	9423	1/1	0.30	0.20	144,144,144,144	0
56	MG	FB	9442	1/1	0.30	0.28	137,137,137,137	0
56	MG	FB	9407	1/1	0.30	0.20	141,141,141,141	0
56	MG	FB	9308	1/1	0.31	0.25	118,118,118,118	0
56	MG	A	1798	1/1	0.31	0.13	123,123,123,123	0
56	MG	FB	9281	1/1	0.33	0.17	151,151,151,151	0
56	MG	A	1648	1/1	0.33	0.31	138,138,138,138	0
56	MG	VC	201	1/1	0.33	0.26	164,164,164,164	0
56	MG	MB	201	1/1	0.33	0.17	148,148,148,148	0
56	MG	EB	1712	1/1	0.34	0.13	182,182,182,182	0
56	MG	EB	1660	1/1	0.34	0.16	171,171,171,171	0
56	MG	D	104	1/1	0.35	0.22	185,185,185,185	0
56	MG	EB	1775	1/1	0.35	0.40	125,125,125,125	0
56	MG	F	302	1/1	0.36	0.11	80,80,80,80	0
56	MG	B	9018	1/1	0.36	0.39	87,87,87,87	0
56	MG	GB	213	1/1	0.37	0.29	117,117,117,117	0
56	MG	EB	1749	1/1	0.39	0.37	92,92,92,92	0
56	MG	FB	9324	1/1	0.39	0.17	153,153,153,153	0
56	MG	MC	102	1/1	0.39	0.20	144,144,144,144	0
56	MG	EB	1791	1/1	0.39	0.42	120,120,120,120	0
56	MG	FB	9099	1/1	0.39	0.23	144,144,144,144	0
56	MG	A	1806	1/1	0.39	0.19	153,153,153,153	0
56	MG	GB	203	1/1	0.41	0.35	113,113,113,113	0
56	MG	EB	1755	1/1	0.41	0.20	155,155,155,155	0
56	MG	EB	1663	1/1	0.41	0.13	168,168,168,168	0
56	MG	FB	9355	1/1	0.41	0.20	226,226,226,226	0
56	MG	FB	9059	1/1	0.41	0.33	102,102,102,102	0
56	MG	B	9300	1/1	0.42	0.26	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FB	9283	1/1	0.42	0.30	116,116,116,116	0
56	MG	EB	1673	1/1	0.42	0.24	139,139,139,139	0
56	MG	B	9226	1/1	0.42	0.24	128,128,128,128	0
56	MG	IA	102	1/1	0.42	0.21	158,158,158,158	0
56	MG	FB	9379	1/1	0.43	0.24	117,117,117,117	0
56	MG	A	1701	1/1	0.43	0.22	120,120,120,120	0
56	MG	EB	1670	1/1	0.43	0.34	125,125,125,125	0
56	MG	C	204	1/1	0.43	0.22	113,113,113,113	0
56	MG	FB	9317	1/1	0.43	0.21	143,143,143,143	0
56	MG	FB	9040	1/1	0.43	0.21	134,134,134,134	0
56	MG	A	1647	1/1	0.43	0.25	157,157,157,157	0
56	MG	FB	9321	1/1	0.44	0.18	98,98,98,98	0
56	MG	D	105	1/1	0.44	0.18	126,126,126,126	0
56	MG	SA	202	1/1	0.45	0.13	144,144,144,144	0
56	MG	MC	104	1/1	0.45	0.29	115,115,115,115	0
56	MG	B	9356	1/1	0.45	0.21	91,91,91,91	0
56	MG	EB	1789	1/1	0.45	0.25	108,108,108,108	0
56	MG	MC	105	1/1	0.46	0.21	135,135,135,135	0
56	MG	EB	1769	1/1	0.46	0.20	149,149,149,149	0
56	MG	FB	9211	1/1	0.46	0.14	144,144,144,144	0
56	MG	CC	106	1/1	0.47	0.25	103,103,103,103	0
56	MG	A	1759	1/1	0.47	0.26	123,123,123,123	0
56	MG	FB	9047	1/1	0.47	0.26	85,85,85,85	0
56	MG	A	1651	1/1	0.47	0.34	129,129,129,129	0
56	MG	A	1678	1/1	0.47	0.15	158,158,158,158	0
56	MG	FB	9377	1/1	0.47	0.17	142,142,142,142	0
56	MG	OC	302	1/1	0.47	0.25	122,122,122,122	0
56	MG	A	1795	1/1	0.47	0.21	123,123,123,123	0
56	MG	A	1751	1/1	0.47	0.37	143,143,143,143	0
56	MG	FB	9307	1/1	0.48	0.27	215,215,215,215	0
56	MG	A	1683	1/1	0.48	0.24	146,146,146,146	0
56	MG	FB	9207	1/1	0.48	0.25	126,126,126,126	0
56	MG	LA	302	1/1	0.48	0.16	113,113,113,113	0
56	MG	FB	9177	1/1	0.49	0.30	133,133,133,133	0
56	MG	GB	209	1/1	0.49	0.27	121,121,121,121	0
56	MG	FB	9432	1/1	0.49	0.15	153,153,153,153	0
56	MG	EB	1632	1/1	0.49	0.17	136,136,136,136	0
56	MG	MB	202	1/1	0.50	0.17	169,169,169,169	0
56	MG	B	9363	1/1	0.50	0.19	111,111,111,111	0
56	MG	EB	1691	1/1	0.50	0.16	116,116,116,116	0
56	MG	B	9238	1/1	0.50	0.23	136,136,136,136	0
56	MG	A	1662	1/1	0.50	0.27	144,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	A	1624	1/1	0.51	0.28	131,131,131,131	0
56	MG	B	9444	1/1	0.51	0.17	110,110,110,110	0
56	MG	A	1610	1/1	0.51	0.34	128,128,128,128	0
56	MG	A	1699	1/1	0.51	0.17	140,140,140,140	0
56	MG	B	9370	1/1	0.51	0.22	73,73,73,73	0
56	MG	EB	1617	1/1	0.51	0.23	134,134,134,134	0
56	MG	A	1718	1/1	0.51	0.15	109,109,109,109	0
56	MG	D	101	1/1	0.51	0.17	137,137,137,137	0
56	MG	FB	9021	1/1	0.52	0.18	103,103,103,103	0
56	MG	FB	9361	1/1	0.52	0.21	118,118,118,118	0
56	MG	EB	1746	1/1	0.52	0.20	126,126,126,126	0
56	MG	C	212	1/1	0.52	0.25	109,109,109,109	0
56	MG	BA	102	1/1	0.52	0.16	147,147,147,147	0
56	MG	FB	9393	1/1	0.52	0.13	108,108,108,108	0
56	MG	EB	1672	1/1	0.52	0.31	122,122,122,122	0
56	MG	FB	9149	1/1	0.52	0.31	121,121,121,121	0
56	MG	FB	9153	1/1	0.52	0.25	123,123,123,123	0
56	MG	FB	9425	1/1	0.52	0.17	119,119,119,119	0
56	MG	FB	9336	1/1	0.52	0.28	77,77,77,77	0
56	MG	EB	1773	1/1	0.53	0.11	149,149,149,149	0
56	MG	FB	9233	1/1	0.53	0.10	117,117,117,117	0
56	MG	B	9172	1/1	0.53	0.20	78,78,78,78	0
56	MG	A	1690	1/1	0.53	0.29	133,133,133,133	0
56	MG	A	1737	1/1	0.53	0.28	97,97,97,97	0
56	MG	A	1741	1/1	0.53	0.17	111,111,111,111	0
56	MG	A	1663	1/1	0.53	0.32	94,94,94,94	0
56	MG	D	103	1/1	0.53	0.11	158,158,158,158	0
56	MG	EB	1796	1/1	0.53	0.45	109,109,109,109	0
56	MG	OC	304	1/1	0.53	0.29	122,122,122,122	0
56	MG	EB	1764	1/1	0.53	0.24	107,107,107,107	0
56	MG	B	9509	1/1	0.53	0.10	146,146,146,146	0
56	MG	B	9364	1/1	0.54	0.19	136,136,136,136	0
56	MG	A	1671	1/1	0.54	0.26	145,145,145,145	0
56	MG	FB	9278	1/1	0.54	0.30	66,66,66,66	0
56	MG	A	1688	1/1	0.54	0.17	112,112,112,112	0
56	MG	FB	9139	1/1	0.54	0.12	146,146,146,146	0
56	MG	GB	201	1/1	0.55	0.51	93,93,93,93	0
56	MG	A	1771	1/1	0.55	0.23	122,122,122,122	0
56	MG	FB	9198	1/1	0.55	0.22	128,128,128,128	0
56	MG	EB	1788	1/1	0.55	0.13	107,107,107,107	0
56	MG	A	1619	1/1	0.55	0.24	135,135,135,135	0
56	MG	B	9343	1/1	0.55	0.15	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9539	1/1	0.55	0.11	143,143,143,143	0
56	MG	FB	9423	1/1	0.55	0.22	137,137,137,137	0
56	MG	HB	106	1/1	0.55	0.16	107,107,107,107	0
56	MG	A	1744	1/1	0.55	0.20	150,150,150,150	0
56	MG	EB	1700	1/1	0.55	0.15	110,110,110,110	0
56	MG	A	1657	1/1	0.55	0.19	145,145,145,145	0
56	MG	A	1606	1/1	0.56	0.34	118,118,118,118	0
56	MG	A	1733	1/1	0.56	0.15	161,161,161,161	0
56	MG	FB	9052	1/1	0.56	0.20	89,89,89,89	0
56	MG	B	9134	1/1	0.56	0.43	53,53,53,53	0
56	MG	A	1736	1/1	0.56	0.24	122,122,122,122	0
56	MG	FB	9403	1/1	0.56	0.24	82,82,82,82	0
56	MG	B	9174	1/1	0.56	0.16	69,69,69,69	0
56	MG	B	9438	1/1	0.56	0.18	102,102,102,102	0
56	MG	A	1629	1/1	0.56	0.24	151,151,151,151	0
56	MG	FB	9349	1/1	0.56	0.18	139,139,139,139	0
56	MG	A	1754	1/1	0.56	0.29	123,123,123,123	0
56	MG	FB	9280	1/1	0.56	0.20	115,115,115,115	0
56	MG	A	1627	1/1	0.57	0.38	103,103,103,103	0
56	MG	JB	302	1/1	0.57	0.21	100,100,100,100	0
56	MG	FB	9322	1/1	0.57	0.20	132,132,132,132	0
56	MG	FB	9178	1/1	0.57	0.33	94,94,94,94	0
56	MG	EB	1605	1/1	0.57	0.31	98,98,98,98	0
56	MG	A	1801	1/1	0.57	0.22	126,126,126,126	0
56	MG	EB	1718	1/1	0.57	0.15	125,125,125,125	0
56	MG	FB	9299	1/1	0.58	0.24	89,89,89,89	0
56	MG	EB	1681	1/1	0.58	0.11	107,107,107,107	0
56	MG	FB	9165	1/1	0.58	0.24	124,124,124,124	0
56	MG	A	1717	1/1	0.58	0.20	119,119,119,119	0
56	MG	FB	9030	1/1	0.58	0.24	83,83,83,83	0
56	MG	EB	1693	1/1	0.58	0.16	176,176,176,176	0
56	MG	A	1791	1/1	0.58	0.26	110,110,110,110	0
56	MG	XA	106	1/1	0.58	0.13	109,109,109,109	0
56	MG	FB	9222	1/1	0.59	0.14	97,97,97,97	0
56	MG	FB	9282	1/1	0.59	0.25	92,92,92,92	0
56	MG	FB	9471	1/1	0.59	0.15	114,114,114,114	0
56	MG	HA	102	1/1	0.59	0.37	105,105,105,105	0
56	MG	A	1693	1/1	0.59	0.23	121,121,121,121	0
56	MG	B	9286	1/1	0.59	0.20	105,105,105,105	0
56	MG	B	9485	1/1	0.59	0.15	84,84,84,84	0
56	MG	FB	9427	1/1	0.60	0.20	105,105,105,105	0
56	MG	FB	9187	1/1	0.60	0.28	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FB	9357	1/1	0.60	0.13	94,94,94,94	0
56	MG	FB	9195	1/1	0.60	0.33	113,113,113,113	0
56	MG	FB	9027	1/1	0.60	0.30	97,97,97,97	0
56	MG	GB	202	1/1	0.60	0.53	99,99,99,99	0
56	MG	FB	9300	1/1	0.60	0.16	94,94,94,94	0
56	MG	EB	1766	1/1	0.60	0.27	125,125,125,125	0
56	MG	B	9041	1/1	0.60	0.26	71,71,71,71	0
56	MG	B	9465	1/1	0.60	0.14	111,111,111,111	0
56	MG	A	1609	1/1	0.60	0.18	129,129,129,129	0
56	MG	EB	1629	1/1	0.60	0.20	115,115,115,115	0
56	MG	FB	9060	1/1	0.60	0.24	97,97,97,97	0
56	MG	UC	202	1/1	0.60	0.15	108,108,108,108	0
56	MG	IA	105	1/1	0.60	0.28	121,121,121,121	0
56	MG	FB	9106	1/1	0.60	0.26	83,83,83,83	0
56	MG	EB	1610	1/1	0.61	0.32	96,96,96,96	0
56	MG	EB	1671	1/1	0.61	0.14	156,156,156,156	0
56	MG	B	9503	1/1	0.61	0.29	92,92,92,92	0
56	MG	FB	9344	1/1	0.61	0.21	72,72,72,72	0
56	MG	FB	9006	1/1	0.61	0.46	74,74,74,74	0
56	MG	B	9277	1/1	0.61	0.14	145,145,145,145	0
56	MG	CC	102	1/1	0.61	0.19	116,116,116,116	0
56	MG	B	9233	1/1	0.61	0.15	96,96,96,96	0
56	MG	YC	205	1/1	0.61	0.27	82,82,82,82	0
56	MG	B	9328	1/1	0.61	0.29	111,111,111,111	0
56	MG	SB	201	1/1	0.62	0.41	91,91,91,91	0
56	MG	FB	9402	1/1	0.62	0.24	118,118,118,118	0
56	MG	A	1691	1/1	0.62	0.11	240,240,240,240	0
56	MG	EB	1800	1/1	0.62	0.47	150,150,150,150	0
56	MG	B	9100	1/1	0.62	0.23	88,88,88,88	0
56	MG	FB	9011	1/1	0.62	0.29	66,66,66,66	0
56	MG	FB	9284	1/1	0.62	0.23	95,95,95,95	0
56	MG	A	1660	1/1	0.62	0.23	117,117,117,117	0
56	MG	B	9139	1/1	0.62	0.12	97,97,97,97	0
56	MG	B	9427	1/1	0.62	0.17	96,96,96,96	0
56	MG	PC	301	1/1	0.62	0.14	137,137,137,137	0
56	MG	A	1682	1/1	0.62	0.32	127,127,127,127	0
56	MG	EB	1732	1/1	0.62	0.13	142,142,142,142	0
56	MG	EB	1744	1/1	0.62	0.25	117,117,117,117	0
56	MG	FB	9053	1/1	0.62	0.31	105,105,105,105	0
56	MG	B	9292	1/1	0.63	0.17	88,88,88,88	0
56	MG	B	9336	1/1	0.63	0.14	70,70,70,70	0
