

wwPDB X-ray Structure Validation Summary Report (i)

Jan 2, 2024 – 04:29 pm GMT

PDB ID	:	4WRA
Title	:	Complex of 70S ribosome with tRNA-Tyr and mRNA with A-A mismatch in
		the first position in the A-site and with antibiotic paromomycin.
Authors	:	Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on	:	2014-10-23
Resolution	:	3.05 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.05 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)
RNA backbone	3102	1036 (3.32-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain							
1	13	1522	33%	44%	17%	•••				
1	1G	1522	38%	42%	17%					
2	12	256	3% 41%	39%	12%	7%				
2	1E	256	2% 	41%	12%	7%				



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Mol	Chain	Length	Quality of chain						
3	22	239	3%	36%	8% 14%				
3	2E	239	4%	31%	8% 14%				
4	32	209	2% 5 0%	39%	9% •				
4	3E	209	44%	45%	11%				
5	42	162	9%	36%	9% 7%				
5	4E	162	49%	36%	8% 7%				
6	52	101	50%	43%	7% •				
6	$5\mathrm{E}$	101	51%	40%	9%				
7	62	156	54%	38%	6% •				
7	6E	156	54%	37%	6% •				
8	72	138	47%	9% •					
8	7E	138	43%	10% •					
9	82	128	48%	8% • 5%					
9	8E	128	38%	48%	13% •				
10	1A	105	38%	44%	12% 6%				
10	1I	105	40%	44%	10% 6%				
11	2A	129	46%	32%	12% • 9%				
11	2I	129	43%	38%	9% 10%				
12	3A	132	53%	32%	10% 5%				
12	3I	132	52%	32%	9% 8%				
13	4A	126	43%	37%	13% • 7%				
13	4I	126	46%	37%	10% 8%				
14	5A	61	48%	33%	11% • 5%				
14	5I	61	30%	54%	13% •				
15	6A	89	²⁰ 62%	31%	6% •				



Continued from previous page... Chain Length Quality of chain Mol 3% 6I 89 1553% 42% . . 32% 167A88 43% 42% 10% 5% 47% 16 7I88 38% 50% 5% 8% 11% 178A 10548% 43% 5% 5% 7% 178I1055% 37% 50% 9% 189A 88 43% 30% 7% • 19% 18 9I88 39% 38% 18% . . 5% 19AA 9340% 32% 10% 16% • 6% AI 93 1945% 34% 9% 11% • 22% 20BA 10649% 34% 8% 7% • 44% 20 BI 10638% 42% 13% 7% 78% $1\mathrm{B}$ 272137% 48% 7% 7% 59% 211F277% 33% 59% 6% 221K8519% 45% 33% • 3% . 232K77 31% 47% 21% .% 232L7745% 36% 13% 5% 27% 241L85 35% 36% 26% . 2% 3K2485 32% 47% 20% . 10% 254K30 17% 10% 13% 60% 13% 4L2530 10% 7% 20% 60% % 26142918 42% 33% 21% • $1\mathrm{H}$ 2918 2628% 42% 23% 6% 271612237% 43% 17% • .% 1J2712245% 6% 28% 21% 2811 27654% 36% 8% •



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Mol	Chain	Length	Quality of chain						
28	19	276	9%	31%	10% ••				
29	21	206	36%	46%	17% •				
29	29	206	40%	41%	17% •				
30	31	210	48%	36%	12% •				
30	39	210	37%	40%	20% ••				
31	41	182	47%	42%	10% •				
31	49	182	50%	40%	9% •				
32	51	180	43%	36%	17% ••				
32	59	180	41%	39%	12% • 6%				
33	61	148	29%	53%	16% ••				
33	69	148	36%	49%	10% ••				
34	15	140	52%	31%	15% •				
34	58	140	42%	40%	15% ••				
35	25	122	53%	38%	8% •				
35	68	122	57%	34%	8%				
36	35	150	43%	35%	19% ·				
36	78	150	% 41%	37%	17% •				
37	45	141	42%	42%	13% ••				
37	88	141	% 48%	40%	9% •				
38	55	118	42%	44%	12% ••				
38	98	118	32%	58%	10%				
39	65	112	35%	50%	12% ••				
39	A8	112	41%	44%	12% ••				
40	75	146	40%	39%	14% • 6%				
40	B8	146	46%	30%	16% • 6%				



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Mol	Chain	Length	Quality of chain						
41	95	110	4%	2007					
41	00	110	12%	30%	11% ••				
41	C8	118	44%	42%	12% ••				
42	95	101	37%	41%	20% •				
40	Do	101	7%						
42	D8	101	45% 4%	46%	8% •				
43	A5	113	52%	37%	11%				
43	E8	113	58%	32%	10%				
44	B5	96	45%	44%	7% •				
44	F8	96	48%	40%	9% •				
45	C5	110	35%	42%	17% 5%				
45	G8	110	3%	45%	12% 5%				
10	Dr	200	5%		12,0 0,0				
40	D5	206	35% 2	22% 8% • 3	33%				
46	H8	206	34%	36% 12%	• 15%				
47	E5	85	45%	35%	11% 9%				
47	I8	85	46%	36%	6% • 11%				
48	F5	98	47%	41%	10% ••				
48	J8	98	53%	34%	12% •				
49	G5	72	% 33%	42% 1	4% • 8%				
49	K8	72	4%	42% 18%	6% 8%				
50	H5	60	^{2%}	40%	7% •				
50	L8	60	50%	37%	12%				
51	15	71	39%	400/ 150					
01	10	11	8%	40 /0 15%	o • 11%				
51	M8	71	34%	37% 21	1% • 7%				
52	J5	60	58%	37%	• •				
52	N8	60	50%	35%	13% •				
53	L5	49	2% 5 5%	37%	8%				
				Continued a	on next page				



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Mol	Chain	Length		Quality of chain							
53	P8	49	51%		35%	8%	6%				
54	M5	65	31%	23%	20%	9%	5%				
54	Q8	65	26%	48%	17%	•	6%				
55	3L	85	24%	49%	25	%	•				

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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	13	1623	-	-	-	Х
56	MG	14	3118	-	-	-	Х
56	MG	14	3158	-	-	-	Х
56	MG	14	3280	-	-	-	Х
56	MG	14	3293	-	-	-	Х
56	MG	14	3298	-	-	-	Х
56	MG	1G	1648	-	-	-	Х
56	MG	1H	3076	-	-	-	Х
56	MG	1H	3101	-	-	-	Х
56	MG	1H	3211	-	-	-	Х
56	MG	1H	3217	-	-	-	Х
56	MG	1H	3223	-	-	-	Х
56	MG	1H	3228	-	-	-	Х
56	MG	1H	3273	-	-	-	Х
56	MG	1H	3274	-	-	-	Х
56	MG	1H	3275	-	-	-	Х
56	MG	1H	3293	-	-	-	Х
56	MG	1H	3319	-	-	-	Х
56	MG	1H	3323	-	-	-	Х
56	MG	1H	3326	-	-	-	Х
56	MG	1H	3328	-	-	-	Х
56	MG	1H	3332	-	-	-	Х



4WRA

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 299607 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		I	Atoms		ZeroOcc	AltConf	Trace		
1	12	1505	Total	С	Ν	0	Р	0	0	0	0
1 10	1000	32352	14399	5994	10454	1505	0	0	0		
1	10	1504	Total	С	Ν	0	Р	0	0		
I IG	1504	32327	14389	5989	10446	1503	0	0	0		

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

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
2	9 1F	027	Total	С	Ν	Ο	S	0	Ο	0
	201	1924	1228	344	347	5	0	0	0	
0	10	227	Total	С	Ν	0	S	0	0	0
	12	231	1924	1228	344	347	5	U	0	0

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

Mol	Chain	Residues		Ate	oms		ZeroOcc	AltConf	Trace	
3	$2\mathrm{F}$	205	Total	С	Ν	0	S	0	0	0
J ZE	200	1605	1011	313	280	1	0	0	0	
2	<u></u>	206	Total	С	Ν	0	S	0	0	0
\mathbf{a} \mathbf{b}	200	1612	1016	314	281	1	0	0	0	

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
4	<u>२</u> म	208	Total	С	Ν	Ο	\mathbf{S}	0	0	0
4	515	200	1702	1066	339	290	7	0	0	0
4	20	208	Total	С	Ν	0	S	0	0	0
4	52	208	1702	1066	339	290	7	0	0	0

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



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
5	4F	151	Total	С	Ν	0	S	0	0	0
5	415	101	1155	729	218	204	4	0	0	0
5	49	151	Total	С	Ν	0	S	0	0	0
5	42	101	1155	729	218	204	4			U

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
6	۶F	101	Total	С	Ν	0	S	0	0	0
0	9E	101	842	531	155	153	3	0	0	0
6	50	101	Total	С	Ν	0	S	0	0	0
0	52	101	842	531	155	153	3	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
7	6E	152	Total 1243	С 774	N 249	0 214	S 6	0	0	0
7	62	155	Total 1256	C 781	N 252	0 217	S 6	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	7F	128	Total	С	Ν	0	S	0	0	0
0		130	1115	705	215	192	3	0	0	0
0	79	127	Total	С	Ν	0	S	0	0	0
0	12	107	1107	700	214	191	2		U	U

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

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
0	8F	197	Total	С	Ν	Ο	0	0	0
9	OL	127	1009	639	197	173	0	0	0
0	80	199	Total	С	Ν	Ο	0	0	0
9	02	122	971	616	189	166	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
10	1I	99	Total 801	C 504	N 157	O 139	S 1	0	0	0



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Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
10	1A	99	Total 801	$\begin{array}{c} \mathrm{C} \\ 504 \end{array}$	N 157	0 139	S 1	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
11	2I	116	Total 864	C 537	N 164	0 160	${ m S} { m 3}$	0	0	0
11	2A	117	Total 873	C 543	N 166	O 161	${ m S} { m 3}$	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
19	्य	199	Total	С	Ν	0	S	0	0	0
12	51	122	956	603	193	159	1	0	0	0
10	2 1	195	Total	С	Ν	0	S	0	0	0
	JA	120	975	614	196	164	1			U

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
12	41	116	Total	С	Ν	0	S	0	0	0
10	41	110	928	574	191	161	2	0	0	0
19	4.4	117	Total	С	Ν	0	S	0	0	0
10	4A		933	577	192	162	2			U

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

Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf	Trace
14	51	59	Total 480	C 306	N 100	0 70	$\frac{S}{4}$	0	0	0
14	5A	58	Total 475	C 303	N 99	O 69	S 4	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
15	бI	00	Total	С	Ν	0	\mathbf{S}	0	0	0
1.0	01	00	733	459	147	125	2	0	0	0
15	61	00	Total	С	Ν	0	\mathbf{S}	0	0	0
1.0	UA	00	733	459	147	125	2	0	0	0



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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
16	71	84	Total	С	Ν	0	S	0	0	0
10	11	04	705	446	140	118	1	0	0	0
16	7Λ	84	Total	С	Ν	0	S	0	0	0
10	(A	04	705	446	140	118	1	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
17	्रा	100	Total	С	Ν	0	S	0	0	0
11	01	100	834	534	155	143	2	0	0	0
17	ο ۸	100	Total	С	Ν	0	S	0	0	0
11	ŏА	100	834	534	155	143	2	0	0	0

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

Mol	Chain	Residues		Ator	\mathbf{ns}		ZeroOcc	AltConf	Trace
18	91	72	Total 590	C 376	N 117	O 97	0	0	0
18	9A	71	Total 581	C 370	N 115	O 96	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
10	ΔΤ	83	Total	С	Ν	0	S	0	0	0
19	AI	00	665	424	124	115	2	0	0	0
10	ΛΛ	78	Total	С	Ν	0	S	0	0	0
19	AA	10	624	398	115	109	2	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
20	BI	00	Total	С	Ν	0	S	0	0	0
20	DI	55	762	470	162	128	2	0	0	0
20	ΡA	00	Total	С	Ν	0	\mathbf{S}	0	0	0
_ 20	DA	39	762	470	162	128	2		U	U

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



Mol	Chain	Residues		Aton	ns		ZeroOcc	AltConf	Trace
91	1 F	25	Total	С	Ν	0	0	0	0
21	11	20	217	134	52	31	0	0	0
21	1P	25	Total	С	Ν	0	0	0	0
		2.0	217	134	52	31		U	

• Molecule 22 is a RNA chain called tRNA-Tyr.

Mol	Chain	Residues		_	Atom	IS			ZeroOcc	AltConf	Trace
22	1K	85	Total 1824	C 821	N 323	O 594	Р 85	S 1	0	0	0

• Molecule 23 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues		-	Atom	IS			ZeroOcc	AltConf	Trace
23	2K	77	Total 1645	С 734	N 298	O 535	Р 77	S 1	0	0	0
23	2L	77	Total 1645	С 734	N 298	O 535	Р 77	S 1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2K	18	C	U	conflict	GB 723229079
2L	18	С	U	conflict	GB 723229079

• Molecule 24 is a RNA chain called tRNA-Tyr.

Mol	Chain	Residues		\mathbf{A}	toms			ZeroOcc	AltConf	Trace
24	3K	85	Total 1807	C 807	N 323	O 592	Р 85	0	0	0
24	1L	85	Total 1807	C 807	N 323	O 592	Р 85	0	0	0

• Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
25	416	19	Total	С	Ν	0	Р	0	1	0
20	41	12	283	128	60	82	13	0	L	0
25	41	10	Total	С	Ν	0	Р	0	0	0
20	4L	12	261	118	55	76	12		U	0

• Molecule 26 is a RNA chain called 23S ribosomal RNA.



Mol	Chain	Residues			Atoms			ZeroOcc	AltConf	Trace
26	1日	2012	Total	С	Ν	0	Р	0	0	0
20	111	2912	62707	27911	11722	20163	2911	0	0	0
26	14	2000	Total	С	Ν	Ο	Р	0	0	0
20	14	2909	62647	27884	11716	20139	2908	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	-	insertion	GB 48268
1H	493	G	-	insertion	GB 48268
1H	654A	А	G	conflict	GB 48268
1H	654E	С	G	conflict	GB 48268
1H	654P	G	С	conflict	GB 48268
1H	654T	А	С	conflict	GB 48268
1H	1058	U	G	conflict	GB 48268
1H	1080	А	С	conflict	GB 48268
1H	1228	G	-	insertion	GB 48268
14	158	U	-	insertion	GB 48268
14	493	G	-	insertion	GB 48268
14	654A	А	G	conflict	GB 48268
14	654E	С	G	conflict	GB 48268
14	654P	G	С	conflict	GB 48268
14	654T	А	С	conflict	GB 48268
14	1058	U	G	conflict	GB 48268
14	1080	А	С	conflict	GB 48268
14	1228	G	-	insertion	GB 48268

• Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
27	16	122	Total 2617	C 1166	N 486	0 844	Р 121	0	0	0
27	1J	122	Total 2617	C 1166	N 486	0 844	Р 121	0	0	0

• Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
28	11	973	Total	С	Ν	0	S	0	0	0
20	11	215	2120	1338	421	358	3	0	0	0
<u> </u>	10	072	Total	С	Ν	0	S	0	0	0
20	19	213	2120	1338	421	358	3	0	0	0



• Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
20	91	205	Total	С	Ν	0	S	0	0	0
29	21	205	1568	991	300	271	6	0	0	0
20	20	205	Total	С	Ν	0	S	0	0	0
29	29	205	1568	991	300	271	6	0	0	0

• Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
20	91	202	Total	С	Ν	0	S	0	0	0
- 50	- 31	202	1585	1011	297	275	2	0	0	0
20	20	208	Total	С	Ν	0	S	0	0	0
- 50	- 59	200	1627	1037	304	283	3	0	0	0

• Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
31	41	181	Total 1473	C 942	N 268	O 259	$\frac{S}{4}$	0	0	0
31	49	181	Total 1473	C 942	N 268	O 259	$\begin{array}{c} \mathrm{S} \\ \mathrm{4} \end{array}$	0	0	0

• Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
20	51	172	Total	С	Ν	0	S	0	0	0
32	51	175	1321	837	248	235	1	0	0	0
20	50	170	Total	С	Ν	0	S	0	0	0
32	- 59	170	1307	829	245	232	1	0	0	0

• Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
22	61	146	Total	С	Ν	0	S	0	0	0
00	01	140	1136	726	201	208	1	0	0	0
22	60	146	Total	С	Ν	0	S	0	0	0
- 55	09	140	1136	726	201	208	1	0	0	0

• Molecule 34 is a protein called 50S ribosomal protein L13.



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
24	59	128	Total	С	Ν	0	\mathbf{S}	0	0	0
04	- 50	130	1104	712	206	182	4	0	0	0
24	15	120	Total	С	Ν	0	S	0	0	0
04	10	130	1104	712	206	182	4	0	0	0

• Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
25	68	199	Total	С	Ν	0	S	0	0	0
50	00	122	932	588	171	169	4	0	0	0
25	25	199	Total	С	Ν	0	S	0	0	0
- 55	20	122	932	588	171	169	4			U

• Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
36	78	150	Total	С	Ν	0	S	0	0	0
- 30	10	150	1144	712	232	197	3	0	0	0
36	35	150	Total	С	Ν	0	S	0	0	0
- 30	- 55	150	1144	712	232	197	3	0	0	0

• Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
37	88	1.41	Total	С	Ν	0	\mathbf{S}	0	0	0
- 57	00	141	1121	715	212	187	7	0	0	0
27	45	120	Total	С	Ν	0	S	0	0	0
- 57	40	139	1107	707	209	184	7	0	0	0

• Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
38	98	118	Total C N O S 967 604 203 159 1	0	0	0
38	55	117	Total C N O 959 599 202 158	0	0	0

• Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
39	A8	110	Total 876	C 553	N 175	0 148	0	0	0



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Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
39	65	111	Total 881	$\begin{array}{c} \mathrm{C} \\ 556 \end{array}$	N 176	O 149	0	0	0

• Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
40	B8	137	Total	С	Ν	0	S	0	0	0
40	Do	107	1141	710	234	196	1	0	0	0
40	75	127	Total	С	Ν	0	S	0	0	0
40	10	107	1141	710	234	196	1	0	0	0

• Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
41	C e	117	Total	С	Ν	0	S	0	0	0
41	0	111	963	610	202	150	1	0	0	0
41	95	117	Total	С	Ν	0	S	0	0	0
41	00	111	963	610	202	150	1	0	0	0

• Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
42	D8	101	Total 778	C 501	N 142	0 134	S 1	0	0	0
42	95	101	Total 778	C 501	N 142	O 134	S 1	0	0	0

• Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
43	F8	112	Total	С	Ν	Ο	\mathbf{S}	0	0	0
40	Eo	115	899	566	177	154	2	0	0	0
43	Λ.5	112	Total	С	Ν	Ο	S	0	0	0
40	АЭ	113	899	566	177	154	2			U

• Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
44	F8	03	Total	С	Ν	Ο	0	0	0
44	ГО	90	730	474	132	124	0	0	0
4.4	D2	02	Total	С	Ν	Ο	0	0	0
44	D0	92	725	471	131	123	0	0	0



• Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
15	<u>C</u> 8	104	Total	С	Ν	0	S	0	0	0
40	Go	104	791	510	149	127	5	0	0	0
15	C5	104	Total	С	Ν	0	S	0	0	0
40	0.5	104	794	510	152	127	5	0	0	0

• Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
46	Цо	175	Total	С	Ν	0	S	0	0	0
40	110	175	1397	892	251	251	3	0	0	0
46	D5	128	Total	С	Ν	0	S	0	0	0
40	D0	130	1139	732	205	199	3	0	0	0

• Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
47	I8	76	Total 606	C 376	N 128	0 101	S 1	0	0	0
47	E5	77	Total 612	C 379	N 129	0 103	S 1	0	0	0

• Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
18	18	J8 97	Total	С	Ν	Ο	S	0	0	0
40	10		762	481	150	130	1	0	0	
19	٣ĸ	07	Total	С	Ν	0	S	0	0	0
48	гэ	97	762	481	150	130	1	0	0	0

• Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
49 K8	66	Total	С	Ν	Ο	\mathbf{S}	0	0	0	
	Кo	00	558	346	113	98	1	0	0	0
40	C5	66	Total	С	Ν	Ο	S	0	0	0
49	G9		558	346	113	98	1	0	0	

• Molecule 50 is a protein called 50S ribosomal protein L30.



Mol	Chain	Residues		Aton	ns		ZeroOcc	AltConf	Trace
50	18	50	Total	С	Ν	0	0	0	0
50	Lo	- 59	468	298	90	80	0	0	0
50	ЦΕ	50	Total	С	Ν	0	0	0	0
50	сп	ПЭ	468	298	90	80	0	0	

• Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	Mo	66	Total	С	Ν	Ο	S	0	0	0
51	MO	00	533	335	96	97	5	0		
51	ΤĘ	62	Total	С	Ν	Ο	S	0	0	0
51	19	10 03	515	326	93	91	5	0	0	U

• Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52 N8	50	Total	С	Ν	Ο	S	0	0	0	
	110		458	288	90	75	5	0	0	0
52	15	50	Total	С	Ν	Ο	S	0	0	0
32	10	- 59	458	288	90	75	5	0	0	

• Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	D8	46	Total	С	Ν	Ο	S	0	0	0
- 55	10		396	243	98	53	2	0		
52	ТБ	45	Total	С	Ν	Ο	S	0	0	0
53	LЭ	L0 40	391	240	97	52	2	0	0	U

• Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
54 Q8	61	Total	С	Ν	0	S	0	0	0	
	QO	01	488	312	99	75	2	0	0	0
54	M5	62	Total	С	Ν	Ο	\mathbf{S}	0	0	0
54	MD	02	495	317	100	76	2	0	0	

 $\bullet\,$ Molecule 55 is a RNA chain called tRNA-Tyr.

Mol	Chain	Residues		_	Atom	IS	ZeroOcc	AltConf	Trace		
55	3L	85	Total 1814	C 813	N 323	O 592	Р 85	S 1	0	0	0



• Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg	(g).
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	13	146	Total Mg 146 146	0	0
56	3E	1	Total Mg 1 1	0	0
56	$5\mathrm{E}$	1	Total Mg 1 1	0	0
56	3I	1	Total Mg 1 1	0	0
56	1K	1	Total Mg 1 1	0	0
56	2K	7	Total Mg 7 7	0	0
56	1H	481	Total Mg 481 481	0	0
56	16	12	TotalMg1212	0	0
56	11	2	Total Mg 2 2	0	0
56	21	2	Total Mg 2 2	0	0
56	31	1	Total Mg 1 1	0	0
56	41	1	Total Mg 1 1	0	0
56	78	1	Total Mg 1 1	0	0
56	88	1	Total Mg 1 1	0	0
56	I8	1	Total Mg 1 1	0	0
56	L8	1	Total Mg 1 1	0	0
56	P8	1	Total Mg 1 1	0	0
56	1G	86	Total Mg 86 86	0	0
56	2L	4	Total Mg 4 4	0	0
56	14	391	Total Mg 391 391	0	0
56	1J	6	Total Mg 6 6	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	29	3	Total Mg 3 3	0	0
56	39	1	Total Mg 1 1	0	0
56	25	1	Total Mg 1 1	0	0
56	35	1	Total Mg 1 1	0	0
56	45	1	Total Mg 1 1	0	0
56	85	1	Total Mg 1 1	0	0
56	C5	1	Total Mg 1 1	0	0
56	L5	1	Total Mg 1 1	0	0

• Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	At	tom	ıs		ZeroOcc	AltConf
57	13	1	Total 42 2	С 23	N 5	0 14	0	0
57	1G	1	Total 42	C 23	N 5	0 14	0	0

• Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).



4WRA

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	3E	1	Total Zn 1 1	0	0
58	51	1	Total Zn 1 1	0	0
58	G8	1	Total Zn 1 1	0	0
58	32	1	Total Zn 1 1	0	0
58	5A	1	Total Zn 1 1	0	0
58	C5	1	Total Zn 1 1	0	0

• Molecule 59 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	13	141	Total O 141 141	0	0
59	3E	1	Total O 1 1	0	0
59	1I	1	Total O 1 1	0	0
59	31	2	Total O 2 2	0	0
59	5I	1	Total O 1 1	0	0
59	1K	1	Total O 1 1	0	0
59	2K	6	Total O 6 6	0	0
59	4K	3	Total O 3 3	0	0
59	1H	633	Total O 633 633	0	0
59	16	11	Total O 11 11	0	0
59	11	10	Total O 10 10	0	0
59	21	5	Total O 5 5	0	0
59	31	5	Total O 5 5	0	0
59	78	4	Total O 4 4	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	F8	1	Total O 1 1	0	0
59	G8	2	Total O 2 2	0	0
59	J8	1	Total O 1 1	0	0
59	L8	2	Total O 2 2	0	0
59	1G	87	Total O 87 87	0	0
59	5A	1	Total O 1 1	0	0
59	6A	1	Total O 1 1	0	0
59	ВА	1	Total O 1 1	0	0
59	14	474	Total O 474 474	0	0
59	1J	6	Total O 6 6	0	0
59	19	9	Total O 9 9	0	0
59	29	3	Total O 3 3	0	0
59	39	5	Total O 5 5	0	0
59	55	1	Total O 1 1	0	0
59	75	1	Total O 1 1	0	0
59	85	1	Total O 1 1	0	0
59	A5	1	Total O 1 1	0	0
59	M5	2	Total O 2 2	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: 16S ribosomal RNA







679 780	G81	U82 II84	U85	086 A87	C88 U89	COO	C91	695	696	A101	C106	G107	G108 A100	C110	G111	G113	U114	6115 A116		C121	G126	G127	0129 U129	<mark>G129A</mark> A130	C131	C132 U133	A134	A141	G142 A143	G144	G145	G147 G147	G148 A140	A149 C150	A151 A152		1919	A160 A161
A162	0164 U164	C165 G166	G167	0015	C174 C175	C176		A179	0180 G181	U182	G183 G184	A185	C186	C186B	187	U188	U189	G190 G191A		U191D 6101F	TETA	0192	C194	A195 A196	A197	G198 G199	G200	U208	U209 1121.0	G216		G220 G220	C221	U223	11229	6230	6231 6232	C233 C234
C235 C736	C237	5 VCV	U244	6245 A246	G247	A250	G251 U252	U253	G255 G255	U256	G257	U261	A262	0264	G265 C266	C267		C2/2 A273		C277	A279	C280 C781	TOZĐ	6289	G297	A298 G299	A300	TOSP	6305 6306	C307		C311	C312	6314 C314	A315 G316	G317	6318 6319	C320 A321
C322		G326	C328	A329 C330	6331 6332		C337 A338	<mark>C339</mark>	A344	C345	G346 G347		G350 C3E1	C352	A353 C354		U359	A360 G361	G362	A363 A364	1365 U365	C366 113.67	U368	C369 C370	G371	C372 A373	A374	0376 G376	G377		A382	C386	U387 7388	4300 A389	C390 G391	G392	A393 G394	C395 G396
A397 7308		6406	A408	G410 G410	A411 A412	G413	G416	C417	C418 C419	U420	0421 0422	G423	G424	G426	0427	U429	A430	A431 A432	C433	U 36	0437 U437	G438 1130	A440	C442	G445	G446 G447	A448	G450	A451 A452	A453	CAER	C450 C457	C458 C464	4404 A465	C466 G467	A468	G4/4 G475	G476 G477
A478	U480	G481	G484	0485 U486	A487 C488	C489	6490 6491	G492	G493 U494	A495	A496 11497	A498	G500	G502	C503	G505	G506		A509	A510 C511	U512	C513	U516	G517 C518	C5 19	A520 G521	C522	CZ CH	C526 C527	C528	G529 CE30	u530 U531	A532 A532	0004	C536 G537	G538	4539 G540	G541 G542
C543 C543	C545	G546 A547			A553 C554	C555	C556	A559	U560 U561	C562	A563 C564	USG5	G566 CE67	G568	C569	A572	A573	A5/4 G575	G576	G577 C578		G581 ITEPO	A583	G584	G587	G589 C589	C590	0091 G592	CEQE	CE96	G597	00390 CE99	C600 C601		G604 11605	G606	A608	A614
C615 C616	G617	C618 11619	C620	A021 A622	C623 C624	G625	0626 G627	<mark>G628</mark>	G629 G630	G631	A 632 G 633	C634	G635 11626	0000	G649 C650	C651	U652	A653	C656	G657 C658	0000 0659	G660 C661	G662	A663 G664	A665	G666 G667	G668	U672	G673 C674	A675	A676 11677		C680	G683	A684 G685	U686	A68/ G688	C689 G690
G691	A696	1697	A7 02	A7 04	U7 05 A7 06	C707	G7 09	G7 10	G713	G714	G718		6721	U7 23	G7.24 C7.25	C726	G727	A/28 A729	G730	G731	C735	C736 4737	C738	C739 U740	G741	G742 U743	C7 44	C747	C748	G750	U751	4753 A753	C754 C755	G756	U757 G758	A759	G761	C762
G765 A766	A767	A768	G771	7/10	A777 G778	C779	A780	C784	G785 G786	A787	67 <u>9</u> 1	A792	U793 A704		6799 C800	U801	A802	6803	C811	C812 11813	0100	A816 Ce17	1100	G821 C822		6825 C826	U827 A 0 2 0	A0.20	6836 6837	G 838	U841 CoAD	U843	C848	U850	G853	G854	A859	A865
C866 C867		U870 11871	A872	4873 G874	C875 G876	C877	G878 C879	C880	G881 C882	-	G885	<mark>6888</mark>	A889	U891	A892 7803	G894	G895	8085	C899	A900	C904	0905 7906	A907	A908 A909		A913 A914	4 010	A910 A919	U920 11924	G922	A923	6926	G927	6933	C934 4935	C936	A937	G942
G947		G951	G954	0956 0956	U957 A958	A959	U960 U961	C962	G963 A964	A965	G966 C967	A968	A969	G971	C972	A974	A975	6976 A977	A978	C979 C080	0360 1981	U982 A983	C984	C985 A986	G987	C990	U991	6993	A994	C998A	1999	G1001	G1002 C1003	A1004	A1005 C1006		61008	G1013 A1014
A1015 A1016	G1017	C1018 C1019	U1020	G1022	G1023 G1024	U1025	G1026 C1027	C1028	C1 028A C1 028B	G1029	C1030 G1031	A1032	G1032A	G1033	G1034 A1035	G1036	C1037	C1038 C1039	U1040	A1041	75075	G1050	G1053	C1054 A1055	U1056	C1059	C1060	01062 U1062	C1063 C1064		C1069	G1072	U1073	C1075	111 078	G1079	61081	U1086
G1087 G1088	G1089	A1007	A1093	01095	C1096 C1097			G1104	A1105 G1106	C1107	G1108 C1109	A1110	A1111	C1113	C1114	C1116 C1116	G1117	C1118 C1119	G1120	U1121 11123	01122 A1123	G1124 11125	U1126	G1127 C1128	C1129	A1130 G1131	C1132	G1134	U1135 111136	C1137	G1138	C1140	C1141	G1143	G1144 C1145	A1146	C114/ U1148	C1149 U1150









1.7.9 M1 886 M1 889 M2 896 M2 897 L10 896 M2 897 L10 896 M2 897 L13 898 M2 899 K54 891 L14 892 M3 893 M3 894 M3 895 K54 841 L46 842 M3 843 L46 843 L46 843 M3 844 L46 845 L46 846 L46 868 L46 869 L76 869 M7 860 L76 860 L76 860 M7 860 L76

• Molecule 6: 30S ribosomal protein S6







• Molecule 10: 30S ribosomal protein S10 23% Chain 1A: 38% 44% 12% 6% MET 196 E97 198 K99 K99 C98 C19 GLY GLY ARG • Molecule 11: 30S ribosomal protein S11 Chain 2I: 43% 38% 9% 10% MET LYS LYS LYS PRO SER LYS LYS • Molecule 11: 30S ribosomal protein S11 10% Chain 2A: 46% 32% 12% 9% MET ALA LYS LYS LYS PRO SER LYS LYS LYS LYS A100 S101 G102 L103 **Q104** V105 K106 S107 D111 D111 T112 P113 V114 P115 H116 N117 388 489 R91 • Molecule 12: 30S ribosomal protein S12 Chain 3I: 52% 32% 9% 8% K124 P125 GLU GLU ALA ALA ALA ALA ALA LYS LYS LYS • Molecule 12: 30S ribosomal protein S12 14% Chain 3A: 53% 32% 10% 5%









• Molecule 18: 30S ribosomal protein S18 Chain 9I: 39% 38% 18% 818 819 820 821 MET SER LYS ALN ALA ALA PRO LYS PRO LYS CLYS GLU SGLU ALA ARG PRO **LRG** • Molecule 18: 30S ribosomal protein S18 Chain 9A: 43% 30% 7% • 19% R87 LYS • Molecule 19: 30S ribosomal protein S19 Chain AI: 45% 34% 11% 9% A5C L5 K6 LYS GLU ALA LYS ALA ALA THR LYS LYS LYS • Molecule 19: 30S ribosomal protein S19 Chain AA: 40% 32% 10% 16% MET PRO ARG SER LEU LYS LYS GLU GLU ALA ALA ALA ALA ALA LYS LYS LYS • Molecule 20: 30S ribosomal protein S20 44% Chain BI: 38% 42% 13% 7% MET ALA GLN LYS LYS PRO LYS LYS