56	MG	A	1721	1/1	0.63	0.40	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FB	9152	1/1	0.63	0.28	99,99,99,99	0
56	MG	FB	9472	1/1	0.63	0.27	98,98,98,98	0
56	MG	EB	1793	1/1	0.63	0.12	140,140,140,140	0
56	MG	B	9240	1/1	0.63	0.17	156,156,156,156	0
56	MG	EB	1633	1/1	0.63	0.29	96,96,96,96	0
56	MG	FB	9410	1/1	0.63	0.09	83,83,83,83	0
56	MG	JA	403	1/1	0.63	0.29	114,114,114,114	0
56	MG	B	9317	1/1	0.63	0.21	126,126,126,126	0
56	MG	B	9437	1/1	0.63	0.19	117,117,117,117	0
56	MG	EB	1638	1/1	0.64	0.30	83,83,83,83	0
56	MG	FB	9310	1/1	0.64	0.19	80,80,80,80	0
56	MG	B	9482	1/1	0.64	0.19	124,124,124,124	0
56	MG	B	9422	1/1	0.64	0.24	64,64,64,64	0
56	MG	FB	9272	1/1	0.64	0.20	124,124,124,124	0
56	MG	FB	9323	1/1	0.64	0.14	177,177,177,177	0
56	MG	B	9166	1/1	0.64	0.33	96,96,96,96	0
56	MG	A	1677	1/1	0.64	0.17	104,104,104,104	0
56	MG	B	9244	1/1	0.64	0.19	68,68,68,68	0
56	MG	HB	105	1/1	0.64	0.12	151,151,151,151	0
56	MG	B	9256	1/1	0.64	0.13	92,92,92,92	0
56	MG	B	9137	1/1	0.64	0.17	103,103,103,103	0
56	MG	B	9563	1/1	0.64	0.16	117,117,117,117	0
56	MG	A	1779	1/1	0.64	0.26	101,101,101,101	0
56	MG	FB	9219	1/1	0.64	0.18	123,123,123,123	0
56	MG	FB	9221	1/1	0.64	0.33	96,96,96,96	0
56	MG	EB	1615	1/1	0.65	0.27	90,90,90,90	0
56	MG	A	1603	1/1	0.65	0.32	69,69,69,69	0
56	MG	QA	202	1/1	0.65	0.30	111,111,111,111	0
56	MG	B	9254	1/1	0.65	0.11	94,94,94,94	0
56	MG	FB	9169	1/1	0.65	0.17	106,106,106,106	0
56	MG	UB	201	1/1	0.65	0.12	86,86,86,86	0
56	MG	A	1659	1/1	0.65	0.24	85,85,85,85	0
56	MG	B	9478	1/1	0.65	0.17	121,121,121,121	0
56	MG	A	1680	1/1	0.65	0.22	89,89,89,89	0
56	MG	FB	9296	1/1	0.65	0.20	71,71,71,71	0
56	MG	A	1720	1/1	0.65	0.16	84,84,84,84	0
56	MG	FB	9387	1/1	0.65	0.30	77,77,77,77	0
56	MG	B	9017	1/1	0.65	0.29	94,94,94,94	0
56	MG	FB	9070	1/1	0.65	0.28	89,89,89,89	0
56	MG	B	9486	1/1	0.65	0.15	71,71,71,71	0
56	MG	EB	1703	1/1	0.65	0.10	98,98,98,98	0
56	MG	QC	304	1/1	0.65	0.29	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FB	9127	1/1	0.65	0.37	111,111,111,111	0
56	MG	EB	1801	1/1	0.65	0.12	129,129,129,129	0
56	MG	B	9183	1/1	0.65	0.27	125,125,125,125	0
56	MG	EB	1612	1/1	0.65	0.27	101,101,101,101	0
56	MG	GB	215	1/1	0.66	0.32	120,120,120,120	0
56	MG	FB	9290	1/1	0.66	0.27	91,91,91,91	0
56	MG	FB	9218	1/1	0.66	0.23	150,150,150,150	0
56	MG	EB	1738	1/1	0.66	0.16	99,99,99,99	0
56	MG	A	1666	1/1	0.66	0.17	142,142,142,142	0
56	MG	A	1667	1/1	0.66	0.31	101,101,101,101	0
56	MG	FB	9416	1/1	0.66	0.26	79,79,79,79	0
56	MG	FB	9227	1/1	0.66	0.21	74,74,74,74	0
56	MG	A	1757	1/1	0.66	0.17	135,135,135,135	0
56	MG	FB	9181	1/1	0.66	0.29	75,75,75,75	0
56	MG	FB	9366	1/1	0.67	0.26	110,110,110,110	0
56	MG	FB	9418	1/1	0.67	0.18	108,108,108,108	0
56	MG	FB	9376	1/1	0.67	0.23	94,94,94,94	0
56	MG	FB	9124	1/1	0.67	0.22	118,118,118,118	0
56	MG	EB	1628	1/1	0.67	0.21	126,126,126,126	0
56	MG	FB	9429	1/1	0.67	0.11	107,107,107,107	0
56	MG	FB	9134	1/1	0.67	0.25	91,91,91,91	0
56	MG	A	1687	1/1	0.67	0.25	107,107,107,107	0
56	MG	EB	1651	1/1	0.67	0.18	124,124,124,124	0
56	MG	EB	1684	1/1	0.67	0.17	96,96,96,96	0
56	MG	EB	1767	1/1	0.67	0.17	128,128,128,128	0
56	MG	FB	9266	1/1	0.67	0.26	86,86,86,86	0
56	MG	C	214	1/1	0.67	0.26	110,110,110,110	0
56	MG	EB	1692	1/1	0.67	0.26	129,129,129,129	0
56	MG	C	210	1/1	0.67	0.21	102,102,102,102	0
56	MG	B	9012	1/1	0.68	0.17	52,52,52,52	0
56	MG	FB	9172	1/1	0.68	0.27	91,91,91,91	0
56	MG	FC	102	1/1	0.68	0.14	122,122,122,122	0
56	MG	FB	9032	1/1	0.68	0.40	90,90,90,90	0
56	MG	A	1702	1/1	0.68	0.20	131,131,131,131	0
56	MG	EB	1751	1/1	0.68	0.15	130,130,130,130	0
56	MG	FB	9051	1/1	0.68	0.29	91,91,91,91	0
56	MG	FB	9148	1/1	0.68	0.20	89,89,89,89	0
56	MG	EB	1754	1/1	0.68	0.11	84,84,84,84	0
56	MG	A	1782	1/1	0.68	0.21	159,159,159,159	0
56	MG	C	219	1/1	0.68	0.23	91,91,91,91	0
56	MG	B	9303	1/1	0.68	0.25	76,76,76,76	0
56	MG	FB	9158	1/1	0.68	0.31	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	IA	101	1/1	0.68	0.22	131,131,131,131	0
56	MG	FB	9352	1/1	0.68	0.18	131,131,131,131	0
56	MG	B	9392	1/1	0.68	0.23	125,125,125,125	0
56	MG	B	9186	1/1	0.69	0.31	94,94,94,94	0
56	MG	FB	9226	1/1	0.69	0.36	100,100,100,100	0
56	MG	FB	9381	1/1	0.69	0.08	117,117,117,117	0
56	MG	FB	9077	1/1	0.69	0.34	95,95,95,95	0
56	MG	D	102	1/1	0.69	0.18	120,120,120,120	0
56	MG	EB	1735	1/1	0.69	0.21	85,85,85,85	0
56	MG	GB	206	1/1	0.69	0.20	114,114,114,114	0
56	MG	FB	9259	1/1	0.69	0.16	79,79,79,79	0
56	MG	A	1617	1/1	0.69	0.18	101,101,101,101	0
56	MG	FB	9267	1/1	0.69	0.14	89,89,89,89	0
56	MG	EB	1739	1/1	0.69	0.23	116,116,116,116	0
56	MG	B	9249	1/1	0.69	0.25	95,95,95,95	0
56	MG	B	9222	1/1	0.69	0.26	64,64,64,64	0
56	MG	A	1743	1/1	0.69	0.29	108,108,108,108	0
56	MG	A	1765	1/1	0.69	0.21	81,81,81,81	0
56	MG	A	1753	1/1	0.69	0.17	132,132,132,132	0
56	MG	B	9352	1/1	0.69	0.29	103,103,103,103	0
56	MG	B	9501	1/1	0.69	0.23	76,76,76,76	0
56	MG	EB	1714	1/1	0.69	0.19	112,112,112,112	0
56	MG	A	1716	1/1	0.69	0.24	131,131,131,131	0
56	MG	EB	1676	1/1	0.70	0.21	99,99,99,99	0
56	MG	GB	210	1/1	0.70	0.18	121,121,121,121	0
56	MG	EB	1620	1/1	0.70	0.23	90,90,90,90	0
56	MG	EB	1770	1/1	0.70	0.15	97,97,97,97	0
56	MG	FB	9235	1/1	0.70	0.19	124,124,124,124	0
56	MG	FB	9302	1/1	0.70	0.10	109,109,109,109	0
56	MG	EB	1621	1/1	0.70	0.23	119,119,119,119	0
56	MG	FB	9057	1/1	0.70	0.32	83,83,83,83	0
56	MG	B	9294	1/1	0.70	0.16	118,118,118,118	0
56	MG	B	9386	1/1	0.70	0.10	115,115,115,115	0
56	MG	OC	303	1/1	0.70	0.15	115,115,115,115	0
56	MG	XA	102	1/1	0.70	0.22	101,101,101,101	0
56	MG	FB	9209	1/1	0.70	0.16	110,110,110,110	0
56	MG	MA	301	1/1	0.70	0.12	130,130,130,130	0
56	MG	C	205	1/1	0.70	0.30	102,102,102,102	0
56	MG	A	1805	1/1	0.70	0.12	136,136,136,136	0
56	MG	YC	201	1/1	0.70	0.30	82,82,82,82	0
56	MG	FB	9120	1/1	0.70	0.21	79,79,79,79	0
56	MG	EB	1646	1/1	0.70	0.21	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FB	9163	1/1	0.71	0.27	75,75,75,75	0
56	MG	B	9477	1/1	0.71	0.12	101,101,101,101	0
56	MG	B	9116	1/1	0.71	0.18	102,102,102,102	0
56	MG	EB	1790	1/1	0.71	0.16	130,130,130,130	0
56	MG	B	9520	1/1	0.71	0.10	90,90,90,90	0
56	MG	AA	102	1/1	0.71	0.15	75,75,75,75	0
56	MG	EB	1756	1/1	0.71	0.17	90,90,90,90	0
56	MG	FB	9094	1/1	0.71	0.31	73,73,73,73	0
56	MG	EB	1639	1/1	0.71	0.20	102,102,102,102	0
56	MG	NA	201	1/1	0.71	0.12	107,107,107,107	0
56	MG	B	9261	1/1	0.71	0.15	69,69,69,69	0
56	MG	FB	9009	1/1	0.71	0.21	78,78,78,78	0
56	MG	EB	1722	1/1	0.71	0.38	146,146,146,146	0
56	MG	FB	9210	1/1	0.71	0.27	99,99,99,99	0
56	MG	EB	1723	1/1	0.71	0.10	99,99,99,99	0
56	MG	OC	301	1/1	0.71	0.26	118,118,118,118	0
56	MG	GB	212	1/1	0.71	0.35	98,98,98,98	0
56	MG	FB	9023	1/1	0.71	0.23	95,95,95,95	0
56	MG	EB	1648	1/1	0.71	0.31	93,93,93,93	0
56	MG	A	1672	1/1	0.71	0.19	102,102,102,102	0
56	MG	A	1770	1/1	0.71	0.39	107,107,107,107	0
56	MG	B	9311	1/1	0.71	0.16	99,99,99,99	0
56	MG	IA	103	1/1	0.71	0.26	101,101,101,101	0
56	MG	FB	9411	1/1	0.71	0.14	75,75,75,75	0
56	MG	A	1725	1/1	0.71	0.33	109,109,109,109	0
56	MG	EB	1748	1/1	0.71	0.09	105,105,105,105	0
56	MG	BD	101	1/1	0.71	0.16	97,97,97,97	0
56	MG	FB	9404	1/1	0.72	0.16	101,101,101,101	0
56	MG	B	9209	1/1	0.72	0.29	73,73,73,73	0
56	MG	C	218	1/1	0.72	0.18	115,115,115,115	0
56	MG	A	1676	1/1	0.72	0.15	72,72,72,72	0
56	MG	FB	9116	1/1	0.72	0.14	92,92,92,92	0
56	MG	B	9135	1/1	0.72	0.34	100,100,100,100	0
56	MG	B	9369	1/1	0.72	0.33	101,101,101,101	0
56	MG	B	9291	1/1	0.72	0.15	100,100,100,100	0
56	MG	A	1732	1/1	0.72	0.22	122,122,122,122	0
56	MG	B	9230	1/1	0.72	0.27	69,69,69,69	0
56	MG	A	1712	1/1	0.72	0.30	95,95,95,95	0
56	MG	B	9143	1/1	0.72	0.19	117,117,117,117	0
56	MG	A	1785	1/1	0.72	0.12	79,79,79,79	0
56	MG	EB	1608	1/1	0.72	0.39	72,72,72,72	0
56	MG	B	9043	1/1	0.72	0.26	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FB	9046	1/1	0.72	0.39	74,74,74,74	0
56	MG	FB	9159	1/1	0.72	0.16	117,117,117,117	0
56	MG	B	9092	1/1	0.72	0.25	92,92,92,92	0
56	MG	B	9248	1/1	0.72	0.19	100,100,100,100	0
56	MG	FB	9276	1/1	0.72	0.20	76,76,76,76	0
56	MG	EB	1728	1/1	0.72	0.16	109,109,109,109	0
56	MG	A	1705	1/1	0.72	0.26	93,93,93,93	0
56	MG	B	9102	1/1	0.72	0.30	69,69,69,69	0
56	MG	B	9476	1/1	0.72	0.09	83,83,83,83	0
56	MG	EB	1618	1/1	0.72	0.29	74,74,74,74	0
56	MG	FB	9064	1/1	0.72	0.32	98,98,98,98	0
56	MG	A	1707	1/1	0.72	0.14	124,124,124,124	0
56	MG	LA	301	1/1	0.72	0.18	136,136,136,136	0
56	MG	FB	9081	1/1	0.72	0.16	139,139,139,139	0
56	MG	FB	9093	1/1	0.73	0.22	71,71,71,71	0
56	MG	H	201	1/1	0.73	0.15	103,103,103,103	0
56	MG	B	9202	1/1	0.73	0.29	101,101,101,101	0
56	MG	A	1783	1/1	0.73	0.13	90,90,90,90	0
56	MG	B	9323	1/1	0.73	0.16	92,92,92,92	0
56	MG	FB	9412	1/1	0.73	0.20	104,104,104,104	0
56	MG	B	9217	1/1	0.73	0.17	128,128,128,128	0
56	MG	A	1706	1/1	0.73	0.14	100,100,100,100	0
56	MG	FB	9125	1/1	0.73	0.19	101,101,101,101	0
56	MG	A	1812	1/1	0.73	0.25	104,104,104,104	0
56	MG	A	1679	1/1	0.73	0.28	103,103,103,103	0
56	MG	EB	1721	1/1	0.73	0.19	87,87,87,87	0
56	MG	B	9250	1/1	0.73	0.31	108,108,108,108	0
56	MG	CB	201	1/1	0.73	0.10	128,128,128,128	0
56	MG	FB	9440	1/1	0.73	0.19	93,93,93,93	0
56	MG	FB	9313	1/1	0.73	0.22	102,102,102,102	0
56	MG	B	9075	1/1	0.73	0.17	54,54,54,54	0