CG6	067 G68	C69	G70 A71	U72	A73 A74	G75 C76	C77		G81 C82	607 (183	A84	G 85	<mark>688</mark>	689 1190	090 A91	G92	CG3	698 698	660	6101 6102		C105	C106 C107	U108	G109	A111	0112	0114 U114	C115	G117 G117	A118 4119	U120	G121	G123	G124	6125 A126	A127	C128 C129	C130	6132 6132	CI 33
C134	G138	G139	A140 A141	C141A	G142 C143	C144	C148	A149	G1 50	C153	G154	C155 U161	U162	U163 11164	010 1 0105	G171	C172 G173	C174	G175	G176 G177	G178	G179	G180 A181	A182	C183	010 1 0185	G186	G188	G189 A100	A191	C192 111 93	G194	A195	A190 A197	C198	A199 U200	C201	0202 C203	A204	A207	C208
C209	C210	G214	G215 A216	G217	A218 G219	G220	A221 A222	A223	6224 4775	G226	A227	A228 A229	U230	C231 C231	A233		C237 C238	U239	G240	A241 G242	U243	A244	G245 C246	G247	G248	G250	A251 C257	C253	G254	A256	A257 С258	G259	G260	TOZD	A265	6266	02 <mark>69</mark>	C270C	C270D	U270F	C27.0G
C270H	C270K	U270L	G270N	U2700	C270P C2700	TOTON	C270U	G270V	G270W	G270Y		G271B U271C	G271	110735	C273F	G274	G275 A776	C277	A278	C279	A282		C286 C287	C288	A289	C291	CJOE		62 <mark>98</mark> 4200	A300	11305	U306	G307	G 309	A310	A311 G312	C313	A314 G315	C316	C319	A320
G321	A322 G323	A324	U328	G329	A330 A331	A332	6334 C334	C335	C336	6338 6338	U339	A340 G341	G342	C343 C344	110 D	G348	G349 11350	G351	G352	G353 G354	G355	G356	A357 11358	A359	G360	U362	G363 A363 A	G363B	G363C	U363E	A363F	1000	G370	A3/1 G372		C3/6	U380	G381 G382	U383 11384	C385	G386
U387	G389 G389		C392	<mark>G396</mark>	6397 6398	G399	00 #5	C404	U405	G407	G408	C409 G410	G411	A412	A415	C416	<mark>C417</mark> ه	G418		A422 A423	G424	G425	C426 11427	A428	A429	0431 U431	A432		G4 40	G442	A443 C444	C445	G446	A44/ U448	A449	G450 C451	G452	C453 A454	C455 C456	A457	G458
U459	A460 C461	C462	G463 U464	G465	A466 G467	G468	A470	A471	A472 C473	0,15	A478	A479 A480	G481	A482 A483	C484	C485	C486	G491	A492	6493 6494	G495		A501 A502		A505	A507	G508	C510	U511 CE10	7105	C516 C517	G518	U519 GEOO	0205	U524	0525 A526	<mark>C527</mark>	A528 A529	G530	4532	G533
U534	C535 A536	CE37	G539	C543	C544 G545	C546	A548	G549	CEF.6	U557	G558	U562	G563	C564	U566	A567	U568 11569	G570	A571	A572 G573	C574	A575	0576 G577	A578	G579	C581	G582 C583	C584	G585 AF06	C587	U588 CERG	A590		4593 U594		G599 G599	G600	<mark>G602</mark>	A603	C605	U606
U607	A608 A609	G609A	C610 C611	G612	U613 U614	G615 A616	G617	G618	C618A	G620	A621	G622 G623	C624	A677	170W	G630	A631 A632	A633	C634	C635 G636	A637	G638	0639 C640	C641	G642	A644	C645 A646	6647 G647	G648 G640	C650	G651	A654	A654A	G654C	G654D	C654G	G654H	C6541 A654J	C654K	C654M	G654N
G6540	G654D C654Q		A654T	A655	C658	C659	C661	G662	G663 C664	1000	U667	G668 G669	A670	C671	C673	G674	A675 A676	A677	C678	C679 G680	G681	G682	C683 G684	A685	G686	U688	A689 C600	C691	C692 C603	0694 U694	G695 C696	C697	C698	G7 00	G701	G/02 U703	G704	A7 05 A7 06		G7 10	G711
	A/16 G717	A718	U724	G725	G726 A727	G728	C730	C731	C732	A734	A735	C736 C737	G738	G739 11740	6741	G742	G743 G744	G745	A746	0748 G748	C749	A750	A751 A752	C753	C754	C756	U757 C768	0000	A761	G763	A764 C765	C766	U767	6/08	U773	A//4 G775	G776	A/// G778	07790	A781	A782
A783	A784 G785	C786	U787 A788	A789	C790 C791	G792 A703	0014	C796	C797	6190 6799	A 800	G801 A802	<mark>U803</mark>	A804 C805	C806	U807	6808 6809	U810	U811	C812 U813	C814	C815	C816 C817	G818	A 0.0 4	N021 U822	6823 A 274	C825	U826 11677	U828	4829 C830	G831	G832 11633	0834 C834	A835	G836 C837	<mark>C838</mark>	U839 C840	A841	6843 2011	C844
G845	C846 U847	G848	A849	G852	G853 G854	G855	C857	U858	G859 11860	0000 A861	G862	A863 G864	C865	A866	A870	U871	A872	C876	U877	A878 G879	G880	G881	G882 G883	C884	C885	A887	C888 C888	A890	G892 C002	C894	U895 <u>A896</u>	C897	C898	A 639	A901	C904	U905	6906 U907	C908	A910	-
U913	C915 C915	<mark>G916</mark>	A917 A918	G919	C925	A926	G929 G929	0830	6931 6932	4933 A933		G938 G939	G940	A941	U943	<mark>G944</mark>	A945 G946	G947	G948	C949 G950	C951	G952	A953 G954	C955		4959	A960 C961	G962	U963	C965	G966 C967	6968 6968	1200	G972 G972	A973	G974A C974A	G975	C976 G977	G978 C070		A983
A984	C985 C986	1987 1987	A988 G989	A990	C991 C992	G993	C995	A996	0997 7008	666N	A1000	A1001 G1002	G1003	C1004	C1006		A1010 G1011	U1012	C1013	01014	C1018	U1019	A1020 A1021	G1022	U1023	G1025	U1026	A1028	A1029		01033 61034	U1035	G1036	G1037 C1038	G1039	C1040 C1041	G1042	A1045	A1046	A1048	C1049





A1050		A1054	G1055 G1056	A1057	G1059	U1060 111061	G1062	G1063	C1064 U1065	U1066	A1067	G1068 A1069	A1070	G1071	C1072	A1073 G1074	C1075	C1076	A1077	C1079	A1080	U1081	U1082	01003 A1084	A1085	A1086	A1088	G1089	01090 21001	C1092	G1093	01094 A1095	A1096	U1097 A1098	G1099	C1100	U1101 C1103	A1103	C1104	U1105	G1107	U1108	C1109 G1110
	61112 U1113	G1114	G1115 C1116	G1117 C1118		G1122 C1123	C1124	G1125	A1126 A1127	A1128	A1129	U1130 C1131	A1132	U1133	ъ	C1135 G1136	G1137	G1138	G1139 C1140	01140 U1141	U1142	A1142A	A1143	G1145 C1145		G1149	G1151 G1151		G1154 A1155	A1156	G1157	01159 U1159	G1160	C1161 C1162	G1163	G1164	U1165	U1167	G1168	G1169	G1171	G1173	A1174 U1175
61176	ALL/ C1178	C1179	C1180 C1181	A1182	G1184 G1184	C1185 C1186	G1187	U1188	A1189 G1190	G1191 G1191	G1192	G1193 A1194	G1195	-	U1198	01199 C1200	C1201	C1202	G1203	A1 204 U1 205		A1210	01211	41212 A1213	A1214	G1215 C1216	01710	G1219	A1220	C1221 C1222	C1223	G1225	G1226	A1227 G1228	G1229	G1229A	C1230	G1232		G1238	01240	A1241	G1244
61245 11776	A1240 A1247	G1248	01249 G1250	C1251	A1253	A1254 111255	G1256	C1257	C1258 G1259	G1260	C1261	A1262 111263	G1264	A1265	G1266	01267 41268	A1269	C1270	61271	A12/2 U1273	A1274		A1278	G1280 G1280	G1281	41704	LOZIV	A1287	U1288	C1290 C1290	C1291	C1295	G1296	C1297 C1298	G1299	U1300	A1301	G1303	C1304	C1305	01200 A1307	A1308	G1309 G1310
G1311	U1313	C1314	C1315 U1316	A1317	61319 61319	C1320 A1321	A1322	U1323	G1324 G1325	U1326	C1327	G1328 II1329	C1330	A1331	G1332	C1333 61334	U1335	A1336	G1337	G1339 G1339	U1340	U1341	A1342	G1344	C1345	G1346	G1348	A1349	111 36.0	20010	G1355	01357 U1357	G1358	A1359 A1360		C1363	G1364	A1305 A1366	A1367	G1368 61260	C1370	G1371	01372 A1373
613/4 01375	C1375 C1376	G1377	A1378 A1379	G1380 61384	61382	C1383	G1385	C1386	C1387 G1388	G1389	U1390	01391 41392	A1393	U1394	A1395	U1396 II1397	C1398	C1399	G1400	G1402 C1402	C1403	C1404	01405	01406 C1407	C1408	0 1 / 1 /	G1413		G1416 C1/17	G1418 G1418	A1419	01420 G1421	G1422	G1423 G1424	G1425	G1426	A1427	G1429 G1429	C1430	U1431	01433	A1434	G1435 G1436
C1 43 /	G1440	G1441	G1442 G1443	G1444	C1445	C1446 C1447	G1448	A1449	G1449A	A1453	U1454	G1455 C1456	A1457	C1458	G1459	A1460 G1461	C1462	C1463	C1464	C1467	C1468	A1469	G1470	A14/1 A1472	G1473	C1474	C1476	A1477	61478 61470	G1480	U1482	G1483 G1484	G1485	A1486 C1487	G1488	U1489	C1 100	01493 A1494	A1495	A1496	01450	C1502	C1505
C1506		C1509	A1510 A1511	G1512 C1513	01514 01514	C1515 11516	G1517	C1518	G1519 U1520	G1521	G1522	C1505	G1526	G1527	A1528	A1529 G1530	C1531	C1532	C1533	u1535	A1536	C1537	G1538	G1540	U1541	G1542 A1E43	C1544	A1545	A1545A	C1547	C1548	C1550		A1554 G1555	C1556	C1557	A1558	G1560	G1561	A1562	C1564	C1565	A1566 A1567
61568 41560	ROCTH	G1573	C1574 C1575	U1576	U1578	A1579 A1580	G1581	C1582	A1586	A1587	C1588	C1589 111590	G1591	C1592	G1593	G1594 G1595	A1596	A1597	C1598	C1600	G1601	U1602	A1603	C1605	G1606	C1607	A1000 A1609	A1610	C1611	G1613 G1613	A1614	C1015 A1616	C1617	A1618 G1619	G1620	U1621	G1622	G1624	C1625	G1626	G1630	C1630A	A1631 A1632
G1633	A1034 G1635	C1636	A1637 C1638	U1639	01040 A1641	G1642	C1644	G1645	C1646 G1647	C1648	G1649	G1650 C1651	A1652	G1653	A1654	A1655 C1656	C1657	C1658	01659 71660	C1660 G1661	C1662	C1663	A1664	A1000 G1666	G1667	A1668	C1670	U1671	C1672	G1674 G1674	C1675	A1677	G1678	U1679 111680	G1681	G1682	C1683	C1685		A1689	C1691	U1692	U1693 C1694
61695	61697 61697	A1698	G1699 A1700		01706 U1706	111 716	G1717		01727 G1728	A1729	U1730	G1731	20110	G1743	G1746	G1747 G1748	A1749	G1750	C1751	G1753	C1754	A1755	G1756 111757	01/5/ G1758	A1759	A1760	A1762	G1763	G1764	C1767	U1768	G1770	C1771	G1772 A1773	C1774	U1775	G1776 111 777	U1778	U1779	A1780	C1782	A1783	A1784 A1785
A1 / 86		C1790	A1791 G1792	C1793	01795 C1795	01796 01797	U1798	G1799	C1800 G1801	A1802	A1803	C1804 111805	C1806	G1807	U1808	A1809 A1810	G1811		G1814 A101E	61816 G1816	G1817	U1818	A1819	07910	A1825	G1826	G1828	A1829	C1830	U1833	U1834	61835 C1836	C1837	C1838 C1838	G1840		C1843	A1847	-	G1850	A1854	G1855	G1856 G1857
G1858	A1859 G1860		01864 01869	C1870	G1878	C1879	C1882	G1883	A1884 A1885	C1886	C1887	G1888	C1895	G1896	G1897	01898 G1899	A1900	A1901	C1902	G1904	C1905	G1906	G1907	0000	A1912	A1913	U1915		A1918 A1919	C1920		576T0	G1 <mark>9</mark> 29	G1930 11931	A1932	G1933	C1934	A1936	A1937	A 1938	01940	C1941	C1942 U1943
01944	01946 01946	C1947	G1950	U1951	ZOGTH	U1955 111956	C1957	C1958	G1959 A1960	00014	U1963	G1964 C1965	A1966	C1967	G1968	A1969 A1970	A1971	A1972	G1973	C19/4 G1975	-	C1979	G1980 A1001	C1982	C1983	G1984 C1005	A1986	G1987	C1988 C1080	C1990	U1991	U1993	C1994	U1995 C1996	G1997	G1998	C1999	42000 A2001	G2002	G2003	C2007	C2008	G2009 G2010









C1005 C1006	C1007 C1008	A1009	A1010 G1011	U1012	C1013 U1014	G1015	G1016	C1018	U1019	A1020	A1021 G1022	U1023	G1024	G1025	A1027	A1028	61030	-	U1033	G1034 111035	G1036	G1037	C1038 G1039	C1040	C1041 G1042	C1043	G1044 A1045	A1046	G1047 A1048	C1049	A1050 G1051	C1052	C1053 A1054	G1055	G1056	A105/ U1058	G1059	U1060 U1061	G1062	01003 01064 01065	
U1066 A1067	G1068 A1069	A1070	G1071 C1072	A1073	G1074 C1075	C1076	A1077	C1079	-	A1084	A1085 A1086	G1087	A1088	G1089 111090	G1091	C1092	U1094	A1095	A1096	01097 A1098	G1099		01104 01105		01108 C1109	G1110	A1111 G1112	U1113	G1122		62115	A1128	A1129 U1130	G1131	A1132	55110	C1135	61136 61137	G1138	C1140 C1140 U1141	
U1142 A1142A	A1143 G1144	C1145	A1148	G1149	C1150 G1151		G1154 A1155	A1155	G1157	C1 158	01159 G1160	C1161	10	01165 C1166	U1167	G1168	G1170 G1170	G1171	G1173	A1174 U1175	G1176	A1177	C11/8 C1179	C1 180	G1183		G1186 G1187	U1 188	A1189 G1190	G1191	26119	C1 196	C1200	C1201	C1202	41204 A1204	U1205	G1206 C1207	C 7 7 7 7	01211 01211 61212	
C1217	A1 220	C1221	C1222	C1225	G1229A		G1236	U1240	A1241		G1244	A1247	G1248	01249 G1250	C1251	G1252	A1253 A1254	U1 255	G1256	C1257 C1258	G1259	G1260	C1 261 A1 262	U1263	G1264 A1265	G1266	U1267 A1268	A1269	C1270 G1271	A1272	012/3 A1274	A1275	A1 278	G1279	G1280	01282 U1282	G1283	A1.284	A1287	C1291	
U1292 C1293	U1294 C1295	G1296	C1297 C1298	G1299	01300 A1301	A1302	G1303	C1305	C1306		G1310 G1311	U1312	U1313	C1314	A1317	C1318	G1319 C1320	A1321	A1322	01323 G1324	G1325	U1326	61327 61328	U1329	C1330 A1331	G1332	C1333 G1334	U1335	A1336 G1337	G1338	U1341	A1342	C1345	G1346	G1347	41340 A1349		A1353	01357	41359 A1359 A1360	
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<mark>G1426</mark> A1427	C1428 C1429	C1430	U1431 C1432	U1433	A1434 G1435	G1436	C1437	G1443	G1444	A1444A	C1445 C1446	G1447	G1448	A1449 G1449A	C1450	C1451	G1455	-	C1458	G1459 A1460	G1461	C1462	C1463 C1464	G1465	G1466 C1467	C1468	A1469 G1470	A1471	G1475		G1478 G1479	G1480	01482 G1483		A1486	G148/ G1488	U1489	A1490 G1491	G1492	01493 A1496	
U1497 C1498	C1499 G1500	C1501	C1502	C1505	C1506 A1507	A1508	C1509		G1512		01516 G1517	C1518	G1519	01520 G1521	G1522	U1523	A1528	A1529	G1530	C1531 C1532	C1533	G1534	01535 A1536	C1537	G1538 G1538		G1542 A1543	C1544	A1545	C1547	C1548	G1555	C1556 C1557	A1558	G1559 C1550	00019	C1564	C1565 A1566	A1567	A1569 A1569 A1570	
A1571 A1572	G1573	C1577	U1578 A1579	A1580	G1581 C1582	A1583	C1585	A1587	C1588	C1589	G1593	G1594	G1595	A1596 A1597	C1598	C1599	G1601	U1602	A1603	C1604	C1607	A1608	A1609 A1610	C1611	C1612 G1613	A1614	C1615 A1616	C1617	A1618 G1619	G1620	01621 G1622	G1623	G1624 C1625		G1630	CTOSON	G1633	A1634 G1635	C1636	C1638 U1639 U1639	
G1642	G1643 C1644		G1647 C1648		A1652 G1653	A1654	C1 6F 7	C1658	U1659	C1660	G1661 C1662	C1663	A1664	A1665 G1666	G1667	A1668	A1009 C1670	U1671		G1674 C1675	A1676	A1677	G1678	G1681	G1682 C1683	C1684	C1685 C1686	G1687	U1688 A1689		01693 C1694	G1695	G1696 G1697	A1698	G1699 11700	A1701	G1702	G1703 G1704	111 200	C1710 C1710 C1711	
C1712 U1716	61717 61718	G1725	G1726 U1727	G1728	A1729 U1730	G1731	A1732	00 119	C1742	G1743	G1746	G1753	C1754	A1755 G1756	U1757	G1758	AC / TH	A1762	G1763	G1764	C1767	U1768	G1769 G1770	C1771	G1772 A1773	C1774	01775 G1776	U1777	U1778 U1779	A1780	C1781 C1782	A1783	A1784 A1785	A1786	A1787	01/00 A1789	C1790	16/1V	U1794	01796 01796 01797	
U1798 G1799	C1800 C1801	A1802	A1803 C1804	U1805	C1806 G1807	U1808	01014	61813	G1814	A1815	G1816 G1817	U1818	A1819	01820 A1821	G1822	G1823	41624 A1825	G1826	C1827	G1828 A1829	C1830		01833 01834	G1835	C1836 C1837	C1838	G1839 G1840		A1847 A1848	G1849	61850	G1856	G1857 G1858	A1859	G1860	G1863	U1864	A1871	A1872	C1882	
G1883 A1884	A1885 C1886	C1887	G1888 A1889	A1890	G1891 C1892	C1893	C1894	G1896	G1897	U1898	G1899 A1900	A1901	C1902	G1903 G1904	C1905	G1906	C1908	-	A1913	C1914 U1915		A1918	C1920	G1921	61922 11923	C1924	C1925 U1926	A1927	A1928 G1929	G1930	01931 A1932	G1933	C1934 G1935	A1936	A1937	A1936 U1939	U1940	C1941 C1942	U1943	01344 01945 U1946	
C1947 G1948	G1949 C1950	U1951	A1952	U1955	C1958		C1961	U1963	G1964	C1965	A1966 C1967	G1968	A1969	A1970 A1971	A1972	G1973		A1978	C1979	G1980	G1987	C1988	G1989 C1990	U1991	G1992 111993	C1994	01995 C1996		C1999 G2000	A2001	6.500.5	A2005	G2010		A2014	A2015 U2016	U2017	G2018 A2019		62023 62023 62024	





• Molecule 27. 55 115050

Chain 16:

37%

17%







R268 F269 1270 1271 A272 R273 R273 LYS LYS

 \bullet Molecule 29: 50S ribosomal protein L3











• Molecule 32: 50S ribosomal protein L6







A150

 \bullet Molecule 36: 50S ribosomal protein L15



 \bullet Molecule 37: 50S ribosomal protein L16







 \bullet Molecule 38: 50S ribosomal protein L17













• Molecule 43: 50S ribosomal protein L22







 \bullet Molecule 45: 50S ribosomal protein L24



 \bullet Molecule 46: 50S ribosomal protein L25







 \bullet Molecule 47: 50S ribosomal protein L27





• Molecule 48: 50S ribosomal protein L28





E89 190 K91 K92 E93 E93 E93 E94 L94 L95 L97 L97

 \bullet Molecule 48: 50S ribosomal protein L28



• Molecule 49: 50S ribosomal protein L29















4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	209.90Å 450.90Å 622.70Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	225.45 - 3.05	Depositor
Resolution (A)	225.45 - 3.05	EDS
% Data completeness	99.9(225.45-3.05)	Depositor
(in resolution range)	$92.8\ (225.45-3.05)$	EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.76 (at 3.07 \text{\AA})$	Xtriage
Refinement program	PHENIX	Depositor
P. P.	0.195 , 0.249	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.196 , 0.248	DCC
R_{free} test set	1999 reflections (0.18%)	wwPDB-VP
Wilson B-factor $(Å^2)$	77.5	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.27, 77.3	EDS
L-test for $twinning^2$	$ < L >=0.43, < L^2>=0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	299607	wwPDB-VP
Average B, all atoms $(Å^2)$	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, MG, PSU, OMC, ZN, MIA, 5MU, QUO, PAR

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| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Chain	B	ond lengths]]	Bond angles
MIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	13	0.75	4/36215~(0.0%)	1.42	401/56524~(0.7%)
1	1G	0.66	1/36187~(0.0%)	1.30	253/56481~(0.4%)
2	12	0.38	0/1959	0.66	0/2642
2	$1\mathrm{E}$	0.42	0/1959	0.70	1/2642~(0.0%)
3	22	0.42	0/1636	0.65	0/2205
3	$2\mathrm{E}$	0.52	0/1629	0.72	0/2195
4	32	0.50	0/1732	0.76	2/2318~(0.1%)
4	3E	0.60	1/1732~(0.1%)	0.76	1/2318~(0.0%)
5	42	0.47	0/1171	0.70	0/1576
5	$4\mathrm{E}$	0.54	0/1171	0.72	1/1576~(0.1%)
6	52	0.52	0/855	0.68	2/1154~(0.2%)
6	$5\mathrm{E}$	0.54	0/855	0.70	0/1154
7	62	0.45	0/1275	0.64	0/1709
7	6E	0.45	0/1261	0.60	0/1689
8	72	0.44	0/1127	0.65	0/1517
8	$7\mathrm{E}$	0.51	0/1135	0.74	1/1527~(0.1%)
9	82	0.40	0/988	0.66	0/1324
9	$8\mathrm{E}$	0.44	0/1028	0.67	0/1379
10	1A	0.37	0/814	0.62	0/1095
10	1I	0.45	0/814	0.66	0/1095
11	2A	0.47	0/888	0.67	1/1198~(0.1%)
11	2I	0.51	0/879	0.74	1/1187~(0.1%)
12	3A	0.58	0/991	0.80	0/1327
12	3I	0.73	0/972	0.91	0/1301
13	4A	0.38	0/943	0.65	1/1265~(0.1%)
13	4I	0.49	0/938	0.71	0/1258
14	5A	0.44	0/484	0.74	0/643
14	5I	0.69	2/489~(0.4%)	0.86	1/650~(0.2%)
15	6A	0.47	0/744	0.65	0/992
15	6I	0.54	0/744	0.73	0/992
16	7A	0.53	0/721	0.71	0/970
16	7I	0.51	0/721	0.75	0/970



	<u> </u>	B	ond lengths		Bond angles
NIOI	Chain	RMSZ	# Z > 5	RMSZ	$ \widetilde{Z} >5$
17	8A	0.50	0/847	0.65	0/1131
17	8I	0.55	0/847	0.74	0/1131
18	9A	0.50	0/586	0.72	1/779~(0.1%)
18	9I	0.49	0/595	0.79	1/790~(0.1%)
19	AA	0.44	0/638	0.72	1/860~(0.1%)
19	AI	0.53	0/680	0.81	0/915
20	BA	0.48	0/764	0.78	1/1007~(0.1%)
20	BI	0.41	0/764	0.68	0/1007
21	1B	0.52	0/221	0.66	0/288
21	1F	0.49	0/221	0.70	0/288
22	1K	0.49	0/1899	1.15	11/2952~(0.4%)
23	2K	0.81	0/1747	1.41	18/2723~(0.7%)
23	2L	0.69	0/1747	1.26	9/2723~(0.3%)
24	1L	0.47	1/1996~(0.1%)	1.08	5/3108~(0.2%)
24	3K	0.41	0/1996	1.01	1/3108~(0.0%)
25	4K	0.78	0/319	1.31	3/495~(0.6%)
25	4L	0.78	0/294	1.50	5/456~(1.1%)
26	14	0.89	62/70167~(0.1%)	1.58	1423/109541 (1.3%)
26	1H	1.03	114/70233~(0.2%)	1.76	2174/109643~(2.0%)
27	16	0.83	1/2928~(0.0%)	1.57	49/4568~(1.1%)
27	1J	0.70	0/2928	1.37	27/4568~(0.6%)
28	11	0.77	2/2170~(0.1%)	0.93	1/2926~(0.0%)
28	19	0.73	0/2170	0.94	6/2926~(0.2%)
29	21	0.70	0/1601	0.96	1/2160~(0.0%)
29	29	0.66	0/1601	0.98	3/2160~(0.1%)
30	31	0.72	0/1620	0.90	2/2194~(0.1%)
30	39	0.61	1/1662~(0.1%)	0.89	4/2249~(0.2%)
31	41	0.52	0/1498	0.75	1/2016~(0.0%)
31	49	0.42	0/1498	0.70	0/2016
32	51	0.65	0/1346	0.93	1/1821~(0.1%)
32	59	0.40	0/1332	0.74	3/1802~(0.2%)
33	61	0.52	0/1151	0.82	2/1558~(0.1%)
33	69	0.51	0/1151	0.77	3/1558~(0.2%)
34	15	0.49	0/1131	0.76	2/1525~(0.1%)
34	58	0.60	0/1131	0.83	0/1525
35	25	0.62	0/942	0.76	1/1269~(0.1%)
35	68	0.66	0/942	0.76	0/1269
36	35	0.67	0/1161	1.12	7/1544~(0.5%)
36	78	0.71	0/1161	1.13	7/1544~(0.5%)
37	45	0.70	$\overline{2/1128}~(0.2\%)$	0.98	3/1508~(0.2%)
37	88	0.82	1/1142~(0.1%)	1.11	4/1527~(0.3%)
38	55	0.65	0/973	0.84	1/1302~(0.1%)
38	98	0.57	0/981	0.79	1/1312~(0.1%)



Mal	Chain	E	Bond lengths		Bond angles
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
39	65	0.54	0/891	0.90	2/1187~(0.2%)
39	A8	0.62	0/886	0.89	2/1180~(0.2%)
40	75	0.58	0/1155	0.76	0/1542
40	B8	0.62	0/1155	0.83	1/1542~(0.1%)
41	85	0.59	0/981	0.78	1/1306~(0.1%)
41	C8	0.71	1/981~(0.1%)	0.89	2/1306~(0.2%)
42	95	0.66	0/789	0.88	1/1057~(0.1%)
42	D8	0.60	0/789	0.82	2/1057~(0.2%)
43	A5	0.72	0/910	0.86	1/1220~(0.1%)
43	E8	0.65	0/910	0.84	0/1220
44	B5	0.80	1/739~(0.1%)	0.88	0/993
44	F8	0.73	0/744	0.83	0/1000
45	C5	0.61	0/807	0.89	1/1076~(0.1%)
45	G8	0.65	0/804	0.94	3/1073~(0.3%)
46	D5	0.43	0/1165	0.72	0/1574
46	H8	0.50	0/1427	0.80	1/1935~(0.1%)
47	E5	0.63	0/620	0.85	0/827
47	I8	0.71	0/614	0.89	0/819
48	F5	0.64	0/769	0.96	2/1022~(0.2%)
48	J8	0.70	0/769	0.86	0/1022
49	G5	0.60	0/560	0.81	0/741
49	K8	0.78	1/560~(0.2%)	0.98	2/741~(0.3%)
50	H5	0.48	0/473	0.69	0/635
50	L8	0.61	0/473	0.78	1/635~(0.2%)
51	I5	0.52	0/527	0.84	0/709
51	M8	0.50	0/545	0.87	0/733
52	J5	0.59	0/472	0.84	0/639
52	N8	0.65	0/472	0.86	1/639~(0.2%)
53	L5	0.70	0/399	0.88	0/526
53	P8	0.88	1/404~(0.2%)	0.97	0/533
54	M5	0.88	0/502	1.22	$\overline{6/661} (0.9\%)$
54	Q8	0.85	0/494	1.10	1/649~(0.2%)
55	3L	0.39	0/1970	1.00	4/3065~(0.1%)
All	All	0.80	$19\overline{6}/3227\overline{22}~(0.1\%)$	1.40	$44\overline{82/483529}\ (0.9\%)$

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	13	1	0



Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	1
2	1E	0	3
4	32	0	2
4	3E	0	1
9	82	0	1
10	1A	0	1
11	2A	0	1
12	3I	0	2
13	4A	0	1
13	4I	0	2
14	5A	0	2
19	AA	0	1
19	AI	0	1
20	BA	0	2
26	14	1	0
28	11	0	1
28	19	0	4
29	21	0	5
29	29	0	4
30	39	0	6
31	41	0	1
31	49	0	2
32	51	0	3
32	59	0	1
33	61	0	4
33	69	0	2
34	58	0	1
36	35	0	4
36	78	0	7
37	45	0	8
37	88	0	2
38	55	0	1
38	98	0	1
39	A8	0	1
40	75	0	2
40	B8	0	2
41	85	0	4
41	C8	0	4
42	95	0	1
42	D8	0	2
43	A5	0	1
44	B5	0	1



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Mol	Chain	#Chirality outliers	#Planarity outliers
45	C5	0	2
45	G8	0	3
46	D5	0	1
46	H8	0	3
47	E5	0	1
47	I8	0	1
48	F5	0	1
48	J8	0	2
49	G5	0	3
49	K8	0	3
51	I5	0	2
51	M8	0	1
52	N8	0	1
54	M5	0	5
54	Q8	0	3
All	All	2	128

The worst 5 of 196 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
26	1H	783	A	N3-C4	-11.75	1.27	1.34
26	1H	2430	А	N9-C4	-11.09	1.31	1.37
26	14	783	А	N9-C4	-10.86	1.31	1.37
26	1H	71	А	N9-C4	-10.78	1.31	1.37
26	1H	676	А	N9-C4	-10.74	1.31	1.37

The worst 5 of 4482 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
26	1H	1899	G	N3-C4-N9	-20.97	113.42	126.00
26	14	1899	G	N3-C4-N9	-17.93	115.24	126.00
26	1H	1899	G	N3-C2-N2	-17.01	107.99	119.90
26	1H	2430	А	O5'-P-OP2	-17.00	90.30	110.70
26	1H	676	А	C2-N3-C4	-16.89	102.15	110.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	13	792	А	C1'
26	14	945	А	C1'

5 of 128 planarity outliers are listed below:



Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	194	PRO	Peptide
2	1E	237	ALA	Peptide
4	3E	29	PRO	Peptide
12	3I	47	LYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32352	0	16325	789	1
1	1G	32327	0	16316	749	3
2	12	1924	0	1975	103	0
2	1E	1924	0	1975	102	0
3	22	1612	0	1677	70	0
3	2E	1605	0	1668	56	0
4	32	1702	0	1763	78	0
4	3E	1702	0	1761	94	0
5	42	1155	0	1213	55	0
5	4E	1155	0	1213	49	0
6	52	842	0	857	32	0
6	$5\mathrm{E}$	842	0	857	37	0
7	62	1256	0	1296	49	0
7	6E	1243	0	1284	50	0
8	72	1107	0	1165	53	0
8	7E	1115	0	1177	59	0
9	82	971	0	1001	55	0
9	8E	1009	0	1037	68	0
10	1A	801	0	849	52	0
10	1I	801	0	849	46	0
11	2A	873	0	894	47	0
11	2I	864	0	881	41	0
12	3A	975	0	1062	40	0
12	3I	956	0	1046	41	0
13	4A	933	0	992	53	0
13	4I	928	0	987	42	0
14	5A	475	0	511	25	0
14	5I	480	0	513	36	0
15	6A	733	0	771	30	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	6I	733	0	771	27	0
16	7A	705	0	725	37	0
16	7I	705	0	725	49	0
17	8A	834	0	904	39	0
17	8I	834	0	904	54	0
18	9A	581	0	649	33	0
18	9I	590	0	662	29	0
19	AA	624	0	636	31	0
19	AI	665	0	686	39	0
20	BA	762	0	861	30	0
20	BI	762	0	861	52	0
21	1B	217	0	234	13	0
21	1F	217	0	234	12	0
22	1K	1824	0	945	57	0
23	2K	1645	0	841	30	0
23	2L	1645	0	841	33	0
24	1L	1807	0	920	32	0
24	3K	1807	0	920	47	0
25	4K	283	0	143	9	0
25	4L	261	0	132	6	0
26	14	62647	0	31582	1375	1
26	1H	62707	0	31612	1450	1
27	16	2617	0	1328	55	0
27	1J	2617	0	1328	80	0
28	11	2120	0	2197	92	0
28	19	2120	0	2197	89	0
29	21	1568	0	1634	111	0
29	29	1568	0	1634	113	0
30	31	1585	0	1632	87	0
30	39	1627	0	1680	110	0
31	41	1473	0	1535	72	0
31	49	1473	0	1535	63	0
32	51	1321	0	1388	82	0
32	59	1307	0	1382	64	1
33	61	1136	0	1223	65	1
33	69	1136	0	1223	50	0
34	15	1104	0	1180	57	0
34	58	1104	0	1180	81	0
35	25	932	0	996	42	0
35	68	932	0	996	40	0
36	35	1144	0	1228	92	0
36	78	1144	0	1228	89	0
					Continu	ued on next page



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	45	1107	0	1166	74	0
37	88	1121	0	1179	57	0
38	55	959	0	1021	47	0
38	98	967	0	1033	64	0
39	65	881	0	943	62	0
39	A8	876	0	938	47	0
40	75	1141	0	1202	71	0
40	B8	1141	0	1202	64	0
41	85	963	0	1022	44	0
41	C8	963	0	1022	66	0
42	95	778	0	852	69	0
42	D8	778	0	852	40	0
43	A5	899	0	964	27	0
43	E8	899	0	964	32	0
44	B5	725	0	778	36	0
44	F8	730	0	780	31	0
45	C5	794	0	884	54	0
45	G8	791	0	882	54	0
46	D5	1139	0	1163	53	0
46	H8	1397	0	1430	79	0
47	E5	612	0	633	31	0
47	I8	606	0	628	24	0
48	F5	762	0	848	36	0
48	J8	762	0	848	34	0
49	G5	558	0	610	30	0
49	K8	558	0	610	37	0
50	H5	468	0	518	13	0
50	L8	468	0	518	20	0
51	I5	515	0	514	54	0
51	M8	533	0	526	37	0
52	J5	458	0	480	21	0
52	N8	458	0	480	25	0
53	L5	391	0	432	9	0
53	P8	396	0	434	14	0
54	M5	495	0	567	62	0
54	Q8	488	0	560	55	0
55	3L	1814	0	932	51	0
56	11	2	0	0		0
56	13	146	0	0		0
56	14	391	0	0		0
56	16	12	0	0		0
56	1G	86	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1H	/81				
56	111	6	0	0	0	0
56	10 1K	1	0	0	0	0
56	21	2	0	0	0	0
56	25	1	0	0	0	0
56	29	3	0	0	0	0
56	2K	7	0	0	0	0
56	2L	4	0	0	0	0
56	31	1	0	0	0	0
56	35	1	0	0	0	0
56	39	1	0	0	0	0
56	3E	1	0	0	0	0
56	3I	1	0	0	0	0
56	41	1	0	0	0	0
56	45	1	0	0	0	0
56	5E	1	0	0	0	0
56	78	1	0	0	0	0
56	85	1	0	0	0	0
56	88	1	0	0	0	0
56	C5	1	0	0	0	0
56	I8	1	0	0	0	0
56	L5	1	0	0	0	0
56	L8	1	0	0	0	0
56	P8	1	0	0	0	0
57	13	42	0	45	2	0
57	1G	42	0	45	0	0
58	32	1	0	0	0	0
58	3E	1	0	0	0	0
58	5A	1	0	0	0	0
58	51	1	0	0	0	0
58	C5	1	0	0	0	0
58	G8	10	0	0	0	0
59	11	10	0	0	1	0
59	13	141	0	0	20 120	0
59	14	4/4	0	0	139	0
50	10	0	0	0		0
59	19 1C	9 97	0		4	0
50	1G 1H	622	0	0	19	0
50	111 1T	1	0	0	100	0
59	11 1 T	6	0	0	0	0
50	15 1K	1	0	0	0	0
- 09	117		U	U	U U	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	21	5	0	0	3	0
59	29	3	0	0	1	0
59	2K	6	0	0	0	0
59	31	5	0	0	0	0
59	39	5	0	0	0	0
59	3E	1	0	0	0	0
59	3I	2	0	0	0	0
59	4K	3	0	0	0	0
59	55	1	0	0	0	0
59	5A	1	0	0	0	0
59	5I	1	0	0	0	0
59	6A	1	0	0	0	0
59	75	1	0	0	0	0
59	78	4	0	0	2	0
59	85	1	0	0	1	0
59	A5	1	0	0	0	0
59	BA	1	0	0	0	0
59	F8	1	0	0	0	0
59	G8	2	0	0	0	0
59	J8	1	0	0	0	0
59	L8	2	0	0	1	0
59	M5	2	0	0	0	0
All	All	299607	0	199932	8541	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 8541 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1K:35:QUO:N3	22:1K:35:QUO:C4	1.70	1.51
4:32:26:CYS:HB3	4:32:31:CYS:SG	1.85	1.17
26:14:2701:C:H3'	26:14:2702:U:H5"	1.31	1.12
26:14:2711:A:OP2	59:14:3464:HOH:O	1.70	1.09
26:1H:229:A:H4'	26:1H:230:U:H5'	1.33	1.08

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:13:85:U:O2'	32:59:100:GLY:O[3_555]	1.97	0.23
1:1G:86:U:N3	26:14:275:G:OP2[3_545]	2.14	0.06
26:1H:2137:C:OP1	1:1G:999:U:O2'[4_555]	2.19	0.01
33:61:91:SER:OG	1:1G:368:U:OP1[4_555]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
2	12	235/256~(92%)	195 (83%)	35~(15%)	5(2%)	7	26
2	1E	235/256~(92%)	200 (85%)	34~(14%)	1 (0%)	34	64
3	22	204/239~(85%)	184 (90%)	20~(10%)	0	100	100
3	2E	203/239~(85%)	180 (89%)	22~(11%)	1 (0%)	29	60
4	32	206/209~(99%)	181 (88%)	24 (12%)	1 (0%)	29	60
4	3E	206/209~(99%)	191 (93%)	15 (7%)	0	100	100
5	42	149/162~(92%)	140 (94%)	9~(6%)	0	100	100
5	4E	149/162~(92%)	141 (95%)	7~(5%)	1 (1%)	22	52
6	52	99/101~(98%)	94 (95%)	5(5%)	0	100	100
6	5E	99/101~(98%)	94 (95%)	5(5%)	0	100	100
7	62	153/156~(98%)	144 (94%)	9~(6%)	0	100	100
7	6E	148/156~(95%)	140 (95%)	8~(5%)	0	100	100
8	72	135/138~(98%)	122 (90%)	11 (8%)	2 (2%)	10	35
8	7E	136/138~(99%)	126 (93%)	9~(7%)	1 (1%)	22	52
9	82	118/128~(92%)	105 (89%)	12~(10%)	1 (1%)	19	50
9	8E	125/128~(98%)	106 (85%)	19~(15%)	0	100	100
10	1A	97/105~(92%)	90 (93%)	7 (7%)	0	100	100
10	1I	97/105~(92%)	90 (93%)	7 (7%)	0	100	100
11	2A	115/129~(89%)	104 (90%)	8 (7%)	3 (3%)	5	22



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
11	2I	114/129~(88%)	101 (89%)	12~(10%)	1 (1%)	17	47
12	3A	123/132~(93%)	101 (82%)	19~(15%)	3~(2%)	6	23
12	3I	120/132~(91%)	103~(86%)	16~(13%)	1 (1%)	19	50
13	4A	115/126~(91%)	95~(83%)	18~(16%)	2 (2%)	9	32
13	4I	114/126~(90%)	96 (84%)	16 (14%)	2 (2%)	8	30
14	5A	56/61~(92%)	46 (82%)	9 (16%)	1 (2%)	8	30
14	5I	57/61~(93%)	46 (81%)	9 (16%)	2 (4%)	3	17
15	6A	86/89~(97%)	78 (91%)	8 (9%)	0	100	100
15	6I	86/89~(97%)	76 (88%)	10 (12%)	0	100	100
16	7A	82/88~(93%)	76 (93%)	6 (7%)	0	100	100
16	7I	82/88~(93%)	72 (88%)	10 (12%)	0	100	100
17	8A	98/105~(93%)	92 (94%)	6 (6%)	0	100	100
17	8I	98/105~(93%)	90 (92%)	8 (8%)	0	100	100
18	9A	69/88~(78%)	66 (96%)	3(4%)	0	100	100
18	9I	70/88~(80%)	62 (89%)	7 (10%)	1 (1%)	11	36
19	AA	76/93~(82%)	62 (82%)	11 (14%)	3 (4%)	3	15
19	AI	81/93~(87%)	67~(83%)	12~(15%)	2 (2%)	5	22
20	BA	97/106~(92%)	83 (86%)	13~(13%)	1 (1%)	15	45
20	BI	97/106~(92%)	83~(86%)	13~(13%)	1 (1%)	15	45
21	1B	23/27~(85%)	21 (91%)	1 (4%)	1 (4%)	2	13
21	$1\mathrm{F}$	23/27~(85%)	21 (91%)	2 (9%)	0	100	100
28	11	271/276~(98%)	249 (92%)	18 (7%)	4 (2%)	10	35
28	19	271/276~(98%)	253~(93%)	13~(5%)	5 (2%)	8	30
29	21	203/206~(98%)	161 (79%)	33 (16%)	9 (4%)	2	12
29	29	203/206~(98%)	158 (78%)	36~(18%)	9 (4%)	2	12
30	31	200/210~(95%)	178 (89%)	21 (10%)	1 (0%)	29	60
30	39	206/210~(98%)	161 (78%)	38~(18%)	7 (3%)	3	17
31	41	179/182~(98%)	157 (88%)	19~(11%)	3 (2%)	9	32
31	49	179/182~(98%)	158 (88%)	20 (11%)	1 (1%)	25	55
32	51	171/180~(95%)	137 (80%)	21 (12%)	13 (8%)	1	4
32	59	168/180~(93%)	128 (76%)	31 (18%)	9 (5%)	2	9



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
33	61	144/148~(97%)	113 (78%)	28~(19%)	3 (2%)	7	26
33	69	144/148~(97%)	113 (78%)	27~(19%)	4 (3%)	5	21
34	15	136/140~(97%)	121 (89%)	14 (10%)	1 (1%)	22	52
34	58	136/140~(97%)	117 (86%)	15 (11%)	4 (3%)	4	20
35	25	120/122~(98%)	112 (93%)	7~(6%)	1 (1%)	19	50
35	68	120/122~(98%)	112 (93%)	8 (7%)	0	100	100
36	35	148/150~(99%)	113 (76%)	32 (22%)	3 (2%)	7	27
36	78	148/150~(99%)	110 (74%)	30 (20%)	8 (5%)	2	9
37	45	137/141~(97%)	110 (80%)	25~(18%)	2 (2%)	10	35
37	88	139/141~(99%)	107 (77%)	26 (19%)	6 (4%)	2	13
38	55	115/118~(98%)	106 (92%)	7~(6%)	2 (2%)	9	32
38	98	116/118~(98%)	106 (91%)	9~(8%)	1 (1%)	17	47
39	65	109/112~(97%)	85 (78%)	22 (20%)	2 (2%)	8	30
39	A8	108/112~(96%)	89 (82%)	18 (17%)	1 (1%)	17	47
40	75	135/146~(92%)	121 (90%)	14 (10%)	0	100	100
40	B8	135/146~(92%)	123 (91%)	12 (9%)	0	100	100
41	85	115/118~(98%)	98~(85%)	17 (15%)	0	100	100
41	C8	115/118~(98%)	107 (93%)	4 (4%)	4 (4%)	3	17
42	95	99/101~(98%)	77 (78%)	18 (18%)	4 (4%)	3	14
42	D8	99/101~(98%)	90 (91%)	6~(6%)	3 (3%)	4	19
43	A5	111/113~(98%)	101 (91%)	7~(6%)	3 (3%)	5	21
43	E8	111/113~(98%)	102 (92%)	9~(8%)	0	100	100
44	B5	90/96~(94%)	76 (84%)	12 (13%)	2 (2%)	6	25
44	F8	91/96~(95%)	83 (91%)	6 (7%)	2 (2%)	6	25
45	C5	102/110~(93%)	76 (74%)	24 (24%)	2 (2%)	7	27
45	G8	102/110~(93%)	83 (81%)	13 (13%)	6 (6%)	1	8
46	D5	132/206~(64%)	104 (79%)	24 (18%)	4 (3%)	4	19
46	H8	173/206~(84%)	133 (77%)	33 (19%)	7 (4%)	3	14
47	E5	75/85~(88%)	68 (91%)	5 (7%)	2 (3%)	5	21
47	I8	74/85~(87%)	66 (89%)	6 (8%)	2 (3%)	5	21
48	F5	95/98~(97%)	86 (90%)	8 (8%)	1 (1%)	14	42



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perc	entiles
48	J8	95/98~(97%)	85~(90%)	8 (8%)	2(2%)	7	26
49	G5	64/72~(89%)	60 (94%)	2(3%)	2(3%)	4	19
49	K8	64/72~(89%)	59 (92%)	2 (3%)	3~(5%)	2	12
50	H5	57/60~(95%)	52 (91%)	5~(9%)	0	100	100
50	L8	57/60~(95%)	54 (95%)	3~(5%)	0	100	100
51	I5	61/71~(86%)	36 (59%)	21 (34%)	4 (7%)	1	6
51	M8	64/71~(90%)	36~(56%)	25~(39%)	3(5%)	2	12
52	J5	57/60~(95%)	52 (91%)	4 (7%)	1 (2%)	8	30
52	N8	57/60~(95%)	50 (88%)	7 (12%)	0	100	100
53	L5	43/49~(88%)	41 (95%)	2(5%)	0	100	100
53	P8	44/49~(90%)	42 (96%)	2(4%)	0	100	100
54	M5	60/65~(92%)	46 (77%)	11 (18%)	3 (5%)	2	11
54	Q8	59/65~(91%)	52 (88%)	3~(5%)	4 (7%)	1	6
All	All	11183/11946 (94%)	9677 (86%)	1306 (12%)	200 (2%)	8	30

5 of 200 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	9I	22	VAL
29	21	83	ASP
32	51	172	LYS
32	51	173	PRO
36	78	19	VAL

5.3.2Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	12	205/220~(93%)	161 (78%)	44 (22%)	1 3
2	$1\mathrm{E}$	205/220~(93%)	159 (78%)	46 (22%)	1 3
3	22	160/188~(85%)	121 (76%)	39~(24%)	0 2



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	$2\mathrm{E}$	159/188~(85%)	119 (75%)	40~(25%)	0 1
4	32	180/181~(99%)	139 (77%)	41 (23%)	1 3
4	3E	180/181~(99%)	138 (77%)	42 (23%)	1 2
5	42	116/123~(94%)	89 (77%)	27~(23%)	1 2
5	$4\mathrm{E}$	116/123~(94%)	94 (81%)	22~(19%)	1 5
6	52	90/90~(100%)	71 (79%)	19 (21%)	1 4
6	$5\mathrm{E}$	90/90~(100%)	71 (79%)	19~(21%)	1 4
7	62	126/127~(99%)	101 (80%)	25~(20%)	1 5
7	6E	126/127~(99%)	106 (84%)	20~(16%)	2 9
8	72	118/119 (99%)	96 (81%)	22 (19%)	1 6
8	7E	119/119~(100%)	92 (77%)	27 (23%)	1 3
9	82	95/99~(96%)	76 (80%)	19 (20%)	1 4
9	8E	98/99~(99%)	74 (76%)	24 (24%)	0 2
10	1A	89/92~(97%)	68 (76%)	21 (24%)	1 2
10	1I	89/92~(97%)	70 (79%)	19 (21%)	1 4
11	2A	89/99~(90%)	69 (78%)	20 (22%)	1 3
11	2I	88/99~(89%)	70 (80%)	18 (20%)	1 4
12	3A	104/109~(95%)	81 (78%)	23~(22%)	1 3
12	3I	103/109~(94%)	85 (82%)	18 (18%)	2 7
13	4A	94/101~(93%)	70 (74%)	24 (26%)	0 1
13	4I	94/101~(93%)	72 (77%)	22 (23%)	1 2
14	5A	48/50~(96%)	34 (71%)	14 (29%)	0 0
14	5I	48/50~(96%)	35 (73%)	13 (27%)	0 1
15	6A	79/80~(99%)	68 (86%)	11 (14%)	3 13
15	6I	79/80~(99%)	65 (82%)	14 (18%)	2 7
16	7A	72/74~(97%)	58 (81%)	14 (19%)	1 5
16	7I	72/74~(97%)	60 (83%)	12 (17%)	2 8
17	8A	95/97~(98%)	80 (84%)	15 (16%)	2 9
17	8I	95/97~(98%)	78 (82%)	17 (18%)	2 6
18	9A	62/77~(80%)	46 (74%)	16 (26%)	0 1
18	9I	63/77~(82%)	53 (84%)	10 (16%)	2 9


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Mol	Chain	Analysed	Rotameric	tameric Outliers		Percentiles		
19	AA	67/80~(84%)	50 (75%)	17~(25%)	0	1		
19	AI	72/80~(90%)	56 (78%)	16~(22%)	1	3		
20	BA	76/82~(93%)	58 (76%)	18 (24%)	1	2		
20	BI	76/82~(93%)	54 (71%)	22~(29%)	0	1		
21	1B	20/22~(91%)	18 (90%)	2~(10%)	7	25		
21	$1\mathrm{F}$	20/22~(91%)	18 (90%)	2(10%)	7	25		
28	11	214/218~(98%)	172 (80%)	42 (20%)	1	5		
28	19	214/218~(98%)	170 (79%)	44 (21%)	1	4		
29	21	165/166~(99%)	121 (73%)	44 (27%)	0	1		
29	29	165/166~(99%)	124 (75%)	41 (25%)	0	2		
30	31	161/166~(97%)	125 (78%)	36~(22%)	1	3		
30	39	165/166~(99%)	121 (73%)	44 (27%)	0	1		
31	41	155/156~(99%)	124 (80%)	31 (20%)	1	4		
31	49	155/156~(99%)	123 (79%)	32 (21%)	1	4		
32	51	142/148~(96%)	108 (76%)	34 (24%)	0	2		
32	59	142/148~(96%)	107 (75%)	35~(25%)	0	2		
33	61	122/124~(98%)	90 (74%)	32 (26%)	0	1		
33	69	122/124~(98%)	86 (70%)	36 (30%)	0	0		
34	15	117/119~(98%)	90 (77%)	27~(23%)	1	2		
34	58	117/119~(98%)	91 (78%)	26~(22%)	1	3		
35	25	100/100~(100%)	77 (77%)	23~(23%)	1	2		
35	68	100/100~(100%)	82 (82%)	18 (18%)	1	6		
36	35	116/116~(100%)	76~(66%)	40 (34%)	0	0		
36	78	116/116~(100%)	81 (70%)	35~(30%)	0	0		
37	45	110/111 (99%)	81 (74%)	29~(26%)	0	1		
37	88	111/111 (100%)	85 (77%)	26~(23%)	1	2		
38	55	100/101~(99%)	72 (72%)	28 (28%)	0	1		
38	98	101/101 (100%)	76 (75%)	25 (25%)	0	2		
39	65	87/88~(99%)	61 (70%)	26 (30%)	0	0		
39	A8	87/88~(99%)	62 (71%)	25 (29%)	0	1		
40	75	120/127~(94%)	86 (72%)	34 (28%)	0	1		



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Mol	Chain	Analysed	Rotameric	otameric Outliers		Percentiles		
40	B8	120/127~(94%)	89 (74%)	31 (26%)	0	1		
41	85	93/94~(99%)	69 (74%)	24 (26%)	0	1		
41	C8	93/94~(99%)	75 (81%)	18 (19%)	1	5		
42	95	82/82~(100%)	55~(67%)	27 (33%)	0	0		
42	D8	82/82~(100%)	63~(77%)	19(23%)	1	2		
43	A5	92/92~(100%)	69~(75%)	23~(25%)	0	1		
43	E8	92/92~(100%)	72~(78%)	20~(22%)	1	3		
44	B5	74/78~(95%)	59~(80%)	15 (20%)	1	4		
44	F8	74/78~(95%)	62 (84%)	12 (16%)	2	9		
45	C5	85/91~(93%)	59~(69%)	26 (31%)	0	0		
45	G8	85/91~(93%)	60 (71%)	25 (29%)	0	0		
46	D5	127/179~(71%)	102 (80%)	25 (20%)	1	5		
46	H8	154/179~(86%)	118 (77%)	36 (23%)	1	2		
47	E5	62/67~(92%)	50 (81%)	12 (19%)	1	5		
47	I8	61/67~(91%)	50 (82%)	11 (18%)	1	6		
48	F5	82/83~(99%)	57 (70%)	25 (30%)	0	0		
48	J8	82/83~(99%)	67~(82%)	15 (18%)	1	6		
49	G5	62/67~(92%)	42 (68%)	20 (32%)	0	0		
49	K8	62/67~(92%)	41 (66%)	21 (34%)	0	0		
50	H5	51/52~(98%)	37~(72%)	14 (28%)	0	1		
50	L8	51/52~(98%)	38 (74%)	13 (26%)	0	1		
51	I5	57/63~(90%)	44 (77%)	13 (23%)	1	3		
51	M8	59/63~(94%)	42 (71%)	17 (29%)	0	1		
52	J5	51/52~(98%)	45 (88%)	6 (12%)	5	18		
52	N8	51/52~(98%)	39 (76%)	12 (24%)	1	2		
53	L5	38/42~(90%)	31 (82%)	7 (18%)	1	6		
53	P8	38/42~(90%)	30 (79%)	8 (21%)	1	4		
54	M5	52/55~(94%)	36 (69%)	16 (31%)	0	0		
54	Q8	51/55~(93%)	38 (74%)	13 (26%)	0	1		
All	All	9444/9894 (96%)	7253 (77%)	2191 (23%)	1	2		

 $5~{\rm of}~2191$ residues with a non-rotameric side chain are listed below:



Mol	Chain	Res	Type
38	55	24	GLN
40	75	11	GLU
38	55	17	ARG
47	E5	12	ASN
39	A8	20	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
18	9A	36	ASN
33	69	104	GLN
51	I5	6	HIS
29	29	60	ASN
37	88	13	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1504/1522~(98%)	381 (25%)	35~(2%)
1	1G	1503/1522~(98%)	361 (24%)	37~(2%)
22	1K	82/85~(96%)	37~(45%)	8 (9%)
23	2K	76/77~(98%)	21 (27%)	3~(3%)
23	2L	76/77~(98%)	17 (22%)	1 (1%)
24	1L	84/85~(98%)	35~(41%)	8(9%)
24	3K	84/85~(98%)	27 (32%)	4(4%)
25	4K	11/30~(36%)	3(27%)	1 (9%)
25	4L	12/30~(40%)	6 (50%)	3~(25%)
26	14	2908/2918~(99%)	759~(26%)	56 (1%)
26	1H	2911/2918~(99%)	725 (24%)	60 (2%)
27	16	121/122~(99%)	20 (16%)	0
27	1J	121/122~(99%)	33 (27%)	3~(2%)
55	3L	83/85~(97%)	34 (40%)	4 (4%)
All	All	9576/9678~(98%)	2459 (25%)	223 (2%)

5 of 2459 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	5	U
1	13	6	G
1	13	8	А
1	13	9	G



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Mol	Chain	Res	Type
1	13	13	U

5 of 223 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	197	А
27	1J	56	G
1	1G	1300	G
26	14	2893	G
26	14	2173	А

5.4 Non-standard residues in protein, DNA, RNA chains (i)

17 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	Bos	Link	B	ond leng	gths	B	Bond ang	gles
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
22	QUO	1K	35	$22,\!25$	$29,\!35,\!36$	5.17	10 (34%)	$31,\!52,\!55$	4.02	10 (32%)
23	PSU	2K	56	23	18,21,22	1.23	2 (11%)	22,30,33	1.72	3 (13%)
23	5MU	2L	55	23	19,22,23	<mark>3.89</mark>	5 (26%)	28,32,35	<mark>3.35</mark>	9 (32%)
23	4SU	2K	8	23	18,21,22	1.94	3 (16%)	26,30,33	2.67	6 (23%)
23	OMC	2L	33	23	19,22,23	1.78	4 (21%)	26,31,34	1.20	2 (7%)
55	PSU	3L	40	55	18,21,22	1.15	1 (5%)	22,30,33	1.47	2 (9%)
22	MIA	1K	38	22	24,31,32	2.33	4 (16%)	26,44,47	<mark>3.09</mark>	6 (23%)
23	OMC	2K	33	23	19,22,23	1.71	3 (15%)	26,31,34	0.62	0
22	PSU	1K	40	22	18,21,22	1.02	1 (5%)	22,30,33	1.54	3 (13%)
23	PSU	2L	56	23	18,21,22	1.16	1 (5%)	22,30,33	1.79	2 (9%)
23	4SU	2L	8	23	18,21,22	1.77	3 (16%)	26,30,33	2.81	5 (19%)
22	PSU	1K	64	22	18,21,22	1.22	1 (5%)	22,30,33	1.68	4 (18%)
24	PSU	1L	40	24	18,21,22	1.22	1 (5%)	22,30,33	1.61	3 (13%)
23	5MU	2K	55	23	19,22,23	<mark>3.93</mark>	5 (26%)	28,32,35	3.21	7 (25%)



Mal	Mol Tuno Choin Dog		Tink	Bond lengths			Bond angles							
	туре	Chain	Ullain	Ullalli	Chain	Chann Res	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
24	PSU	3K	40	24	18,21,22	1.17	1 (5%)	22,30,33	1.66	2 (9%)				
55	MIA	3L	38	55	24,31,32	2.44	3 (12%)	26,44,47	2.60	10 (38%)				
22	5MU	1K	63	22	19,22,23	<mark>3.77</mark>	5 (26%)	28,32,35	3.13	7 (25%)				

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	QUO	1K	35	22,25	-	4/6/43/44	0/4/4/4
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	2/9/27/28	0/2/2/2
55	PSU	3L	40	55	-	0/7/25/26	0/2/2/2
22	MIA	1K	38	22	-	3/11/33/34	0/3/3/3
23	OMC	2K	33	23	-	0/9/27/28	0/2/2/2
22	PSU	1K	40	22	-	1/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	1/7/25/26	0/2/2/2
23	$4\mathrm{SU}$	2L	8	23	-	0/7/25/26	0/2/2/2
22	PSU	1K	64	22	-	0/7/25/26	0/2/2/2
24	PSU	1L	40	24	-	0/7/25/26	0/2/2/2
23	5 MU	2K	55	23	-	3/7/25/26	0/2/2/2
24	PSU	3K	40	24	-	0/7/25/26	0/2/2/2
55	MIA	3L	38	55	-	4/11/33/34	0/3/3/3
22	5MU	1K	63	22	_	3/7/25/26	0/2/2/2

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1K	35	QUO	C6-N1	-14.81	1.15	1.37
22	1K	35	QUO	C4-N3	13.48	1.70	1.37
23	2K	55	5MU	C2-N1	13.09	1.59	1.38
23	2L	55	5MU	C2-N1	12.54	1.58	1.38
22	1K	63	5MU	C2-N1	12.26	1.58	1.38

The worst 5 of 81 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
22	1K	35	QUO	C5-C6-N1	14.32	127.49	115.36
22	1K	35	QUO	C8-N9-C1'	-13.50	113.53	125.48
23	2L	55	5MU	C5-C4-N3	10.76	124.50	115.31
22	1K	63	5MU	C5-C4-N3	10.74	124.48	115.31
22	1K	38	MIA	C11-S10-C2	-10.67	94.30	102.27

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	35	QUO	O4'-C4'-C5'-O5'
22	1K	35	QUO	C16-C12-N11-C10
22	1K	38	MIA	N6-C12-C13-C14
22	1K	38	MIA	C12-C13-C14-C15
22	1K	38	MIA	C12-C13-C14-C16

There are no ring outliers.

10 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	35	QUO	5	0
23	2K	56	PSU	1	0
23	2K	8	4SU	1	0
23	2L	33	OMC	6	0
22	1K	38	MIA	6	0
22	1K	40	PSU	2	0
23	2L	56	PSU	1	0
23	2L	8	4SU	1	0
22	1K	64	PSU	1	0
23	2K	55	5MU	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1166 ligands modelled in this entry, 1164 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).

Mal	Turne	Chain	Dog Link		Bog Link Bond lengths				Bond angles		
INIOI	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
57	PAR	13	1745	-	45,45,45	0.83	2 (4%)	64,67,67	2.07	18 (28%)	
57	PAR	1G	1686	-	45,45,45	0.72	1 (2%)	64,67,67	1.85	12 (18%)	

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	PAR	13	1745	-	-	6/18/94/94	0/4/4/4
57	PAR	1G	1686	-	-	5/18/94/94	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
57	1G	1686	PAR	C24-N24	-2.32	1.43	1.47
57	13	1745	PAR	C21-N21	-2.19	1.44	1.47
57	13	1745	PAR	C24-N24	-2.19	1.44	1.47

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
57	1G	1686	PAR	C13-O52-C52	-6.63	101.57	117.96
57	13	1745	PAR	C11-O51-C51	5.23	123.95	113.69
57	13	1745	PAR	C14-O54-C54	5.04	123.58	113.69
57	1G	1686	PAR	C11-O51-C51	4.98	123.46	113.69
57	1G	1686	PAR	C14-O54-C54	4.89	123.29	113.69

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	1G	1686	PAR	O51-C51-C61-O61
57	1G	1686	PAR	C33-C43-C53-O53
57	1G	1686	PAR	C41-C51-C61-O61
57	1G	1686	PAR	O51-C11-O11-C42



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Mol	Chain	\mathbf{Res}	Type	Atoms
57	13	1745	PAR	O43-C43-C53-O53

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	13	1745	PAR	2	0

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 then 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.