56	MG	FB	9204	1/1	0.73	0.23	88,88,88,88	0
56	MG	B	9188	1/1	0.73	0.36	84,84,84,84	0
56	MG	OB	201	1/1	0.73	0.13	104,104,104,104	0
56	MG	FB	9086	1/1	0.73	0.26	70,70,70,70	0
56	MG	FB	9004	1/1	0.74	0.27	79,79,79,79	0
56	MG	FB	9391	1/1	0.74	0.18	107,107,107,107	0
56	MG	EB	1657	1/1	0.74	0.14	99,99,99,99	0
56	MG	FB	9289	1/1	0.74	0.18	124,124,124,124	0
56	MG	EB	1659	1/1	0.74	0.33	87,87,87,87	0
56	MG	B	9339	1/1	0.74	0.07	103,103,103,103	0
56	MG	A	1794	1/1	0.74	0.14	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FB	9202	1/1	0.74	0.11	94,94,94,94	0
56	MG	I	201	1/1	0.74	0.10	89,89,89,89	0
56	MG	A	1641	1/1	0.74	0.24	123,123,123,123	0
56	MG	B	9106	1/1	0.74	0.17	63,63,63,63	0
56	MG	FB	9128	1/1	0.74	0.37	85,85,85,85	0
56	MG	DA	103	1/1	0.74	0.32	95,95,95,95	0
56	MG	A	1618	1/1	0.74	0.20	126,126,126,126	0
56	MG	FB	9319	1/1	0.74	0.07	99,99,99,99	0
56	MG	TA	203	1/1	0.74	0.12	107,107,107,107	0
56	MG	A	1626	1/1	0.74	0.25	91,91,91,91	0
56	MG	FB	9428	1/1	0.74	0.24	111,111,111,111	0
56	MG	EB	1734	1/1	0.74	0.14	101,101,101,101	0
56	MG	EB	1783	1/1	0.74	0.09	111,111,111,111	0
56	MG	FB	9438	1/1	0.74	0.26	97,97,97,97	0
56	MG	A	1664	1/1	0.74	0.11	121,121,121,121	0
56	MG	AB	102	1/1	0.74	0.11	95,95,95,95	0
56	MG	FB	9468	1/1	0.74	0.17	88,88,88,88	0
56	MG	A	1749	1/1	0.74	0.12	119,119,119,119	0
56	MG	FB	9160	1/1	0.74	0.14	98,98,98,98	0
56	MG	EB	1740	1/1	0.74	0.22	112,112,112,112	0
56	MG	IA	104	1/1	0.74	0.34	118,118,118,118	0
56	MG	A	1623	1/1	0.74	0.25	105,105,105,105	0
56	MG	B	9560	1/1	0.74	0.15	100,100,100,100	0
56	MG	FB	9171	1/1	0.74	0.12	117,117,117,117	0
56	MG	EB	1647	1/1	0.74	0.24	97,97,97,97	0
56	MG	FB	9176	1/1	0.74	0.13	81,81,81,81	0
56	MG	B	9140	1/1	0.74	0.55	69,69,69,69	0
56	MG	B	9205	1/1	0.74	0.17	80,80,80,80	0
58	ZN	FC	101	1/1	0.74	0.18	176,176,176,176	0
56	MG	FB	9003	1/1	0.75	0.30	64,64,64,64	0
56	MG	A	1813	1/1	0.75	0.13	127,127,127,127	0
56	MG	B	9262	1/1	0.75	0.09	97,97,97,97	0
56	MG	B	9447	1/1	0.75	0.07	78,78,78,78	0
56	MG	FB	9462	1/1	0.75	0.20	113,113,113,113	0
56	MG	TB	201	1/1	0.75	0.20	117,117,117,117	0
56	MG	FB	9463	1/1	0.75	0.12	83,83,83,83	0
56	MG	HA	101	1/1	0.75	0.36	95,95,95,95	0
56	MG	B	9007	1/1	0.75	0.34	61,61,61,61	0
56	MG	FB	9162	1/1	0.75	0.16	93,93,93,93	0
56	MG	B	9521	1/1	0.75	0.13	125,125,125,125	0
56	MG	A	1799	1/1	0.75	0.15	99,99,99,99	0
56	MG	EB	1668	1/1	0.75	0.15	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FB	9031	1/1	0.75	0.35	60,60,60,60	0
56	MG	FB	9118	1/1	0.75	0.21	87,87,87,87	0
56	MG	A	1756	1/1	0.75	0.14	94,94,94,94	0
56	MG	FB	9243	1/1	0.75	0.11	69,69,69,69	0
56	MG	B	9556	1/1	0.75	0.17	87,87,87,87	0
56	MG	A	1802	1/1	0.75	0.32	82,82,82,82	0
56	MG	A	1752	1/1	0.75	0.28	101,101,101,101	0
56	MG	A	1709	1/1	0.75	0.14	97,97,97,97	0
56	MG	RC	203	1/1	0.75	0.09	103,103,103,103	0
56	MG	FB	9183	1/1	0.75	0.30	89,89,89,89	0
56	MG	B	9059	1/1	0.75	0.35	85,85,85,85	0
56	MG	A	1661	1/1	0.75	0.35	112,112,112,112	0
56	MG	EB	1759	1/1	0.75	0.13	81,81,81,81	0
56	MG	EB	1643	1/1	0.75	0.53	91,91,91,91	0
56	MG	J	201	1/1	0.75	0.16	99,99,99,99	0
56	MG	FB	9364	1/1	0.75	0.11	74,74,74,74	0
56	MG	FB	9015	1/1	0.76	0.34	63,63,63,63	0
56	MG	A	1774	1/1	0.76	0.20	111,111,111,111	0
56	MG	FB	9236	1/1	0.76	0.12	76,76,76,76	0
56	MG	B	9562	1/1	0.76	0.12	75,75,75,75	0
56	MG	FB	9331	1/1	0.76	0.14	89,89,89,89	0
56	MG	FB	9104	1/1	0.76	0.18	96,96,96,96	0
56	MG	A	1764	1/1	0.76	0.24	99,99,99,99	0
56	MG	B	9263	1/1	0.76	0.17	60,60,60,60	0
56	MG	B	9395	1/1	0.76	0.27	59,59,59,59	0
56	MG	K	204	1/1	0.76	0.06	89,89,89,89	0
56	MG	FB	9434	1/1	0.76	0.10	102,102,102,102	0
56	MG	FB	9035	1/1	0.76	0.26	73,73,73,73	0
56	MG	FB	9036	1/1	0.76	0.28	66,66,66,66	0
56	MG	A	1633	1/1	0.76	0.25	94,94,94,94	0
56	MG	LC	101	1/1	0.76	0.36	86,86,86,86	0
56	MG	B	9210	1/1	0.76	0.15	85,85,85,85	0
56	MG	B	9337	1/1	0.76	0.28	111,111,111,111	0
56	MG	FB	9199	1/1	0.76	0.26	78,78,78,78	0
56	MG	B	9287	1/1	0.76	0.10	76,76,76,76	0
56	MG	FB	9380	1/1	0.76	0.20	87,87,87,87	0
56	MG	A	1790	1/1	0.76	0.24	104,104,104,104	0
56	MG	UA	201	1/1	0.76	0.37	92,92,92,92	0
56	MG	EB	1715	1/1	0.76	0.17	85,85,85,85	0
56	MG	B	9181	1/1	0.76	0.13	74,74,74,74	0
56	MG	B	9221	1/1	0.76	0.24	88,88,88,88	0
56	MG	FB	9395	1/1	0.76	0.15	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FB	9214	1/1	0.76	0.08	150,150,150,150	0
56	MG	FB	9401	1/1	0.76	0.13	98,98,98,98	0
56	MG	A	1711	1/1	0.76	0.25	88,88,88,88	0
56	MG	WC	201	1/1	0.76	0.49	116,116,116,116	0
56	MG	A	1745	1/1	0.76	0.16	115,115,115,115	0
56	MG	A	1704	1/1	0.76	0.25	114,114,114,114	0
56	MG	FB	9078	1/1	0.76	0.18	82,82,82,82	0
56	MG	EB	1677	1/1	0.76	0.18	83,83,83,83	0
56	MG	EB	1604	1/1	0.76	0.48	87,87,87,87	0
56	MG	FB	9179	1/1	0.77	0.12	95,95,95,95	0
56	MG	EB	1662	1/1	0.77	0.36	89,89,89,89	0
56	MG	B	9535	1/1	0.77	0.21	84,84,84,84	0
56	MG	B	9479	1/1	0.77	0.28	57,57,57,57	0
56	MG	EB	1799	1/1	0.77	0.24	82,82,82,82	0
56	MG	FB	9192	1/1	0.77	0.11	93,93,93,93	0
56	MG	FB	9194	1/1	0.77	0.15	109,109,109,109	0
56	MG	EB	1622	1/1	0.77	0.32	95,95,95,95	0
56	MG	B	9546	1/1	0.77	0.09	108,108,108,108	0
56	MG	B	9167	1/1	0.77	0.26	92,92,92,92	0
56	MG	FB	9370	1/1	0.77	0.11	77,77,77,77	0
56	MG	B	9109	1/1	0.77	0.29	78,78,78,78	0
56	MG	FB	9203	1/1	0.77	0.13	96,96,96,96	0
56	MG	B	9439	1/1	0.77	0.10	83,83,83,83	0
56	MG	EB	1636	1/1	0.77	0.35	82,82,82,82	0
56	MG	B	9200	1/1	0.77	0.33	67,67,67,67	0
56	MG	JA	402	1/1	0.77	0.29	103,103,103,103	0
56	MG	B	9488	1/1	0.77	0.15	115,115,115,115	0
56	MG	A	1792	1/1	0.77	0.14	100,100,100,100	0
56	MG	B	9176	1/1	0.77	0.26	90,90,90,90	0
56	MG	C	209	1/1	0.77	0.22	119,119,119,119	0
56	MG	B	9475	1/1	0.77	0.19	84,84,84,84	0
56	MG	B	9120	1/1	0.77	0.22	71,71,71,71	0
56	MG	FB	9315	1/1	0.77	0.24	84,84,84,84	0
56	MG	FB	9170	1/1	0.77	0.23	103,103,103,103	0
56	MG	FB	9114	1/1	0.77	0.16	82,82,82,82	0
56	MG	DA	102	1/1	0.77	0.24	104,104,104,104	0
56	MG	FB	9408	1/1	0.77	0.17	105,105,105,105	0
56	MG	A	1788	1/1	0.77	0.09	91,91,91,91	0
56	MG	A	1604	1/1	0.77	0.41	99,99,99,99	0
56	MG	EB	1704	1/1	0.77	0.14	110,110,110,110	0
56	MG	FB	9413	1/1	0.77	0.18	87,87,87,87	0
56	MG	FB	9329	1/1	0.77	0.13	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FB	9092	1/1	0.78	0.22	84,84,84,84	0
56	MG	A	1787	1/1	0.78	0.11	116,116,116,116	0
56	MG	EB	1623	1/1	0.78	0.30	80,80,80,80	0
56	MG	FB	9098	1/1	0.78	0.32	99,99,99,99	0
56	MG	EB	1806	1/1	0.78	0.21	105,105,105,105	0
56	MG	B	9171	1/1	0.78	0.10	52,52,52,52	0
56	MG	NA	202	1/1	0.78	0.19	122,122,122,122	0
56	MG	FB	9107	1/1	0.78	0.32	79,79,79,79	0
56	MG	B	9105	1/1	0.78	0.16	55,55,55,55	0
56	MG	A	1803	1/1	0.78	0.19	108,108,108,108	0
56	MG	EB	1634	1/1	0.78	0.14	77,77,77,77	0
56	MG	B	9449	1/1	0.78	0.13	104,104,104,104	0
56	MG	KB	303	1/1	0.78	0.13	100,100,100,100	0
56	MG	B	9550	1/1	0.78	0.15	82,82,82,82	0
56	MG	FB	9312	1/1	0.78	0.32	92,92,92,92	0
56	MG	A	1804	1/1	0.78	0.09	138,138,138,138	0
56	MG	RB	201	1/1	0.78	0.26	92,92,92,92	0
56	MG	FB	9314	1/1	0.78	0.18	64,64,64,64	0
56	MG	EB	1640	1/1	0.78	0.11	110,110,110,110	0
56	MG	V	502	1/1	0.78	0.14	82,82,82,82	0
56	MG	B	9114	1/1	0.78	0.19	78,78,78,78	0
56	MG	A	1735	1/1	0.78	0.11	128,128,128,128	0
56	MG	FB	9140	1/1	0.78	0.27	81,81,81,81	0
56	MG	FB	9216	1/1	0.78	0.18	72,72,72,72	0
56	MG	A	1639	1/1	0.78	0.15	108,108,108,108	0
56	MG	C	201	1/1	0.78	0.40	86,86,86,86	0
56	MG	FB	9330	1/1	0.78	0.14	72,72,72,72	0
56	MG	B	9050	1/1	0.78	0.29	74,74,74,74	0
56	MG	EB	1774	1/1	0.78	0.10	129,129,129,129	0
56	MG	A	1681	1/1	0.78	0.20	121,121,121,121	0
56	MG	B	9060	1/1	0.78	0.22	53,53,53,53	0
56	MG	B	9065	1/1	0.78	0.29	71,71,71,71	0
56	MG	B	9314	1/1	0.78	0.10	76,76,76,76	0
56	MG	B	9415	1/1	0.78	0.08	79,79,79,79	0
56	MG	A	1740	1/1	0.78	0.20	96,96,96,96	0
56	MG	B	9491	1/1	0.78	0.21	86,86,86,86	0
56	MG	A	1638	1/1	0.78	0.17	96,96,96,96	0
56	MG	B	9145	1/1	0.78	0.16	70,70,70,70	0
56	MG	JA	404	1/1	0.78	0.10	111,111,111,111	0
56	MG	EB	1795	1/1	0.78	0.24	78,78,78,78	0
56	MG	GB	208	1/1	0.78	0.35	97,97,97,97	0
56	MG	B	9434	1/1	0.78	0.13	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9008	1/1	0.78	0.34	67,67,67,67	0
56	MG	FB	9088	1/1	0.78	0.27	69,69,69,69	0
56	MG	B	9359	1/1	0.79	0.17	70,70,70,70	0
56	MG	FB	9020	1/1	0.79	0.26	60,60,60,60	0
56	MG	EB	1765	1/1	0.79	0.24	99,99,99,99	0
56	MG	K	202	1/1	0.79	0.22	73,73,73,73	0
56	MG	EB	1619	1/1	0.79	0.47	83,83,83,83	0
56	MG	FB	9389	1/1	0.79	0.22	93,93,93,93	0
56	MG	FB	9188	1/1	0.79	0.18	69,69,69,69	0
56	MG	FB	9115	1/1	0.79	0.22	81,81,81,81	0
56	MG	FB	9028	1/1	0.79	0.40	67,67,67,67	0
56	MG	B	9272	1/1	0.79	0.24	98,98,98,98	0
56	MG	EB	1667	1/1	0.79	0.11	84,84,84,84	0
56	MG	T	201	1/1	0.79	0.06	65,65,65,65	0
56	MG	B	9313	1/1	0.79	0.10	93,93,93,93	0
56	MG	B	9201	1/1	0.79	0.28	73,73,73,73	0
56	MG	EB	1724	1/1	0.79	0.20	102,102,102,102	0
56	MG	FB	9042	1/1	0.79	0.21	65,65,65,65	0
56	MG	EB	1726	1/1	0.79	0.20	95,95,95,95	0
56	MG	B	9281	1/1	0.79	0.18	80,80,80,80	0
56	MG	OB	203	1/1	0.79	0.12	104,104,104,104	0
56	MG	FB	9049	1/1	0.79	0.18	70,70,70,70	0
56	MG	B	9378	1/1	0.79	0.21	107,107,107,107	0
56	MG	A	1808	1/1	0.79	0.27	108,108,108,108	0
56	MG	A	1758	1/1	0.79	0.07	133,133,133,133	0