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95^{th} 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	$OWAB(A^2)$	Q < 0.9
1	13	1505/1522~(98%)	0.12	30 (1%) 65 41	53, 96, 178, 280	0
1	1G	1504/1522~(98%)	0.10	34 (2%) 60 36	67, 108, 172, 272	0
2	12	237/256~(92%)	0.03	7 (2%) 50 25	122, 156, 179, 190	0
2	1E	237/256~(92%)	-0.04	5 (2%) 63 39	101, 137, 165, 175	0
3	22	206/239~(86%)	-0.00	8 (3%) 39 19	114, 132, 162, 173	0
3	2E	205/239~(85%)	0.16	10 (4%) 29 13	81, 103, 132, 138	0
4	32	208/209~(99%)	0.28	5 (2%) 59 34	88, 109, 130, 142	0
4	3E	208/209~(99%)	0.67	21 (10%) 7 2	77, 98, 122, 131	0
5	42	151/162~(93%)	0.53	15 (9%) 7 2	99, 115, 136, 155	0
5	4E	151/162~(93%)	0.42	13 (8%) 10 4	72, 91, 112, 150	0
6	52	101/101 (100%)	-0.39	0 100 100	78, 94, 114, 144	0
6	5E	101/101 (100%)	-0.12	2 (1%) 65 41	75, 94, 115, 132	0
7	62	155/156~(99%)	0.49	20 (12%) 3 1	105, 120, 143, 157	0
7	6E	152/156~(97%)	0.27	11 (7%) 15 5	96, 114, 137, 148	0
8	72	137/138~(99%)	1.22	37 (27%) 0 0	98, 119, 131, 137	0
8	7E	138/138~(100%)	1.00	28 (20%) 1 0	81, 100, 114, 126	0
9	82	122/128~(95%)	2.19	61 (50%) 0 0	102, 149, 166, 170	0
9	8E	127/128~(99%)	1.39	42 (33%) 0 0	81, 135, 158, 168	0
10	1A	99/105~(94%)	0.93	24 (24%) 0 0	111, 148, 164, 171	0
10	1I	99/105~(94%)	1.34	29 (29%) 0 0	73, 128, 159, 161	0
11	2A	117/129~(90%)	0.72	13 (11%) 5 2	81, 103, 120, 147	0
11	2I	116/129~(89%)	0.27	7 (6%) 21 9	72, 98, 120, 150	0
12	3A	125/132~(94%)	0.71	19 (15%) 2 1	78, 96, 129, 157	0
12	3I	122/132~(92%)	0.32	7 (5%) 23 10	61, 71, 97, 126	0



Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
13	4A	117/126~(92%)	0.93	25 (21%) 0 0	102, 137, 157, 170	0
13	4I	116/126~(92%)	0.09	5 (4%) 35 16	78, 117, 136, 144	0
14	5A	58/61~(95%)	2.78	34~(58%) 0 0	116, 131, 146, 154	0
14	5I	59/61~(96%)	1.26	11 (18%) 1 0	82, 92, 108, 118	0
15	6A	88/89~(98%)	0.15	1 (1%) 80 60	80, 105, 121, 127	0
15	6I	88/89~(98%)	0.31	3 (3%) 45 22	67, 93, 110, 123	0
16	7A	84/88~(95%)	1.63	28 (33%) 0 0	85, 98, 124, 154	0
16	7I	84/88~(95%)	1.88	41 (48%) 0 0	90, 104, 132, 160	0
17	8A	100/105~(95%)	0.50	12 (12%) 4 1	91, 106, 124, 128	0
17	8I	100/105~(95%)	0.09	7 (7%) 16 6	81, 99, 111, 121	0
18	9A	71/88~(80%)	-0.33	0 100 100	84, 107, 134, 164	0
18	9I	72/88~(81%)	-0.02	0 100 100	80, 98, 126, 161	0
19	AA	78/93~(83%)	0.35	5 (6%) 19 7	124, 142, 171, 180	0
19	AI	83/93~(89%)	0.22	6 (7%) 15 5	90, 116, 137, 145	0
20	BA	99/106~(93%)	0.99	23 (23%) 0 0	83, 105, 133, 143	0
20	BI	99/106~(93%)	1.75	47 (47%) 0 0	101, 115, 146, 151	0
21	1B	25/27~(92%)	3.83	21 (84%) 0 0	110, 126, 143, 163	0
21	$1\mathrm{F}$	25/27~(92%)	2.86	16 (64%) 0 0	90, 102, 116, 142	0
22	1K	80/85~(94%)	0.11	5 (6%) 20 8	81, 190, 249, 257	0
23	2K	73/77~(94%)	-0.05	2 (2%) 54 28	68, 96, 122, 140	0
23	2L	73/77~(94%)	-0.29	1 (1%) 75 53	76, 105, 138, 160	0
24	1L	84/85~(98%)	1.36	23 (27%) 0 0	107, 214, 302, 318	0
24	3K	84/85~(98%)	-0.18	2 (2%) 59 34	68, 209, 252, 259	0
25	4K	12/30~(40%)	1.37	$3\ (25\%)\ 0\ 0$	64, 94, 132, 145	0
25	4L	12/30~(40%)	1.32	4 (33%) 0 0	85, 117, 155, 188	0
26	14	2909/2918~(99%)	0.11	39 (1%) 77 56	48, 80, 223, 333	0
26	1H	2912/2918~(99%)	0.14	22 (0%) 86 70	38, 71, 216, 270	0
27	16	122/122~(100%)	-0.20	0 100 100	65, 91, 113, 185	0
27	1J	$\overline{122/122}\ (100\%)$	-0.32	1 (0%) 86 70	73, 107, 128, 182	0
28	11	$\overline{273/276}\ (98\%)$	0.34	3 (1%) 80 60	39, 62, 80, 92	0
28	19	273/276~(98%)	0.75	24 (8%) 10 3	42, 70, 88, 102	0



Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
29	21	205/206~(99%)	0.80	21 (10%) 6 2	48, 85, 125, 137	0
29	29	205/206~(99%)	0.84	38 (18%) 1 0	56, 87, 129, 148	0
30	31	202/210~(96%)	0.02	0 100 100	38, 74, 110, 127	0
30	39	208/210~(99%)	0.20	7 (3%) 45 22	54, 95, 146, 178	0
31	41	181/182~(99%)	0.27	10 (5%) 25 10	79, 102, 133, 149	0
31	49	181/182~(99%)	1.02	33 (18%) 1 0	104, 125, 154, 169	0
32	51	173/180~(96%)	-0.03	2 (1%) 79 58	79, 102, 115, 151	0
32	59	170/180~(94%)	1.82	58 (34%) 0 0	134, 183, 210, 241	0
33	61	146/148~(98%)	-0.07	2 (1%) 75 53	74, 122, 140, 145	0
33	69	146/148~(98%)	0.47	20 (13%) 3 1	77, 118, 142, 146	0
34	15	138/140~(98%)	1.04	31 (22%) 0 0	75, 100, 129, 137	0
34	58	138/140~(98%)	0.47	9 (6%) 18 7	61, 88, 126, 143	0
35	25	122/122~(100%)	0.43	5 (4%) 37 18	61, 84, 102, 110	0
35	68	122/122~(100%)	0.49	3 (2%) 57 32	55, 74, 92, 101	0
36	35	150/150~(100%)	0.85	26 (17%) 1 0	54, 96, 133, 159	0
36	78	150/150~(100%)	0.24	1 (0%) 87 72	45, 81, 111, 152	0
37	45	139/141~(98%)	1.85	59 (42%) 0 0	69, 98, 116, 136	0
37	88	141/141 (100%)	0.36	2 (1%) 75 53	52, 77, 101, 129	0
38	55	117/118~(99%)	0.63	8 (6%) 17 6	56, 75, 92, 108	0
38	98	118/118 (100%)	0.51	4 (3%) 45 22	56, 80, 101, 107	0
39	65	111/112~(99%)	0.71	14 (12%) 3 1	75, 102, 120, 132	0
39	A8	110/112~(98%)	0.28	6 (5%) 25 10	70, 86, 110, 125	0
40	75	137/146~(93%)	0.34	11 (8%) 12 4	75, 91, 148, 185	0
40	B8	137/146~(93%)	0.50	14 (10%) 6 2	70, 89, 136, 159	0
41	85	117/118~(99%)	0.41	5 (4%) 35 16	62, 88, 122, 143	0
41	C8	117/118~(99%)	0.84	14 (11%) 4 1	50, 76, 107, 141	0
42	95	101/101 (100%)	0.28	7 (6%) 16 6	61, 116, 131, 136	0
42	D8	101/101~(100%)	0.29	7 (6%) 16 6	53, 100, 124, 139	0
43	A5	113/113 (100%)	0.40	4 (3%) 44 22	56, 71, 100, 159	0
43	E8	113/113 (100%)	0.16	0 100 100	52, 72, 105, 140	0
44	B5	92/96~(95%)	0.12	2 (2%) 62 38	64, 79, 106, 119	0



Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
44	F8	93/96~(96%)	-0.05	0 100 100	51,67,93,102	0
45	C5	104/110~(94%)	0.99	17 (16%) 1 0	89, 119, 158, 166	0
45	G8	104/110~(94%)	0.45	3 (2%) 51 26	69, 96, 140, 148	0
46	D5	138/206~(66%)	0.40	11 (7%) 12 4	103, 134, 178, 186	0
46	H8	175/206~(84%)	-0.21	1 (0%) 89 76	84, 119, 190, 195	0
47	E5	77/85~(90%)	1.24	15 (19%) 1 0	64, 81, 99, 131	0
47	I8	76/85~(89%)	0.68	5 (6%) 18 7	52, 69, 85, 113	0
48	F5	97/98~(98%)	1.41	16 (16%) 1 0	57, 77, 122, 143	0
48	J8	97/98~(98%)	0.88	11 (11%) 5 1	48, 72, 124, 150	0
49	G5	66/72~(91%)	0.15	1 (1%) 73 51	74, 96, 114, 135	0
49	K8	66/72~(91%)	0.36	3 (4%) 33 15	59, 77, 90, 124	0
50	H5	59/60~(98%)	0.51	1 (1%) 70 46	74, 94, 132, 157	0
50	L8	59/60~(98%)	0.40	0 100 100	56, 78, 114, 137	0
51	I5	63/71~(88%)	2.20	28 (44%) 0 0	138, 171, 190, 192	0
51	M8	66/71~(92%)	0.50	6 (9%) 9 3	105, 154, 174, 184	0
52	J5	59/60~(98%)	0.50	3 (5%) 28 12	56, 80, 147, 187	0
52	N8	59/60~(98%)	0.66	6 (10%) 6 2	51, 86, 152, 158	0
53	L5	45/49~(91%)	0.45	1 (2%) 62 38	47, 56, 69, 84	0
53	P8	46/49~(93%)	0.10	0 100 100	40, 48, 66, 81	0
54	M5	62/65~(95%)	1.56	20 (32%) 0 0	65, 77, 93, 107	0
54	Q8	61/65~(93%)	1.01	8 (13%) 3 1	56, 66, 80, 98	0
55	3L	83/85~(97%)	0.32	9 (10%) 5 2	72, 217, 260, 269	0
All	All	20954/21624~(96%)	0.37	1450 (6%) 16 6	38, 95, 175, 333	0

The worst 5 of 1450 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	59	99	VAL	15.8
48	F5	98	LEU	14.8
48	F5	97	LEU	11.8
32	59	96	ALA	11.0
11	2A	11	LYS	10.3



6.2 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, 95^{th} 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
23	4SU	2L	8	20/21	0.91	0.14	99,106,113,117	0
23	OMC	2L	33	21/22	0.91	0.22	86,95,99,102	0
23	PSU	2L	56	20/21	0.91	0.10	101,108,114,119	0
22	5MU	1K	63	21/22	0.92	0.16	106,124,138,141	0
22	PSU	1K	64	20/21	0.92	0.14	106,129,138,140	0
24	PSU	1L	40	20/21	0.92	0.26	99,116,121,124	0
55	MIA	3L	38	29/30	0.93	0.26	102,116,135,141	0
55	PSU	3L	40	20/21	0.93	0.24	110,117,123,123	0
22	QUO	1K	35	32/33	0.94	0.37	67,86,101,111	0
23	4SU	2K	8	20/21	0.94	0.16	83,89,99,107	0
22	MIA	1K	38	29/30	0.95	0.29	67,84,98,112	0
23	5MU	2K	55	21/22	0.95	0.14	88,99,104,112	0
23	5MU	2L	55	21/22	0.95	0.11	101,110,116,118	0
23	PSU	2K	56	20/21	0.95	0.12	93,98,101,113	0
24	PSU	3K	40	20/21	0.95	0.12	106,113,117,119	0
22	PSU	1K	40	20/21	0.95	0.15	78,96,104,105	0
23	OMC	2K	33	21/22	0.98	0.26	70,74,82,85	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 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, 95^{th} 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
58	ZN	G8	201	1/1	0.23	0.14	178,178,178,178	0
56	MG	25	201	1/1	0.43	0.38	107,107,107,107	0
56	MG	14	3261	1/1	0.44	0.38	93,93,93,93	0
56	MG	14	3182	1/1	0.49	0.24	72,72,72,72	0
56	MG	1G	1641	1/1	0.49	0.26	73,73,73,73	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors(A^2)	Q < 0.9
56	MG	1H	3223	1/1	0.51	0.58	102,102,102,102	0
56	MG	14	3289	1/1	0.53	0.28	79,79,79,79	0
56	MG	2L	102	1/1	0.54	0.22	79,79,79,79	0
56	MG	14	3254	1/1	0.54	0.27	102,102,102,102	0
58	ZN	C5	202	1/1	0.57	0.14	192,192,192,192	0
56	MG	1G	1684	1/1	0.58	0.12	122,122,122,122	0
56	MG	13	1685	1/1	0.59	0.22	91,91,91,91	0
56	MG	13	1647	1/1	0.59	0.21	77,77,77,77	0
56	MG	13	1743	1/1	0.61	0.36	102,102,102,102	0
56	MG	13	1617	1/1	0.62	0.26	86,86,86,86	0
56	MG	14	3148	1/1	0.62	0.22	82,82,82,82	0
56	MG	1H	3416	1/1	0.62	0.12	77,77,77,77	0
56	MG	14	3118	1/1	0.63	0.42	86,86,86,86	0
56	MG	1H	3239	1/1	0.63	0.22	$72,\!72,\!72,\!72$	0
56	MG	1G	1646	1/1	0.63	0.23	$79,\!79,\!79,\!79$	0
56	MG	14	3151	1/1	0.64	0.23	$72,\!72,\!72,\!72$	0
56	MG	$1\mathrm{H}$	3275	1/1	0.64	0.44	75, 75, 75, 75, 75	0
56	MG	$1\mathrm{H}$	3300	1/1	0.64	0.31	77, 77, 77, 77	0
56	MG	1H	3185	1/1	0.64	0.19	71,71,71,71	0
56	MG	13	1715	1/1	0.65	0.14	83,83,83,83	0
56	MG	1H	3274	1/1	0.65	0.47	80,80,80,80	0
56	MG	14	3144	1/1	0.65	0.39	79,79,79,79	0
56	MG	14	3265	1/1	0.66	0.34	121,121,121,121	0
56	MG	14	3199	1/1	0.66	0.20	69,69,69,69	0
56	MG	14	3249	1/1	0.66	0.19	77,77,77,77	0
56	MG	14	3180	1/1	0.66	0.18	$71,\!71,\!71,\!71$	0
56	MG	$1\mathrm{H}$	3451	1/1	0.66	0.13	46, 46, 46, 46	0
56	MG	1H	3178	1/1	0.67	0.27	$63,\!63,\!63,\!63$	0
56	MG	1H	3467	1/1	0.67	0.09	75,75,75,75	0
56	MG	14	3293	1/1	0.67	0.48	88,88,88,88	0
56	MG	1H	3319	1/1	0.68	0.56	92,92,92,92	0
56	MG	13	1688	1/1	0.68	0.26	77,77,77,77	0
56	MG	13	1623	1/1	0.68	0.44	94,94,94,94	0
56	MG	14	3139	1/1	0.69	0.20	81,81,81,81	0
56	MG	1H	3326	1/1	0.69	0.55	96,96,96,96	0
56	MG	1H	3030	1/1	0.69	0.34	81,81,81,81	0
56	MG	1H	3295	1/1	0.69	0.17	76,76,76,76	0
56	MG	1H	3098	1/1	0.70	0.20	87,87,87,87	0
56	MG	1H	3248	1/1	0.70	0.32	80,80,80,80	0
56	MG	14	3260	1/1	0.70	0.27	85,85,85,85	0
56	MG	1H	3273	1/1	0.70	0.41	87,87,87,87	0
56	MG	13	1673	1/1	0.70	0.23	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1H	3228	1/1	0.71	0.42	74,74,74,74	0
56	MG	1H	3201	1/1	0.71	0.20	59,59,59,59	0
56	MG	1H	3144	1/1	0.71	0.27	66,66,66,66	0
56	MG	14	3132	1/1	0.71	0.30	86,86,86,86	0
56	MG	14	3377	1/1	0.71	0.12	96,96,96,96	0
56	MG	1H	3282	1/1	0.71	0.40	83,83,83,83	0
56	MG	1H	3330	1/1	0.71	0.21	67,67,67,67	0
56	MG	1G	1667	1/1	0.71	0.25	80,80,80,80	0
56	MG	16	203	1/1	0.72	0.17	68,68,68,68	0
56	MG	1H	3207	1/1	0.72	0.21	73,73,73,73	0
56	MG	2K	102	1/1	0.72	0.23	83,83,83,83	0
56	MG	1H	3459	1/1	0.72	0.08	77,77,77,77	0
56	MG	1H	3339	1/1	0.72	0.30	88,88,88,88	0
56	MG	14	3282	1/1	0.72	0.32	86,86,86,86	0
56	MG	1H	3349	1/1	0.73	0.35	85,85,85,85	0
56	MG	14	3167	1/1	0.73	0.14	59,59,59,59	0
56	MG	14	3264	1/1	0.73	0.28	67,67,67,67	0
56	MG	14	3169	1/1	0.73	0.14	77,77,77,77	0
56	MG	1H	3171	1/1	0.73	0.14	79,79,79,79	0
56	MG	14	3286	1/1	0.73	0.23	78,78,78,78	0
56	MG	1H	3243	1/1	0.74	0.23	69,69,69,69	0
56	MG	14	3094	1/1	0.74	0.18	69,69,69,69	0
56	MG	1H	3217	1/1	0.74	0.46	93,93,93,93	0
56	MG	1G	1620	1/1	0.74	0.34	78,78,78,78	0
56	MG	1H	3299	1/1	0.74	0.38	82,82,82,82	0
56	MG	14	3226	1/1	0.74	0.18	82,82,82,82	0
56	MG	13	1658	1/1	0.74	0.24	70,70,70,70	0
56	MG	1H	3076	1/1	0.74	0.41	75,75,75,75	0
56	MG	13	1741	1/1	0.74	0.09	110,110,110,110	0
56	MG	14	3158	1/1	0.74	0.41	$67,\!67,\!67,\!67$	0
56	MG	13	1720	1/1	0.75	0.11	62,62,62,62	0
56	MG	31	301	1/1	0.75	0.10	56, 56, 56, 56	0
56	MG	14	3149	1/1	0.75	0.33	84,84,84,84	0
56	MG	1H	3386	1/1	0.75	0.12	$53,\!53,\!53,\!53$	0
56	MG	14	3290	1/1	0.75	0.22	82,82,82,82	0
56	MG	1H	3314	1/1	0.76	0.37	90,90,90,90	0
56	MG	13	1616	1/1	0.76	0.37	93,93,93,93	0
56	MG	14	3217	1/1	0.76	0.28	$68,\!68,\!68,\!68$	0
56	MG	1H	3293	1/1	0.76	0.46	90,90,90,90	0
56	MG	1H	$3\overline{205}$	1/1	0.76	0.36	$62, \overline{62}, \overline{62}, \overline{62}$	0
56	MG	14	3250	1/1	0.76	0.22	74,74,74,74	0
56	MG	13	1687	1/1	0.76	0.21	70,70,70,70	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors(A^2)	Q<0.9
56	MG	1H	3163	1/1	0.76	0.34	87,87,87,87	0
56	MG	1H	3366	1/1	0.76	0.40	74,74,74,74	0
56	MG	1H	3311	1/1	0.76	0.27	78,78,78,78	0
56	MG	14	3275	1/1	0.77	0.27	60,60,60,60	0
56	MG	1H	3264	1/1	0.77	0.22	58,58,58,58	0
56	MG	14	3284	1/1	0.77	0.11	88,88,88,88	0
56	MG	1H	3305	1/1	0.77	0.29	75,75,75,75	0
56	MG	1H	3222	1/1	0.77	0.36	80,80,80,80	0
56	MG	1H	3101	1/1	0.77	0.43	62,62,62,62	0
56	MG	1H	3298	1/1	0.77	0.29	79,79,79,79	0
56	MG	14	3298	1/1	0.77	0.40	103,103,103,103	0
56	MG	14	3305	1/1	0.77	0.17	79,79,79,79	0
56	MG	13	1697	1/1	0.77	0.15	82,82,82,82	0
56	MG	39	301	1/1	0.77	0.23	71,71,71,71	0
56	MG	1H	3328	1/1	0.77	0.47	91,91,91,91	0
56	MG	14	3190	1/1	0.77	0.26	85,85,85,85	0
56	MG	1H	3453	1/1	0.77	0.12	76,76,76,76	0
56	MG	1G	1665	1/1	0.78	0.13	94,94,94,94	0
56	MG	14	3267	1/1	0.78	0.22	81,81,81,81	0
56	MG	1H	3332	1/1	0.78	0.47	88,88,88,88	0
56	MG	13	1692	1/1	0.78	0.17	79,79,79,79	0
56	MG	13	1707	1/1	0.78	0.25	96,96,96,96	0
56	MG	14	3077	1/1	0.78	0.30	68,68,68,68	0
56	MG	1H	3250	1/1	0.78	0.16	68,68,68,68	0
56	MG	13	1696	1/1	0.78	0.26	116,116,116,116	0
56	MG	14	3283	1/1	0.79	0.12	102,102,102,102	0
56	MG	14	3218	1/1	0.79	0.19	77,77,77,77	0
56	MG	1G	1648	1/1	0.79	0.43	121,121,121,121	0
56	MG	1H	3211	1/1	0.79	0.43	64,64,64,64	0
56	MG	1H	3233	1/1	0.79	0.21	53,53,53,53	0
56	MG	1H	3461	1/1	0.79	0.09	108,108,108,108	0
56	MG	1H	3368	1/1	0.79	0.27	74,74,74,74	0
56	MG	14	3302	1/1	0.79	0.15	72,72,72,72	0
56	MG	1H	3477	1/1	0.79	0.06	106,106,106,106	0
56	MG	14	3365	1/1	0.79	0.07	85,85,85,85	0
56	MG	1H	3322	1/1	0.79	0.36	80,80,80,80	0
56	MG	1H	3393	1/1	0.79	0.10	65,65,65,65	0
56	MG	13	1649	1/1	0.79	0.21	85,85.85.85	0
56	MG	1H	3431	1/1	0.79	0.21	99,99,99,99	0
56	MG	1H	3341	1/1	0.79	0.33	67.67.67.67	0
56	MG	14	3096	1/1	0.80	0.19	78,78.78.78	0
56	MG	14	3117	1/1	0.80	0.34	76,76,76,76	0

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56 MG 111 3203 $1/1$ 0.80 0.40 80,80,80,80,80 0 56 MG 14 3287 $1/1$ 0.80 0.20 $79,79,79,79,79,79,79,79,79,79,79,79,79,7$	Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors(A^2)	Q<0.9
56 MG 1G 1622 1/1 0.80 0.16 72,72,72,72 0 56 MG 14 3287 1/1 0.80 0.20 79,79,79,79 0 56 MG 1H 3358 1/1 0.80 0.22 80,80,80,80 0 56 MG 1H 3323 1/1 0.80 0.02 88,88,88 0 56 MG 1H 3423 1/1 0.80 0.06 92,92,92,92 0 56 MG 1H 3423 1/1 0.80 0.02 53,53,53,53 0 56 MG 1H 3424 1/1 0.80 0.30 98,98,98,98 0 56 MG 1H 3421 1/1 0.80 0.31 79,79,79,79 0 56 MG 1H 3421 1/1 0.80 0.43 87,87,87,87 0 56 MG 1H 3135 1/1	56	MG	1H	3203	1/1	0.80	0.40	80,80,80,80	0
56 MG 14 3287 1/1 0.80 0.20 $79, 79, 79, 79$ 0 56 MG 1H 3358 1/1 0.80 0.25 80,80,80,80 0 56 MG 11 3068 1/1 0.80 0.29 67,67,67,67 0 56 MG 1H 3323 1/1 0.80 0.012 88,88,88 0 56 MG 1H 3462 1/1 0.80 0.06 92,92,92,92 0 56 MG 1H 3422 1/1 0.80 0.21 54,54,54,4 0 56 MG 1H 3424 1/1 0.80 0.30 98,98,98 0 56 MG 1H 3422 1/1 0.80 0.43 87,87,87,87 0 56 MG 1H 3433 1/1 0.81 0.30 73,73,73 0 56 MG 14 3133 1/1 <	56	MG	IG	1622	1/1	0.80	0.16	72,72,72,72	0
56 MG 1H 3358 1/1 0.80 0.25 80,80,80,80 0 56 MG 1H 3068 1/1 0.80 0.29 67,67,67,67 0 56 MG 1H 323 1/1 0.80 0.50 82,82,82,82 0 56 MG 1H 3462 1/1 0.80 0.06 92,92,92,92 0 56 MG 1H 3432 1/1 0.80 0.21 54,54,54,54 0 56 MG 1H 3409 1/1 0.80 0.30 98,98,98 0 56 MG 1H 3421 1/1 0.80 0.31 79,79,79,79 0 56 MG 14 3135 1/1 0.80 0.43 87,87,87,87 0 56 MG 14 3137 1/1 0.81 0.10 78,78,78,7 0 56 MG 13 1662 1/1 <t< td=""><td>56</td><td>MG</td><td>14</td><td>3287</td><td>1/1</td><td>0.80</td><td>0.20</td><td>79,79,79,79</td><td>0</td></t<>	56	MG	14	3287	1/1	0.80	0.20	79,79,79,79	0
56 MG 1H 3068 1/1 0.80 0.29 67,67,67,67 0 56 MG 1H 3323 1/1 0.80 0.12 88,88,88 0 56 MG 1H 3323 1/1 0.80 0.06 92,92,92,92 0 56 MG 1H 3462 1/1 0.80 0.06 92,92,92,92 0 56 MG 1H 3238 1/1 0.80 0.21 54,54,54,54 0 56 MG 1H 3349 1/1 0.80 0.30 98,98,98,98 0 56 MG 1H 3421 1/1 0.80 0.31 79,79,79,79 0 56 MG 14 3135 1/1 0.80 0.43 87,87,87,87 0 56 MG 14 3135 1/1 0.81 0.30 73,73,73 0 56 MG 13 1662 1/1 <td< td=""><td>56</td><td>MG</td><td>1H</td><td>3358</td><td>1/1</td><td>0.80</td><td>0.25</td><td>80,80,80,80</td><td>0</td></td<>	56	MG	1H	3358	1/1	0.80	0.25	80,80,80,80	0
56 MG 13 1663 1/1 0.80 0.12 88.88,88,88 0 56 MG 1H 3323 1/1 0.80 0.50 82,82,82,82 0 56 MG 1H 3462 1/1 0.80 0.06 92,92,92,92,90 0 56 MG 1H 3238 1/1 0.80 0.21 54,54,54,54 0 56 MG 1H 3423 1/1 0.80 0.20 53,53,53,53 0 56 MG 1H 342 1/1 0.80 0.31 79,79,79,79 0 56 MG 14 3170 1/1 0.80 0.43 87,87,87,87 0 56 MG 14 3135 1/1 0.81 0.10 78,78,78,7 0 56 MG 13 1662 1/1 0.81 0.21 65,65,65,65 0 56 MG 13 1662 1/1	56	MG	1H	3068	1/1	0.80	0.29	67,67,67,67	0
56 MG 1H 3323 1/1 0.80 0.50 82,82,82,82 0 56 MG 1H 3462 1/1 0.80 0.06 92,92,92 0 56 MG 14 3153 1/1 0.80 0.17 94,94,94,94,94 0 56 MG 1H 3238 1/1 0.80 0.21 54,54,54,54,54 0 56 MG 1H 3420 1/1 0.80 0.30 98,98,98,98 0 56 MG 1H 3421 1/1 0.80 0.31 79,79,79,79,79 0 56 MG 14 3130 1/1 0.81 0.10 78,78,78,78 0 56 MG 14 3137 1/1 0.81 0.34 69,69,69 0 56 MG 1H 3313 1/1 0.81 0.32 83,83,80 0 56 MG 13 1662 1/1	56	MG	13	1663	1/1	0.80	0.12	88,88,88,88	0
56 MG 1H 3462 $1/1$ 0.80 0.06 92,92,92,92 0 56 MG 14 3153 $1/1$ 0.80 0.17 94,94,94,94 0 56 MG 1H 3238 $1/1$ 0.80 0.21 54,54,54,54,54 0 56 MG 1H 3342 $1/1$ 0.80 0.20 53,53,53,53 0 56 MG 1H 3342 $1/1$ 0.80 0.31 79,79,79,79 0 56 MG 1H 3421 $1/1$ 0.80 0.43 87,87,87,87 0 56 MG 14 3135 $1/1$ 0.81 0.34 69,69,69,09 0 56 MG 14 3137 $1/1$ 0.81 0.30 73,73,73 0 56 MG 13 1662 $1/1$ 0.81 0.30 73,73,73,73 0 56 MG 13 16650	56	MG	1H	3323	1/1	0.80	0.50	82,82,82,82	0
56 MG 14 3153 $1/1$ 0.80 0.17 94,94,94,94 0 56 MG 1H 3238 $1/1$ 0.80 0.21 54,54,54,54 0 56 MG 1H 3409 $1/1$ 0.80 0.20 53,53,53,53 0 56 MG 1H 3421 $1/1$ 0.80 0.31 79,79,79 0 56 MG 1H 3421 $1/1$ 0.80 0.07 57,57,57,57 0 56 MG 14 3137 $1/1$ 0.81 0.10 78,78,78,78 0 56 MG 14 3137 $1/1$ 0.81 0.34 69,69,69 0 56 MG 13 1662 $1/1$ 0.81 0.30 73,73,73 0 56 MG 13 1662 $1/1$ 0.81 0.40 87,87,87,87 0 56 MG 13 1637 $1/1$	56	MG	1H	3462	1/1	0.80	0.06	92,92,92,92	0
56 MG 1H 3238 $1/1$ 0.80 0.21 54,54,54,54,54 0 56 MG 1H 3409 $1/1$ 0.80 0.20 53,53,53,53 0 56 MG 1H 3342 $1/1$ 0.80 0.31 79,79,79,79 0 56 MG 1H 3421 $1/1$ 0.80 0.07 57,57,57,57 0 56 MG 14 3135 $1/1$ 0.81 0.10 78,78,78,78 0 56 MG 14 3135 $1/1$ 0.81 0.34 69,69,69,69 0 56 MG 14 3137 $1/1$ 0.81 0.21 65,65,65 0 56 MG 13 1662 $1/1$ 0.81 0.40 87,87,87,87 0 56 MG 13 1637 $1/1$ 0.81 0.40 87,87,87,87 0 56 MG 14 3139	56	MG	14	3153	1/1	0.80	0.17	94,94,94,94	0
56 MG 1H 3409 $1/1$ 0.80 0.20 53,53,53,53 0 56 MG 1H 3342 $1/1$ 0.80 0.30 98,98,98,98 0 56 MG 1H 3421 $1/1$ 0.80 0.07 57,57,57,57 0 56 MG 14 3135 $1/1$ 0.80 0.43 87,87,87,87 0 56 MG 14 3135 $1/1$ 0.81 0.34 69,69,69,69 0 56 MG 14 3137 $1/1$ 0.81 0.34 69,69,69,69 0 56 MG 13 1662 $1/1$ 0.81 0.30 73,73,73,73 0 56 MG 13 1671 $1/1$ 0.81 0.40 87,87,87,87 0 56 MG 13 1637 $1/1$ 0.81 0.17 66,66,66,66 0 56 MG 1H 3139	56	MG	1H	3238	1/1	0.80	0.21	54,54,54,54	0
56MG1H33421/10.800.3098,98,98,98056MG1431701/10.800.3179,79,79,79056MG1H34211/10.800.0757,57,57,57,57056MG1431351/10.800.4387,87,87,87056MG1431371/10.810.1078,78,78,78056MG1H31311/10.810.3469,69,69,69056MG1131311/10.810.3073,73,73,73056MG1316621/10.810.4087,87,87,87056MG1316621/10.810.4087,87,87,87056MG1316631/10.810.4087,87,87,87056MG1G16501/10.810.4087,87,87,87056MG1316371/10.810.1280,80,80,80056MG1H31391/10.810.1766,66,66,66056MG1H32401/10.810.1873,73,73,73056MG1430201/10.810.1873,73,73,73,73056MG1430201/10.810.1248,84,84,84056MG1430911/1<	56	MG	1H	3409	1/1	0.80	0.20	53,53,53,53	0
56MG143170 $1/1$ 0.800.3179,79,79,79056MG1H3421 $1/1$ 0.800.0757,57,57,57056MG143280 $1/1$ 0.800.4387,87,87,87056MG143135 $1/1$ 0.810.1078,78,78,78056MG143137 $1/1$ 0.810.3469,69,69,69056MG1H3313 $1/1$ 0.810.2165,65,65,65056MG131662 $1/1$ 0.810.3073,73,73,73056MG1G1050 $1/1$ 0.810.4087,87,87,87056MG131637 $1/1$ 0.810.2461,61,61,61056MG113139 $1/1$ 0.810.1766,66,66,66056MG1G1675 $1/1$ 0.810.1873,73,73,73056MG1G1675 $1/1$ 0.810.1873,73,73,73056MG1H3240 $1/1$ 0.810.1873,73,73,73056MG1H3200 $1/1$ 0.810.1568,68,68056MG143020 $1/1$ 0.810.1280,80,80,80056MG143091 $1/1$ 0.810.1285,85,85,85056MG14 <td< td=""><td>56</td><td>MG</td><td>1H</td><td>3342</td><td>1/1</td><td>0.80</td><td>0.30</td><td>$98,\!98,\!98,\!98$</td><td>0</td></td<>	56	MG	1H	3342	1/1	0.80	0.30	$98,\!98,\!98,\!98$	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3170	1/1	0.80	0.31	$79,\!79,\!79,\!79$	0
56MG14 3280 $1/1$ 0.80 0.43 $87,87,87,87,87$ 0 56 MG14 3135 $1/1$ 0.81 0.10 $78,78,78,78$ 0 56 MG14 3137 $1/1$ 0.81 0.34 $69,69,69,69$ 0 56 MG11 3313 $1/1$ 0.81 0.21 $65,65,65,65$ 0 56 MG13 1662 $1/1$ 0.81 0.30 $73,73,73,73$ 0 56 MG13 1701 $1/1$ 0.81 0.12 $80,80,80,80$ 0 56 MG13 1650 $1/1$ 0.81 0.40 $87,87,87,87,87$ 0 56 MG13 1637 $1/1$ 0.81 0.40 $87,87,87,87,87$ 0 56 MG13 1637 $1/1$ 0.81 0.12 $80,80,80,80$ 0 56 MG14 3139 $1/1$ 0.81 0.14 $87,87,87,87,87,87,87,87,87,87,87,87,87,8$	56	MG	1H	3421	1/1	0.80	0.07	$57,\!57,\!57,\!57$	0
56MG14 3135 $1/1$ 0.81 0.10 $78,78,78,78$ 0 56 MG14 3137 $1/1$ 0.81 0.34 $69,69,69,69$ 0 56 MG1H 3313 $1/1$ 0.81 0.21 $65,65,65,65$ 0 56 MG13 1662 $1/1$ 0.81 0.30 $73,73,73,73$ 0 56 MG13 1701 $1/1$ 0.81 0.40 $87,87,87,87,87$ 0 56 MG13 1637 $1/1$ 0.81 0.40 $87,87,87,87,87$ 0 56 MG13 1637 $1/1$ 0.81 0.40 $87,87,87,87,87,87,87,87,87,87,87,87,87,8$	56	MG	14	3280	1/1	0.80	0.43	87,87,87,87	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3135	1/1	0.81	0.10	78,78,78,78	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3137	1/1	0.81	0.34	69,69,69,69	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3313	1/1	0.81	0.21	$65,\!65,\!65,\!65$	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	13	1662	1/1	0.81	0.30	73,73,73,73	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	13	1701	1/1	0.81	0.12	80,80,80,80	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1G	1650	1/1	0.81	0.40	87,87,87,87	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	13	1637	1/1	0.81	0.24	61,61,61,61	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3139	1/1	0.81	0.17	66,66,66,66	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1G	1675	1/1	0.81	0.08	110,110,110,110	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3240	1/1	0.81	0.18	73,73,73,73	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	3E	301	1/1	0.81	0.11	112,112,112,112	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3020	1/1	0.81	0.15	68,68,68,68	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3171	1/1	0.81	0.24	80,80,80,80	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3146	1/1	0.81	0.24	75,75,75,75	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3091	1/1	0.81	0.22	84,84,84,84	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	13	1708	1/1	0.81	0.22	85,85,85,85	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	P8	101	1/1	0.81	0.29	68,68,68,68	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3216	1/1	0.81	0.17	83,83,83,83	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3342	1/1	0.81	0.13	74,74,74,74	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	13	1710	1/1	0.81	0.12	128,128,128,128	0
56 MG 13 1670 1/1 0.81 0.13 78,78,78,78 0 56 MG 14 3122 1/1 0.81 0.14 68,68,68,68 0 56 MG 14 3122 1/1 0.81 0.14 68,68,68,68 0 56 MG 14 3127 1/1 0.81 0.17 64,64,64,64 0 56 MG C5 201 1/1 0.81 0.28 104,104,104,104 0	56	MG	14	3369	1/1	0.81	0.12	97,97,97,97	0
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	56	MG	13	1670	1/1	0.81	0.13	78,78,78,78	0
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	56	MG	14	3122	1/1	0.81	0.14	68,68,68,68	0
56 MG C5 201 1/1 0.81 0.28 104,104,104 0	56	MG	14	3127	1/1	0.81	0.17	64,64,64,64	0
	56	MG	C5	201	1/1	0.81	0.28	104,104,104,104	0
56 MG 1G 1623 1/1 0.81 0.22 73,73,73,73 0	56	MG	1G	1623	1/1	0.81	0.22	73,73,73,73	0
56 MG 14 3133 1/1 0.81 0.19 86,86,86,86 0	56	MG	14	3133	1/1	0.81	0.19	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors(A^2)	Q < 0.9
56	MG	14	3303	1/1	0.82	0.15	101,101,101,101	0
56	MG	1H	3321	1/1	0.82	0.42	86,86,86,86	0
56	MG	14	3332	1/1	0.82	0.17	73,73,73,73	0
56	MG	1H	3281	1/1	0.82	0.37	74,74,74,74	0
56	MG	1H	3170	1/1	0.82	0.22	61,61,61,61	0
56	MG	14	3033	1/1	0.82	0.17	64,64,64,64	0
56	MG	1H	3288	1/1	0.82	0.13	$54,\!54,\!54,\!54$	0
56	MG	14	3378	1/1	0.82	0.10	79,79,79,79	0
56	MG	1H	3290	1/1	0.82	0.41	84,84,84,84	0
56	MG	1H	3067	1/1	0.82	0.25	49,49,49,49	0
56	MG	14	3272	1/1	0.82	0.35	82,82,82,82	0
56	MG	13	1679	1/1	0.82	0.28	77,77,77,77	0
56	MG	13	1703	1/1	0.82	0.20	89,89,89,89	0
56	MG	1H	3249	1/1	0.83	0.26	85,85,85,85	0
56	MG	14	3214	1/1	0.83	0.17	$65,\!65,\!65,\!65$	0
56	MG	1G	1670	1/1	0.83	0.20	77,77,77,77	0
56	MG	16	207	1/1	0.83	0.28	71,71,71,71	0
56	MG	1H	3338	1/1	0.83	0.23	60,60,60,60	0
56	MG	1H	3053	1/1	0.83	0.36	72,72,72,72	0
56	MG	1H	3259	1/1	0.83	0.20	81,81,81,81	0
56	MG	13	1704	1/1	0.83	0.20	80,80,80,80	0
56	MG	1H	3172	1/1	0.83	0.40	84,84,84,84	0
56	MG	1H	3129	1/1	0.83	0.20	68,68,68,68	0
56	MG	1G	1642	1/1	0.83	0.34	81,81,81,81	0
56	MG	14	3161	1/1	0.83	0.24	86,86,86,86	0
56	MG	1H	3138	1/1	0.83	0.35	66,66,66,66	0
56	MG	1H	3168	1/1	0.83	0.44	79,79,79,79	0
56	MG	1H	3202	1/1	0.83	0.17	66,66,66,66	0
56	MG	14	3121	1/1	0.83	0.17	58,58,58,58	0
56	MG	1G	1652	1/1	0.83	0.30	74,74,74,74	0
56	MG	1G	1656	1/1	0.83	0.28	72,72,72,72	0
56	MG	14	3189	1/1	0.83	0.16	60,60,60,60	0
56	MG	1H	3331	1/1	0.83	0.23	76,76,76,76	0
56	MG	1H	3359	1/1	0.84	0.53	84,84,84,84	0
56	MG	1G	1654	1/1	0.84	0.42	101,101,101,101	0
56	MG	1H	3209	1/1	0.84	0.31	77,77,77,77	0
56	MG	14	3104	1/1	0.84	0.28	84,84,84,84	0
56	MG	1G	1659	1/1	0.84	0.20	93,93,93,93	0
56	MG	14	3159	1/1	0.84	0.22	73,73,73,73	0
56	MG	1G	1664	1/1	0.84	0.42	102,102,102,102	0
56	MG	1H	3334	1/1	0.84	0.23	60,60,60,60	0
56	MG	1H	3197	1/1	0.84	0.29	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(A ²)	Q<0.9
56	MG	IH	3271	1/1	0.84	0.30	65,65,65,65	0
56	MG	1G	1636	1/1	0.84	0.16	84,84,84,84	0
56	MG	14	3173	1/1	0.84	0.16	62,62,62,62	0
56	MG	1H	3057	1/1	0.84	0.36	57,57,57,57	0
56	MG	1H	3221	1/1	0.84	0.24	80,80,80,80	0
56	MG	1H	3125	1/1	0.84	0.20	49,49,49,49	0
56	MG	16	205	1/1	0.84	0.30	77,77,77,77	0
56	MG	14	3195	1/1	0.84	0.25	$65,\!65,\!65,\!65$	0
56	MG	14	3142	1/1	0.84	0.21	59,59,59,59	0
56	MG	1H	3280	1/1	0.84	0.20	59,59,59,59	0
56	MG	1H	3312	1/1	0.85	0.47	78,78,78,78	0
56	MG	14	3220	1/1	0.85	0.22	82,82,82,82	0
56	MG	14	3223	1/1	0.85	0.24	$62,\!62,\!62,\!62$	0
56	MG	1H	3177	1/1	0.85	0.30	$55,\!55,\!55,\!55$	0
56	MG	14	3069	1/1	0.85	0.27	78,78,78,78	0
56	MG	1H	3117	1/1	0.85	0.31	80,80,80,80	0
56	MG	14	3136	1/1	0.85	0.28	73,73,73,73	0
56	MG	1H	3316	1/1	0.85	0.15	74,74,74,74	0
56	MG	13	1728	1/1	0.85	0.11	85,85,85,85	0
56	MG	1H	3435	1/1	0.85	0.05	90,90,90,90	0
56	MG	1H	3128	1/1	0.85	0.28	57,57,57,57	0
56	MG	14	3145	1/1	0.85	0.16	81,81,81,81	0
56	MG	14	3268	1/1	0.85	0.19	57,57,57,57	0
56	MG	14	3115	1/1	0.85	0.36	88,88,88,88	0
56	MG	1H	3077	1/1	0.85	0.23	73,73,73,73	0
56	MG	1H	3153	1/1	0.85	0.33	64,64,64,64	0
56	MG	1G	1609	1/1	0.85	0.35	81,81,81,81	0
56	MG	14	3154	1/1	0.85	0.12	82,82,82,82	0
56	MG	2L	103	1/1	0.85	0.23	89,89,89,89	0
56	MG	14	3285	1/1	0.85	0.40	74,74,74,74	0
56	MG	13	1716	1/1	0.86	0.14	92,92,92,92	0
56	MG	1H	3199	1/1	0.86	0.31	57,57,57,57	0
56	MG	1H	3438	1/1	0.86	0.12	54,54,54,54	0
56	MG	1H	3156	1/1	0.86	0.11	54,54,54,54	0
56	MG	13	1628	1/1	0.86	0.13	48,48,48,48	0
56	MG	1H	3276	1/1	0.86	0.34	55,55,55,55	0
56	MG	14	3042	1/1	0.86	0.16	72,72,72,72	0
56	MG	1G	1643	1/1	0.86	0.37	88,88,88,88	0
56	MG	14	3292	1/1	0.86	0.24	82,82,82,82	0
56	MG	13	1643	1/1	0.86	0.35	80,80,80.80	0
56	MG	13	1730	1/1	0.86	0.11	86,86,86,86	0
56	MG	13	1733	1/1	0.86	0.06	73,73,73,73	0