56	MG	BC	101	1/1	0.79	0.14	93,93,93,93	0
56	MG	FB	9055	1/1	0.79	0.29	74,74,74,74	0
56	MG	B	9227	1/1	0.79	0.22	76,76,76,76	0
56	MG	C	215	1/1	0.79	0.21	123,123,123,123	0
56	MG	B	9208	1/1	0.79	0.24	82,82,82,82	0
56	MG	FB	9325	1/1	0.79	0.15	117,117,117,117	0
56	MG	B	9525	1/1	0.79	0.07	130,130,130,130	0
56	MG	FB	9232	1/1	0.79	0.31	75,75,75,75	0
56	MG	B	9528	1/1	0.79	0.12	126,126,126,126	0
56	MG	A	1608	1/1	0.79	0.31	99,99,99,99	0
56	MG	FB	9339	1/1	0.79	0.13	87,87,87,87	0
56	MG	FB	9441	1/1	0.79	0.23	133,133,133,133	0
56	MG	A	1739	1/1	0.79	0.12	101,101,101,101	0
56	MG	FB	9347	1/1	0.79	0.30	83,83,83,83	0
56	MG	EB	1644	1/1	0.79	0.19	93,93,93,93	0
56	MG	FB	9242	1/1	0.79	0.15	61,61,61,61	0
56	MG	B	9125	1/1	0.79	0.17	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	SC	201	1/1	0.79	0.13	104,104,104,104	0
56	MG	TC	201	1/1	0.79	0.13	117,117,117,117	0
56	MG	B	9480	1/1	0.79	0.06	83,83,83,83	0
56	MG	FB	9476	1/1	0.79	0.15	93,93,93,93	0
56	MG	FB	9264	1/1	0.79	0.07	61,61,61,61	0
56	MG	A	1636	1/1	0.79	0.21	84,84,84,84	0
56	MG	EB	1650	1/1	0.79	0.24	84,84,84,84	0
56	MG	B	9431	1/1	0.79	0.13	57,57,57,57	0
56	MG	FB	9275	1/1	0.79	0.29	71,71,71,71	0
56	MG	B	9484	1/1	0.79	0.15	129,129,129,129	0
56	MG	EB	1786	1/1	0.80	0.14	103,103,103,103	0
56	MG	FB	9303	1/1	0.80	0.27	77,77,77,77	0
56	MG	I	203	1/1	0.80	0.09	92,92,92,92	0
56	MG	A	1686	1/1	0.80	0.33	101,101,101,101	0
56	MG	B	9329	1/1	0.80	0.11	76,76,76,76	0
56	MG	B	9077	1/1	0.80	0.14	67,67,67,67	0
56	MG	Q	202	1/1	0.80	0.06	78,78,78,78	0
56	MG	FB	9155	1/1	0.80	0.15	87,87,87,87	0
56	MG	B	9079	1/1	0.80	0.26	65,65,65,65	0
56	MG	EB	1645	1/1	0.80	0.23	84,84,84,84	0
56	MG	B	9390	1/1	0.80	0.23	61,61,61,61	0
56	MG	FB	9067	1/1	0.80	0.18	89,89,89,89	0
56	MG	A	1708	1/1	0.80	0.16	93,93,93,93	0
56	MG	B	9048	1/1	0.80	0.16	71,71,71,71	0
56	MG	B	9396	1/1	0.80	0.13	116,116,116,116	0
56	MG	FB	9080	1/1	0.80	0.25	75,75,75,75	0
56	MG	B	9247	1/1	0.80	0.25	75,75,75,75	0
56	MG	EB	1652	1/1	0.80	0.13	108,108,108,108	0
56	MG	EB	1757	1/1	0.80	0.13	108,108,108,108	0
56	MG	FB	9332	1/1	0.80	0.11	89,89,89,89	0
56	MG	EB	1655	1/1	0.80	0.17	100,100,100,100	0
56	MG	FB	9173	1/1	0.80	0.13	92,92,92,92	0
56	MG	FB	9261	1/1	0.80	0.17	84,84,84,84	0
56	MG	B	9498	1/1	0.80	0.27	89,89,89,89	0
56	MG	EB	1707	1/1	0.80	0.17	103,103,103,103	0
56	MG	EB	1658	1/1	0.80	0.37	90,90,90,90	0
56	MG	B	9561	1/1	0.80	0.19	91,91,91,91	0
56	MG	NC	404	1/1	0.80	0.13	119,119,119,119	0
56	MG	A	1669	1/1	0.80	0.19	95,95,95,95	0
56	MG	FB	9359	1/1	0.80	0.31	91,91,91,91	0
56	MG	EB	1661	1/1	0.80	0.39	90,90,90,90	0
56	MG	UA	203	1/1	0.80	0.26	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	UA	204	1/1	0.80	0.07	100,100,100,100	0
56	MG	EB	1771	1/1	0.80	0.11	94,94,94,94	0
56	MG	EB	1666	1/1	0.80	0.24	97,97,97,97	0
56	MG	B	9014	1/1	0.80	0.21	79,79,79,79	0
56	MG	EB	1631	1/1	0.80	0.22	83,83,83,83	0
56	MG	A	1723	1/1	0.80	0.17	99,99,99,99	0
56	MG	B	9518	1/1	0.80	0.10	132,132,132,132	0
56	MG	FB	9295	1/1	0.80	0.12	58,58,58,58	0
56	MG	FB	9043	1/1	0.80	0.26	81,81,81,81	0
56	MG	FB	9388	1/1	0.80	0.20	73,73,73,73	0
56	MG	A	1637	1/1	0.80	0.17	106,106,106,106	0
56	MG	AD	102	1/1	0.80	0.14	106,106,106,106	0
56	MG	I	202	1/1	0.80	0.07	79,79,79,79	0
56	MG	FB	9301	1/1	0.80	0.20	86,86,86,86	0
56	MG	M	203	1/1	0.81	0.20	87,87,87,87	0
56	MG	FB	9316	1/1	0.81	0.23	87,87,87,87	0
56	MG	FB	9072	1/1	0.81	0.29	79,79,79,79	0
56	MG	FB	9074	1/1	0.81	0.24	76,76,76,76	0
56	MG	MA	302	1/1	0.81	0.11	111,111,111,111	0
56	MG	FB	9409	1/1	0.81	0.22	74,74,74,74	0
56	MG	A	1695	1/1	0.81	0.31	111,111,111,111	0
56	MG	B	9211	1/1	0.81	0.11	72,72,72,72	0
56	MG	A	1645	1/1	0.81	0.17	122,122,122,122	0
56	MG	FB	9022	1/1	0.81	0.35	72,72,72,72	0
56	MG	B	9083	1/1	0.81	0.20	79,79,79,79	0
56	MG	OB	202	1/1	0.81	0.16	99,99,99,99	0
56	MG	EB	1680	1/1	0.81	0.17	90,90,90,90	0
56	MG	PB	201	1/1	0.81	0.18	85,85,85,85	0
56	MG	C	217	1/1	0.81	0.11	85,85,85,85	0
56	MG	FB	9421	1/1	0.81	0.17	118,118,118,118	0
56	MG	SB	202	1/1	0.81	0.13	81,81,81,81	0
56	MG	FB	9029	1/1	0.81	0.34	78,78,78,78	0
56	MG	FB	9333	1/1	0.81	0.13	74,74,74,74	0
56	MG	ZB	702	1/1	0.81	0.13	94,94,94,94	0
56	MG	FB	9097	1/1	0.81	0.22	65,65,65,65	0
56	MG	A	1653	1/1	0.81	0.21	84,84,84,84	0
56	MG	EB	1686	1/1	0.81	0.35	78,78,78,78	0
56	MG	DC	101	1/1	0.81	0.07	93,93,93,93	0
56	MG	B	9366	1/1	0.81	0.17	60,60,60,60	0
56	MG	A	1674	1/1	0.81	0.10	90,90,90,90	0
56	MG	A	1622	1/1	0.81	0.36	101,101,101,101	0
56	MG	FB	9113	1/1	0.81	0.33	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	EB	1694	1/1	0.81	0.34	90,90,90,90	0
56	MG	B	9016	1/1	0.81	0.17	58,58,58,58	0
56	MG	FB	9449	1/1	0.81	0.11	107,107,107,107	0
56	MG	FB	9360	1/1	0.81	0.16	83,83,83,83	0
56	MG	EB	1747	1/1	0.81	0.19	90,90,90,90	0
56	MG	B	9293	1/1	0.81	0.17	78,78,78,78	0
56	MG	EB	1702	1/1	0.81	0.20	94,94,94,94	0
56	MG	FB	9123	1/1	0.81	0.20	80,80,80,80	0
56	MG	OC	305	1/1	0.81	0.15	120,120,120,120	0
56	MG	FB	9048	1/1	0.81	0.26	74,74,74,74	0
56	MG	QC	301	1/1	0.81	0.26	94,94,94,94	0
56	MG	B	9441	1/1	0.81	0.15	67,67,67,67	0
56	MG	EB	1752	1/1	0.81	0.15	78,78,78,78	0
56	MG	B	9489	1/1	0.81	0.16	98,98,98,98	0
56	MG	FB	9131	1/1	0.81	0.21	66,66,66,66	0
56	MG	A	1601	1/1	0.81	0.28	62,62,62,62	0
56	MG	B	9494	1/1	0.81	0.14	76,76,76,76	0
56	MG	B	9445	1/1	0.81	0.10	101,101,101,101	0
56	MG	FB	9143	1/1	0.81	0.16	103,103,103,103	0
56	MG	B	9338	1/1	0.81	0.12	75,75,75,75	0
56	MG	A	1703	1/1	0.81	0.11	98,98,98,98	0
56	MG	B	9180	1/1	0.81	0.12	57,57,57,57	0
56	MG	B	9403	1/1	0.81	0.28	77,77,77,77	0
58	ZN	BA	101	1/1	0.81	0.17	162,162,162,162	0
56	MG	FB	9069	1/1	0.81	0.23	88,88,88,88	0
56	MG	EB	1776	1/1	0.82	0.25	98,98,98,98	0
56	MG	FB	9248	1/1	0.82	0.31	83,83,83,83	0
56	MG	FB	9255	1/1	0.82	0.34	89,89,89,89	0
56	MG	B	9531	1/1	0.82	0.13	58,58,58,58	0
56	MG	FB	9108	1/1	0.82	0.23	68,68,68,68	0
56	MG	FB	9111	1/1	0.82	0.20	77,77,77,77	0
56	MG	FB	9420	1/1	0.82	0.10	99,99,99,99	0
56	MG	A	1761	1/1	0.82	0.17	85,85,85,85	0
56	MG	FB	9338	1/1	0.82	0.22	104,104,104,104	0
56	MG	FB	9424	1/1	0.82	0.10	97,97,97,97	0
56	MG	B	9428	1/1	0.82	0.07	70,70,70,70	0
56	MG	B	9543	1/1	0.82	0.08	63,63,63,63	0
56	MG	A	1775	1/1	0.82	0.08	70,70,70,70	0
56	MG	FB	9348	1/1	0.82	0.12	107,107,107,107	0
56	MG	A	1762	1/1	0.82	0.18	103,103,103,103	0
56	MG	E	301	1/1	0.82	0.04	78,78,78,78	0
56	MG	EB	1690	1/1	0.82	0.13	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	EB	1745	1/1	0.82	0.16	89,89,89,89	0
56	MG	A	1747	1/1	0.82	0.08	99,99,99,99	0
56	MG	B	9375	1/1	0.82	0.09	51,51,51,51	0
56	MG	JC	101	1/1	0.82	0.36	89,89,89,89	0
56	MG	B	9025	1/1	0.82	0.20	49,49,49,49	0
56	MG	FB	9451	1/1	0.82	0.14	73,73,73,73	0
56	MG	FB	9453	1/1	0.82	0.13	85,85,85,85	0
56	MG	JA	405	1/1	0.82	0.13	111,111,111,111	0
56	MG	B	9030	1/1	0.82	0.22	72,72,72,72	0
56	MG	B	9251	1/1	0.82	0.15	72,72,72,72	0
56	MG	NC	401	1/1	0.82	0.13	114,114,114,114	0
56	MG	NC	403	1/1	0.82	0.15	93,93,93,93	0
56	MG	EB	1701	1/1	0.82	0.42	98,98,98,98	0
56	MG	B	9081	1/1	0.82	0.21	68,68,68,68	0
56	MG	FB	9474	1/1	0.82	0.07	87,87,87,87	0
56	MG	B	9393	1/1	0.82	0.14	70,70,70,70	0
56	MG	B	9448	1/1	0.82	0.12	78,78,78,78	0
56	MG	FB	9150	1/1	0.82	0.19	84,84,84,84	0
56	MG	A	1673	1/1	0.82	0.14	104,104,104,104	0
56	MG	C	207	1/1	0.82	0.13	99,99,99,99	0
56	MG	S	202	1/1	0.82	0.13	89,89,89,89	0
56	MG	B	9452	1/1	0.82	0.06	93,93,93,93	0
56	MG	B	9231	1/1	0.82	0.31	89,89,89,89	0
56	MG	A	1726	1/1	0.82	0.24	97,97,97,97	0
56	MG	FB	9224	1/1	0.82	0.24	73,73,73,73	0
56	MG	B	9354	1/1	0.82	0.12	71,71,71,71	0
56	MG	EB	1768	1/1	0.82	0.15	90,90,90,90	0
56	MG	B	9306	1/1	0.82	0.11	61,61,61,61	0
56	MG	A	1694	1/1	0.82	0.35	107,107,107,107	0
56	MG	FB	9320	1/1	0.82	0.12	67,67,67,67	0
56	MG	A	1728	1/1	0.82	0.15	108,108,108,108	0
56	MG	XA	104	1/1	0.82	0.21	101,101,101,101	0
56	MG	EB	1674	1/1	0.82	0.27	84,84,84,84	0
56	MG	XA	105	1/1	0.82	0.15	97,97,97,97	0
56	MG	A	1814	1/1	0.83	0.12	171,171,171,171	0
56	MG	FB	9024	1/1	0.83	0.33	60,60,60,60	0
56	MG	B	9182	1/1	0.83	0.33	81,81,81,81	0
56	MG	B	9214	1/1	0.83	0.13	57,57,57,57	0
56	MG	FB	9417	1/1	0.83	0.16	99,99,99,99	0
56	MG	FB	9246	1/1	0.83	0.29	73,73,73,73	0
56	MG	FB	9247	1/1	0.83	0.14	79,79,79,79	0
56	MG	FB	9095	1/1	0.83	0.30	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FB	9253	1/1	0.83	0.22	67,67,67,67	0
56	MG	A	1797	1/1	0.83	0.12	83,83,83,83	0
56	MG	B	9312	1/1	0.83	0.28	103,103,103,103	0
56	MG	A	1807	1/1	0.83	0.17	92,92,92,92	0
56	MG	FB	9343	1/1	0.83	0.15	72,72,72,72	0
56	MG	B	9095	1/1	0.83	0.14	64,64,64,64	0
56	MG	EB	1683	1/1	0.83	0.27	84,84,84,84	0
56	MG	EB	1782	1/1	0.83	0.08	93,93,93,93	0
56	MG	A	1634	1/1	0.83	0.22	79,79,79,79	0
56	MG	B	9487	1/1	0.83	0.09	72,72,72,72	0
56	MG	B	9446	1/1	0.83	0.15	55,55,55,55	0
56	MG	EB	1743	1/1	0.83	0.10	86,86,86,86	0
56	MG	B	9408	1/1	0.83	0.15	73,73,73,73	0
56	MG	EB	1653	1/1	0.83	0.20	77,77,77,77	0
56	MG	B	9409	1/1	0.83	0.09	66,66,66,66	0
56	MG	B	9070	1/1	0.83	0.23	57,57,57,57	0
56	MG	B	9136	1/1	0.83	0.25	64,64,64,64	0
56	MG	EB	1624	1/1	0.83	0.11	96,96,96,96	0
56	MG	FB	9054	1/1	0.83	0.30	76,76,76,76	0
56	MG	FB	9126	1/1	0.83	0.15	84,84,84,84	0