$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$		nuea fro		is page.		DCCC	DCD	D f_{2} (λ^{2})	0 (0 0
56MG131644 $1/1$ 0.860.3476,76,76,76,76056MG1317111/10.860.2179,79,79056MG1431101/10.860.1964,64,64056MG1432581/10.860.1473,73,73,73056MG1316861/10.860.1869,69,69,69056MG1433721/10.860.0758,58,58,58056MG162081/10.860.3366,66,66,66056MG1433891/10.860.3276,76,76,76056MG1433891/10.860.2462,62,62,62056MG1G16681/10.860.2269,69,69,9056MG1G16681/10.860.2269,69,69,9056MG1431291/10.860.2463,63,63,63056MG1431201/10.870.2449,49,49,49056MG1432761/10.870.3867,67,67,6056MG1432761/10.870.2556,56,56,56056MG1432761/10.870.2973,73,73056MG1432761/10.87 <t< th=""><th>Mol</th><th>Type</th><th>Chain</th><th>Res</th><th>Atoms</th><th>RSCC</th><th>RSR</th><th>$\frac{\text{B-factors}(A^2)}{76.76.76}$</th><th>Q<0.9</th></t<>	Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\frac{\text{B-factors}(A^2)}{76.76.76}$	Q<0.9
56 MG 13 1711 $1/1$ 0.86 0.21 79,79,79,79,79 0 56 MG 14 3110 $1/1$ 0.86 0.19 64,64,64 0 56 MG 14 3258 $1/1$ 0.86 0.14 73,73,73 0 56 MG 13 1686 $1/1$ 0.86 0.18 69,69,69,69 0 56 MG 14 3372 $1/1$ 0.86 0.07 58,58,58,58 0 56 MG 16 208 $1/1$ 0.86 0.33 66,66,66 0 56 MG 1H 3263 $1/1$ 0.86 0.32 76,76,76,76 0 56 MG 1H 3194 $1/1$ 0.86 0.24 62,62,62,62 0 56 MG 1G 1668 $1/1$ 0.86 0.26 71,71,71 0 56 MG 14 3129 $1/1$ <	56	MG	13	1644	1/1	0.86	0.34	76,76,76,76	0
56 MG 14 3110 1/1 0.86 0.19 64,64,64,64 0 56 MG 13 1686 1/1 0.86 0.14 73,73,73,73 0 56 MG 13 1686 1/1 0.86 0.18 69,69,69,69 0 56 MG 31 201 1/1 0.86 0.07 58,58,58,58 0 56 MG 14 3372 1/1 0.86 0.22 84,84,84,84 0 56 MG 1H 3263 1/1 0.86 0.32 76,76,76,76 0 56 MG 1H 3194 1/1 0.86 0.24 62,62,62,62 0 56 MG 1G 1668 1/1 0.86 0.26 82,82,82,82 0 56 MG 14 3129 1/1 0.86 0.26 71,71,71,71 0 56 MG 14 3129 1/1	56	MG	13	1711	1/1	0.86	0.21	79,79,79,79	0
56 MG 14 3258 1/1 0.86 0.14 73,73,73,73 0 56 MG 13 1686 1/1 0.86 0.18 69,69,69,69 0 56 MG 31 201 1/1 0.86 0.07 58,58,58,58 0 56 MG 14 3372 1/1 0.86 0.03 66,66,66 0 56 MG 14 3389 1/1 0.86 0.32 76,76,76,76 0 56 MG 1H 3194 1/1 0.86 0.24 62,62,62,62 0 56 MG 1G 1668 1/1 0.86 0.26 82,82,82,82 0 56 MG 14 3129 1/1 0.86 0.26 71,71,71,71 0 56 MG 1H 3122 1/1 0.86 0.36 62,62,62,62 0 56 MG 1H 3229 1/1 <	56	MG	14	3110	1/1	0.86	0.19	64,64,64,64	0
56 MG 13 1686 1/1 0.86 0.18 69,69,69,69 0 56 MG 31 201 1/1 0.86 0.07 58,58,58,58 0 56 MG 14 3372 1/1 0.86 0.22 84,84,84,84 0 56 MG 16 208 1/1 0.86 0.33 66,66,66,66 0 56 MG 1H 3263 1/1 0.86 0.32 76,76,76,76 0 56 MG 1H 3194 1/1 0.86 0.24 62,62,62,62 0 56 MG 1G 1668 1/1 0.86 0.26 82,82,82,82,82 0 56 MG 14 3129 1/1 0.86 0.26 71,71,71,71 0 56 MG 1H 3269 1/1 0.86 0.36 62,62,62,62 0 56 MG 1H 3269 1/1	56	MG	14	3258	1/1	0.86	0.14	73,73,73,73	0
56 MG 31 201 $1/1$ 0.86 0.07 58,58,58,58 0 56 MG 14 3372 $1/1$ 0.86 0.22 84,84,84,84 0 56 MG 16 208 $1/1$ 0.86 0.33 66,66,66,66 0 56 MG 1H 3263 $1/1$ 0.86 0.32 76,76,76,76 0 56 MG 1H 3194 $1/1$ 0.86 0.24 62,62,62,62 0 56 MG 1G 1668 $1/1$ 0.86 0.24 62,62,62,62 0 56 MG 14 3129 $1/1$ 0.86 0.22 69,69,69,69 0 56 MG 14 3129 $1/1$ 0.86 0.24 63,63,63,63 0 56 MG 1H 3269 $1/1$ 0.87 0.24 49,49,49,49 0 56 MG 1H 3274 <t< td=""><td>56</td><td>MG</td><td>13</td><td>1686</td><td>1/1</td><td>0.86</td><td>0.18</td><td>69,69,69,69</td><td>0</td></t<>	56	MG	13	1686	1/1	0.86	0.18	69,69,69,69	0
56MG14 3372 $1/1$ 0.86 0.22 $84,84,84,84$ 0 56 MG16 208 $1/1$ 0.86 0.33 $66,66,66,66$ 0 56 MG1H 3263 $1/1$ 0.86 0.32 $76,76,76,76$ 0 56 MG14 3389 $1/1$ 0.86 0.18 $97,97,97,97,97$ 0 56 MG1H 3194 $1/1$ 0.86 0.24 $62,62,62,62,62$ 0 56 MG1G 1668 $1/1$ 0.86 0.24 $62,62,62,62,62$ 0 56 MG14 3129 $1/1$ 0.86 0.22 $69,69,69,69,69$ 0 56 MG14 3129 $1/1$ 0.86 0.24 $63,63,63,63$ 0 56 MG1H 3129 $1/1$ 0.86 0.24 $63,63,63,63$ 0 56 MG1H 3129 $1/1$ 0.86 0.26 $62,62,62$ 0 56 MG1H 3269 $1/1$ 0.87 0.26 $82,82,82,82$ 0 56 MG1H 3274 $1/1$ 0.87 0.38 $77,77,77,77,77,77,77,77,77,77,77,77,77,$	56	MG	3I	201	1/1	0.86	0.07	58,58,58,58	0
56MG16 208 $1/1$ 0.86 0.33 $66,66,66,66$ 0 56 MG1H 3263 $1/1$ 0.86 0.32 $76,76,76,76$ 0 56 MG14 3389 $1/1$ 0.86 0.18 $97,97,97,97$ 0 56 MG1H 3194 $1/1$ 0.86 0.24 $62,62,62,62$ 0 56 MG1G 1668 $1/1$ 0.86 0.24 $62,62,62,62$ 0 56 MG14 3129 $1/1$ 0.86 0.22 $69,69,69,69$ 0 56 MG14 3129 $1/1$ 0.86 0.24 $63,63,63,63$ 0 56 MG14 3129 $1/1$ 0.86 0.26 $71,71,71,71$ 0 56 MG1H 3269 $1/1$ 0.86 0.36 $62,62,62,62$ 0 56 MG1H 3122 $1/1$ 0.87 0.24 $49,49,49,49$ 0 56 MG14 3274 $1/1$ 0.87 0.26 $82,82,82,82$ 0 56 MG14 3276 $1/1$ 0.87 0.18 $101,101,101,101$ 0 56 MG1H 3463 $1/1$ 0.87 0.25 $56,56,56,56$ 0 56 MG1H 3464 $1/1$ 0.87 0.29 $73,73,73,73$ 0 56 MG1H 3468 $1/1$ 0.87 0.14 $71,71,71,71$ <	56	MG	14	3372	1/1	0.86	0.22	84,84,84,84	0
56MG1H 3263 $1/1$ 0.86 0.32 $76,76,76,76$ 0 56 MG14 3389 $1/1$ 0.86 0.18 $97,97,97,97$ 0 56 MG1H 3194 $1/1$ 0.86 0.24 $62,62,62,62$ 0 56 MG1G 1668 $1/1$ 0.86 0.24 $62,62,62,62$ 0 56 MG85 201 $1/1$ 0.86 0.22 $69,69,69,69$ 0 56 MG14 3129 $1/1$ 0.86 0.24 $63,63,63,63$ 0 56 MG14 3130 $1/1$ 0.86 0.26 $71,71,71,71$ 0 56 MG1H 3229 $1/1$ 0.86 0.36 $62,62,62,62$ 0 56 MG1H 3122 $1/1$ 0.87 0.24 $49,49,49,49$ 0 56 MG14 3274 $1/1$ 0.87 0.38 $77,77,77,77$ 0 56 MG14 3276 $1/1$ 0.87 0.18 $101,101,101,101$ 0 56 MG1H 3463 $1/1$ 0.87 0.29 $73,73,73,3$ 0 56 MG1H 3464 $1/1$ 0.87 0.14 $71,71,71,71$ 0 56 MG1H 3468 $1/1$ 0.87 0.14 $71,71,71,71$ 0 56 MG1H 3468 $1/1$ 0.87 0.29 $73,73,73,73$ </td <td>56</td> <td>MG</td> <td>16</td> <td>208</td> <td>1/1</td> <td>0.86</td> <td>0.33</td> <td>66,66,66,66</td> <td>0</td>	56	MG	16	208	1/1	0.86	0.33	66,66,66,66	0
56MG14 3389 $1/1$ 0.86 0.18 $97,97,97,97$ 0 56 MG1H 3194 $1/1$ 0.86 0.24 $62,62,62,62$ 0 56 MG1G 1668 $1/1$ 0.86 0.26 $82,82,82,82,82$ 0 56 MG85 201 $1/1$ 0.86 0.22 $69,69,69,69$ 0 56 MG14 3129 $1/1$ 0.86 0.22 $69,69,69,69,69$ 0 56 MG14 3129 $1/1$ 0.86 0.24 $63,63,63,63$ 0 56 MG1H 3269 $1/1$ 0.86 0.26 $71,71,71,71$ 0 56 MG1H 3122 $1/1$ 0.87 0.24 $49,49,49,49$ 0 56 MG14 3274 $1/1$ 0.87 0.26 $82,82,82,82$ 0 56 MG14 3274 $1/1$ 0.87 0.38 $77,77,77,77,77$ 0 56 MG14 3276 $1/1$ 0.87 0.18 $101,101,101,101$ 0 56 MG1H 3463 $1/1$ 0.87 0.29 $73,73,73,73$ 0 56 MG1H 3464 $1/1$ 0.87 0.14 $71,71,71,71$ 0 56 MG1H 3468 $1/1$ 0.87 0.14 $71,71,71,71$ 0 56 MG1H 3468 $1/1$ 0.87 0.14 $71,7$	56	MG	1H	3263	1/1	0.86	0.32	76, 76, 76, 76	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3389	1/1	0.86	0.18	$97,\!97,\!97,\!97$	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3194	1/1	0.86	0.24	62,62,62,62	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1G	1668	1/1	0.86	0.26	82,82,82,82	0
56MG14 3129 $1/1$ 0.86 0.24 $63,63,63,63$ 0 56 MG14 3130 $1/1$ 0.86 0.26 $71,71,71,71,71$ 0 56 MG1H 3269 $1/1$ 0.86 0.36 $62,62,62,62$ 0 56 MG1H 3122 $1/1$ 0.87 0.24 $49,49,49,49$ 0 56 MG14 3274 $1/1$ 0.87 0.26 $82,82,82,82$ 0 56 MG13 1633 $1/1$ 0.87 0.38 $77,77,77,77,77,77,77,77,77,77,77,77,77,$	56	MG	85	201	1/1	0.86	0.22	69,69,69,69	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3129	1/1	0.86	0.24	63,63,63,63	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3130	1/1	0.86	0.26	71,71,71,71	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3269	1/1	0.86	0.36	62,62,62,62	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3122	1/1	0.87	0.24	49,49,49,49	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3274	1/1	0.87	0.26	82,82,82,82	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	13	1633	1/1	0.87	0.38	77,77,77,77	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3276	1/1	0.87	0.15	76,76,76,76	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3463	1/1	0.87	0.18	101,101,101,101	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3116	1/1	0.87	0.25	56,56,56,56	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3464	1/1	0.87	0.08	92,92,92,92	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3029	1/1	0.87	0.29	73,73,73,73	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3468	1/1	0.87	0.14	71,71,71,71	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3475	1/1	0.87	0.10	79,79,79,79	0
56 MG 16 202 1/1 0.87 0.38 59,59,59,59 0 56 MG 1H 3078 1/1 0.87 0.14 63,63,63,63 0 56 MG 14 3207 1/1 0.87 0.59 81,81,81,81 0 56 MG 14 3208 1/1 0.87 0.15 68,68,68,68 0 56 MG 14 3208 1/1 0.87 0.15 68,68,68,68 0 56 MG 1H 3173 1/1 0.87 0.32 52,52,52,52 0	56	MG	13	1668	1/1	0.87	0.22	76,76,76,76	0
56 MG 1H 3078 1/1 0.87 0.14 63,63,63,63 0 56 MG 14 3207 1/1 0.87 0.59 81,81,81,81 0 56 MG 14 3208 1/1 0.87 0.15 68,68,68,68 0 56 MG 1H 3173 1/1 0.87 0.32 52,52,52,52 0	56	MG	16	202	1/1	0.87	0.38	59, 59, 59, 59	0
56 MG 14 3207 1/1 0.87 0.59 81,81,81,81 0 56 MG 14 3208 1/1 0.87 0.15 68,68,68,68 0 56 MG 1H 3173 1/1 0.87 0.32 52,52,52,52 0	56	MG	1H	3078	1/1	0.87	0.14	63,63,63,63	0
56 MG 14 3208 1/1 0.87 0.15 68,68,68,68 0 56 MG 1H 3173 1/1 0.87 0.32 52,52,52,52 0	56	MG	14	3207	1/1	0.87	0.59	81,81,81,81	0
56 MC 1H 3173 1/1 0.87 0.39 59.59.59.59 0	56	MG	14	3208	1/1	0.87	0.15	68,68,68,68	0
00 100 111 0.07 0.02 $0.02,02,02,02$	56	MG	1H	3173	1/1	0.87	0.32	52,52,52,52	0
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	56	MG	1G	1669	1/1	0.87	0.20	88,88,88,88	0
56 MG 1H 3213 1/1 0.87 0.32 77,77,77,77 0	56	MG	1H	3213	1/1	0.87	0.32	77,77,77,77	0
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	56	MG	1H	3401	1/1	0.87	0.07	64,64,64,64	0
56 MG 1G 1677 1/1 0.87 0.19 104,104,104,104 0	56	MG	1G	1677	1/1	0.87	0.19	104,104,104,104	0
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	56	MG	11	302	1/1	0.87	0.19	42,42,42,42	0
56 MG 14 3345 1/1 0.87 0.15 81,81,81 0	56	MG	14	3345	1/1	0.87	0.15	81,81,81,81	0
56 MG 1H 3096 1/1 0.87 0.23 54,54,54,54 0	56	MG	1H	3096	1/1	0.87	0.23	54,54,54,54	0
56 MG 13 1698 1/1 0.87 0.15 74,74,74,74 0	56	MG	13	1698	1/1	0.87	0.15	74,74,74,74	0
56 MG 13 1684 1/1 0.87 0.30 62.62.62.62 0	56	MG	13	1684	1/1	0.87	0.30	62,62.62.62	0
56 MG 1H 3150 1/1 0.87 0.20 59,59,59,59 0	56	MG	1H	3150	1/1	0.87	0.20	59,59,59,59	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors(A^2)	Q<0.9
56	MG	1H	3301	1/1	0.87	0.28	79,79,79,79	0
56	MG	1H	3272	1/1	0.87	0.31	69,69,69,69	0
56	MG	1H	3152	1/1	0.87	0.21	75,75,75,75	0
56	MG	14	3089	1/1	0.87	0.38	79,79,79,79	0
56	MG	1H	3106	1/1	0.87	0.17	58,58,58,58	0
56	MG	1H	3458	1/1	0.87	0.15	84,84,84,84	0
56	MG	13	1602	1/1	0.87	0.14	66,66,66,66	0
56	MG	14	3271	1/1	0.87	0.14	87,87,87,87	0
56	MG	13	1705	1/1	0.88	0.36	94,94,94,94	0
56	MG	14	3172	1/1	0.88	0.35	$69,\!69,\!69,\!69$	0
56	MG	1H	3255	1/1	0.88	0.26	76, 76, 76, 76	0
56	MG	14	3175	1/1	0.88	0.15	$56,\!56,\!56,\!56$	0
56	MG	1H	3443	1/1	0.88	0.06	$58,\!58,\!58,\!58$	0
56	MG	1H	3444	1/1	0.88	0.13	$59,\!59,\!59,\!59$	0
56	MG	14	3125	1/1	0.88	0.19	$53,\!53,\!53,\!53$	0
56	MG	41	201	1/1	0.88	0.37	82,82,82,82	0
56	MG	1H	3344	1/1	0.88	0.52	87,87,87,87	0
56	MG	1G	1608	1/1	0.88	0.25	88,88,88,88	0
56	MG	1H	3148	1/1	0.88	0.29	82,82,82,82	0
56	MG	1G	1685	1/1	0.88	0.08	111,111,111,111	0
56	MG	1H	3353	1/1	0.88	0.24	73,73,73,73	0
56	MG	1H	3261	1/1	0.88	0.15	61,61,61,61	0
56	MG	13	1653	1/1	0.88	0.09	75,75,75,75	0
56	MG	14	3300	1/1	0.88	0.27	109,109,109,109	0
56	MG	1H	3227	1/1	0.88	0.49	74,74,74,74	0
56	MG	14	3034	1/1	0.88	0.10	86,86,86,86	0
56	MG	13	1641	1/1	0.88	0.16	59,59,59,59	0
56	MG	1H	3384	1/1	0.88	0.07	57,57,57,57	0
56	MG	14	3241	1/1	0.88	0.26	91,91,91,91	0
56	MG	1H	3174	1/1	0.88	0.27	63,63,63,63	0
56	MG	13	1717	1/1	0.88	0.23	74,74,74,74	0
56	MG	14	3367	1/1	0.88	0.13	70,70,70,70	0
56	MG	13	1660	1/1	0.88	0.13	91,91,91,91	0
56	MG	14	3256	1/1	0.88	0.30	66,66,66,66	0
56	MG	1H	3110	1/1	0.88	0.37	57,57,57,57	0
56	MG	14	3095	1/1	0.88	0.20	56,56,56,56	0
56	MG	14	3381	1/1	0.88	0.09	62,62,62,62	0
56	MG	14	3155	1/1	0.88	0.24	75,75,75,75	0
56	MG	1J	203	1/1	0.88	0.29	81,81,81,81	0
56	MG	16	201	1/1	0.88	0.24	78,78.78.78	0
56	MG	14	3102	1/1	0.88	0.15	49,49,49,49	0
56	MG	1H	3186	1/1	0.88	0.20	83,83.83.83	0
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(A ²)	Q<0.9
56	MG	IH	3189	1/1	0.88	0.34	63,63,63,63	0
56	MG	16	204	1/1	0.88	0.19	86,86,86,86	0
56	MG	1H	3042	1/1	0.88	0.30	74,74,74,74	0
56	MG	14	3059	1/1	0.89	0.23	52,52,52,52	0
56	MG	1H	3113	1/1	0.89	0.13	41,41,41,41	0
56	MG	1G	1610	1/1	0.89	0.37	77,77,77,77	0
56	MG	13	1666	1/1	0.89	0.12	58,58,58,58	0
56	MG	1H	3234	1/1	0.89	0.22	75,75,75,75	0
56	MG	1H	3192	1/1	0.89	0.19	72,72,72,72	0
56	MG	1G	1633	1/1	0.89	0.25	76,76,76,76	0
56	MG	1H	3446	1/1	0.89	0.15	78,78,78,78	0
56	MG	1H	3336	1/1	0.89	0.26	$79,\!79,\!79,\!79$	0
56	MG	1H	3154	1/1	0.89	0.34	74,74,74,74	0
56	MG	1H	3454	1/1	0.89	0.12	$98,\!98,\!98,\!98$	0
56	MG	14	3177	1/1	0.89	0.19	$72,\!72,\!72,\!72$	0
56	MG	13	1631	1/1	0.89	0.28	$73,\!73,\!73,\!73$	0
56	MG	1H	3159	1/1	0.89	0.12	$71,\!71,\!71,\!71$	0
56	MG	1H	3161	1/1	0.89	0.26	$55,\!55,\!55,\!55$	0
56	MG	13	1609	1/1	0.89	0.35	86,86,86,86	0
56	MG	14	3119	1/1	0.89	0.22	69,69,69,69	0
56	MG	1H	3165	1/1	0.89	0.23	61,61,61,61	0
56	MG	1H	3167	1/1	0.89	0.15	67,67,67,67	0
56	MG	1H	3257	1/1	0.89	0.42	85,85,85,85	0
56	MG	13	1719	1/1	0.89	0.24	89,89,89,89	0
56	MG	1H	3470	1/1	0.89	0.12	106,106,106,106	0
56	MG	14	3306	1/1	0.89	0.15	69,69,69,69	0
56	MG	1H	3364	1/1	0.89	0.09	$68,\!68,\!68,\!68$	0
56	MG	14	3341	1/1	0.89	0.11	48,48,48,48	0
56	MG	1H	3091	1/1	0.89	0.21	55,55,55,55	0
56	MG	1H	3210	1/1	0.89	0.43	77,77,77,77	0
56	MG	1H	3372	1/1	0.89	0.08	37,37,37,37	0
56	MG	1H	3137	1/1	0.89	0.20	49,49,49,49	0
56	MG	13	1747	1/1	0.89	0.21	64,64,64,64	0
56	MG	14	3243	1/1	0.89	0.22	72,72,72,72	0
56	MG	14	3138	1/1	0.89	0.33	79,79,79,79	0
56	MG	1H	3054	1/1	0.89	0.33	59,59,59,59	0
56	MG	14	3379	1/1	0.89	0.12	72,72,72,72	0
56	MG	1H	3394	1/1	0.89	0.10	57,57,57,57	0
56	MG	14	3388	1/1	0.89	0.06	88,88,88,88	0
56	MG	13	1693	1/1	0.89	0.15	65,65.65.65	0
56	MG	1J	202	1/1	0.89	0.34	73,73.73.73	0
56	MG	1H	3406	1/1	0.89	0.10	45,45,45,45	0
56	MG	1H	3406	1/1	0.89	0.10	45,45,45,45	0

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Mol Type Chain Res Atoms RSCC RSR B-factors(A ²) Q<)))))))))
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$)))))))
56 MG 1H 3058 1/1 0.89 0.17 61,61,61,61 0 56 MG 14 3263 1/1 0.89 0.32 71,71,71,71 0 56 MG 1H 3109 1/1 0.89 0.15 60,60,60,60 0 56 MG 1H 3224 1/1 0.89 0.22 61,61,61,61 0 56 MG 13 1642 1/1 0.89 0.29 72,72,72,72 72))))))
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$)))))
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$)))))
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$))))
1 56 MC 1 31 1649 171 1080 1090 179797979 100)))
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56 MG 13 1700 1/1 0.90 0.26 71,71,71,71)
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	-
56 MG 13 1651 1/1 0.90 0.20 87,87,87,87 0)
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$)
56 MG 14 3088 1/1 0.90 0.43 71,71,71,71)
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$)
56 MG 1G 1628 1/1 0.90 0.22 77,77,77,77)
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$)
56 MG 14 3278 1/1 0.90 0.19 98,98,98,98 0)
56 MG 13 1689 1/1 0.90 0.38 120,120,120,120 0)
56 MG 2K 105 1/1 0.90 0.35 78,78,78,78 0)
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$)
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$)
56 MG 1H 3081 1/1 0.90 0.22 61,61,61,61 0)
$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$)
$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$)
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$)
56 MG 13 1634 1/1 0.90 0.25 74,74,74,74)
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$)
56 MG 14 3291 1/1 0.90 0.26 55,55,55,55 0)
56 MG 1H 3033 1/1 0.90 0.15 67,67,67,67 0.13 0.15)
56 MG 14 3192 1/1 0.90 0.35 80,80,80,80 0.35)
56 MG 1H 3379 1/1 0.90 0.10 46,46,46,46)
56 MG 14 3299 1/1 0.90 0.32 70,70,70,70)
56 MG 1H 3147 1/1 0.90 0.47 68,68,68,68 0)
56 MG 1G 1662 1/1 0.90 0.19 73,73,73,73)
56 MG 1G 1663 1/1 0.90 0.20 75,75,75,75)
56 MG 14 3210 1/1 0.90 0.26 71,71,71,71)
56 MG 14 3213 1/1 0.90 0.27 85,85,85,85)
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$)
56 MG 13 1665 1/1 0.90 0.24 67,67,67,67)
56 MG 14 3339 1/1 0.90 0.17 94,94,94,94)
56 MG 1H 3050 1/1 0.90 0.28 36,36,36,36)
56 MG 13 1694 1/1 0.90 0.20 82,82,82)
56 MG 1H 3325 1/1 0.90 0.39 96.96.96.96 0)
56 MG 13 1740 1/1 0.90 0.12 88,88,88,88)



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(A ²)	Q<0.9
56	MG	13	1648	1/1	0.90	0.19	69,69,69,69	0
56	MG	1G	1671	1/1	0.90	0.09	73,73,73,73	0
56	MG	14	3228	1/1	0.90	0.46	98,98,98,98	0
56	MG	14	3233	1/1	0.90	0.11	61,61,61,61	0
56	MG	16	206	1/1	0.90	0.40	60,60,60,60	0
56	MG	13	1659	1/1	0.90	0.21	66,66,66,66	0
56	MG	14	3247	1/1	0.90	0.11	$67,\!67,\!67,\!67$	0
56	MG	14	3387	1/1	0.90	0.09	$97,\!97,\!97,\!97$	0
56	MG	1H	3158	1/1	0.90	0.15	70,70,70,70	0
56	MG	1H	3425	1/1	0.90	0.07	67,67,67,67	0
56	MG	1H	3426	1/1	0.90	0.13	59, 59, 59, 59	0
56	MG	1H	3118	1/1	0.90	0.26	52,52,52,52	0
56	MG	1J	205	1/1	0.90	0.10	82,82,82,82	0
56	MG	L8	101	1/1	0.90	0.24	70,70,70,70	0
56	MG	14	3259	1/1	0.90	0.23	82,82,82,82	0
56	MG	14	3018	1/1	0.90	0.13	68,68,68,68	0
56	MG	1H	3285	1/1	0.90	0.21	61,61,61,61	0
56	MG	13	1646	1/1	0.90	0.18	95,95,95,95	0
56	MG	1H	3241	1/1	0.90	0.26	65,65,65,65	0
56	MG	1H	3034	1/1	0.91	0.12	51,51,51,51	0
56	MG	1H	3333	1/1	0.91	0.46	93,93,93,93	0
56	MG	14	3296	1/1	0.91	0.15	74,74,74,74	0
56	MG	1H	3140	1/1	0.91	0.45	63,63,63,63	0
56	MG	1H	3450	1/1	0.91	0.05	67,67,67,67	0
56	MG	1H	3335	1/1	0.91	0.26	87,87,87,87	0
56	MG	1H	3284	1/1	0.91	0.18	62,62,62,62	0
56	MG	1H	3045	1/1	0.91	0.35	66,66,66,66	0
56	MG	1H	3226	1/1	0.91	0.27	69,69,69,69	0
56	MG	1H	3151	1/1	0.91	0.20	66,66,66,66	0
56	MG	14	3184	1/1	0.91	0.15	53,53,53,53	0
56	MG	14	3185	1/1	0.91	0.11	52,52,52,52	0
56	MG	1H	3246	1/1	0.91	0.26	79,79,79,79	0
56	MG	14	3340	1/1	0.91	0.10	59,59,59,59	0
56	MG	1H	3215	1/1	0.91	0.22	85,85,85,85	0
56	MG	1H	3231	1/1	0.91	0.14	31,31,31,31	0
56	MG	14	3140	1/1	0.91	0.31	92,92,92,92	0
56	MG	14	3348	1/1	0.91	0.09	54,54,54,54	0
56	MG	14	3350	1/1	0.91	0.11	83,83.83.83	0
56	MG	14	3353	1/1	0.91	0.23	83,83.83.83	0
56	MG	14	3359	1/1	0.91	0.09	87.87.87.87	0
56	MG	14	3269	1/1	0.91	0.19	59.59.59.59	0
56	MG	14	3270	1/1	0.91	0.11	56.56.56.56	0
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INIOI	Type		Res	Atoms	RSCC	RSR	$\mathbf{B}\text{-factors}(\mathbf{A}^{-})$	Q<0.9
56	MG	14	3196		0.91	0.20	90,90,90,90	0
50	MG		3340		0.91	0.21		0
50	MG	14	3375		0.91	0.06	91,91,91,91	0
56	MG	14	3273		0.91	0.09		0
56	MG		3092		0.91	0.11	50,50,50,50	0
56	MG	IH	3424		0.91	0.14	58,58,58,58	0
56	MG	IH	3254	1/1	0.91	0.19	77,77,77,77	0
56	MG	IH	3469	1/1	0.91	0.10	90,90,90,90	0
56	MG	1H	3356	1/1	0.91	0.14	79,79,79,79	0
56	MG	1G	1625	1/1	0.91	0.38	84,84,84,84	0
56	MG	14	3113	1/1	0.91	0.13	42,42,42,42	0
56	MG	1G	1626	1/1	0.91	0.27	79,79,79,79	0
56	MG	1G	1680	1/1	0.91	0.27	94,94,94,94	0
56	MG	1H	3145	1/1	0.91	0.25	49,49,49,49	0
56	MG	14	3160	1/1	0.91	0.12	73,73,73,73	0
56	MG	1H	3103	1/1	0.91	0.16	30,30,30,30	0
56	MG	1H	3478	1/1	0.91	0.10	102,102,102,102	0
56	MG	14	3238	1/1	0.91	0.23	85,85,85,85	0
56	MG	1H	3308	1/1	0.91	0.22	$65,\!65,\!65,\!65$	0
56	MG	13	1736	1/1	0.92	0.07	73,73,73,73	0
56	MG	14	3257	1/1	0.92	0.18	79,79,79,79	0
56	MG	1H	3270	1/1	0.92	0.30	94,94,94,94	0
56	MG	13	1699	1/1	0.92	0.20	75,75,75,75	0
56	MG	1H	3016	1/1	0.92	0.22	45,45,45,45	0
56	MG	1G	1644	1/1	0.92	0.18	70,70,70,70	0
56	MG	1H	3028	1/1	0.92	0.27	67,67,67,67	0
56	MG	1H	3105	1/1	0.92	0.15	56, 56, 56, 56	0
56	MG	1H	3180	1/1	0.92	0.18	59, 59, 59, 59, 59	0
56	MG	1H	3183	1/1	0.92	0.38	66,66,66,66	0
56	MG	1H	3278	1/1	0.92	0.25	76,76,76,76	0
56	MG	1H	3279	1/1	0.92	0.16	73,73,73,73	0
56	MG	1H	3337	1/1	0.92	0.18	94,94,94,94	0
56	MG	1H	3066	1/1	0.92	0.17	67,67,67,67	0
56	MG	13	1677	1/1	0.92	0.17	71,71,71,71	0
56	MG	1H	3188	1/1	0.92	0.15	60,60,60,60	0
56	MG	13	1742	1/1	0.92	0.10	115,115,115,115	0
56	MG	1G	1666	1/1	0.92	0.16	74,74,74,74	0
56	MG	1H	3465	1/1	0.92	0.10	94,94,94,94	0
56	MG	1H	3236	1/1	0.92	0.18	68,68,68,68	0
56	MG	1H	3237	1/1	0.92	0.15	57,57,57,57	0
56	MG	1H	3289	1/1	0.92	0.32	62,62,62,62	0
56	MG	14	3156	1/1	0.92	0.18	60,60,60,60	0
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MoiTypeChainResAtomsRSCCRSRB-factors(A^{-}) $Q<0.9$ 56MG1H33471/10.920.56 $85,85,85,85$ 056MG1H31121/10.920.11 $64,64,64,64$ 056MG1H31121/10.920.24 $66,66,66,66$ 056MG1H30701/10.920.16 $46,46,46,46$ 056MG1G16831/10.920.10104,104,104,104056MG1H33541/10.920.29 $89,89,89,89,89$ 056MG1H31681/10.920.2972,72,72,72056MG1H31981/10.920.43 $82,82,82,82$ 056MG1H31551/10.920.1574,74,74,74056MG1316721/10.920.1774,04,04,04056MG1316721/10.920.1740,40,40,40056MG1430231/10.920.27 $86,86,86,86$ 056MG1430291/10.920.1976,76,76,76056MG1H33041/10.920.1976,76,76,76056MG1430071/10.920.17 $86,86,86,86$ 056MG <td< th=""></td<>
56MG1H 3347 $1/1$ 0.92 0.56 $85,85,85,85$ 0 56MG1H 3474 $1/1$ 0.92 0.11 $64,64,64,64$ 0 56MG1H 3112 $1/1$ 0.92 0.24 $66,66,66,66$ 0 56MG1H 3070 $1/1$ 0.92 0.16 $46,46,46,46$ 0 56MG1G 1683 $1/1$ 0.92 0.10 $104,104,104,104$ 0 56MG1H 3354 $1/1$ 0.92 0.29 $89,89,89,89$ 0 56MG1H 3354 $1/1$ 0.92 0.29 $89,89,89,89$ 0 56MG1H 3168 $1/1$ 0.92 0.29 $72,72,72,72$ 0 56MG1H 3198 $1/1$ 0.92 0.29 $72,72,72,72$ 0 56MG1H 3198 $1/1$ 0.92 0.15 $74,74,74,74$ 0 56MG1H 3155 $1/1$ 0.92 0.15 $74,74,74,74$ 0 56MG13 1672 $1/1$ 0.92 0.17 $40,40,40,40$ 0 56MG14 3023 $1/1$ 0.92 0.27 $86,86,86,86$ 0 56MG14 302 $1/1$ 0.92 0.17 $40,40,40,40$ 0 56MG1H 3304 $1/1$ 0.92 0.12 $80,80,80,80$ 0 5
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56 MG 14 3051 1/1 0.92 0.14 78.78.78.78 0
56 MG 14 3054 1/1 0.92 0.35 74,74,74,74 0
56 MG 16 210 1/1 0.92 0.28 89,89,89,89 0
56 MG 14 3067 1/1 0.92 0.18 48,48,48,48 0
56 MG 16 212 1/1 0.92 0.14 73,73,73,73 0
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56 MG 14 3205 1/1 0.92 0.25 71,71,71,71 0
56 MG 1H 3204 1/1 0.92 0.25 59,59,59,59 0
56 MG 1H 3310 1/1 0.92 0.28 69,69,69,69 0
56 MG 1H 3083 1/1 0.92 0.12 69,69,69,69 0
56 MG 78 201 1/1 0.92 0.18 59,59,59,59 0
56 MG 88 201 1/1 0.92 0.20 78,78,78,78 0
56 MG 1H 3085 1/1 0.92 0.21 66,66,66,66 0
56 MG 1H 3134 1/1 0.92 0.12 61,61,61,61 0
56 MG 1H 3135 1/1 0.92 0.23 54,54,54,54 0
56 MG 14 3373 1/1 0.92 0.11 69,69,69,69 0
56 MG 1H 3088 1/1 0.92 0.33 73,73,73 0
56 MG 1H 3317 1/1 0.92 0.18 61,61,61,61 0
56 MG 14 3224 1/1 0.92 0.48 48,48,48,48 0
56 MG 1H 3318 1/1 0.92 0.15 56.56.56.56 0
56 MG 1H 3089 1/1 0.92 0.26 45,45,45,45 0



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56 MG 1H 3265 1/1 0.92 0.84 54.54.54.54 0
56 MG 14 3246 1/1 0.92 0.12 66,66,66,66 0
56 MG 1G 1629 1/1 0.92 0.24 79,79,79,79 0
56 MG 1H 3437 1/1 0.92 0.11 59,59,59,59 0
56 MG 1G 1634 1/1 0.92 0.33 76,76,76,76 0
56 MG L5 101 1/1 0.92 0.21 73,73,73,73 0
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56 MG 13 1613 1/1 0.93 0.27 71,71,71,71 0
56 MG 14 3281 1/1 0.93 0.22 73,73,73,73 0
56 MG 1G 1657 1/1 0.93 0.17 126,126,126,126 0
56 MG 1H 3429 1/1 0.93 0.08 40,40,40,40 0
56 MG 1H 3247 1/1 0.93 0.24 64,64,64,64 0
56 MG 14 3186 1/1 0.93 0.28 54,54,54,54 0
56 MG 1H 3434 1/1 0.93 0.08 75,75,75,75 0
56 MG 1H 3216 1/1 0.93 0.24 67,67,67,67 0
56 MG 1H 3348 1/1 0.93 0.53 80,80,80,80 0
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56 MG 13 1691 1/1 0.93 0.12 64,64,64,64 0
56 MG 21 302 1/1 0.93 0.32 66,66,66,66 0
56 MG 14 3197 1/1 0.93 0.28 89,89,89,89 0
56 MG 14 3198 1/1 0.93 0.25 78,78,78,78 0
56 MG 1H 3350 1/1 0.93 0.08 67,67,67,67 0
56 MG 14 3297 1/1 0.93 0.08 74.74.74.74 0
56 MG 14 3201 1/1 0.93 0.25 72.72.72 0
56 MG 1H 3351 1/1 0.93 0.25 70.70.70.70 0
56 MG 14 3120 1/1 0.93 0.28 75.75.75 0
56 MG 1H 3131 1/1 0.93 0.28 67.67.67 0
56 MG 1H 3157 1/1 0.93 0.37 72.72.72.72 0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors(A^2)	Q<0.9
56	MG	1G	1672	1/1	0.93	0.10	78,78,78,78	0
56	MG	13	1721	1/1	0.93	0.14	90,90,90,90	0
56	MG	13	1722	1/1	0.93	0.11	76,76,76,76	0
56	MG	1H	3097	1/1	0.93	0.15	67,67,67,67	0
56	MG	1G	1681	1/1	0.93	0.18	110,110,110,110	0
56	MG	14	3131	1/1	0.93	0.17	70,70,70,70	0
56	MG	1H	3360	1/1	0.93	0.32	$73,\!73,\!73,\!73$	0
56	MG	1H	3361	1/1	0.93	0.21	$53,\!53,\!53,\!53$	0
56	MG	1H	3065	1/1	0.93	0.20	54,54,54,54	0
56	MG	1H	3327	1/1	0.93	0.47	79,79,79,79	0
56	MG	14	3229	1/1	0.93	0.14	$65,\!65,\!65,\!65$	0
56	MG	14	3231	1/1	0.93	0.22	74,74,74,74	0
56	MG	1H	3032	1/1	0.93	0.30	78,78,78,78	0
56	MG	1G	1624	1/1	0.93	0.18	63,63,63,63	0
56	MG	14	3352	1/1	0.93	0.08	84,84,84,84	0
56	MG	14	3011	1/1	0.93	0.18	43,43,43,43	0
56	MG	14	3017	1/1	0.93	0.17	49,49,49,49	0
56	MG	14	3363	1/1	0.93	0.07	74,74,74,74	0
56	MG	14	3141	1/1	0.93	0.11	76,76,76,76	0
56	MG	13	1682	1/1	0.93	0.11	86,86,86,86	0
56	MG	13	1713	1/1	0.93	0.16	70,70,70,70	0
56	MG	1G	1627	1/1	0.93	0.18	57,57,57,57	0
56	MG	14	3147	1/1	0.93	0.18	78,78,78,78	0
56	MG	14	3026	1/1	0.93	0.13	$65,\!65,\!65,\!65$	0
56	MG	14	3251	1/1	0.93	0.15	48,48,48,48	0
56	MG	1H	3037	1/1	0.93	0.21	62,62,62,62	0
56	MG	1H	3039	1/1	0.93	0.19	47,47,47,47	0
56	MG	1G	1631	1/1	0.93	0.21	86,86,86,86	0
56	MG	1H	3388	1/1	0.93	0.14	64,64,64,64	0
56	MG	1H	3390	1/1	0.93	0.10	66,66,66,66	0
56	MG	1H	3041	1/1	0.93	0.28	87,87,87,87	0
56	MG	14	3058	1/1	0.93	0.19	61,61,61,61	0
56	MG	14	3391	1/1	0.93	0.71	58,58,58,58	0
56	MG	13	1671	1/1	0.93	0.11	98,98,98,98	0
56	MG	1H	3307	1/1	0.93	0.21	80,80,80,80	0
56	MG	1K	101	1/1	0.93	0.19	75,75,75,75	0
56	MG	14	3072	1/1	0.93	0.15	45,45,45,45	0
56	MG	1J	206	1/1	0.93	0.13	73,73,73,73	0
56	MG	14	3266	1/1	0.93	0.21	68,68,68,68	0
56	MG	14	3166	1/1	0.93	0.21	70,70,70,70	0
56	MG	35	201	1/1	0.93	0.20	60,60,60,60	0
56	MG	1H	3047	1/1	0.93	0.21	70,70,70,70	0



Mol	Type	Chain	ls page.	 Atoms	BSCC	RSR	B -factors (\mathbf{A}^2)	0<0.9
56	MC	13	1706	1/1	0.03	0.17	70 70 70 70 70	Q<0.5
56	MG	10	3087	1/1	0.95	0.17	62 62 62 62	0
56	MG	1G	1647	1/1	0.93	0.00	$\frac{02,02,02,02}{102\ 102\ 102\ 102}$	0
56	MG	10 1H	3086	1/1	0.93	0.10	66 66 66 66	0
56	MG	1H	3062	1/1	0.94	0.20	65 65 65 65	0
56	MG	13	1681	1/1	0.94	0.30	81 81 81 81	0
56	MG	14	3037	1/1	0.94	0.20	61 61 61 61	0
56	MG	1H	3179	1/1	0.94	0.10	55 55 55 55	0
56	MG	14	3045	1/1	0.94	0.32	57.57.57.57	0
56	MG	1H	3220	1/1	0.94	0.11	50.50.50.50	0
56	MG	13	1709	1/1	0.94	0.22	89 89 89 89	0
56	MG	1H	3181	1/1	0.94	0.14	54 54 54 54	0
56	MG	13	1607	1/1	0.94	0.18	77.77.77.77	0
56	MG	14	3174	1/1	0.94	0.18	66.66.66.66	0
56	MG	1H	3457	1/1	0.94	0.06	92,92,92,92	0
56	MG	1H	3355	1/1	0.94	0.22	60.60.60.60	0
56	MG	1G	1632	1/1	0.94	0.20	70,70,70,70	0
56	MG	1H	3315	1/1	0.94	0.28	66.66.66.66	0
56	MG	1H	3460	1/1	0.94	0.13	55,55,55,55	0
56	MG	1H	3038	1/1	0.94	0.13	55,55,55,55	0
56	MG	1H	3069	1/1	0.94	0.09	44,44,44,44	0
56	MG	1H	3187	1/1	0.94	0.30	56,56,56,56	0
56	MG	13	1611	1/1	0.94	0.30	70,70,70,70	0
56	MG	1H	3229	1/1	0.94	0.33	95,95,95,95	0
56	MG	13	1729	1/1	0.94	0.06	97,97,97,97	0
56	MG	1H	3190	1/1	0.94	0.14	67,67,67,67	0
56	MG	2K	101	1/1	0.94	0.34	79,79,79,79	0
56	MG	1H	3373	1/1	0.94	0.15	45,45,45,45	0
56	MG	1H	3471	1/1	0.94	0.09	68,68,68,68	0
56	MG	1H	3377	1/1	0.94	0.07	44,44,44,44	0
56	MG	14	3106	1/1	0.94	0.13	50,50,50,50	0
56	MG	14	3107	1/1	0.94	0.24	40,40,40,40	0
56	MG	1H	3324	1/1	0.94	0.26	87,87,87,87	0
56	MG	1H	3043	1/1	0.94	0.45	84,84,84,84	0
56	MG	1G	1658	1/1	0.94	0.17	79,79,79,79	0
56	MG	14	3304	1/1	0.94	0.10	$68,\!68,\!68,\!68$	0
56	MG	14	3209	1/1	0.94	0.16	74,74,74,74	0
56	MG	13	1612	1/1	0.94	0.16	63,63,63,63	0
56	MG	13	1714	1/1	0.94	0.34	99,99,99,99	0
56	MG	14	3308	1/1	0.94	0.12	46,46,46,46	0
56	MG	14	3310	1/1	0.94	0.09	$50,\!50,\!50,\!50$	0
56	MG	1H	3283	1/1	0.94	0.31	74,74,74,74	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(A ²)	Q<0.9
56	MG	14	3315		0.94	0.13	68,68,68,68	0
56	MG	14	3322		0.94	0.10		0
50	MG	14	3215		0.94	0.12	50,50,50,50	0
56	MG	14	3327		0.94	0.10	58,58,58,58	0
56	MG	IH	3329		0.94	0.39		0
56	MG	14	3338	1/1	0.94	0.13	53,53,53,53	0
56	MG	1H	3048	1/1	0.94	0.24	48,48,48,48	0
56	MG	1H	3397	1/1	0.94	0.11	66,66,66,66	0
56	MG	1H	3399	1/1	0.94	0.08	47,47,47,47	0
56	MG	2K	106	1/1	0.94	0.06	84,84,84,84	0
56	MG	1H	3130	1/1	0.94	0.24	54,54,54,54	0
56	MG	14	3346	1/1	0.94	0.12	59,59,59,59	0
56	MG	14	3225	1/1	0.94	0.20	78,78,78,78	0
56	MG	14	3349	1/1	0.94	0.20	63,63,63,63	0
56	MG	13	1655	1/1	0.94	0.13	73,73,73,73	0
56	MG	1H	3244	1/1	0.94	0.17	39,39,39,39	0
56	MG	1H	3420	1/1	0.94	0.16	48,48,48,48	0
56	MG	14	3354	1/1	0.94	0.10	71,71,71,71	0
56	MG	1G	1673	1/1	0.94	0.06	74, 74, 74, 74	0
56	MG	1G	1674	1/1	0.94	0.11	$70,\!70,\!70,\!70$	0
56	MG	1H	3292	1/1	0.94	0.21	$60,\!60,\!60,\!60$	0
56	MG	14	3237	1/1	0.94	0.13	$54,\!54,\!54,\!54$	0
56	MG	21	301	1/1	0.94	0.15	$53,\!53,\!53,\!53$	0
56	MG	14	3239	1/1	0.94	0.16	76,76,76,76	0
56	MG	1G	1679	1/1	0.94	0.10	90,90,90,90	0
56	MG	13	1657	1/1	0.94	0.27	69,69,69,69	0
56	MG	14	3376	1/1	0.94	0.13	87,87,87,87	0
56	MG	13	1632	1/1	0.94	0.18	63,63,63,63	0
56	MG	1H	3055	1/1	0.94	0.11	61,61,61,61	0
56	MG	1H	3094	1/1	0.94	0.28	41,41,41,41	0
56	MG	14	3380	1/1	0.94	0.10	93,93,93,93	0
56	MG	1H	3340	1/1	0.94	0.14	74,74,74,74	0
56	MG	14	3383	1/1	0.94	0.10	86,86,86,86	0
56	MG	I8	101	1/1	0.94	0.39	$53,\!53,\!53,\!53$	0
56	MG	1H	3095	1/1	0.94	0.41	49,49,49,49	0
56	MG	13	1718	1/1	0.94	0.20	90,90,90,90	0
56	MG	14	3146	1/1	0.94	0.29	69,69,69,69	0
56	MG	14	3390	1/1	0.94	0.15	90,90,90,90	0
56	MG	14	3255	1/1	0.94	0.14	$65,\!65,\!65,\!65$	0
56	MG	1J	201	1/1	0.94	0.16	87,87,87,87	0
56	MG	14	3002	1/1	0.94	0.18	43,43,43,43	0
56	MG	14	3008	1/1	0.94	0.21	54,54,54,54	0



Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
56	MG	1H	3141	1/1	0.94	0.38	60.60.60.60	0
56	MG	14	3015	1/1	0.94	0.18	71,71,71,71	0
56	MG	13	1622	1/1	0.94	0.35	79,79,79,79	0
56	MG	1H	3345	1/1	0.94	0.11	60,60,60,60	0
56	MG	1G	1617	1/1	0.94	0.16	80,80,80,80	0
56	MG	14	3022	1/1	0.94	0.14	72,72,72,72	0
56	MG	14	3157	1/1	0.94	0.12	88,88,88,88	0
56	MG	1G	1619	1/1	0.94	0.19	84,84,84,84	0
56	MG	1H	3060	1/1	0.94	0.20	74,74,74,74	0
56	MG	14	3028	1/1	0.94	0.18	73,73,73,73	0
56	MG	1G	1621	1/1	0.94	0.15	81,81,81,81	0
56	MG	1H	3382	1/1	0.95	0.09	45,45,45,45	0
56	MG	1H	3383	1/1	0.95	0.18	52,52,52,52	0
56	MG	14	3074	1/1	0.95	0.17	66,66,66,66	0
56	MG	14	3075	1/1	0.95	0.15	$53,\!53,\!53,\!53$	0
56	MG	1H	3286	1/1	0.95	0.21	70,70,70,70	0
56	MG	14	3181	1/1	0.95	0.18	$55,\!55,\!55,\!55$	0
56	MG	1H	3119	1/1	0.95	0.29	52,52,52,52	0
56	MG	1H	3120	1/1	0.95	0.13	60,60,60,60	0
56	MG	1H	3121	1/1	0.95	0.18	64,64,64,64	0
56	MG	1G	1653	1/1	0.95	0.23	90,90,90,90	0
56	MG	1H	3214	1/1	0.95	0.34	$68,\!68,\!68,\!68$	0
56	MG	1H	3063	1/1	0.95	0.44	$65,\!65,\!65,\!65$	0
56	MG	1H	3396	1/1	0.95	0.18	$57,\!57,\!57,\!57$	0
56	MG	1H	3294	1/1	0.95	0.19	$47,\!47,\!47,\!47$	0
56	MG	14	3194	1/1	0.95	0.16	$52,\!52,\!52,\!52$	0
56	MG	14	3294	1/1	0.95	0.24	74, 74, 74, 74	0
56	MG	1H	3064	1/1	0.95	0.26	56, 56, 56, 56	0
56	MG	1G	1660	1/1	0.95	0.10	74,74,74,74	0
56	MG	1G	1661	1/1	0.95	0.20	73,73,73,73	0
56	MG	14	3103	1/1	0.95	0.21	67,67,67,67	0
56	MG	1H	3251	1/1	0.95	0.10	61,61,61,61	0
56	MG	1H	3253	1/1	0.95	0.15	78,78,78,78	0
56	MG	14	3204	1/1	0.95	0.19	51,51,51,51	0
56	MG	13	1635	1/1	0.95	0.12	59,59,59,59	0
56	MG	14	3206	1/1	0.95	0.15	48,48,48,48	0
56	MG	1H	3044	1/1	0.95	0.16	51,51,51,51	0
56	MG	1H	3303	1/1	0.95	0.18	65,65,65,65	0
56	MG	14	3114	1/1	0.95	0.25	44,44,44,44	0
56	MG	16	209	1/1	0.95	0.20	56,56,56,56	0
56	MG	1H	3256	1/1	0.95	0.20	57,57,57,57	0
56	MG	1H	3219	1/1	0.95	0.15	$53,\!53,\!53,\!53$	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors(A^2)	$\mathbf{Q} < 0.9$
56	MG	13	1661	1/1	0.95	0.29	54,54,54,54	0
56	MG	5E	201	1/1	0.95	0.18	70,70,70,70	0
56	MG	1H	3262	1/1	0.95	0.39	56,56,56,56	0
56	MG	14	3326	1/1	0.95	0.14	$65,\!65,\!65,\!65$	0
56	MG	1H	3427	1/1	0.95	0.23	76, 76, 76, 76	0
56	MG	14	3219	1/1	0.95	0.14	56, 56, 56, 56	0
56	MG	14	3337	1/1	0.95	0.06	$55,\!55,\!55,\!55$	0
56	MG	1H	3309	1/1	0.95	0.48	98,98,98,98	0
56	MG	1H	3430	1/1	0.95	0.07	76,76,76,76	0
56	MG	1H	3132	1/1	0.95	0.21	45,45,45,45	0
56	MG	1H	3432	1/1	0.95	0.12	$65,\!65,\!65,\!65$	0
56	MG	14	3128	1/1	0.95	0.29	58,58,58,58	0
56	MG	14	3343	1/1	0.95	0.14	46,46,46,46	0
56	MG	13	1737	1/1	0.95	0.07	62,62,62,62	0
56	MG	1H	3191	1/1	0.95	0.18	75,75,75,75	0
56	MG	1G	1604	1/1	0.95	0.12	77,77,77,77	0
56	MG	1G	1606	1/1	0.95	0.25	79,79,79,79	0
56	MG	1H	3436	1/1	0.95	0.10	60,60,60,60	0
56	MG	14	3235	1/1	0.95	0.26	72,72,72,72	0
56	MG	14	3134	1/1	0.95	0.17	64,64,64,64	0
56	MG	1H	3031	1/1	0.95	0.17	71,71,71,71	0
56	MG	14	3356	1/1	0.95	0.09	72,72,72,72	0
56	MG	1H	3352	1/1	0.95	0.13	61,61,61,61	0
56	MG	1G	1611	1/1	0.95	0.13	72,72,72,72	0
56	MG	1H	3439	1/1	0.95	0.10	69,69,69,69	0
56	MG	14	3366	1/1	0.95	0.13	66,66,66,66	0
56	MG	14	3007	1/1	0.95	0.13	48,48,48,48	0
56	MG	14	3244	1/1	0.95	0.15	$65,\!65,\!65,\!65$	0
56	MG	1H	3162	1/1	0.95	0.25	68,68,68,68	0
56	MG	1H	3195	1/1	0.95	0.27	$65,\!65,\!65,\!65$	0
56	MG	1H	3196	1/1	0.95	0.08	68,68,68,68	0
56	MG	1H	3073	1/1	0.95	0.27	63,63,63,63	0
56	MG	13	1723	1/1	0.95	0.08	86,86,86,86	0
56	MG	13	1726	1/1	0.95	0.13	77,77,77,77	0
56	MG	14	3253	1/1	0.95	0.30	74,74,74,74	0
56	MG	1H	3235	1/1	0.95	0.14	38,38,38,38	0
56	MG	13	1678	1/1	0.95	0.21	74,74,74,74	0
56	MG	14	3382	1/1	0.95	0.08	69,69,69,69	0
56	MG	14	3024	1/1	0.95	0.15	74,74,74,74	0
56	MG	14	3384	1/1	0.95	0.09	62,62,62,62	0
56	MG	2K	103	1/1	0.95	0.18	81,81,81,81	0
56	MG	1H	3082	1/1	0.95	0.27	70,70,70,70	0