56	MG	EB	1625	1/1	0.83	0.17	98,98,98,98	0
56	MG	EB	1798	1/1	0.83	0.17	97,97,97,97	0
56	MG	EB	1626	1/1	0.83	0.23	90,90,90,90	0
56	MG	XA	101	1/1	0.83	0.28	99,99,99,99	0
56	MG	FB	9384	1/1	0.83	0.14	120,120,120,120	0
56	MG	GB	204	1/1	0.83	0.14	118,118,118,118	0
56	MG	B	9499	1/1	0.83	0.08	51,51,51,51	0
56	MG	EB	1665	1/1	0.83	0.29	95,95,95,95	0
56	MG	FB	9141	1/1	0.83	0.28	82,82,82,82	0
56	MG	FB	9068	1/1	0.83	0.15	64,64,64,64	0
56	MG	FB	9144	1/1	0.83	0.25	65,65,65,65	0
56	MG	FB	9311	1/1	0.83	0.22	89,89,89,89	0
56	MG	B	9454	1/1	0.83	0.28	70,70,70,70	0
56	MG	B	9502	1/1	0.83	0.23	74,74,74,74	0
56	MG	JA	401	1/1	0.83	0.16	108,108,108,108	0
56	MG	FB	9073	1/1	0.83	0.35	74,74,74,74	0
56	MG	EB	1713	1/1	0.83	0.14	96,96,96,96	0
56	MG	A	1605	1/1	0.83	0.25	68,68,68,68	0
56	MG	B	9015	1/1	0.83	0.34	77,77,77,77	0
56	MG	EB	1637	1/1	0.83	0.21	107,107,107,107	0
56	MG	B	9373	1/1	0.83	0.09	60,60,60,60	0
56	MG	A	1665	1/1	0.83	0.14	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	A	1729	1/1	0.84	0.13	71,71,71,71	0
56	MG	B	9265	1/1	0.84	0.06	74,74,74,74	0
56	MG	A	1742	1/1	0.84	0.19	110,110,110,110	0
56	MG	B	9365	1/1	0.84	0.16	104,104,104,104	0
56	MG	GB	214	1/1	0.84	0.16	82,82,82,82	0
56	MG	A	1621	1/1	0.84	0.34	93,93,93,93	0
56	MG	EB	1779	1/1	0.84	0.11	102,102,102,102	0
56	MG	B	9315	1/1	0.84	0.24	112,112,112,112	0
56	MG	B	9279	1/1	0.84	0.20	87,87,87,87	0
56	MG	FB	9394	1/1	0.84	0.17	72,72,72,72	0
56	MG	B	9027	1/1	0.84	0.22	73,73,73,73	0
56	MG	B	9011	1/1	0.84	0.35	58,58,58,58	0
56	MG	EB	1727	1/1	0.84	0.15	99,99,99,99	0
56	MG	FB	9212	1/1	0.84	0.12	103,103,103,103	0
56	MG	K	201	1/1	0.84	0.32	76,76,76,76	0
56	MG	B	9376	1/1	0.84	0.22	68,68,68,68	0
56	MG	KB	301	1/1	0.84	0.10	80,80,80,80	0
56	MG	B	9035	1/1	0.84	0.23	49,49,49,49	0
56	MG	B	9149	1/1	0.84	0.12	60,60,60,60	0
56	MG	M	204	1/1	0.84	0.16	89,89,89,89	0
56	MG	EB	1630	1/1	0.84	0.27	81,81,81,81	0
56	MG	C	202	1/1	0.84	0.17	80,80,80,80	0
56	MG	C	203	1/1	0.84	0.14	80,80,80,80	0
56	MG	A	1772	1/1	0.84	0.16	101,101,101,101	0
56	MG	T	202	1/1	0.84	0.08	69,69,69,69	0
56	MG	A	1713	1/1	0.84	0.17	99,99,99,99	0
56	MG	FB	9234	1/1	0.84	0.21	108,108,108,108	0
56	MG	B	9253	1/1	0.84	0.07	87,87,87,87	0
56	MG	B	9169	1/1	0.84	0.20	69,69,69,69	0
56	MG	WB	201	1/1	0.84	0.15	106,106,106,106	0
56	MG	FB	9326	1/1	0.84	0.38	94,94,94,94	0
56	MG	B	9349	1/1	0.84	0.15	93,93,93,93	0
56	MG	FB	9240	1/1	0.84	0.15	99,99,99,99	0
56	MG	CC	104	1/1	0.84	0.18	79,79,79,79	0
56	MG	B	9397	1/1	0.84	0.13	104,104,104,104	0
56	MG	ZA	201	1/1	0.84	0.10	94,94,94,94	0
56	MG	B	9453	1/1	0.84	0.12	68,68,68,68	0
56	MG	B	9516	1/1	0.84	0.17	102,102,102,102	0
56	MG	FB	9019	1/1	0.84	0.22	59,59,59,59	0
56	MG	A	1614	1/1	0.84	0.12	82,82,82,82	0
56	MG	FB	9437	1/1	0.84	0.09	99,99,99,99	0
56	MG	FB	9254	1/1	0.84	0.18	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9462	1/1	0.84	0.08	69,69,69,69	0
56	MG	FB	9345	1/1	0.84	0.10	92,92,92,92	0
56	MG	FB	9258	1/1	0.84	0.09	126,126,126,126	0
56	MG	FB	9445	1/1	0.84	0.20	72,72,72,72	0
56	MG	FB	9447	1/1	0.84	0.38	96,96,96,96	0
56	MG	NC	405	1/1	0.84	0.19	82,82,82,82	0
56	MG	B	9353	1/1	0.84	0.14	67,67,67,67	0
56	MG	EB	1606	1/1	0.84	0.26	77,77,77,77	0
56	MG	EB	1649	1/1	0.84	0.54	81,81,81,81	0
56	MG	FB	9454	1/1	0.84	0.10	81,81,81,81	0
56	MG	FB	9455	1/1	0.84	0.13	83,83,83,83	0
56	MG	EB	1607	1/1	0.84	0.41	85,85,85,85	0
56	MG	FB	9103	1/1	0.84	0.28	78,78,78,78	0
56	MG	FB	9358	1/1	0.84	0.11	75,75,75,75	0
56	MG	FB	9470	1/1	0.84	0.11	86,86,86,86	0
56	MG	FB	9269	1/1	0.84	0.07	97,97,97,97	0
56	MG	A	1766	1/1	0.84	0.12	95,95,95,95	0
56	MG	FB	9473	1/1	0.84	0.10	107,107,107,107	0
56	MG	B	9413	1/1	0.84	0.21	62,62,62,62	0
56	MG	B	9527	1/1	0.84	0.09	82,82,82,82	0
56	MG	B	9057	1/1	0.84	0.18	62,62,62,62	0
56	MG	EB	1656	1/1	0.84	0.20	78,78,78,78	0
56	MG	FB	9033	1/1	0.84	0.45	76,76,76,76	0
56	MG	EB	1613	1/1	0.84	0.32	71,71,71,71	0
56	MG	GB	205	1/1	0.84	0.23	103,103,103,103	0
56	MG	FB	9191	1/1	0.84	0.31	90,90,90,90	0
56	MG	EB	1614	1/1	0.84	0.23	88,88,88,88	0
56	MG	FB	9356	1/1	0.85	0.17	89,89,89,89	0
56	MG	B	9280	1/1	0.85	0.30	84,84,84,84	0
56	MG	FB	9433	1/1	0.85	0.45	90,90,90,90	0
56	MG	NB	203	1/1	0.85	0.16	129,129,129,129	0
56	MG	B	9154	1/1	0.85	0.18	68,68,68,68	0
56	MG	FB	9435	1/1	0.85	0.37	72,72,72,72	0
56	MG	FB	9090	1/1	0.85	0.28	95,95,95,95	0
56	MG	B	9515	1/1	0.85	0.19	81,81,81,81	0
56	MG	FB	9154	1/1	0.85	0.18	71,71,71,71	0
56	MG	A	1612	1/1	0.85	0.30	83,83,83,83	0
56	MG	B	9351	1/1	0.85	0.14	82,82,82,82	0
56	MG	A	1796	1/1	0.85	0.07	81,81,81,81	0
56	MG	FB	9375	1/1	0.85	0.14	80,80,80,80	0
56	MG	B	9038	1/1	0.85	0.13	53,53,53,53	0
56	MG	FB	9044	1/1	0.85	0.40	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	ZB	703	1/1	0.85	0.23	91,91,91,91	0
56	MG	A	1724	1/1	0.85	0.13	80,80,80,80	0
56	MG	FB	9228	1/1	0.85	0.09	115,115,115,115	0
56	MG	CC	103	1/1	0.85	0.18	72,72,72,72	0
56	MG	FB	9229	1/1	0.85	0.36	69,69,69,69	0
56	MG	B	9144	1/1	0.85	0.19	79,79,79,79	0
56	MG	B	9391	1/1	0.85	0.16	81,81,81,81	0
56	MG	B	9457	1/1	0.85	0.37	102,102,102,102	0
56	MG	B	9196	1/1	0.85	0.18	70,70,70,70	0
56	MG	FB	9002	1/1	0.85	0.37	62,62,62,62	0
56	MG	EB	1730	1/1	0.85	0.08	97,97,97,97	0
56	MG	KA	301	1/1	0.85	0.13	119,119,119,119	0
56	MG	EB	1733	1/1	0.85	0.16	109,109,109,109	0
56	MG	B	9111	1/1	0.85	0.26	64,64,64,64	0
56	MG	FB	9058	1/1	0.85	0.26	68,68,68,68	0
56	MG	FB	9400	1/1	0.85	0.09	88,88,88,88	0
56	MG	Q	201	1/1	0.85	0.16	121,121,121,121	0
56	MG	FB	9013	1/1	0.85	0.30	56,56,56,56	0
56	MG	FB	9251	1/1	0.85	0.25	77,77,77,77	0
56	MG	FB	9122	1/1	0.85	0.10	64,64,64,64	0
56	MG	GB	207	1/1	0.85	0.27	109,109,109,109	0
56	MG	EB	1737	1/1	0.85	0.10	113,113,113,113	0
56	MG	FB	9066	1/1	0.85	0.34	69,69,69,69	0
56	MG	B	9537	1/1	0.85	0.13	59,59,59,59	0
56	MG	B	9497	1/1	0.85	0.12	69,69,69,69	0
56	MG	FB	9189	1/1	0.85	0.13	93,93,93,93	0
56	MG	B	9101	1/1	0.85	0.21	61,61,61,61	0
56	MG	B	9544	1/1	0.85	0.12	68,68,68,68	0
56	MG	FB	9071	1/1	0.85	0.28	73,73,73,73	0
56	MG	B	9153	1/1	0.85	0.21	85,85,85,85	0
56	MG	FB	9340	1/1	0.85	0.09	76,76,76,76	0
56	MG	FB	9135	1/1	0.85	0.09	93,93,93,93	0
56	MG	FB	9136	1/1	0.85	0.16	84,84,84,84	0
56	MG	EB	1780	1/1	0.85	0.20	101,101,101,101	0
56	MG	B	9547	1/1	0.85	0.18	127,127,127,127	0
56	MG	B	9179	1/1	0.85	0.19	58,58,58,58	0
56	MG	B	9553	1/1	0.85	0.12	63,63,63,63	0
56	MG	IB	302	1/1	0.85	0.20	64,64,64,64	0
56	MG	B	9554	1/1	0.85	0.12	75,75,75,75	0
56	MG	B	9368	1/1	0.85	0.20	78,78,78,78	0
56	MG	A	1689	1/1	0.86	0.33	78,78,78,78	0
56	MG	FB	9256	1/1	0.86	0.30	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9051	1/1	0.86	0.23	67,67,67,67	0
56	MG	B	9223	1/1	0.86	0.26	93,93,93,93	0
56	MG	B	9121	1/1	0.86	0.17	54,54,54,54	0
56	MG	FB	9341	1/1	0.86	0.21	75,75,75,75	0
56	MG	FB	9342	1/1	0.86	0.14	92,92,92,92	0
56	MG	FB	9263	1/1	0.86	0.18	78,78,78,78	0
56	MG	FB	9190	1/1	0.86	0.32	79,79,79,79	0
56	MG	B	9500	1/1	0.86	0.09	88,88,88,88	0
56	MG	FB	9431	1/1	0.86	0.24	86,86,86,86	0
56	MG	FB	9007	1/1	0.86	0.36	69,69,69,69	0
56	MG	FB	9008	1/1	0.86	0.34	63,63,63,63	0
56	MG	B	9324	1/1	0.86	0.07	78,78,78,78	0
56	MG	FB	9350	1/1	0.86	0.13	91,91,91,91	0
56	MG	EB	1717	1/1	0.86	0.16	90,90,90,90	0
56	MG	B	9325	1/1	0.86	0.10	53,53,53,53	0
56	MG	FB	9014	1/1	0.86	0.27	64,64,64,64	0
56	MG	B	9036	1/1	0.86	0.17	68,68,68,68	0
56	MG	FB	9017	1/1	0.86	0.16	85,85,85,85	0
56	MG	FB	9443	1/1	0.86	0.19	96,96,96,96	0
56	MG	FB	9205	1/1	0.86	0.21	84,84,84,84	0
56	MG	EB	1601	1/1	0.86	0.46	79,79,79,79	0
56	MG	FB	9208	1/1	0.86	0.28	78,78,78,78	0
56	MG	FB	9288	1/1	0.86	0.09	73,73,73,73	0
56	MG	B	9559	1/1	0.86	0.12	71,71,71,71	0
56	MG	B	9128	1/1	0.86	0.17	72,72,72,72	0
56	MG	FB	9291	1/1	0.86	0.12	65,65,65,65	0
56	MG	FB	9457	1/1	0.86	0.09	77,77,77,77	0
56	MG	A	1800	1/1	0.86	0.10	116,116,116,116	0
56	MG	A	1632	1/1	0.86	0.17	100,100,100,100	0
56	MG	FB	9465	1/1	0.86	0.11	94,94,94,94	0
56	MG	B	9297	1/1	0.86	0.18	57,57,57,57	0
56	MG	EB	1678	1/1	0.86	0.20	74,74,74,74	0
56	MG	B	9519	1/1	0.86	0.12	75,75,75,75	0
56	MG	FB	9089	1/1	0.86	0.12	76,76,76,76	0
56	MG	NC	402	1/1	0.86	0.11	125,125,125,125	0
56	MG	B	9155	1/1	0.86	0.22	76,76,76,76	0
56	MG	B	9091	1/1	0.86	0.09	71,71,71,71	0
56	MG	EB	1682	1/1	0.86	0.27	90,90,90,90	0
56	MG	B	9344	1/1	0.86	0.23	74,74,74,74	0
56	MG	B	9523	1/1	0.86	0.16	65,65,65,65	0
56	MG	B	9345	1/1	0.86	0.12	56,56,56,56	0
56	MG	EB	1688	1/1	0.86	0.25	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9301	1/1	0.86	0.18	75,75,75,75	0
56	MG	FB	9102	1/1	0.86	0.17	79,79,79,79	0
56	MG	FB	9164	1/1	0.86	0.15	67,67,67,67	0
56	MG	A	1730	1/1	0.86	0.14	73,73,73,73	0
56	MG	S	201	1/1	0.86	0.13	80,80,80,80	0
56	MG	QA	201	1/1	0.86	0.21	111,111,111,111	0
56	MG	B	9243	1/1	0.86	0.12	73,73,73,73	0
56	MG	FB	9405	1/1	0.86	0.17	73,73,73,73	0
56	MG	C	211	1/1	0.86	0.11	111,111,111,111	0
56	MG	B	9273	1/1	0.86	0.12	52,52,52,52	0
56	MG	XC	201	1/1	0.86	0.11	97,97,97,97	0
56	MG	FB	9244	1/1	0.86	0.25	86,86,86,86	0
56	MG	YC	202	1/1	0.86	0.19	76,76,76,76	0
56	MG	A	1649	1/1	0.86	0.29	103,103,103,103	0
56	MG	W	301	1/1	0.86	0.13	104,104,104,104	0
56	MG	W	302	1/1	0.86	0.15	87,87,87,87	0
56	MG	B	9538	1/1	0.86	0.18	74,74,74,74	0
56	MG	FB	9117	1/1	0.86	0.14	96,96,96,96	0
56	MG	B	9170	1/1	0.86	0.17	75,75,75,75	0
56	MG	B	9468	1/1	0.87	0.16	62,62,62,62	0
56	MG	GB	211	1/1	0.87	0.19	104,104,104,104	0
56	MG	FB	9038	1/1	0.87	0.20	70,70,70,70	0
56	MG	FB	9197	1/1	0.87	0.41	74,74,74,74	0
56	MG	EB	1664	1/1	0.87	0.36	83,83,83,83	0
56	MG	FB	9294	1/1	0.87	0.10	118,118,118,118	0
56	MG	B	9330	1/1	0.87	0.07	81,81,81,81	0
56	MG	B	9536	1/1	0.87	0.15	71,71,71,71	0
56	MG	FB	9119	1/1	0.87	0.09	84,84,84,84	0
56	MG	B	9335	1/1	0.87	0.11	77,77,77,77	0
56	MG	FB	9045	1/1	0.87	0.52	79,79,79,79	0
56	MG	FB	9206	1/1	0.87	0.13	91,91,91,91	0
56	MG	EB	1781	1/1	0.87	0.17	95,95,95,95	0
56	MG	B	9033	1/1	0.87	0.26	75,75,75,75	0
56	MG	B	9129	1/1	0.87	0.10	65,65,65,65	0
56	MG	B	9401	1/1	0.87	0.14	66,66,66,66	0
56	MG	FB	9050	1/1	0.87	0.15	87,87,87,87	0
56	MG	B	9402	1/1	0.87	0.10	60,60,60,60	0
56	MG	B	9290	1/1	0.87	0.16	63,63,63,63	0
56	MG	B	9407	1/1	0.87	0.10	75,75,75,75	0
56	MG	B	9052	1/1	0.87	0.26	60,60,60,60	0
56	MG	A	1607	1/1	0.87	0.41	84,84,84,84	0
56	MG	A	1616	1/1	0.87	0.15	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	EB	1792	1/1	0.87	0.24	76,76,76,76	0
56	MG	TA	202	1/1	0.87	0.15	90,90,90,90	0
56	MG	FB	9225	1/1	0.87	0.17	71,71,71,71	0
56	MG	EB	1736	1/1	0.87	0.10	85,85,85,85	0
56	MG	FB	9061	1/1	0.87	0.24	66,66,66,66	0
56	MG	FB	9422	1/1	0.87	0.12	104,104,104,104	0
56	MG	FB	9145	1/1	0.87	0.16	66,66,66,66	0
56	MG	B	9175	1/1	0.87	0.16	64,64,64,64	0
56	MG	UB	203	1/1	0.87	0.24	91,91,91,91	0
56	MG	B	9296	1/1	0.87	0.14	72,72,72,72	0
56	MG	B	9037	1/1	0.87	0.23	65,65,65,65	0
56	MG	B	9252	1/1	0.87	0.14	69,69,69,69	0
56	MG	A	1715	1/1	0.87	0.28	113,113,113,113	0
56	MG	CC	101	1/1	0.87	0.17	82,82,82,82	0
56	MG	EB	1802	1/1	0.87	0.06	108,108,108,108	0
56	MG	B	9039	1/1	0.87	0.27	56,56,56,56	0
56	MG	FB	9334	1/1	0.87	0.21	65,65,65,65	0
56	MG	B	9040	1/1	0.87	0.24	57,57,57,57	0
56	MG	B	9357	1/1	0.87	0.20	62,62,62,62	0
56	MG	EB	1687	1/1	0.87	0.26	95,95,95,95	0
56	MG	B	9304	1/1	0.87	0.15	72,72,72,72	0
56	MG	B	9110	1/1	0.87	0.24	58,58,58,58	0
56	MG	AA	101	1/1	0.87	0.17	80,80,80,80	0
56	MG	B	9309	1/1	0.87	0.19	73,73,73,73	0
56	MG	FB	9250	1/1	0.87	0.25	75,75,75,75	0
56	MG	FB	9083	1/1	0.87	0.32	82,82,82,82	0
56	MG	A	1625	1/1	0.87	0.15	96,96,96,96	0
56	MG	FB	9168	1/1	0.87	0.18	85,85,85,85	0
56	MG	A	1748	1/1	0.87	0.18	82,82,82,82	0
56	MG	B	9510	1/1	0.87	0.06	120,120,120,120	0
56	MG	EB	1697	1/1	0.87	0.09	98,98,98,98	0
56	MG	B	9047	1/1	0.87	0.22	68,68,68,68	0
56	MG	B	9270	1/1	0.87	0.23	57,57,57,57	0
56	MG	FB	9458	1/1	0.87	0.13	85,85,85,85	0
56	MG	FB	9459	1/1	0.87	0.07	92,92,92,92	0
56	MG	FB	9461	1/1	0.87	0.13	71,71,71,71	0
56	MG	FB	9175	1/1	0.87	0.35	87,87,87,87	0
56	MG	B	9082	1/1	0.87	0.23	69,69,69,69	0
56	MG	EB	1761	1/1	0.87	0.24	82,82,82,82	0
56	MG	QC	303	1/1	0.87	0.19	101,101,101,101	0
56	MG	EB	1763	1/1	0.87	0.07	85,85,85,85	0
56	MG	A	1731	1/1	0.87	0.13	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FB	9362	1/1	0.87	0.06	84,84,84,84	0
56	MG	B	9320	1/1	0.87	0.35	85,85,85,85	0
56	MG	B	9122	1/1	0.87	0.21	79,79,79,79	0
56	MG	A	1750	1/1	0.87	0.10	79,79,79,79	0
56	MG	FB	9371	1/1	0.87	0.09	79,79,79,79	0
56	MG	FB	9277	1/1	0.87	0.44	65,65,65,65	0
56	MG	B	9239	1/1	0.87	0.14	94,94,94,94	0
56	MG	EB	1711	1/1	0.87	0.20	85,85,85,85	0
56	MG	YC	204	1/1	0.87	0.16	74,74,74,74	0
56	MG	C	220	1/1	0.87	0.15	99,99,99,99	0
56	MG	B	9326	1/1	0.87	0.20	69,69,69,69	0
56	MG	B	9168	1/1	0.87	0.11	64,64,64,64	0
56	MG	FB	9382	1/1	0.87	0.21	80,80,80,80	0
56	MG	B	9284	1/1	0.87	0.20	65,65,65,65	0
56	MG	FB	9287	1/1	0.87	0.25	72,72,72,72	0
56	MG	FB	9079	1/1	0.88	0.24	73,73,73,73	0
56	MG	B	9308	1/1	0.88	0.23	70,70,70,70	0
56	MG	FB	9016	1/1	0.88	0.41	75,75,75,75	0
56	MG	B	9405	1/1	0.88	0.05	73,73,73,73	0
56	MG	B	9093	1/1	0.88	0.23	60,60,60,60	0
56	MG	B	9530	1/1	0.88	0.19	71,71,71,71	0
56	MG	A	1722	1/1	0.88	0.18	126,126,126,126	0
56	MG	JB	301	1/1	0.88	0.19	69,69,69,69	0
56	MG	FB	9238	1/1	0.88	0.08	68,68,68,68	0
56	MG	FB	9239	1/1	0.88	0.08	111,111,111,111	0
56	MG	B	9056	1/1	0.88	0.23	63,63,63,63	0
56	MG	FB	9241	1/1	0.88	0.29	84,84,84,84	0
56	MG	B	9034	1/1	0.88	0.31	84,84,84,84	0
56	MG	B	9481	1/1	0.88	0.08	58,58,58,58	0
56	MG	A	1773	1/1	0.88	0.13	98,98,98,98	0
56	MG	A	1643	1/1	0.88	0.19	73,73,73,73	0
56	MG	B	9361	1/1	0.88	0.08	56,56,56,56	0
56	MG	EB	1772	1/1	0.88	0.24	102,102,102,102	0
56	MG	B	9061	1/1	0.88	0.14	64,64,64,64	0
56	MG	FB	9337	1/1	0.88	0.18	78,78,78,78	0
56	MG	B	9545	1/1	0.88	0.13	99,99,99,99	0
56	MG	B	9151	1/1	0.88	0.27	66,66,66,66	0
56	MG	B	9321	1/1	0.88	0.15	77,77,77,77	0
56	MG	B	9062	1/1	0.88	0.24	70,70,70,70	0
56	MG	A	1734	1/1	0.88	0.07	89,89,89,89	0
56	MG	FB	9257	1/1	0.88	0.25	76,76,76,76	0
56	MG	EB	1725	1/1	0.88	0.10	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9435	1/1	0.88	0.09	63,63,63,63	0
56	MG	FB	9260	1/1	0.88	0.20	70,70,70,70	0
56	MG	FB	9182	1/1	0.88	0.23	60,60,60,60	0
56	MG	FB	9112	1/1	0.88	0.33	91,91,91,91	0
56	MG	B	9288	1/1	0.88	0.09	58,58,58,58	0
56	MG	A	1776	1/1	0.88	0.12	93,93,93,93	0
56	MG	FB	9354	1/1	0.88	0.13	69,69,69,69	0
56	MG	B	9327	1/1	0.88	0.30	90,90,90,90	0
56	MG	EB	1731	1/1	0.88	0.16	79,79,79,79	0
56	MG	B	9156	1/1	0.88	0.21	79,79,79,79	0
56	MG	FB	9273	1/1	0.88	0.08	76,76,76,76	0
56	MG	FB	9274	1/1	0.88	0.15	78,78,78,78	0
56	MG	A	1719	1/1	0.88	0.09	105,105,105,105	0
56	MG	A	1635	1/1	0.88	0.30	103,103,103,103	0
56	MG	B	9382	1/1	0.88	0.24	66,66,66,66	0
56	MG	FB	9196	1/1	0.88	0.27	84,84,84,84	0
56	MG	FB	9279	1/1	0.88	0.18	70,70,70,70	0
56	MG	B	9019	1/1	0.88	0.19	44,44,44,44	0
56	MG	FB	9466	1/1	0.88	0.13	74,74,74,74	0
56	MG	B	9023	1/1	0.88	0.29	48,48,48,48	0
56	MG	FB	9469	1/1	0.88	0.19	74,74,74,74	0
56	MG	U	102	1/1	0.88	0.13	69,69,69,69	0
56	MG	EB	1794	1/1	0.88	0.10	88,88,88,88	0
56	MG	A	1780	1/1	0.88	0.13	79,79,79,79	0
56	MG	B	9511	1/1	0.88	0.07	77,77,77,77	0
56	MG	EB	1742	1/1	0.88	0.17	82,82,82,82	0
56	MG	FB	9129	1/1	0.88	0.22	87,87,87,87	0
56	MG	B	9026	1/1	0.88	0.14	53,53,53,53	0
56	MG	Z	103	1/1	0.88	0.18	82,82,82,82	0
56	MG	FB	9292	1/1	0.88	0.22	85,85,85,85	0
56	MG	B	9084	1/1	0.88	0.10	61,61,61,61	0
56	MG	C	208	1/1	0.88	0.18	99,99,99,99	0
56	MG	FB	9065	1/1	0.88	0.32	75,75,75,75	0
56	MG	B	9340	1/1	0.88	0.35	64,64,64,64	0
56	MG	B	9085	1/1	0.88	0.23	67,67,67,67	0
56	MG	B	9460	1/1	0.88	0.08	76,76,76,76	0
56	MG	EB	1695	1/1	0.88	0.11	77,77,77,77	0
56	MG	B	9088	1/1	0.88	0.31	59,59,59,59	0
56	MG	C	213	1/1	0.88	0.11	103,103,103,103	0
56	MG	EB	1698	1/1	0.88	0.15	82,82,82,82	0
56	MG	EB	1699	1/1	0.88	0.07	81,81,81,81	0
56	MG	A	1697	1/1	0.88	0.11	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FB	9075	1/1	0.88	0.21	62,62,62,62	0
56	MG	A	1738	1/1	0.88	0.16	103,103,103,103	0
56	MG	EB	1609	1/1	0.88	0.27	86,86,86,86	0
56	MG	B	9278	1/1	0.89	0.20	67,67,67,67	0
56	MG	FB	9156	1/1	0.89	0.30	89,89,89,89	0
56	MG	FB	9450	1/1	0.89	0.11	71,71,71,71	0
56	MG	A	1810	1/1	0.89	0.05	110,110,110,110	0
56	MG	FB	9012	1/1	0.89	0.46	78,78,78,78	0
56	MG	FB	9262	1/1	0.89	0.08	61,61,61,61	0
56	MG	B	9316	1/1	0.89	0.18	58,58,58,58	0
56	MG	EB	1741	1/1	0.89	0.17	87,87,87,87	0
56	MG	B	9118	1/1	0.89	0.15	64,64,64,64	0
56	MG	B	9130	1/1	0.89	0.27	53,53,53,53	0
56	MG	FB	9460	1/1	0.89	0.13	73,73,73,73	0
56	MG	VB	201	1/1	0.89	0.30	69,69,69,69	0
56	MG	FB	9392	1/1	0.89	0.10	77,77,77,77	0
56	MG	FB	9213	1/1	0.89	0.21	61,61,61,61	0
56	MG	B	9203	1/1	0.89	0.36	57,57,57,57	0
56	MG	FB	9063	1/1	0.89	0.19	63,63,63,63	0
56	MG	B	9053	1/1	0.89	0.18	48,48,48,48	0
56	MG	FB	9397	1/1	0.89	0.14	85,85,85,85	0
56	MG	V	503	1/1	0.89	0.14	66,66,66,66	0
56	MG	B	9207	1/1	0.89	0.16	57,57,57,57	0
56	MG	B	9162	1/1	0.89	0.15	71,71,71,71	0
56	MG	Y	101	1/1	0.89	0.10	66,66,66,66	0
56	MG	EC	101	1/1	0.89	0.17	78,78,78,78	0
56	MG	B	9346	1/1	0.89	0.33	68,68,68,68	0
56	MG	B	9268	1/1	0.89	0.18	49,49,49,49	0
56	MG	FB	9475	1/1	0.89	0.17	77,77,77,77	0
56	MG	FB	9174	1/1	0.89	0.25	90,90,90,90	0
56	MG	B	9184	1/1	0.89	0.26	76,76,76,76	0
56	MG	F	301	1/1	0.89	0.15	60,60,60,60	0
56	MG	A	1760	1/1	0.89	0.09	74,74,74,74	0
56	MG	UA	202	1/1	0.89	0.17	88,88,88,88	0
56	MG	B	9112	1/1	0.89	0.17	66,66,66,66	0
56	MG	FB	9076	1/1	0.89	0.32	72,72,72,72	0
56	MG	A	1642	1/1	0.89	0.23	69,69,69,69	0
56	MG	EB	1689	1/1	0.89	0.11	81,81,81,81	0
56	MG	B	9493	1/1	0.89	0.09	71,71,71,71	0
56	MG	FB	9185	1/1	0.89	0.13	104,104,104,104	0
56	MG	B	9383	1/1	0.89	0.12	74,74,74,74	0
56	MG	B	9385	1/1	0.89	0.22	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FB	9041	1/1	0.89	0.24	61,61,61,61	0
56	MG	EB	1729	1/1	0.89	0.19	77,77,77,77	0
56	MG	B	9355	1/1	0.89	0.04	74,74,74,74	0
56	MG	EB	1804	1/1	0.89	0.15	79,79,79,79	0
56	MG	B	9463	1/1	0.89	0.09	72,72,72,72	0
56	MG	B	9464	1/1	0.89	0.13	78,78,78,78	0
56	MG	FB	9249	1/1	0.89	0.14	88,88,88,88	0
56	MG	FB	9309	1/1	0.89	0.09	70,70,70,70	0
56	MG	M	201	1/1	0.89	0.26	78,78,78,78	0
56	MG	M	202	1/1	0.89	0.16	83,83,83,83	0
56	MG	FB	9005	1/1	0.89	0.35	53,53,53,53	0
56	MG	FB	9372	1/1	0.89	0.17	81,81,81,81	0
56	MG	FB	9373	1/1	0.89	0.10	76,76,76,76	0
56	MG	IB	303	1/1	0.89	0.17	59,59,59,59	0