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56 MG 1H 3143 1/1 0.95 0.13 49,49,49,49 0 56 MG 1H 3369 1/1 0.95 0.12 45,45,45,45 0 56 MG 1H 3300 1/1 0.95 0.12 54,54,54,54 0 56 MG 14 3035 1/1 0.95 0.10 79,79,79,79 0 56 MG 13 1645 1/1 0.95 0.34 98,98,98,98 0 56 MG 14 3044 1/1 0.95 0.34 98,98,98,98 0 56 MG 14 3047 1/1 0.95 0.34 98,98,98,98 0 56 MG 14 3047 1/1 0.95 0.11 60,60,60 0 56 MG 14 3056 1/1 0.95 0.16 75,75,75 0 56 MG 14 3056 1/1 <td< th=""><th>Mol</th><th>Type</th><th>Chain</th><th>Res</th><th>Atoms</th><th>RSCC</th><th>RSR</th><th>$\frac{B-factors(A^2)}{40,40,40}$</th><th>Q<0.9</th></td<>	Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\frac{B-factors(A^2)}{40,40,40}$	Q<0.9
56MG1H3369 $1/1$ 0.95 0.12 $45,45,45,45,45$ 056MG1H3370 $1/1$ 0.95 0.12 $54,54,54,54$ 056MG143035 $1/1$ 0.95 0.14 $54,54,54,54$ 056MG13 1645 $1/1$ 0.95 0.10 $79,79,79,79$ 056MG14 3044 $1/1$ 0.95 0.10 $79,79,79,79$ 056MG1G 1635 $1/1$ 0.95 0.34 $98,98,98,98$ 056MG14 3044 $1/1$ 0.95 0.34 $98,98,98,98$ 056MG14 3047 $1/1$ 0.95 0.38 $56,56,56,56$ 056MG1H 3375 $1/1$ 0.95 0.16 $75,75,75$ 056MG14 3056 $1/1$ 0.95 0.16 $75,75,75,75$ 056MG14 3056 $1/1$ 0.95 0.16 $68,68,68,68$ 056MG14 3056 $1/1$ 0.95 0.14 $45,45,45,45$ 056MG14 3056 $1/1$ 0.95 0.14 $55,55,55,55$ 056MG14 3066 $1/1$ 0.95 0.14 $49,49,49,49$ 056MG1H 3391 $1/1$ 0.96 0.97 $71,71,71$ 056MG1H 3392 <td>56</td> <td>MG</td> <td>IH</td> <td>3143</td> <td>1/1</td> <td>0.95</td> <td>0.13</td> <td>49,49,49,49</td> <td>0</td>	56	MG	IH	3143	1/1	0.95	0.13	49,49,49,49	0
56 MG 1H 3370 1/1 0.95 0.12 54,54,54,54 0 56 MG 14 3035 1/1 0.95 0.14 54,54,54,54 0 56 MG 2K 104 1/1 0.95 0.29 98,98,98,98 0 56 MG 14 3044 1/1 0.95 0.08 53,53,53,53 0 56 MG 14 3044 1/1 0.95 0.34 98,98,98,98 0 56 MG 14 3047 1/1 0.95 0.38 56,56,56,56 0 56 MG 14 3047 1/1 0.95 0.16 75,75,75,75 0 56 MG 14 3056 1/1 0.95 0.16 68,68,68 0 56 MG 14 3057 1/1 0.95 0.14 49,49,49,49 0 56 MG 14 3066 1/1 <	56	MG	1H	3369	1/1	0.95	0.12	45,45,45,45	0
56 MG 14 3035 1/1 0.95 0.14 $54,54,54,54,54$ 0 56 MG 2K 104 1/1 0.95 0.29 98,98,98,98 0 56 MG 13 1645 1/1 0.95 0.10 79,79,79,79 0 56 MG 14 3044 1/1 0.95 0.38 55,56,55,56 0 56 MG 14 3162 1/1 0.95 0.38 56,56,56,56 0 56 MG 14 3047 1/1 0.95 0.11 60,60,60 0 56 MG 1H 3375 1/1 0.95 0.16 75,75,75,75 0 56 MG 14 3056 1/1 0.95 0.16 68,68,68,68 0 56 MG 14 3056 1/1 0.95 0.14 45,55,55,55 0 56 MG 1H 307 1/1	56	MG	1H	3370	1/1	0.95	0.12	54,54,54,54	0
56 MG 2K 104 1/1 0.95 0.29 98,98,98,98 0 56 MG 13 1645 1/1 0.95 0.10 79,79,79,79 0 56 MG 14 3044 1/1 0.95 0.08 53,53,53,53 0 56 MG 14 3047 1/1 0.95 0.34 98,98,98,98 0 56 MG 14 3047 1/1 0.95 0.38 56,56,56,56 0 56 MG 14 3047 1/1 0.95 0.10 67,57,57,75 0 56 MG 14 3056 1/1 0.95 0.16 68,68,68,68 0 56 MG 14 3057 1/1 0.95 0.16 68,68,68,68 0 56 MG 14 3057 1/1 0.95 0.14 45,48,48,48 0 56 MG 14 3066 1/1	56	MG	14	3035	1/1	0.95	0.14	54,54,54,54	0
56 MG 13 1645 1/1 0.95 0.10 79,79,79,79 0 56 MG 14 3044 1/1 0.95 0.08 53,53,53,53 0 56 MG 14 3162 1/1 0.95 0.34 98,98,98,98 0 56 MG 14 3047 1/1 0.95 0.38 56,56,56,56 0 56 MG 14 3047 1/1 0.95 0.11 60,60,60 0 56 MG 1H 3375 1/1 0.95 0.16 75,75,75,75 0 56 MG 14 3056 1/1 0.95 0.16 68,68,68,68 0 56 MG 13 1624 1/1 0.95 0.16 68,68,68,68 0 56 MG 1H 307 1/1 0.95 0.14 49,49,49,49 0 56 MG 1H 3004 1/1 <	56	MG	2K	104	1/1	0.95	0.29	98,98,98,98	0
56MG143044 $1/1$ 0.950.0853,53,53,53056MG1G1635 $1/1$ 0.950.3498,98,98,98056MG143162 $1/1$ 0.950.3856,56,56,56056MG143047 $1/1$ 0.950.1160,60,60,60056MG1H3375 $1/1$ 0.950.0937,37,37,37056MG1G1638 $1/1$ 0.950.1675,75,75,75056MG143056 $1/1$ 0.950.1851,51,51,51056MG143057 $1/1$ 0.950.1668,68,68,68056MG1H3378 $1/1$ 0.950.1455,55,55,55056MG1H3378 $1/1$ 0.950.1447,47,47,47056MG1H3004 $1/1$ 0.950.4147,47,47,47056MG1H3391 $1/1$ 0.960.0971,71,71,71056MG1H3392 $1/1$ 0.960.1264,64,64,64056MG1H3011 $1/1$ 0.960.1952,52,52,52056MG1H3127 $1/1$ 0.960.1969,69,69,69056MG1H3012 $1/1$ 0.960.1277,77,77,77056MG1H	56	MG	13	1645	1/1	0.95	0.10	79,79,79,79	0
56MG1G 1635 $1/1$ 0.95 0.34 $98,98,98,98$ 0 56 MG14 3162 $1/1$ 0.95 0.38 $56,56,56,56$ 0 56 MG14 3047 $1/1$ 0.95 0.11 $60,60,60,60$ 0 56 MG1H 3375 $1/1$ 0.95 0.09 $37,37,37,37$ 0 56 MG1G 1638 $1/1$ 0.95 0.16 $75,75,75,75$ 0 56 MG14 3056 $1/1$ 0.95 0.16 $68,68,68,68$ 0 56 MG14 3057 $1/1$ 0.95 0.16 $68,68,68,68$ 0 56 MG1H 3378 $1/1$ 0.95 0.14 $49,49,49,49$ 0 56 MG1H 3378 $1/1$ 0.95 0.14 $47,47,47,47$ 0 56 MG1H 3066 $1/1$ 0.95 0.14 $49,49,49,49$ 0 56 MG1H 3391 $1/1$ 0.96 0.09 $71,71,71,71$ 0 56 MG1H 3392 $1/1$ 0.96 0.12 $64,64,64,64$ 0 56 MG1H 3011 $1/1$ 0.96 0.19 $52,52,52,52$ 0 56 MG1H 3012 $1/1$ 0.96 0.17 $84,84,84,84$ 0 56 MG1H 3012 $1/1$ 0.96 0.19 $52,52,52,52,2$ </td <td>56</td> <td>MG</td> <td>14</td> <td>3044</td> <td>1/1</td> <td>0.95</td> <td>0.08</td> <td>53,53,53,53</td> <td>0</td>	56	MG	14	3044	1/1	0.95	0.08	53,53,53,53	0
56MG14 3162 $1/1$ 0.95 0.38 $56,56,56,56$ 0 56 MG14 3047 $1/1$ 0.95 0.11 $60,60,60,60$ 0 56 MG1H 3375 $1/1$ 0.95 0.09 $37,37,37,37$ 0 56 MG1G 1638 $1/1$ 0.95 0.16 $75,75,75,75$ 0 56 MG14 3056 $1/1$ 0.95 0.18 $51,51,51,51$ 0 56 MG14 3057 $1/1$ 0.95 0.18 $51,51,51,51$ 0 56 MG1H 3378 $1/1$ 0.95 0.14 $48,48,48,48$ 0 56 MG1H 3378 $1/1$ 0.95 0.14 $49,49,49,49$ 0 56 MG1H 3006 $1/1$ 0.95 0.14 $49,49,49,49$ 0 56 MG1H 3004 $1/1$ 0.95 0.14 $47,47,47,47$ 0 56 MG1H 3391 $1/1$ 0.96 0.09 $71,71,71,71$ 0 56 MG1H 3392 $1/1$ 0.96 0.12 $64,64,64,64$ 0 56 MG1H 3011 $1/1$ 0.96 0.19 $52,52,52,52$ 0 56 MG1H 3127 $1/1$ 0.96 0.19 $69,69,69,69$ 0 56 MG1H 3012 $1/1$ 0.96 0.19 $69,69,69,69,69$ <	56	MG	1G	1635	1/1	0.95	0.34	$98,\!98,\!98,\!98$	0
56MG14 3047 $1/1$ 0.95 0.11 $60,60,60,60$ 0 56 MG1H 3375 $1/1$ 0.95 0.09 $37,37,37,37$ 0 56 MG1G 1638 $1/1$ 0.95 0.16 $75,75,75,75$ 0 56 MG14 3056 $1/1$ 0.95 0.16 $68,68,68,68$ 0 56 MG14 3057 $1/1$ 0.95 0.16 $68,68,68,68$ 0 56 MG11 3057 $1/1$ 0.95 0.14 $55,55,55,55$ 0 56 MG1H 3378 $1/1$ 0.95 0.14 $49,49,49,49$ 0 56 MG1H 3066 $1/1$ 0.95 0.14 $49,49,49,49$ 0 56 MG1H 3004 $1/1$ 0.95 0.41 $47,47,47,47$ 0 56 MG1H 3004 $1/1$ 0.95 0.41 $47,47,47,47$ 0 56 MG1H 3391 $1/1$ 0.96 0.09 $71,71,71,71$ 0 56 MG1H 3392 $1/1$ 0.96 0.12 $64,64,64,64$ 0 56 MG1H 3011 $1/1$ 0.96 0.19 $52,52,52,52$ 0 56 MG1H 3012 $1/1$ 0.96 0.19 $69,69,69,69$ 0 56 MG1H 3012 $1/1$ 0.96 0.12 $77,77,77,77$ <td>56</td> <td>MG</td> <td>14</td> <td>3162</td> <td>1/1</td> <td>0.95</td> <td>0.38</td> <td>$56,\!56,\!56,\!56$</td> <td>0</td>	56	MG	14	3162	1/1	0.95	0.38	$56,\!56,\!56,\!56$	0
56MG1H 3375 $1/1$ 0.95 0.09 $37,37,37,37$ 0 56 MG1G 1638 $1/1$ 0.95 0.16 $75,75,75,75$ 0 56 MG14 3056 $1/1$ 0.95 0.18 $51,51,51,51$ 0 56 MG14 3057 $1/1$ 0.95 0.18 $51,51,51,51$ 0 56 MG11 3057 $1/1$ 0.95 0.16 $68,68,68,68$ 0 56 MG1H 3378 $1/1$ 0.95 0.14 $45,55,55,55$ 0 56 MG1H 3066 $1/1$ 0.95 0.14 $49,49,49,49$ 0 56 MG1H 3004 $1/1$ 0.95 0.41 $47,47,47,47,47$ 0 56 MG1H 3391 $1/1$ 0.96 0.09 $71,71,71,71$ 0 56 MG1H 3392 $1/1$ 0.96 0.12 $64,64,64,64$ 0 56 MG1H 3127 $1/1$ 0.96 0.19 $52,52,52,52$ 0 56 MG1H 3127 $1/1$ 0.96 0.19 $69,69,69,69$ 0 56 MG1H 3012 $1/1$ 0.96 0.19 $69,69,69,69$ 0 56 MG1H 3012 $1/1$ 0.96 0.12 $77,77,77,77$ 0 56 MG1H 3013 $1/1$ 0.96 0.39 $79,79,79,79,7$	56	MG	14	3047	1/1	0.95	0.11	60,60,60,60	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3375	1/1	0.95	0.09	37,37,37,37	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1G	1638	1/1	0.95	0.16	75,75,75,75	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3056	1/1	0.95	0.18	51,51,51,51	0
56MG13 1624 $1/1$ 0.95 0.28 $48,48,48,48$ 0 56 MG1H 3378 $1/1$ 0.95 0.14 $55,55,55,55$ 0 56 MG1H 3066 $1/1$ 0.95 0.14 $49,49,49,49$ 0 56 MG1H 3004 $1/1$ 0.95 0.41 $47,47,47,47$ 0 56 MG1H 3391 $1/1$ 0.96 0.09 $71,71,71,71$ 0 56 MG1H 3277 $1/1$ 0.96 0.17 $66,66,66,66$ 0 56 MG1H 3392 $1/1$ 0.96 0.12 $64,64,64,64$ 0 56 MG1H 3011 $1/1$ 0.96 0.12 $64,64,64,64$ 0 56 MG1H 3011 $1/1$ 0.96 0.19 $52,52,52,52$ 0 56 MG1H 3127 $1/1$ 0.96 0.19 $52,52,52,52$ 0 56 MG1H 3012 $1/1$ 0.96 0.17 $84,84,84,84$ 0 56 MG1H 3012 $1/1$ 0.96 0.28 $64,64,64,64$ 0 56 MG1H 3013 $1/1$ 0.96 0.28 $64,64,64,64$ 0 56 MG1H 3013 $1/1$ 0.96 0.12 $77,77,77,77,77,77,77,77,77,77,77,77,77,$	56	MG	14	3057	1/1	0.95	0.16	68,68,68,68	0
56MG1H 3378 $1/1$ 0.95 0.14 $55,55,55,55$ 0 56 MG14 3066 $1/1$ 0.95 0.14 $49,49,49,49$ 0 56 MG1H 3004 $1/1$ 0.95 0.41 $47,47,47,47$ 0 56 MG1H 3391 $1/1$ 0.96 0.09 $71,71,71,71$ 0 56 MG1H 3327 $1/1$ 0.96 0.17 $66,66,66,66$ 0 56 MG1H 3392 $1/1$ 0.96 0.12 $64,64,64,64$ 0 56 MG1H 3011 $1/1$ 0.96 0.12 $64,64,64,64$ 0 56 MG1H 3011 $1/1$ 0.96 0.19 $52,52,52,52$ 0 56 MG1H 3127 $1/1$ 0.96 0.19 $69,69,69,69$ 0 56 MG1H 3012 $1/1$ 0.96 0.17 $84,84,84,84$ 0 56 MG1H 3012 $1/1$ 0.96 0.28 $64,64,64,64$ 0 56 MG1H 3013 $1/1$ 0.96 0.28 $64,64,64,64$ 0 56 MG1H 3013 $1/1$ 0.96 0.12 $77,77,77,77,77,77,77,77,77,77,77,77,77,$	56	MG	13	1624	1/1	0.95	0.28	48,48,48,48	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3378	1/1	0.95	0.14	$55,\!55,\!55,\!55$	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3066	1/1	0.95	0.14	49,49,49,49	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3004	1/1	0.95	0.41	47,47,47,47	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3391	1/1	0.96	0.09	71,71,71,71	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3277	1/1	0.96	0.17	66,66,66,66	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3392	1/1	0.96	0.12	64,64,64,64	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3011	1/1	0.96	0.20	48,48,48,48	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3127	1/1	0.96	0.19	52,52,52,52	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3068	1/1	0.96	0.19	69,69,69,69	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1G	1651	1/1	0.96	0.17	84,84,84,84	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3012	1/1	0.96	0.34	45,45,45,45	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3179	1/1	0.96	0.28	64,64,64,64	0
56 MG 1H 3481 1/1 0.96 0.12 77,77,77,77 0 56 MG 1G 1655 1/1 0.96 0.39 79,79,79,79 0 56 MG 1H 3398 1/1 0.96 0.11 55,55,55,55 0 56 MG 14 3081 1/1 0.96 0.16 67,67,67 67 56 MC 14 3082 1/1 0.96 0.16 67,67,67 0	56	MG	1H	3013	1/1	0.96	0.20	31,31,31,31	0
56 MG 1G 1655 1/1 0.96 0.39 79,79,79,79 0 56 MG 1H 3398 1/1 0.96 0.11 55,55,55,55 0 56 MG 14 3081 1/1 0.96 0.25 52,52,52,52 0 56 MC 14 3082 1/1 0.96 0.16 67,67,67 0	56	MG	1H	3481	1/1	0.96	0.12	77,77,77,77	0
56 MG 1H 3398 1/1 0.96 0.11 55,55,55,55 0 56 MG 14 3081 1/1 0.96 0.25 52,52,52,52 0 56 MC 14 3082 1/1 0.96 0.16 67,67,67 0	56	MG	1G	1655	1/1	0.96	0.39	79,79,79,79	0
56 MG 14 3081 1/1 0.96 0.25 52,52,52,52 0 56 MC 14 3082 1/1 0.96 0.16 67.67.67.67 0	56	MG	1H	3398	1/1	0.96	0.11	55,55,55,55	0
56 MC 14 2082 1/1 0.06 0.16 67.67.67.67 0	56	MG	14	3081	1/1	0.96	0.25	52,52,52,52	0
00 100 14 0002 $1/1$ 0.90 0.10 $0/,0/,0/,0/$	56	MG	14	3082	1/1	0.96	0.16	67,67,67,67	0
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	56	MG	14	3188	1/1	0.96	0.17	56,56,56,56	0
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	56	MG	1H	3164	1/1	0.96	0.18	52,52,52,52	0
56 MG 1H 3015 1/1 0.96 0.22 59,59,59,59 0	56	MG	1H	3015	1/1	0.96	0.22	59,59,59,59	0
56 MG 1H 3405 1/1 0.96 0.20 61,61,61,61 0	56	MG	1H	3405	1/1	0.96	0.20	61,61,61,61	0
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	56	MG	14	3295	1/1	0.96	0.23	64,64,64,64	0
56 MG 1H 3166 1/1 0.96 0.26 72,72,72,72 0	56	MG	1H	3166	1/1	0.96	0.26	72,72,72,72	0
56 MG 1H 3296 1/1 0.96 0.25 90,90,90,90 0	56	MG	1H	3296	1/1	0.96	0.25	90,90,90,90	0
56 MG 1H 3297 1/1 0.96 0.33 71,71,71,71 0	56	MG	1H	3297	1/1	0.96	0.33	71,71,71,71	0
56 MG 13 1695 1/1 0.96 0.21 79,79,79,79 0	56	MG	13	1695	1/1	0.96	0.21	79,79,79,79	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
56	MG	1H	3208	1/1	0.96	0.26	78,78,78,78	0
56	MG	1H	3018	1/1	0.96	0.17	52,52,52,52	0
56	MG	14	3100	1/1	0.96	0.17	63,63,63,63	0
56	MG	14	3200	1/1	0.96	0.13	66,66,66,66	0
56	MG	1H	3133	1/1	0.96	0.17	60,60,60,60	0
56	MG	14	3203	1/1	0.96	0.19	55,55,55,55	0
56	MG	1H	3027	1/1	0.96	0.22	32,32,32,32	0
56	MG	13	1683	1/1	0.96	0.14	69,69,69,69	0
56	MG	13	1732	1/1	0.96	0.12	62,62,62,62	0
56	MG	14	3309	1/1	0.96	0.11	58,58,58,58	0
56	MG	1H	3059	1/1	0.96	0.13	68,68,68,68	0
56	MG	14	3312	1/1	0.96	0.07	67,67,67,67	0
56	MG	14	3108	1/1	0.96	0.21	76,76,76,76	0
56	MG	14	3109	1/1	0.96	0.09	78,78,78,78	0
56	MG	14	3317	1/1	0.96	0.10	41,41,41,41	0
56	MG	14	3321	1/1	0.96	0.08	62,62,62,62	0
56	MG	1H	3258	1/1	0.96	0.22	63,63,63,63	0
56	MG	14	3211	1/1	0.96	0.15	67,67,67,67	0
56	MG	14	3325	1/1	0.96	0.12	63,63,63,63	0
56	MG	14	3212	1/1	0.96	0.12	$65,\!65,\!65,\!65$	0
56	MG	14	3112	1/1	0.96	0.11	$65,\!65,\!65,\!65$	0
56	MG	14	3328	1/1	0.96	0.10	62,62,62,62	0
56	MG	14	3330	1/1	0.96	0.06	48,48,48,48	0
56	MG	13	1712	1/1	0.96	0.16	77,77,77,77	0
56	MG	14	3334	1/1	0.96	0.08	79,79,79,79	0
56	MG	14	3336	1/1	0.96	0.09	52,52,52,52	0
56	MG	1H	3260	1/1	0.96	0.11	72,72,72,72	0
56	MG	1H	3433	1/1	0.96	0.09	83,83,83,83	0
56	MG	1H	3176	1/1	0.96	0.16	60,60,60,60	0
56	MG	13	1734	1/1	0.96	0.07	86,86,86,86	0
56	MG	1G	1603	1/1	0.96	0.12	76,76,76,76	0
56	MG	13	1650	1/1	0.96	0.16	$68,\!68,\!68,\!68$	0
56	MG	13	1603	1/1	0.96	0.15	58,58,58,58	0
56	MG	1G	1682	1/1	0.96	0.08	74,74,74,74	0
56	MG	13	1739	1/1	0.96	0.21	73,73,73,73	0
56	MG	1H	3268	1/1	0.96	0.23	46,46,46,46	0
56	MG	1H	3441	1/1	0.96	0.10	86,86,86,86	0
56	MG	1G	1687	1/1	0.96	0.10	81,81,81,81	0
56	MG	13	1614	1/1	0.96	0.19	79,79,79,79	0
56	MG	14	3232	1/1	0.96	0.29	62,62,62,62	0
56	MG	1G	1612	1/1	0.96	0.18	63,63,63,63	0
56	MG	1G	1614	1/1	0.96	0.27	72,72,72,72	0



MoiTypeChainResAtomsRSCCRSRB-factors(A) $Q <$ 56MG143358 $1/1$ 0.960.2277,77,77,77056MG1G1616 $1/1$ 0.960.1586,86,86,86056MG143362 $1/1$ 0.960.0869,69,69,69056MG143004 $1/1$ 0.960.1746,46,46,46056MG1H3363 $1/1$ 0.960.2368,68,68,68056MG1H3182 $1/1$ 0.960.2087,87,87,87056MG1H3140 $1/1$ 0.960.2087,87,87,870	$ \begin{array}{c} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\$
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	$\begin{array}{c} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 $
56 MG IG I616 I/1 0.96 0.15 86,86,86,86 0 56 MG 14 3362 1/1 0.96 0.08 69,69,69,69 0 56 MG 14 3004 1/1 0.96 0.17 46,46,46,46 0 56 MG 1H 3363 1/1 0.96 0.23 68,68,68,68 0 56 MG 1H 3182 1/1 0.96 0.20 87,87,87,87 0 56 MG 1H 3182 1/1 0.96 0.20 87,87,87,87 0	$\begin{array}{c} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 $
56 MG 14 3362 1/1 0.96 0.08 69,69,69,69 0 56 MG 14 3004 1/1 0.96 0.17 46,46,46,46 0 56 MG 1H 3363 1/1 0.96 0.23 68,68,68,68 0 56 MG 1H 3182 1/1 0.96 0.20 87,87,87,87 0 56 MG 1H 3182 1/1 0.96 0.20 87,87,87,87 0	$\begin{array}{c} 0 \\ 0 \\ \hline \end{array}$
56 MG 14 3004 1/1 0.96 0.17 46,46,46,46 0 56 MG 1H 3363 1/1 0.96 0.23 68,68,68,68 0 56 MG 1H 3182 1/1 0.96 0.20 87,87,87,87 0 56 MG 1H 3182 1/1 0.96 0.20 87,87,87,87 0	$\begin{array}{c} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \end{array}$
56 MG 1H 3363 1/1 0.96 0.23 68,68,68,68 0 56 MG 1H 3182 1/1 0.96 0.20 87,87,87,87 0 56 MG 1H 3182 1/1 0.96 0.20 87,87,87,87 0	$\begin{array}{c} 0 \\ 0 \\ \hline \end{array}$
56 MG 1H 3182 1/1 0.96 0.20 87,87,87,87 0	$\frac{0}{0}$
	$\frac{0}{0}$
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	$\frac{0}{0}$
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	\cap
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0
56 MG 14 3245 $1/1$ 0.96 0.21 $70,70,70,70$ 0	0
56 MG 1H 3184 $1/1$ 0.96 0.19 $45,45,45,45$ 0	0
56 MG 13 1639 $1/1$ 0.96 0.12 56,56,56,56 0	0
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	0
$ \begin{tabular}{ c c c c c c c c c c c c c c c c c c c$	0
$ \begin{tabular}{ c c c c c c c c c c c c c c c c c c c$	0
56 MG 1H 3456 $1/1$ 0.96 0.12 $92,92,92,92$ 0	0
56 MG 1H 3003 $1/1$ 0.96 0.26 $35,35,35,35$ 0	0
56 MG $1H$ 3116 $1/1$ 0.96 0.37 $62,62,62,62$ 0	0
56 MG 1H 3376 $1/1$ 0.96 0.08 $36,36,36,36$ (0
56 MG 1H 3074 $1/1$ 0.96 0.28 $70,70,70,70$ 0	0
$56 \ \mathrm{MG} \ 14 \ 3386 \ 1/1 \ 0.96 \ 0.22 \ 60,60,60,60 \ 0$	0
56 MG 14 3031 $1/1$ 0.96 0.27 $60,60,60,60$ (0
56 MG 1H 3075 $1/1$ 0.96 0.39 $70,70,70,70$ 0	0
56 MG 13 1744 $1/1$ 0.96 0.07 $95,95,95,95$ 0	0
56 MG 1H 3381 $1/1$ 0.96 0.11 $40,40,40,40$ (0
56 MG 14 3036 1/1 0.96 0.16 42,42,42,42 0	0
56 MG 1H 3193 $1/1$ 0.96 0.29 $69,69,69,69$ (0
56 MG 14 3039 1/1 0.96 0.17 38,38,38,38 0	0
56 MG 1H 3005 $1/1$ 0.96 0.23 $53,53,53,53$ 0	0
56 MG 14 3043 1/1 0.96 0.15 67,67,67 0	0
56 MG 1G 1637 1/1 0.96 0.41 81,81,81,81 (0
56 MG 1H 3466 $1/1$ 0.96 0.06 $56,56,56,56$ 0	0
56 MG 29 302 1/1 0.96 0.29 65,65,65,65 0.29	0
56 MG 1H 3008 1/1 0.96 0.33 42,42,42,42	0
56 MG 14 3048 1/1 0.96 0.15 67,67,67 0	0
56 MG 14 3165 1/1 0.96 0.16 58,58,58,58	0
56 MG 1H 3046 1/1 0.96 0.34 67,67,67,67 0	0
56 MG 1H 3123 1/1 0.96 0.23 52.52.52 0	0
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	0
56 MG 1H 3287 1/1 0.96 0.14 50,50,50.50 0	0


Mol	Tvpe	Chain	Res	Atoms	RSCC	RSR	B-factors ($Å^2$)	Q<0.9
56	MG	1G	1645	1/1	0.96	0.12	73 73 73 73	0
56	MG	13	1702	1/1	0.97	0.26	62.62.62.62	0
56	MG	14	3098	1/1	0.97	0.22	54.54.54.54	0
56	MG	1H	3149	1/1	0.97	0.34	65.65.65.65	0
56	MG	14	3101	1/1	0.97	0.26	84,84,84,84	0
56	MG	1H	3071	1/1	0.97	0.16	53,53,53,53	0
56	MG	2L	101	1/1	0.97	0.15	76,76,76,76	0
56	MG	1H	3302	1/1	0.97	0.12	59,59,59,59	0
56	MG	13	1680	1/1	0.97	0.28	69,69,69,69	0
56	MG	13	1626	1/1	0.97	0.29	68,68,68,68	0
56	MG	14	3202	1/1	0.97	0.38	55,55,55,55	0
56	MG	14	3001	1/1	0.97	0.23	53,53,53,53	0
56	MG	13	1731	1/1	0.97	0.10	94,94,94,94	0
56	MG	1H	3014	1/1	0.97	0.27	43,43,43,43	0
56	MG	14	3006	1/1	0.97	0.16	48,48,48,48	0
56	MG	13	1654	1/1	0.97	0.23	75,75,75,75	0
56	MG	1H	3225	1/1	0.97	0.32	57,57,57,57	0
56	MG	1H	3400	1/1	0.97	0.13	47,47,47,47	0
56	MG	14	3012	1/1	0.97	0.26	77,77,77,77	0
56	MG	13	1627	1/1	0.97	0.21	62,62,62,62	0
56	MG	14	3014	1/1	0.97	0.22	58, 58, 58, 58	0
56	MG	1H	3404	1/1	0.97	0.08	45,45,45,45	0
56	MG	14	3313	1/1	0.97	0.06	$50,\!50,\!50,\!50$	0
56	MG	1H	3080	1/1	0.97	0.29	$53,\!53,\!53,\!53$	0
56	MG	1H	3473	1/1	0.97	0.17	73,73,73,73	0
56	MG	14	3316	1/1	0.97	0.10	49,49,49,49	0
56	MG	13	1656	1/1	0.97	0.26	91,91,91,91	0
56	MG	14	3123	1/1	0.97	0.13	60,60,60,60	0
56	MG	1H	3019	1/1	0.97	0.22	38,38,38,38	0
56	MG	1H	3476	1/1	0.97	0.07	$79,\!79,\!79,\!79$	0
56	MG	14	3324	1/1	0.97	0.10	$52,\!52,\!52,\!52$	0
56	MG	14	3126	1/1	0.97	0.31	66,66,66,66	0
56	MG	14	3221	1/1	0.97	0.29	58, 58, 58, 58	0
56	MG	14	3222	1/1	0.97	0.18	83,83,83,83	0
56	MG	1G	1639	1/1	0.97	0.10	85,85,85,85	0
56	MG	14	3329	1/1	0.97	0.12	$45,\!45,\!45,\!45$	0
56	MG	1G	1640	1/1	0.97	0.19	80,80,80,80	0
56	MG	14	3331	1/1	0.97	0.12	70,70,70,70	0
56	MG	1H	3411	1/1	0.97	0.08	$53,\!53,\!53,\!53$	0
56	MG	14	3027	1/1	0.97	0.13	70,70,70,70	0
56	MG	14	3335	1/1	0.97	0.06	$55,\!55,\!55,\!55$	0
56	MG	1H	3414	1/1	0.97	0.13	$53, \overline{53}, \overline{53}, \overline{53}$	0



Mol	Tvpe	Chain	$\frac{15 \text{ page.}}{\text{Res}}$	Atoms	RSCC	RSR	B-factors ($Å^2$)	Q<0.9
56	MG	1H	3415	1/1	0.97	0.17	68.68.68.68	0
56	MG	1H	3160	1/1	0.97	0.14	56.56.56.56	0
56	MG	14	3032	1/1	0.97	0.17	65.65.65.65	0
56	MG	1H	3232	1/1	0.97	0.13	43,43,43,43	0
56	MG	1H	3021	1/1	0.97	0.22	45,45,45,45	0
56	MG	1H	3023	1/1	0.97	0.22	51,51,51,51	0
56	MG	1H	3357	1/1	0.97	0.29	62,62,62,62	0
56	MG	1G	1649	1/1	0.97	0.14	72,72,72,72	0
56	MG	1H	3052	1/1	0.97	0.22	46,46,46,46	0
56	MG	14	3041	1/1	0.97	0.21	39,39,39,39	0
56	MG	1H	3277	1/1	0.97	0.27	70,70,70,70	0
56	MG	14	3242	1/1	0.97	0.17	74,74,74,74	0
56	MG	1H	3024	1/1	0.97	0.32	46,46,46,46	0
56	MG	1H	3025	1/1	0.97	0.23	53,53,53,53	0
56	MG	1H	3200	1/1	0.97	0.19	59, 59, 59, 59, 59	0
56	MG	1H	3026	1/1	0.97	0.23	$53,\!53,\!53,\!53$	0
56	MG	14	3357	1/1	0.97	0.15	$62,\!62,\!62,\!62$	0
56	MG	1H	3365	1/1	0.97	0.17	64,64,64,64	0
56	MG	13	1735	1/1	0.97	0.06	71,71,71,71	0
56	MG	14	3361	1/1	0.97	0.07	60,60,60,60	0
56	MG	14	3052	1/1	0.97	0.24	62,62,62,62	0
56	MG	14	3152	1/1	0.97	0.11	67,67,67,67	0
56	MG	14	3364	1/1	0.97	0.08	75,75,75,75	0
56	MG	1H	3367	1/1	0.97	0.30	66,66,66,66	0
56	MG	13	1664	1/1	0.97	0.21	59,59,59,59	0
56	MG	13	1638	1/1	0.97	0.19	53,53,53,53	0
56	MG	13	1738	1/1	0.97	0.09	72,72,72,72	0
56	MG	1H	3371	1/1	0.97	0.16	46,46,46,46	0
56	MG	1H	3206	1/1	0.97	0.23	63,63,63,63	0
56	MG	14	3060	1/1	0.97	0.15	48,48,48,48	0
56	MG	14	3374		0.97	0.17	76,76,76,76	0
56	MG	14	3065		0.97	0.28	46,46,46	0
50	MG	11	3440		0.97	0.12	61,61,61,61	0
50	MG	13	1070		0.97	0.10	02,02,02,02	0
50	MG	14	3103		0.97	0.20	80,80,80,80	0
00 56	MC	15 1U	2100		0.97	$\begin{array}{c} 0.21 \\ 0.17 \end{array}$	01,01,01,01	0
00 56	MC		3070	1/1 1/1	0.97	$\begin{array}{c} 0.11\\ 0.91 \end{array}$	40,40,40,40	0
- 00 56	MC	14 1U	3070		0.97	0.21	39,39,39,39	0
50	MC		3001 2072		0.97	0.18	49,49,49,49	0
50	MC	14	0070 1605	1/1 1/1	0.97	0.10	74 74 74 74 74	0
00 56	MC	1G 1U	2447		0.97	0.13	14,14,14,14	0
- 00	MG		0447		0.97	0.11	10,10,10,10	



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(A ²)	Q<0.9
56	MG	1H	3448	1/1	0.97	0.06	88,88,88,88	0
56	MG	1H	3102	1/1	0.97	0.14	60,60,60,60	0
56	MG	14	3079	1/1	0.97	0.15	57,57,57,57	0
56	MG	14	3080	1/1	0.97	0.07	69,69,69,69	0
56	MG	13	1724	1/1	0.97	0.18	78,78,78,78	0
56	MG	1H	3252	1/1	0.97	0.12	49,49,49,49	0
56	MG	14	3083	1/1	0.97	0.15	60,60,60,60	0
56	MG	14	3178	1/1	0.97	0.21	80,80,80,80	0
56	MG	14	3085	1/1	0.97	0.13	50,50,50,50	0
56	MG	1H	3036	1/1	0.97	0.33	57,57,57,57	0
56	MG	1G	1676	1/1	0.97	0.07	75,75,75,75	0
56	MG	1G	1613	1/1	0.97	0.08	87,87,87,87	0
56	MG	14	3183	1/1	0.97	0.26	46, 46, 46, 46	0
56	MG	14	3090	1/1	0.97	0.20	$52,\!52,\!52,\!52$	0
56	MG	13	1667	1/1	0.97	0.19	$92,\!92,\!92,\!92$	0
56	MG	1G	1615	1/1	0.97	0.17	87,87,87,87	0
56	MG	45	201	1/1	0.97	0.11	$50,\!50,\!50,\!50$	0
56	MG	14	3093	1/1	0.97	0.26	48,48,48,48	0
56	MG	13	1606	1/1	0.97	0.20	63,63,63,63	0
56	MG	1H	3385	1/1	0.97	0.10	54,54,54,54	0
57	PAR	13	1745	42/42	0.97	0.22	57,66,72,75	0
57	PAR	1G	1686	42/42	0.97	0.25	69,76,87,91	0
58	ZN	3E	302	1/1	0.97	0.35	89,89,89,89	0
56	MG	14	3191	1/1	0.97	0.20	57,57,57,57	0
58	ZN	5A	101	1/1	0.97	0.14	121,121,121,121	0
56	MG	1H	3006	1/1	0.97	0.16	49,49,49,49	0
56	MG	14	3084	1/1	0.98	0.18	43,43,43,43	0
56	MG	1H	3072	1/1	0.98	0.19	43,43,43,43	0
56	MG	14	3086	1/1	0.98	0.06	$65,\!65,\!65,\!65$	0
56	MG	1H	3099	1/1	0.98	0.33	53,53,53,53	0
56	MG	1H	3230	1/1	0.98	0.19	37,37,37,37	0
56	MG	14	3009	1/1	0.98	0.18	51,51,51,51	0
56	MG	14	3010	1/1	0.98	0.22	58,58,58,58	0
56	MG	1H	3428	1/1	0.98	0.15	47,47,47,47	0
56	MG	13	1625	1/1	0.98	0.34	45,45,45,45	0
56	MG	1H	3267	1/1	0.98	0.24	60,60,60,60	0
56	MG	2K	107	1/1	0.98	0.20	59,59,59,59	0
56	MG	14	3333	1/1	0.98	0.12	58,58,58,58	0
56	MG	13	1727	1/1	0.98	0.06	76,76,76,76	0
56	MG	1H	3380	1/1	0.98	0.12	41,41,41,41	0
56	MG	1H	3035	1/1	0.98	0.15	61,61.61.61	0
56	MG	1H	3104	1/1	0.98	0.16	41,41,41,41	0
00	mu	111	0104	1 / 1	0.00	0.10	,,,,	0



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56 MG 14 3019 1/1 0.98 0.12 74,74,74,74 0 56 MG 1H 3017 1/1 0.98 0.19 55,55,55 0 56 MG 16 211 1/1 0.98 0.13 85,85,85,85 0 56 MG 14 3005 1/1 0.98 0.13 85,85,85,85 0 56 MG 14 3056 1/1 0.98 0.09 51,51,51 0 56 MG 14 3025 1/1 0.98 0.20 34,34,34,40 0 56 MG 1H 3025 1/1 0.98 0.22 84,84,844 0 56 MG 1H 307 1/1 0.98 0.22 55,55,55 0 56 MG 1H 317 1/1 0.98 0.22 55,55,55 0 56 MG 14 3187 1/1 0.98	Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors(A^2)	Q<0.9
56 MG 1H 3017 $1/1$ 0.98 0.20 $41,41,41,41$ 0 56 MG 14 3021 $1/1$ 0.98 0.13 $85,55,55,55,55,55,55,55,55,55,55,55,55,5$	56	MG	14	3019	1/1	0.98	0.12	74,74,74,74	0
56 MG 14 3021 $1/1$ 0.98 0.19 55,5,5,5,5,5 0 56 MG 16 211 $1/1$ 0.98 0.13 85,85,85,85 0 56 MG 14 3105 $1/1$ 0.98 0.19 47,47,47,47 0 56 MG 14 3344 $1/1$ 0.98 0.09 51,51,51,51 0 56 MG 14 3025 $1/1$ 0.98 0.22 84,84,84,84 0 56 MG 14 3025 $1/1$ 0.98 0.22 84,84,84,84 0 56 MG 114 3079 $1/1$ 0.98 0.28 67,67,67,67 0 56 MG 14 3175 $1/1$ 0.98 0.21 55,55,55 0 56 MG 14 3187 $1/1$ 0.98 0.11 42,42,42,42 0 56 MG 1H 3389 <t< td=""><td>56</td><td>MG</td><td>1H</td><td>3017</td><td>1/1</td><td>0.98</td><td>0.20</td><td>41,41,41,41</td><td>0</td></t<>	56	MG	1H	3017	1/1	0.98	0.20	41,41,41,41	0
56 MG 16 211 $1/1$ 0.98 0.13 85,85,85,85 0 56 MG 1H 3056 $1/1$ 0.98 0.33 70,70,70,70 0 56 MG 14 3105 $1/1$ 0.98 0.09 51,51,51,51 0 56 MG 1H 3108 $1/1$ 0.98 0.20 34,34,34,34 0 56 MG 1H 3262 $1/1$ 0.98 0.22 84,84,84,84 0 56 MG 1H 3262 $1/1$ 0.98 0.26 45,45,45,45 0 56 MG 1H 3387 $1/1$ 0.98 0.29 67,67,67,67 0 56 MG 14 3187 $1/1$ 0.98 0.29 67,67,67,67 0 56 MG 1H 342 $1/1$ 0.98 0.11 42,42,42,42 0 56 MG 1H 3442 <t< td=""><td>56</td><td>MG</td><td>14</td><td>3021</td><td>1/1</td><td>0.98</td><td>0.19</td><td>55,55,55,55</td><td>0</td></t<>	56	MG	14	3021	1/1	0.98	0.19	55,55,55,55	0
$ 56 \mathrm{MG} 1H 3056 1/1 0.98 0.33 70, 70, 70, 70 0 \\ 56 \mathrm{MG} 14 3105 1/1 0.98 0.19 47, 47, 47, 47 0 \\ 56 \mathrm{MG} 1H 3108 1/1 0.98 0.20 34, 34, 34, 34 0 \\ 56 \mathrm{MG} 1H 3108 1/1 0.98 0.20 34, 34, 34, 34 0 \\ 56 \mathrm{MG} 1H 3025 1/1 0.98 0.22 84, 84, 84, 84 0 \\ 56 \mathrm{MG} 1H 3079 1/1 0.98 0.26 45, 45, 45, 45 0 \\ 56 \mathrm{MG} 1H 3079 1/1 0.98 0.26 45, 45, 45, 454 0 \\ 56 \mathrm{MG} 1H 3079 1/1 0.98 0.29 67, 67, 67, 67 0 \\ 56 \mathrm{MG} 1H 3175 1/1 0.98 0.29 67, 67, 67, 67 0 \\ 56 \mathrm{MG} 1H 3175 1/1 0.98 0.29 67, 67, 67, 67 0 \\ 56 \mathrm{MG} 14 3111 1/1 0.98 0.22 55, 55, 55, 55 0 \\ 56 \mathrm{MG} 14 3187 1/1 0.98 0.21 53, 53, 53, 53 0 \\ 56 \mathrm{MG} 1H 3442 1/1 0.98 0.11 42, 42, 42, 42 0 \\ 56 \mathrm{MG} 1H 3442 1/1 0.98 0.11 42, 42, 42, 42 0 \\ 56 \mathrm{MG} 1H 3445 1/1 0.98 0.10 52, 52, 52, 52 0 \\ 56 \mathrm{MG} 1H 3445 1/1 0.98 0.10 52, 52, 52, 52 0 \\ 56 \mathrm{MG} 1H 3445 1/1 0.98 0.10 52, 52, 52, 52 0 \\ 56 \mathrm{MG} 1H 3445 1/1 0.98 0.10 75, 75, 75, 75 0 \\ 56 \mathrm{MG} 1H 3445 1/1 0.98 0.10 75, 75, 75, 75 0 \\ 56 \mathrm{MG} 1H 3445 1/1 0.98 0.10 75, 75, 75, 75 0 \\ 56 \mathrm{MG} 1H 3445 1/1 0.98 0.10 75, 75, 75, 75 0 \\ 56 \mathrm{MG} 1H 3445 1/1 0.98 0.10 75, 75, 75, 75 0 \\ 56 \mathrm{MG} 1H 3445 1/1 0.98 0.10 75, 75, 75, 75 0 \\ 56 \mathrm{MG} 1G 1601 1/1 0.98 0.10 75, 75, 75, 75 0 \\ 56 \mathrm{MG} 1G 1601 1/1 0.98 0.10 75, 75, 75, 75 0 \\ 56 \mathrm{MG} 14 3038 1/1 0.98 0.10 53, 53, 53, 53 0 \\ 0 \\ 56 \mathrm{MG} 1H 3114 1/1 0.98 0.10 53, 53, 53, 53 0 \\ 0 \\ 56 \mathrm{MG} 1H 3114 1/1 0.98 0.10 73,$	56	MG	16	211	1/1	0.98	0.13	85,85,85,85	0
56 MG 14 3105 $1/1$ 0.98 0.19 $47,47,47,47$ 0 56 MG 14 3344 $1/1$ 0.98 0.09 51,51,51 0 56 MG 1H 3108 $1/1$ 0.98 0.22 34,34,34,34 0 56 MG 14 3262 $1/1$ 0.98 0.22 48,48,48,48 0 56 MG 1H 3079 $1/1$ 0.98 0.26 45,45,45,45 0 56 MG 1H 3175 $1/1$ 0.98 0.22 55,55,55 0 56 MG 14 3187 $1/1$ 0.98 0.21 53,53,53,53 0 56 MG 1H 3385 $1/1$ 0.98 0.11 42,42,42,42 0 56 MG 1H 3389 $1/1$ 0.98 0.11 42,42,42,42 0 56 MG 1H 3442	56	MG	1H	3056	1/1	0.98	0.33	70,70,70,70	0
56 MG 14 3344 1/1 0.98 0.09 51,51,51 0 56 MG 1H 3108 1/1 0.98 0.20 34,34,34,34,34 0 56 MG 14 3025 1/1 0.98 0.22 84,84,84,84 0 56 MG 1H 3079 1/1 0.98 0.26 45,45,45,45 0 56 MG 1H 3387 1/1 0.98 0.29 67,67,67,67 0 56 MG 1H 3175 1/1 0.98 0.22 55,55,55 0 56 MG 14 3187 1/1 0.98 0.21 53,53,53 0 56 MG 1H 3355 1/1 0.98 0.11 42,42,42 0 56 MG 1H 3369 1/1 0.98 0.10 52,52,52,52 0 56 MG 1H 3242 1/1 0.	56	MG	14	3105	1/1	0.98	0.19	47,47,47,47	0
56 MG 1H 3108 $1/1$ 0.98 0.20 34,34,34,34 0 56 MG 14 3025 $1/1$ 0.98 0.22 84,84,84,84 0 56 MG 14 3262 $1/1$ 0.98 0.13 66,66,66,66 0 56 MG 1H 3387 $1/1$ 0.98 0.26 45,45,45,45,45 0 56 MG 1H 3175 $1/1$ 0.98 0.29 67,67,67,67 0 56 MG 14 3187 $1/1$ 0.98 0.22 55,55,55,55 0 56 MG 14 3355 $1/1$ 0.98 0.11 42,42,42,0 0 56 MG 1H 3422 $1/1$ 0.98 0.11 42,42,42,0 0 56 MG 1H 302 $1/1$ 0.98 0.10 52,52,52,52 0 56 MG 1H 3242	56	MG	14	3344	1/1	0.98	0.09	51,51,51,51	0
56 MG 14 3025 $1/1$ 0.98 0.22 84,84,84,84 0 56 MG 14 3262 $1/1$ 0.98 0.13 66,66,66,66 0 56 MG 1H 3079 $1/1$ 0.98 0.26 45,45,45,45 0 56 MG 1H 3175 $1/1$ 0.98 0.29 67,67,67,67 0 56 MG 14 3111 $1/1$ 0.98 0.22 55,55,55,55 0 56 MG 14 3187 $1/1$ 0.98 0.09 47,47,47,47 0 56 MG 1H 3442 $1/1$ 0.98 0.11 42,42,42,42 0 56 MG 1H 3002 $1/1$ 0.98 0.13 63,63,63 0 56 MG 1H 302 $1/1$ 0.98 0.10 52,52,52 0 56 MG 1H 3242 $1/$	56	MG	1H	3108	1/1	0.98	0.20	34,34,34,34	0
56 MG 14 3262 $1/1$ 0.98 0.13 66,66,66,66 0 56 MG 1H 3079 $1/1$ 0.98 0.26 45,45,45,45 0 56 MG 1H 3175 $1/1$ 0.98 0.29 67,67,67,67 0 56 MG 14 3111 $1/1$ 0.98 0.22 55,55,55 0 56 MG 14 3187 $1/1$ 0.98 0.21 53,53,53,53 0 56 MG 1H 3442 $1/1$ 0.98 0.11 42,42,42,42 0 56 MG 1H 3442 $1/1$ 0.98 0.14 68,68,68 0 56 MG 1H 3002 $1/1$ 0.98 0.10 52,52,52 0 56 MG 1H 3445 $1/1$ 0.98 0.10 75,75,75 0 56 MG 1H 3242 $1/1$ <td>56</td> <td>MG</td> <td>14</td> <td>3025</td> <td>1/1</td> <td>0.98</td> <td>0.22</td> <td>84,84,84,84</td> <td>0</td>	56	MG	14	3025	1/1	0.98	0.22	84,84,84,84	0
56MG1H3079 $1/1$ 0.980.2645,45,45,45056MG1H3387 $1/1$ 0.980.08 $54,54,54,54$ 056MG1H3175 $1/1$ 0.980.29 $67,67,67,67$ 056MG143111 $1/1$ 0.980.22 $55,55,55,55$ 056MG143187 $1/1$ 0.980.21 $53,53,53,53$ 056MG1H3355 $1/1$ 0.980.09 $47,47,47,47,47$ 056MG1H3389 $1/1$ 0.980.11 $42,42,42,42$ 056MG1H3002 $1/1$ 0.980.10 $52,52,52,52$ 056MG1H3445 $1/1$ 0.980.10 $52,52,52,52$ 056MG1H3242 $1/1$ 0.980.10 $52,52,52,52$ 056MG1H3242 $1/1$ 0.980.10 $75,75,75,75$ 056MG1G1601 $1/1$ 0.980.10 $75,75,75,75,75$ 056MG1G1601 $1/1$ 0.980.1164,64,64,64056MG143038 $1/1$ 0.980.10 $75,75,75,75,75,75,75,75,75,75,75,75,75,7$	56	MG	14	3262	1/1	0.98	0.13	66,66,66,66	0
56MG1H3387 $1/1$ 0.980.08 $54,54,54,54,54$ 056MG1H3175 $1/1$ 0.980.29 $67,67,67,67$ 056MG143111 $1/1$ 0.980.22 $55,55,55,55$ 056MG143187 $1/1$ 0.980.21 $53,53,53,53,53$ 056MG1H3355 $1/1$ 0.980.09 $47,47,47,47,47$ 056MG1H3442 $1/1$ 0.980.11 $42,42,42,42$ 056MG1H3002 $1/1$ 0.980.14 $68,68,68,68$ 056MG1H3002 $1/1$ 0.980.10 $52,52,52,52$ 056MG1H3002 $1/1$ 0.980.10 $52,52,52,52,52,52$ 056MG1H3445 $1/1$ 0.980.10 $52,52,52,52,52,52,52,52,52,52,52,52,52,5$	56	MG	1H	3079	1/1	0.98	0.26	$45,\!45,\!45,\!45$	0
56MG1H 3175 $1/1$ 0.98 0.29 $67,67,67,67$ 0 56 MG14 3111 $1/1$ 0.98 0.22 $55,55,55,55$ 0 56 MG14 3187 $1/1$ 0.98 0.21 $53,53,53,53$ 0 56 MG14 3355 $1/1$ 0.98 0.09 $47,47,47,47,47$ 0 56 MG1H 3442 $1/1$ 0.98 0.11 $42,42,42,42$ 0 56 MG1H 3302 $1/1$ 0.98 0.14 $68,68,68,68$ 0 56 MG1H 3445 $1/1$ 0.98 0.18 $40,40,40,40$ 0 56 MG1H 3445 $1/1$ 0.98 0.13 $63,63,63,63$ 0 56 MG1H 3242 $1/1$ 0.98 0.10 $52,52,52,52,52$ 0 56 MG1H 3242 $1/1$ 0.98 0.10 $52,57,57,57,57,57,57,55$ 0 56 MG1G 1601 $1/1$ 0.98 0.10 $75,75,75,75,75,75,75,75,75,75,75,75,75,7$	56	MG	1H	3387	1/1	0.98	0.08	$54,\!54,\!54,\!54$	0
56MG14 3111 $1/1$ 0.98 0.22 $55,55,55,55$ 0 56 MG14 3187 $1/1$ 0.98 0.21 $53,53,53,53$ 0 56 MG14 3355 $1/1$ 0.98 0.09 $47,47,47,47,47$ 0 56 MG1H 3442 $1/1$ 0.98 0.11 $42,42,42,42$ 0 56 MG1H 3389 $1/1$ 0.98 0.14 $68,68,68,68$ 0 56 MG1H 3002 $1/1$ 0.98 0.18 $40,40,40,40$ 0 56 MG1H 3445 $1/1$ 0.98 0.10 $52,52,52,52$ 0 56 MG1H 3445 $1/1$ 0.98 0.10 $52,52,52,52$ 0 56 MG1H 3242 $1/1$ 0.98 0.10 $52,52,57,57$ 0 56 MG1H 3242 $1/1$ 0.98 0.10 $75,75,75,75$ 0 56 MG1G1601 $1/1$ 0.98 0.10 $65,65,65,65$ 0 56 MG14 3038 $1/1$ 0.98 0.11 $64,64,64,64$ 0 56 MG14 3038 $1/1$ 0.98 0.10 $53,53,53,53$ 0 56 MG14 3368 $1/1$ 0.98 0.10 $53,53,53,53$ 0 56 MG14 3370 $1/1$ 0.98 0.10 $68,68,68,68$ <td>56</td> <td>MG</td> <td>1H</td> <td>3175</td> <td>1/1</td> <td>0.98</td> <td>0.29</td> <td>$67,\!67,\!67,\!67$</td> <td>0</td>	56	MG	1H	3175	1/1	0.98	0.29	$67,\!67,\!67,\!67$	0
56MG14 3187 $1/1$ 0.98 0.21 $53,53,53,53$ 0 56 MG14 3355 $1/1$ 0.98 0.09 $47,47,47,47$ 0 56 MG1H 3442 $1/1$ 0.98 0.11 $42,42,42,42$ 0 56 MG1H 3389 $1/1$ 0.98 0.14 $68,68,68,68$ 0 56 MG1H 3002 $1/1$ 0.98 0.18 $40,40,40,40$ 0 56 MG1H 3445 $1/1$ 0.98 0.10 $52,52,52,52$ 0 56 MG14 3360 $1/1$ 0.98 0.10 $52,52,52,52$ 0 56 MG1H 3242 $1/1$ 0.98 0.10 $52,52,52,55$ 0 56 MG1H 3242 $1/1$ 0.98 0.29 $58,58,58,58$ 0 56 MG1G 1601 $1/1$ 0.98 0.10 $75,75,75,75$ 0 56 MG1G 1602 $1/1$ 0.98 0.11 $64,64,64,64$ 0 56 MG14 3038 $1/1$ 0.98 0.27 $74,74,74,74$ 0 56 MG14 3040 $1/1$ 0.98 0.23 $48,48,48,48$ 0 56 MG1H 3114 $1/1$ 0.98 0.10 $53,53,53,53$ 0 56 MG1H 3395 $1/1$ 0.98 0.10 $68,68,68,68$ <td>56</td> <td>MG</td> <td>14</td> <td>3111</td> <td>1/1</td> <td>0.98</td> <td>0.22</td> <td>$55,\!55,\!55,\!55$</td> <td>0</td>	56	MG	14	3111	1/1	0.98	0.22	$55,\!55,\!55,\!55$	0
56MG14 3355 $1/1$ 0.98 0.09 $47,47,47,47,47$ 0 56 MG1H 3442 $1/1$ 0.98 0.11 $42,42,42,42$ 0 56 MG1H 3389 $1/1$ 0.98 0.14 $68,68,68,68$ 0 56 MG1H 3002 $1/1$ 0.98 0.14 $68,68,68,68$ 0 56 MG1H 3445 $1/1$ 0.98 0.10 $52,52,52,52$ 0 56 MG14 3360 $1/1$ 0.98 0.13 $63,63,63,63$ 0 56 MG1H 3242 $1/1$ 0.98 0.29 $58,58,58,58$ 0 56 MG13 1640 $1/1$ 0.98 0.10 $75,75,75,75$ 0 56 MG1G 1601 $1/1$ 0.98 0.10 $75,75,75,75$ 0 56 MG14 3038 $1/1$ 0.98 0.11 $64,64,64,64$ 0 56 MG14 3038 $1/1$ 0.98 0.27 $74,74,74,74$ 0 56 MG14 3040 $1/1$ 0.98 0.21 $43,43,43,43$ 0 56 MG1H 3114 $1/1$ 0.98 0.10 $53,53,53,53$ 0 56 MG1H 3395 $1/1$ 0.98 0.23 $48,48,48,48$ 0 56 MG1H 3115 $1/1$ 0.98 0.27 $53,53,53,53$ <	56	MG	14	3187	1/1	0.98	0.21	$53,\!53,\!53,\!53$	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3355	1/1	0.98	0.09	$47,\!47,\!47,\!47$	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3442	1/1	0.98	0.11	42,42,42,42	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3389	1/1	0.98	0.14	$68,\!68,\!68,\!68$	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3002	1/1	0.98	0.18	40,40,40,40	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3445	1/1	0.98	0.10	52,52,52,52	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3360	1/1	0.98	0.13	$63,\!63,\!63,\!63$	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3242	1/1	0.98	0.29	58, 58, 58, 58	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	13	1640	1/1	0.98	0.10	75,75,75,75	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1G	1601	1/1	0.98	0.20	$65,\!65,\!65,\!65$	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1G	1602	1/1	0.98	0.11	64,64,64,64	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3038	1/1	0.98	0.15	34,34,34,34	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	13	1621	1/1	0.98	0.27	74,74,74,74	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3040	1/1	0.98	0.21	43,43,43,43	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3368	1/1	0.98	0.10	53,53,53,53	0
56 MG 14 3370 1/1 0.98 0.10 68,68,68,68 0 56 MG 1H 3395 1/1 0.98 0.09 45,45,45,45 0 56 MG 1H 3115 1/1 0.98 0.34 51,51,51,51 0 56 MG 1G 1607 1/1 0.98 0.34 51,51,51,51 0 56 MG 1G 1607 1/1 0.98 0.16 81,81,81,81 0 56 MG 1H 3022 1/1 0.98 0.27 53,53,53,53 0 56 MG 1H 3084 1/1 0.98 0.28 48,48,48,48 0 56 MG 13 1675 1/1 0.98 0.10 73,73,73,73 0 56 MG 13 1605 1/1 0.98 0.18 67,67,67,67 0 56 MG 1H 3007 1/1	56	MG	1H	3114	1/1	0.98	0.23	48,48,48,48	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	14	3370	1/1	0.98	0.10	68,68,68,68	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3395	1/1	0.98	0.09	45,45,45,45	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	56	MG	1H	3115	1/1	0.98	0.34	51,51,51,51	0
56 MG 1H 3022 1/1 0.98 0.27 53,53,53,53 0 56 MG 1H 3084 1/1 0.98 0.28 48,48,48,48 0 56 MG 13 1675 1/1 0.98 0.10 73,73,73,73 0 56 MG 13 1605 1/1 0.98 0.18 67,67,67,67 0 56 MG 1H 3007 1/1 0.98 0.32 46,46,46,46 0	56	MG	1G	1607	1/1	0.98	0.16	81,81,81,81	0
56 MG 1H 3084 1/1 0.98 0.28 48,48,48,48 0 56 MG 13 1675 1/1 0.98 0.10 73,73,73,73 0 56 MG 13 1605 1/1 0.98 0.10 73,73,73,73 0 56 MG 13 1605 1/1 0.98 0.18 67,67,67,67 0 56 MG 1H 3007 1/1 0.98 0.32 46,46,46,46 0	56	MG	1H	3022	1/1	0.98	0.27	53,53,53,53	0
56 MG 13 1675 1/1 0.98 0.10 73,73,73,73 0 56 MG 13 1605 1/1 0.98 0.18 67,67,67,67 0 56 MG 1H 3007 1/1 0.98 0.32 46,46,46,46 0	56	MG	1H	3084	1/1	0.98	0.28	48,48,48,48	0
56 MG 13 1605 1/1 0.98 0.18 67,67,67,67 0 56 MG 1H 3007 1/1 0.98 0.32 46,46,46,46 0	56	MG	13	1675	1/1	0.98	0.10	73,73,73,73	0
56 MG 1H 3007 1/1 0.98 0.32 46,46,46,46 0	56	MG	13	1605	1/1	0.98	0.18	67,67,67,67	0
	56	MG	1H	3007	1/1	0.98	0.32	46,46,46,46	0
$56 \mid MG \mid 1H \mid 3402 \mid 1/1 \mid 0.98 \mid 0.10 \mid 48.48.48.48 \mid 0$	56	MG	1H	3402	1/1	0.98	0.10	48,48,48,48	0
56 MG 13 1615 1/1 0.98 0.28 92.92.92.92 0	56	MG	13	1615	1/1	0.98	0.28	92,92,92,92	0
56 MG 1H 3090 1/1 0.98 0.21 44,44,44,44 0	56	MG	1H	3090	1/1	0.98	0.21	44,44,44,44	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
56	MG	1H	3362	1/1	0.98	0.23	69,69,69,69	0
56	MG	1H	3407	1/1	0.98	0.07	57,57,57,57	0
56	MG	1G	1618	1/1	0.98	0.13	88,88,88,88	0
56	MG	1H	3408	1/1	0.98	0.11	47,47,47,47	0
56	MG	14	3064	1/1	0.98	0.15	71,71,71,71	0
56	MG	1G	1678	1/1	0.98	0.16	98,98,98,98	0
56	MG	1H	3009	1/1	0.98	0.27	43,43,43,43	0
56	MG	1H	3410	1/1	0.98	0.11	46,46,46,46	0
56	MG	14	3143	1/1	0.98	0.21	67,67,67,67	0
56	MG	1H	3291	1/1	0.98	0.25	40,40,40,40	0
56	MG	1H	3412	1/1	0.98	0.15	32,32,32,32	0
56	MG	1H	3413	1/1	0.98	0.17	44,44,44,44	0
56	MG	1H	3010	1/1	0.98	0.18	54,54,54,54	0
56	MG	1H	3126	1/1	0.98	0.34	60,60,60,60	0
56	MG	1H	3093	1/1	0.98	0.09	47,47,47,47	0
56	MG	14	3150	1/1	0.98	0.18	$51,\!51,\!51,\!51$	0
56	MG	14	3227	1/1	0.98	0.13	88,88,88,88	0
56	MG	1H	3417	1/1	0.98	0.15	61,61,61,61	0
56	MG	1H	3418	1/1	0.98	0.06	42,42,42,42	0
56	MG	1G	1630	1/1	0.98	0.24	75,75,75,75	0
56	MG	14	3311	1/1	0.98	0.12	$51,\!51,\!51,\!51$	0
56	MG	14	3078	1/1	0.98	0.29	$50,\!50,\!50,\!50$	0
56	MG	13	1629	1/1	0.98	0.18	46,46,46,46	0
56	MG	13	1630	1/1	0.98	0.18	43,43,43,43	0
56	MG	1H	3049	1/1	0.98	0.28	60,60,60,60	0
56	MG	14	3236	1/1	0.98	0.23	75, 75, 75, 75	0
56	MG	14	3003	1/1	0.98	0.09	54,54,54,54	0
58	ZN	5I	101	1/1	0.98	0.16	88,88,88,88	0
56	MG	14	3319	1/1	0.98	0.08	62,62,62,62	0
58	ZN	32	301	1/1	0.98	0.36	96,96,96,96	0
56	MG	14	3320	1/1	0.98	0.23	60,60,60,60	0
56	MG	13	1604	1/1	0.98	0.10	68,68,68,68	0
56	MG	14	3061	1/1	0.99	0.22	50,50,50,50	0
56	MG	14	3062	1/1	0.99	0.18	56,56,56,56	0
56	MG	14	3063	1/1	0.99	0.29	66,66,66,66	0
56	MG	14	3347	1/1	0.99	0.07	56,56,56,56	0
56	MG	1H	3061	1/1	0.99	0.12	48,48,48,48	0
56	MG	1H	3419	1/1	0.99	0.10	37,37,37,37	0
56	MG	1H	3136	1/1	0.99	0.27	41,41,41,41	0
56	MG	14	3351	1/1	0.99	0.13	43,43,43,43	0
56	MG	1H	3107	1/1	0.99	0.28	65,65,65,65	0
56	MG	14	3318	1/1	0.99	0.10	$57,\!57,\!57,\!57$	0



4WRA

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\operatorname{\AA}^2)$	Q<0.9
56	MG	13	1608	1/1	0.99	0.17	71,71,71,71	0
56	MG	14	3099	1/1	0.99	0.19	46,46,46,46	0
56	MG	1H	3472	1/1	0.99	0.14	56, 56, 56, 56	0
56	MG	1H	3455	1/1	0.99	0.08	$57,\!57,\!57,\!57$	0
56	MG	14	3071	1/1	0.99	0.19	61,61,61,61	0
56	MG	1H	3423	1/1	0.99	0.07	44,44,44,44	0
56	MG	11	301	1/1	0.99	0.20	48,48,48,48	0
56	MG	1H	3087	1/1	0.99	0.37	43,43,43,43	0
56	MG	14	3230	1/1	0.99	0.30	73,73,73,73	0
56	MG	29	301	1/1	0.99	0.18	44,44,44,44	0
56	MG	13	1601	1/1	0.99	0.23	46,46,46,46	0
56	MG	29	303	1/1	0.99	0.20	71,71,71,71	0
56	MG	14	3046	1/1	0.99	0.09	$53,\!53,\!53,\!53$	0
56	MG	1H	3111	1/1	0.99	0.20	43,43,43,43	0
56	MG	13	1618	1/1	0.99	0.17	58, 58, 58, 58	0
56	MG	14	3049	1/1	0.99	0.18	54,54,54,54	0
56	MG	14	3050	1/1	0.99	0.20	63,63,63,63	0
56	MG	14	3005	1/1	0.99	0.21	$53,\!53,\!53,\!53$	0
56	MG	13	1652	1/1	0.99	0.20	80,80,80,80	0
56	MG	14	3053	1/1	0.99	0.22	52,52,52,52	0
56	MG	1H	3480	1/1	0.99	0.20	56, 56, 56, 56	0
56	MG	1H	3020	1/1	0.99	0.20	47,47,47,47	0
56	MG	14	3030	1/1	0.99	0.14	$55,\!55,\!55,\!55$	0
56	MG	1H	3374	1/1	0.99	0.10	$50,\!50,\!50,\!50$	0
56	MG	1H	3266	1/1	0.99	0.07	64,64,64,64	0
56	MG	1H	3124	1/1	0.99	0.19	52,52,52,52	0
56	MG	1H	3403	1/1	0.99	0.16	43,43,43,43	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.







6.5 Other polymers (i)

There are no such residues in this entry.