56	MG	IB	304	1/1	0.89	0.24	62,62,62,62	0
56	MG	FB	9374	1/1	0.89	0.14	84,84,84,84	0
56	MG	B	9388	1/1	0.89	0.07	71,71,71,71	0
56	MG	B	9389	1/1	0.89	0.16	57,57,57,57	0
56	MG	B	9332	1/1	0.89	0.07	52,52,52,52	0
56	MG	FB	9378	1/1	0.89	0.08	85,85,85,85	0
56	MG	FB	9101	1/1	0.89	0.19	76,76,76,76	0
56	MG	NB	201	1/1	0.89	0.20	124,124,124,124	0
56	MG	B	9271	1/1	0.90	0.10	89,89,89,89	0
56	MG	EB	1762	1/1	0.90	0.15	84,84,84,84	0
56	MG	FB	9137	1/1	0.90	0.47	71,71,71,71	0
56	MG	B	9456	1/1	0.90	0.14	53,53,53,53	0
56	MG	B	9064	1/1	0.90	0.26	73,73,73,73	0
56	MG	A	1668	1/1	0.90	0.12	80,80,80,80	0
56	MG	FB	9142	1/1	0.90	0.24	71,71,71,71	0
56	MG	NB	202	1/1	0.90	0.14	113,113,113,113	0
56	MG	B	9108	1/1	0.90	0.16	71,71,71,71	0
56	MG	B	9147	1/1	0.90	0.12	52,52,52,52	0
56	MG	FB	9439	1/1	0.90	0.13	91,91,91,91	0
56	MG	FB	9018	1/1	0.90	0.26	77,77,77,77	0
56	MG	M	205	1/1	0.90	0.16	75,75,75,75	0
56	MG	EB	1719	1/1	0.90	0.20	121,121,121,121	0
56	MG	B	9204	1/1	0.90	0.09	76,76,76,76	0
56	MG	B	9241	1/1	0.90	0.08	54,54,54,54	0
56	MG	FB	9220	1/1	0.90	0.28	66,66,66,66	0
56	MG	B	9148	1/1	0.90	0.28	65,65,65,65	0
56	MG	B	9472	1/1	0.90	0.12	80,80,80,80	0
56	MG	FB	9084	1/1	0.90	0.11	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	FB	9026	1/1	0.90	0.30	81,81,81,81	0
56	MG	FB	9297	1/1	0.90	0.37	75,75,75,75	0
56	MG	FB	9298	1/1	0.90	0.08	61,61,61,61	0
56	MG	A	1811	1/1	0.90	0.15	100,100,100,100	0
56	MG	A	1809	1/1	0.90	0.13	93,93,93,93	0
56	MG	TA	201	1/1	0.90	0.11	96,96,96,96	0
56	MG	B	9058	1/1	0.90	0.23	59,59,59,59	0
56	MG	B	9049	1/1	0.90	0.16	65,65,65,65	0
56	MG	FB	9305	1/1	0.90	0.14	72,72,72,72	0
56	MG	CC	107	1/1	0.90	0.10	68,68,68,68	0
56	MG	FB	9306	1/1	0.90	0.16	71,71,71,71	0
56	MG	B	9113	1/1	0.90	0.12	64,64,64,64	0
56	MG	B	9080	1/1	0.90	0.17	59,59,59,59	0
56	MG	FB	9467	1/1	0.90	0.10	82,82,82,82	0
56	MG	B	9158	1/1	0.90	0.25	77,77,77,77	0
56	MG	X	101	1/1	0.90	0.18	77,77,77,77	0
56	MG	B	9021	1/1	0.90	0.26	54,54,54,54	0
56	MG	FB	9390	1/1	0.90	0.14	67,67,67,67	0
56	MG	Z	101	1/1	0.90	0.17	82,82,82,82	0
56	MG	EB	1685	1/1	0.90	0.21	71,71,71,71	0
56	MG	Z	102	1/1	0.90	0.13	64,64,64,64	0
56	MG	B	9429	1/1	0.90	0.10	56,56,56,56	0
56	MG	EB	1642	1/1	0.90	0.15	92,92,92,92	0
56	MG	B	9163	1/1	0.90	0.14	54,54,54,54	0
56	MG	B	9164	1/1	0.90	0.32	65,65,65,65	0
56	MG	FB	9110	1/1	0.90	0.36	62,62,62,62	0
56	MG	B	9258	1/1	0.90	0.11	88,88,88,88	0
56	MG	B	9540	1/1	0.90	0.09	65,65,65,65	0
56	MG	B	9260	1/1	0.90	0.09	60,60,60,60	0
56	MG	EB	1602	1/1	0.90	0.39	72,72,72,72	0
56	MG	B	9185	1/1	0.90	0.15	78,78,78,78	0
56	MG	B	9165	1/1	0.90	0.13	53,53,53,53	0
56	MG	HA	103	1/1	0.90	0.24	104,104,104,104	0
56	MG	B	9302	1/1	0.90	0.22	58,58,58,58	0
56	MG	B	9029	1/1	0.90	0.21	46,46,46,46	0
56	MG	EB	1803	1/1	0.90	0.29	88,88,88,88	0
56	MG	FB	9121	1/1	0.90	0.14	53,53,53,53	0
56	MG	B	9229	1/1	0.90	0.10	59,59,59,59	0
56	MG	FB	9414	1/1	0.90	0.17	76,76,76,76	0
56	MG	G	302	1/1	0.90	0.09	83,83,83,83	0
56	MG	EB	1753	1/1	0.90	0.11	93,93,93,93	0
56	MG	FB	9193	1/1	0.90	0.18	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9266	1/1	0.90	0.06	74,74,74,74	0
56	MG	B	9307	1/1	0.90	0.20	72,72,72,72	0
56	MG	B	9193	1/1	0.90	0.19	59,59,59,59	0
56	MG	B	9347	1/1	0.90	0.10	90,90,90,90	0
56	MG	B	9042	1/1	0.90	0.26	61,61,61,61	0
56	MG	FB	9130	1/1	0.90	0.37	76,76,76,76	0
56	MG	B	9350	1/1	0.90	0.13	60,60,60,60	0
56	MG	EB	1710	1/1	0.90	0.15	96,96,96,96	0
56	MG	FB	9056	1/1	0.91	0.37	72,72,72,72	0
56	MG	FB	9268	1/1	0.91	0.12	70,70,70,70	0
56	MG	B	9067	1/1	0.91	0.15	66,66,66,66	0
56	MG	FB	9270	1/1	0.91	0.08	78,78,78,78	0
56	MG	KB	302	1/1	0.91	0.09	84,84,84,84	0
56	MG	O	202	1/1	0.91	0.43	76,76,76,76	0
56	MG	KB	304	1/1	0.91	0.10	93,93,93,93	0
56	MG	B	9495	1/1	0.91	0.12	69,69,69,69	0
56	MG	B	9198	1/1	0.91	0.08	56,56,56,56	0
56	MG	B	9450	1/1	0.91	0.11	58,58,58,58	0
56	MG	FB	9062	1/1	0.91	0.21	87,87,87,87	0
56	MG	EB	1805	1/1	0.91	0.17	84,84,84,84	0
56	MG	B	9032	1/1	0.91	0.20	78,78,78,78	0
56	MG	B	9406	1/1	0.91	0.10	60,60,60,60	0
56	MG	A	1615	1/1	0.91	0.13	63,63,63,63	0
56	MG	A	1763	1/1	0.91	0.15	95,95,95,95	0
56	MG	B	9371	1/1	0.91	0.09	75,75,75,75	0
56	MG	B	9504	1/1	0.91	0.09	59,59,59,59	0
56	MG	B	9508	1/1	0.91	0.08	70,70,70,70	0
56	MG	FB	9286	1/1	0.91	0.15	72,72,72,72	0
56	MG	FB	9446	1/1	0.91	0.06	83,83,83,83	0
56	MG	B	9411	1/1	0.91	0.07	73,73,73,73	0
56	MG	AB	101	1/1	0.91	0.13	92,92,92,92	0
56	MG	FB	9367	1/1	0.91	0.09	70,70,70,70	0
56	MG	B	9412	1/1	0.91	0.17	50,50,50,50	0
56	MG	B	9255	1/1	0.91	0.16	66,66,66,66	0
56	MG	B	9512	1/1	0.91	0.11	59,59,59,59	0
56	MG	B	9514	1/1	0.91	0.12	59,59,59,59	0
56	MG	FB	9293	1/1	0.91	0.14	68,68,68,68	0
56	MG	EB	1708	1/1	0.91	0.09	115,115,115,115	0
56	MG	B	9078	1/1	0.91	0.31	56,56,56,56	0
56	MG	CC	105	1/1	0.91	0.22	67,67,67,67	0
56	MG	A	1644	1/1	0.91	0.24	83,83,83,83	0
56	MG	B	9467	1/1	0.91	0.18	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	A	1698	1/1	0.91	0.15	75,75,75,75	0
56	MG	B	9469	1/1	0.91	0.10	59,59,59,59	0
56	MG	B	9471	1/1	0.91	0.18	74,74,74,74	0
56	MG	FB	9085	1/1	0.91	0.17	71,71,71,71	0
56	MG	C	216	1/1	0.91	0.08	117,117,117,117	0
56	MG	EB	1716	1/1	0.91	0.07	84,84,84,84	0
56	MG	FB	9385	1/1	0.91	0.17	77,77,77,77	0
56	MG	FB	9231	1/1	0.91	0.12	81,81,81,81	0
56	MG	A	1640	1/1	0.91	0.07	84,84,84,84	0
56	MG	B	9473	1/1	0.91	0.06	70,70,70,70	0
56	MG	B	9424	1/1	0.91	0.10	82,82,82,82	0
56	MG	B	9096	1/1	0.91	0.10	55,55,55,55	0
56	MG	B	9152	1/1	0.91	0.13	50,50,50,50	0
56	MG	B	9322	1/1	0.91	0.09	55,55,55,55	0
56	MG	FB	9167	1/1	0.91	0.13	65,65,65,65	0
56	MG	B	9430	1/1	0.91	0.05	68,68,68,68	0
56	MG	B	9533	1/1	0.91	0.10	53,53,53,53	0
56	MG	B	9534	1/1	0.91	0.08	81,81,81,81	0
56	MG	FB	9100	1/1	0.91	0.23	83,83,83,83	0
56	MG	FB	9034	1/1	0.91	0.23	69,69,69,69	0
56	MG	B	9097	1/1	0.91	0.11	67,67,67,67	0
56	MG	B	9099	1/1	0.91	0.06	60,60,60,60	0
56	MG	B	9242	1/1	0.91	0.16	67,67,67,67	0
56	MG	B	9022	1/1	0.91	0.19	47,47,47,47	0
56	MG	B	9216	1/1	0.91	0.10	61,61,61,61	0
56	MG	B	9245	1/1	0.91	0.18	77,77,77,77	0
56	MG	EB	1787	1/1	0.91	0.06	113,113,113,113	0
56	MG	B	9542	1/1	0.91	0.12	54,54,54,54	0
56	MG	B	9394	1/1	0.91	0.08	96,96,96,96	0
56	MG	B	9443	1/1	0.91	0.09	57,57,57,57	0
56	MG	B	9191	1/1	0.91	0.25	67,67,67,67	0
56	MG	B	9192	1/1	0.91	0.22	54,54,54,54	0
56	MG	FB	9186	1/1	0.91	0.13	75,75,75,75	0
56	MG	B	9490	1/1	0.91	0.23	65,65,65,65	0
56	MG	B	9549	1/1	0.91	0.11	59,59,59,59	0
56	MG	B	9305	1/1	0.91	0.09	76,76,76,76	0
56	MG	B	9551	1/1	0.91	0.21	90,90,90,90	0
56	MG	EB	1797	1/1	0.91	0.05	97,97,97,97	0
56	MG	EB	1635	1/1	0.91	0.29	87,87,87,87	0
56	MG	B	9173	1/1	0.91	0.06	69,69,69,69	0
56	MG	FB	9452	1/1	0.92	0.14	67,67,67,67	0
56	MG	B	9044	1/1	0.92	0.25	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9318	1/1	0.92	0.06	79,79,79,79	0
56	MG	B	9212	1/1	0.92	0.11	77,77,77,77	0
56	MG	FB	9365	1/1	0.92	0.06	72,72,72,72	0
56	MG	FB	9200	1/1	0.92	0.18	93,93,93,93	0
56	MG	B	9157	1/1	0.92	0.07	69,69,69,69	0
56	MG	EB	1654	1/1	0.92	0.13	71,71,71,71	0
56	MG	XA	103	1/1	0.92	0.39	96,96,96,96	0
56	MG	B	9517	1/1	0.92	0.08	80,80,80,80	0
56	MG	B	9459	1/1	0.92	0.05	71,71,71,71	0
56	MG	FB	9327	1/1	0.92	0.24	69,69,69,69	0
56	MG	A	1768	1/1	0.92	0.12	78,78,78,78	0
56	MG	EB	1627	1/1	0.92	0.16	73,73,73,73	0
56	MG	A	1777	1/1	0.92	0.10	86,86,86,86	0
56	MG	B	9433	1/1	0.92	0.05	69,69,69,69	0
56	MG	FB	9252	1/1	0.92	0.07	79,79,79,79	0
56	MG	B	9218	1/1	0.92	0.24	58,58,58,58	0
56	MG	B	9150	1/1	0.92	0.16	61,61,61,61	0
56	MG	B	9557	1/1	0.92	0.11	58,58,58,58	0
56	MG	B	9436	1/1	0.92	0.08	70,70,70,70	0
56	MG	B	9374	1/1	0.92	0.09	62,62,62,62	0
56	MG	B	9220	1/1	0.92	0.11	64,64,64,64	0
56	MG	B	9529	1/1	0.92	0.09	62,62,62,62	0
56	MG	A	1655	1/1	0.92	0.15	74,74,74,74	0
56	MG	FB	9105	1/1	0.92	0.15	67,67,67,67	0
56	MG	B	9141	1/1	0.92	0.18	56,56,56,56	0
56	MG	FB	9436	1/1	0.92	0.06	69,69,69,69	0
56	MG	B	9381	1/1	0.92	0.06	71,71,71,71	0
56	MG	FB	9146	1/1	0.92	0.14	61,61,61,61	0
56	MG	B	9187	1/1	0.92	0.11	56,56,56,56	0
56	MG	EB	1705	1/1	0.92	0.12	82,82,82,82	0
56	MG	B	9206	1/1	0.92	0.21	65,65,65,65	0
56	MG	B	9331	1/1	0.92	0.08	63,63,63,63	0
56	MG	B	9131	1/1	0.92	0.23	62,62,62,62	0
56	MG	B	9086	1/1	0.92	0.16	66,66,66,66	0
56	MG	J	202	1/1	0.92	0.06	104,104,104,104	0
56	MG	B	9295	1/1	0.92	0.06	61,61,61,61	0
56	MG	B	9178	1/1	0.92	0.14	65,65,65,65	0
56	MG	B	9020	1/1	0.92	0.22	45,45,45,45	0
56	MG	L	202	1/1	0.92	0.07	81,81,81,81	0
58	ZN	HC	101	1/1	0.92	0.15	135,135,135,135	0
56	MG	UB	202	1/1	0.93	0.05	83,83,83,83	0
56	MG	B	9348	1/1	0.93	0.07	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9066	1/1	0.93	0.17	57,57,57,57	0
56	MG	FB	9037	1/1	0.93	0.09	130,130,130,130	0
56	MG	B	9380	1/1	0.93	0.10	51,51,51,51	0
56	MG	FB	9304	1/1	0.93	0.15	66,66,66,66	0
56	MG	FB	9039	1/1	0.93	0.31	78,78,78,78	0
56	MG	B	9228	1/1	0.93	0.14	62,62,62,62	0
56	MG	B	9009	1/1	0.93	0.46	55,55,55,55	0
56	MG	FB	9419	1/1	0.93	0.11	72,72,72,72	0
56	MG	B	9526	1/1	0.93	0.10	65,65,65,65	0
56	MG	FB	9363	1/1	0.93	0.07	63,63,63,63	0
56	MG	FB	9166	1/1	0.93	0.12	80,80,80,80	0
56	MG	A	1767	1/1	0.93	0.05	94,94,94,94	0
56	MG	B	9417	1/1	0.93	0.18	67,67,67,67	0
56	MG	B	9420	1/1	0.93	0.07	103,103,103,103	0
56	MG	FB	9215	1/1	0.93	0.17	70,70,70,70	0
56	MG	B	9421	1/1	0.93	0.22	57,57,57,57	0
56	MG	FB	9265	1/1	0.93	0.14	69,69,69,69	0
56	MG	B	9195	1/1	0.93	0.16	62,62,62,62	0
56	MG	B	9138	1/1	0.93	0.11	69,69,69,69	0
56	MG	FB	9318	1/1	0.93	0.12	68,68,68,68	0
56	MG	B	9197	1/1	0.93	0.17	65,65,65,65	0
56	MG	B	9257	1/1	0.93	0.14	61,61,61,61	0
56	MG	B	9089	1/1	0.93	0.16	59,59,59,59	0
56	MG	FB	9223	1/1	0.93	0.07	68,68,68,68	0
56	MG	FB	9091	1/1	0.93	0.40	68,68,68,68	0
56	MG	B	9358	1/1	0.93	0.11	64,64,64,64	0
56	MG	B	9466	1/1	0.93	0.05	69,69,69,69	0
56	MG	B	9126	1/1	0.93	0.19	54,54,54,54	0
56	MG	B	9071	1/1	0.93	0.19	49,49,49,49	0
56	MG	FB	9138	1/1	0.93	0.49	66,66,66,66	0
56	MG	FB	9230	1/1	0.93	0.07	70,70,70,70	0
56	MG	B	9142	1/1	0.93	0.28	65,65,65,65	0
56	MG	B	9074	1/1	0.93	0.29	54,54,54,54	0
56	MG	FB	9448	1/1	0.93	0.17	79,79,79,79	0
56	MG	B	9505	1/1	0.93	0.14	60,60,60,60	0
56	MG	B	9264	1/1	0.93	0.28	74,74,74,74	0
56	MG	FB	9335	1/1	0.93	0.23	69,69,69,69	0
56	MG	B	9103	1/1	0.93	0.21	53,53,53,53	0
56	MG	B	9474	1/1	0.93	0.05	75,75,75,75	0
56	MG	B	9548	1/1	0.93	0.12	84,84,84,84	0
56	MG	B	9400	1/1	0.93	0.08	119,119,119,119	0
56	MG	FB	9147	1/1	0.93	0.12	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9003	1/1	0.93	0.32	54,54,54,54	0
56	MG	B	9342	1/1	0.93	0.20	56,56,56,56	0
56	MG	B	9161	1/1	0.93	0.19	67,67,67,67	0
56	MG	FB	9151	1/1	0.93	0.09	127,127,127,127	0
56	MG	B	9319	1/1	0.93	0.18	75,75,75,75	0
56	MG	FB	9109	1/1	0.93	0.18	61,61,61,61	0
56	MG	FB	9406	1/1	0.93	0.13	100,100,100,100	0
56	MG	B	9224	1/1	0.93	0.13	47,47,47,47	0
56	MG	B	9225	1/1	0.93	0.07	52,52,52,52	0
56	MG	B	9013	1/1	0.93	0.34	66,66,66,66	0
56	MG	CA	602	1/1	0.93	0.09	62,62,62,62	0
56	MG	FB	9133	1/1	0.94	0.13	69,69,69,69	0
56	MG	B	9432	1/1	0.94	0.08	67,67,67,67	0
56	MG	Z	104	1/1	0.94	0.05	76,76,76,76	0
56	MG	B	9275	1/1	0.94	0.11	59,59,59,59	0
56	MG	B	9360	1/1	0.94	0.14	63,63,63,63	0
56	MG	B	9552	1/1	0.94	0.06	56,56,56,56	0
56	MG	FB	9184	1/1	0.94	0.16	61,61,61,61	0
56	MG	B	9094	1/1	0.94	0.24	53,53,53,53	0
56	MG	G	301	1/1	0.94	0.03	85,85,85,85	0
56	MG	B	9334	1/1	0.94	0.18	64,64,64,64	0
56	MG	B	9004	1/1	0.94	0.27	40,40,40,40	0
56	MG	FB	9285	1/1	0.94	0.15	73,73,73,73	0
56	MG	B	9005	1/1	0.94	0.30	47,47,47,47	0
56	MG	B	9046	1/1	0.94	0.13	51,51,51,51	0
56	MG	B	9440	1/1	0.94	0.07	55,55,55,55	0
56	MG	FB	9010	1/1	0.94	0.52	60,60,60,60	0
56	MG	B	9115	1/1	0.94	0.20	48,48,48,48	0
56	MG	B	9283	1/1	0.94	0.15	67,67,67,67	0
56	MG	B	9068	1/1	0.94	0.16	52,52,52,52	0
56	MG	B	9341	1/1	0.94	0.15	69,69,69,69	0
56	MG	K	203	1/1	0.94	0.10	71,71,71,71	0
56	MG	B	9189	1/1	0.94	0.07	52,52,52,52	0
56	MG	B	9190	1/1	0.94	0.27	52,52,52,52	0
56	MG	FB	9399	1/1	0.94	0.20	71,71,71,71	0
56	MG	B	9069	1/1	0.94	0.12	63,63,63,63	0
56	MG	B	9235	1/1	0.94	0.09	80,80,80,80	0
56	MG	B	9377	1/1	0.94	0.08	61,61,61,61	0
56	MG	JA	406	1/1	0.94	0.13	74,74,74,74	0
56	MG	FB	9456	1/1	0.94	0.09	76,76,76,76	0
56	MG	B	9236	1/1	0.94	0.26	63,63,63,63	0
56	MG	B	9006	1/1	0.94	0.21	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QC	302	1/1	0.94	0.06	95,95,95,95	0
56	MG	A	1684	1/1	0.94	0.18	74,74,74,74	0
56	MG	B	9419	1/1	0.94	0.06	58,58,58,58	0
56	MG	RC	201	1/1	0.94	0.05	85,85,85,85	0
56	MG	RC	202	1/1	0.94	0.09	92,92,92,92	0
56	MG	B	9215	1/1	0.94	0.05	71,71,71,71	0
56	MG	B	9458	1/1	0.94	0.04	58,58,58,58	0
56	MG	B	9072	1/1	0.94	0.19	55,55,55,55	0
56	MG	UC	201	1/1	0.94	0.24	98,98,98,98	0
56	MG	B	9073	1/1	0.94	0.15	48,48,48,48	0
56	MG	B	9031	1/1	0.94	0.13	60,60,60,60	0
56	MG	U	101	1/1	0.94	0.09	62,62,62,62	0
56	MG	A	1602	1/1	0.94	0.33	60,60,60,60	0
56	MG	B	9425	1/1	0.94	0.15	86,86,86,86	0
56	MG	B	9269	1/1	0.94	0.08	53,53,53,53	0
56	MG	B	9199	1/1	0.94	0.13	54,54,54,54	0
56	MG	B	9146	1/1	0.94	0.06	53,53,53,53	0
56	MG	C	221	1/1	0.94	0.07	100,100,100,100	0
56	MG	FB	9369	1/1	0.94	0.18	63,63,63,63	0
56	MG	FB	9082	1/1	0.94	0.07	62,62,62,62	0
56	MG	A	1714	1/1	0.94	0.12	98,98,98,98	0
56	MG	B	9010	1/1	0.94	0.43	67,67,67,67	0
56	MG	B	9470	1/1	0.94	0.12	97,97,97,97	0
56	MG	B	9117	1/1	0.95	0.41	69,69,69,69	0
56	MG	B	9063	1/1	0.95	0.16	56,56,56,56	0
56	MG	B	9132	1/1	0.95	0.10	46,46,46,46	0
56	MG	FB	9426	1/1	0.95	0.11	71,71,71,71	0
56	MG	B	9274	1/1	0.95	0.14	68,68,68,68	0
56	MG	B	9404	1/1	0.95	0.09	65,65,65,65	0
56	MG	B	9379	1/1	0.95	0.15	54,54,54,54	0
56	MG	FB	9430	1/1	0.95	0.05	75,75,75,75	0
56	MG	FB	9353	1/1	0.95	0.08	76,76,76,76	0
56	MG	B	9461	1/1	0.95	0.29	67,67,67,67	0
56	MG	B	9133	1/1	0.95	0.09	61,61,61,61	0
56	MG	B	9076	1/1	0.95	0.21	53,53,53,53	0
56	MG	B	9492	1/1	0.95	0.09	59,59,59,59	0
56	MG	B	9160	1/1	0.95	0.16	60,60,60,60	0
56	MG	B	9259	1/1	0.95	0.18	61,61,61,61	0
56	MG	B	9410	1/1	0.95	0.05	69,69,69,69	0
56	MG	B	9384	1/1	0.95	0.09	52,52,52,52	0
56	MG	B	9087	1/1	0.95	0.15	60,60,60,60	0
56	MG	B	9362	1/1	0.95	0.27	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9002	1/1	0.95	0.50	45,45,45,45	0
56	MG	B	9442	1/1	0.95	0.13	65,65,65,65	0
56	MG	B	9282	1/1	0.95	0.21	53,53,53,53	0
56	MG	B	9124	1/1	0.95	0.14	55,55,55,55	0
56	MG	FB	9368	1/1	0.95	0.16	74,74,74,74	0
56	MG	B	9418	1/1	0.95	0.17	72,72,72,72	0
56	MG	FB	9025	1/1	0.95	0.23	53,53,53,53	0
56	MG	B	9246	1/1	0.95	0.32	61,61,61,61	0
56	MG	B	9028	1/1	0.95	0.16	54,54,54,54	0
56	MG	B	9232	1/1	0.95	0.07	79,79,79,79	0
56	MG	B	9090	1/1	0.95	0.09	49,49,49,49	0
56	MG	B	9234	1/1	0.95	0.18	59,59,59,59	0
56	MG	FB	9096	1/1	0.95	0.15	73,73,73,73	0
56	MG	L	201	1/1	0.95	0.15	57,57,57,57	0
56	MG	B	9451	1/1	0.95	0.11	55,55,55,55	0
56	MG	EA	101	1/1	0.95	0.15	57,57,57,57	0
56	MG	B	9107	1/1	0.95	0.30	58,58,58,58	0
56	MG	FB	9271	1/1	0.95	0.21	64,64,64,64	0
57	BLS	B	9001	30/30	0.95	0.12	80,80,81,81	0
57	BLS	FB	9001	30/30	0.95	0.12	83,84,84,84	0
56	MG	IB	301	1/1	0.95	0.14	65,65,65,65	0
56	MG	FB	9201	1/1	0.95	0.07	67,67,67,67	0
56	MG	A	1613	1/1	0.95	0.14	76,76,76,76	0
56	MG	B	9054	1/1	0.96	0.32	50,50,50,50	0
56	MG	B	9416	1/1	0.96	0.10	59,59,59,59	0
56	MG	FB	9386	1/1	0.96	0.08	72,72,72,72	0
56	MG	B	9119	1/1	0.96	0.10	49,49,49,49	0
56	MG	FB	9444	1/1	0.96	0.05	84,84,84,84	0
56	MG	FB	9087	1/1	0.96	0.23	65,65,65,65	0
56	MG	EB	1777	1/1	0.96	0.05	116,116,116,116	0
56	MG	B	9194	1/1	0.96	0.19	56,56,56,56	0
56	MG	B	9541	1/1	0.96	0.08	55,55,55,55	0
56	MG	B	9285	1/1	0.96	0.10	61,61,61,61	0
56	MG	B	9213	1/1	0.96	0.09	53,53,53,53	0
56	MG	B	9098	1/1	0.96	0.17	53,53,53,53	0
56	MG	B	9524	1/1	0.96	0.11	62,62,62,62	0
56	MG	B	9276	1/1	0.96	0.09	57,57,57,57	0
56	MG	B	9127	1/1	0.96	0.10	52,52,52,52	0
56	MG	FB	9398	1/1	0.96	0.10	72,72,72,72	0
56	MG	A	1755	1/1	0.96	0.08	110,110,110,110	0
56	MG	B	9367	1/1	0.96	0.08	57,57,57,57	0
56	MG	FB	9245	1/1	0.96	0.14	63,63,63,63	0

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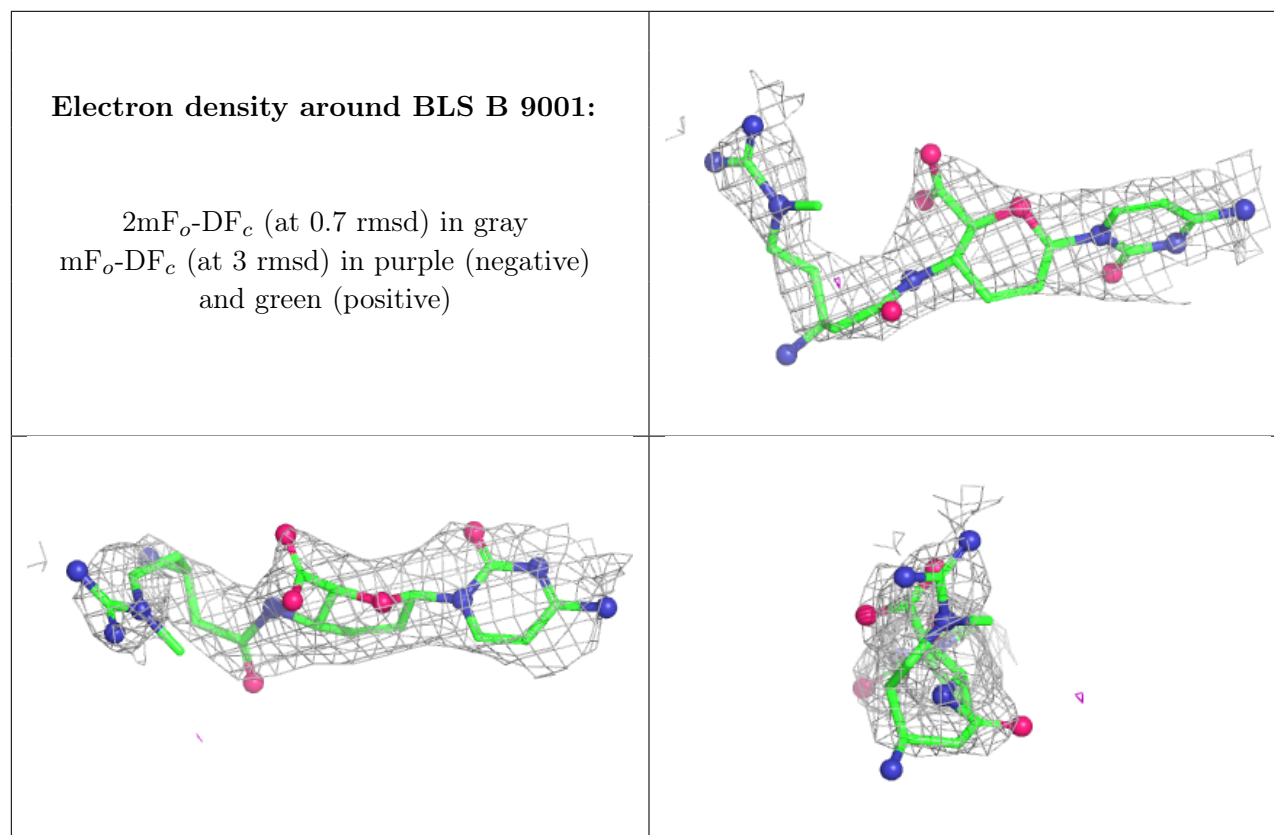
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YC	203	1/1	0.96	0.13	80,80,80,80	0
56	MG	B	9426	1/1	0.96	0.10	48,48,48,48	0
56	MG	A	1786	1/1	0.96	0.05	119,119,119,119	0
56	MG	B	9123	1/1	0.96	0.07	46,46,46,46	0
56	MG	FB	9351	1/1	0.96	0.09	68,68,68,68	0
56	MG	B	9513	1/1	0.96	0.19	61,61,61,61	0
56	MG	CD	101	1/1	0.96	0.20	94,94,94,94	0
56	MG	B	9399	1/1	0.96	0.06	67,67,67,67	0
56	MG	B	9159	1/1	0.96	0.25	65,65,65,65	0
56	MG	B	9496	1/1	0.96	0.06	55,55,55,55	0
56	MG	EB	1750	1/1	0.96	0.12	85,85,85,85	0
56	MG	B	9558	1/1	0.96	0.07	62,62,62,62	0
56	MG	B	9398	1/1	0.97	0.10	54,54,54,54	0
56	MG	FB	9346	1/1	0.97	0.19	83,83,83,83	0
56	MG	FB	9464	1/1	0.97	0.13	76,76,76,76	0
56	MG	B	9310	1/1	0.97	0.23	54,54,54,54	0
56	MG	B	9507	1/1	0.97	0.11	64,64,64,64	0
56	MG	B	9532	1/1	0.97	0.24	62,62,62,62	0
56	MG	B	9387	1/1	0.97	0.05	56,56,56,56	0
56	MG	FB	9132	1/1	0.97	0.21	67,67,67,67	0
56	MG	O	201	1/1	0.97	0.12	63,63,63,63	0
56	MG	B	9372	1/1	0.97	0.18	55,55,55,55	0
56	MG	A	1630	1/1	0.97	0.07	66,66,66,66	0
56	MG	B	9055	1/1	0.97	0.23	57,57,57,57	0
58	ZN	ZB	701	1/1	0.97	0.04	106,106,106,106	0
56	MG	B	9555	1/1	0.97	0.11	79,79,79,79	0
56	MG	B	9024	1/1	0.97	0.23	57,57,57,57	0
56	MG	FB	9328	1/1	0.98	0.03	70,70,70,70	0
56	MG	B	9506	1/1	0.98	0.07	61,61,61,61	0
56	MG	FB	9217	1/1	0.98	0.08	138,138,138,138	0
56	MG	B	9104	1/1	0.98	0.03	78,78,78,78	0
56	MG	B	9267	1/1	0.98	0.23	56,56,56,56	0
58	ZN	V	501	1/1	0.98	0.06	100,100,100,100	0
56	MG	B	9333	1/1	0.98	0.33	64,64,64,64	0
58	ZN	DA	101	1/1	0.98	0.11	133,133,133,133	0
56	MG	B	9045	1/1	0.98	0.20	49,49,49,49	0
56	MG	B	9455	1/1	0.98	0.11	67,67,67,67	0
56	MG	T	203	1/1	0.98	0.03	72,72,72,72	0
58	ZN	GA	101	1/1	0.99	0.02	94,94,94,94	0
56	MG	B	9289	1/1	0.99	0.08	62,62,62,62	0
58	ZN	CA	601	1/1	0.99	0.03	82,82,82,82	0
58	ZN	GC	101	1/1	0.99	0.03	104,104,104,104	0

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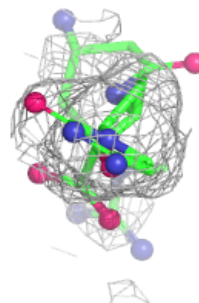
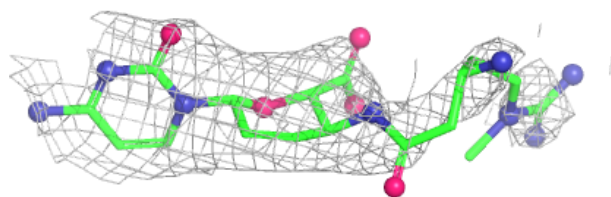
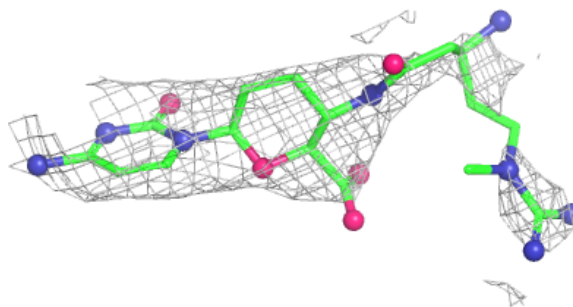
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B	9299	1/1	0.99	0.17	49,49,49,49	0
58	ZN	KC	101	1/1	0.99	0.03	121,121,121,121	0

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 BLS FB 9001:

$2mF_o-DF_c$ (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.