Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 04:20 AM EST

PDB ID	:	6N9F
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with a short substrate mimic ACCA-DPhe and bound to mRNA and P-site tRNA at 3.7A resolution
Authors	:	Melnikov, S.V.; Khabibullina, N.F.; Mairhofer, E.; Vargas-Rodriguez, O.; Reynolds, N.M.; Micura, R.; Soll, D.; Polikanov, Y.S.
Deposited on	:	2018-12-03
Resolution	:	3.70 Å(reported)

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

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

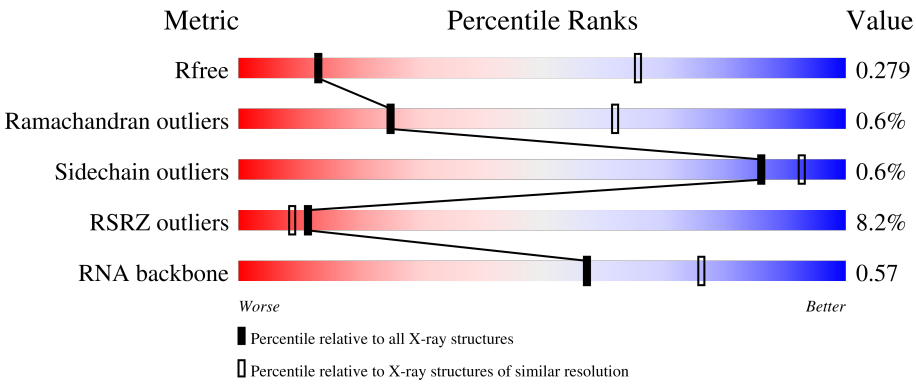
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1049 (3.88-3.52)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)
RNA backbone	3102	1027 (4.40-3.00)

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	1A	2915	3%, 83%, 15%, •
1	2A	2915	5%, 80%, 16%, •
2	1B	121	90%, 8%, ••
2	2B	121	88%, 11%, ••

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Mol	Chain	Length	Quality of chain
3	1D	276	6% 99%
3	2D	276	22% 99%
4	1E	206	13% 98%
4	2E	206	14% 98%
5	1F	210	6% 96%
5	2F	210	15% 96%
6	1G	182	98%
6	2G	182	13% 97%
7	1H	180	% 96%
7	2H	180	7% 96%
8	1I	148	2% 97%
8	2I	148	8% 97%
9	1N	140	7% 100%
9	2N	140	15% 99%
10	1O	122	30% 100%
10	2O	122	16% 99%
11	1P	150	5% 96%
11	2P	150	22% 97%
12	1Q	141	23% 99%
12	2Q	141	11% 100%
13	1R	118	3% 99%
13	2R	118	8% 100%
14	1S	112	98%
14	2S	112	% 97%
15	1T	146	8% 90% 10%

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Mol	Chain	Length	Quality of chain
15	2T	146	14% 90% 10%
16	1U	118	3% 98%
16	2U	118	27% 98%
17	1V	101	% 98%
17	2V	101	11% 97%
18	1W	113	9% 98%
18	2W	113	17% 99%
19	1X	96	8% 99%
19	2X	96	8% 99%
20	1Y	110	3% 95%
20	2Y	110	19% 96%
21	1Z	206	73% 25%
21	2Z	206	76% 22%
22	10	85	15% 96%
22	20	85	21% 98%
23	11	98	22% 96%
23	21	98	39% 98%
24	12	72	97%
24	22	72	% 97%
25	13	60	98%
25	23	60	18% 98%
26	14	71	89% 8%
26	24	71	% 89% 7%
27	15	60	17% 97%
27	25	60	8% 97%

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Mol	Chain	Length	Quality of chain
28	16	54	2%, 98%
28	26	54	26%, 98%
29	17	49	16%, 98%
29	27	49	47%, 98%
30	18	65	5%, 98%
30	28	65	54%, 98%
31	19	37	100%
31	29	37	38%, 100%
32	1a	1521	3%, 82%, 17%
32	2a	1521	2%, 82%, 17%
33	1b	256	2%, 89%, 10%
33	2b	256	5%, 87%, 10%
34	1c	239	21%, 85%, 14%
34	2c	239	10%, 86%, 14%
35	1d	209	15%, 98%
35	2d	209	8%, 99%
36	1e	162	20%, 91%, 9%
36	2e	162	20%, 91%, 9%
37	1f	101	2%, 99%
37	2f	101	5%, 99%
38	1g	156	5%, 96%
38	2g	156	7%, 97%
39	1h	138	5%, 99%
39	2h	138	9%, 98%
40	1i	128	23%, 98%

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Mol	Chain	Length	Quality of chain
40	2i	128	25% 98%
41	1j	105	21% 91% 8%
41	2j	105	13% 90% 9%
42	1k	129	6% 88% 12%
42	2k	129	20% 87% 12%
43	1l	132	16% 92% 8%
43	2l	132	20% 92% 8%
44	1m	126	8% 97%
44	2m	126	17% 97%
45	1n	61	23% 97%
45	2n	61	15% 97%
46	1o	89	8% 98%
46	2o	89	2% 99%
47	1p	88	22% 91% 7%
47	2p	88	3% 92% 7%
48	1q	105	5% 94% 6%
48	2q	105	13% 94% 6%
49	1r	88	77% 23%
49	2r	88	7% 77% 23%
50	1s	93	87% 11%
50	2s	93	14% 87% 11%
51	1t	106	15% 88% 9%
51	2t	106	13% 87% 9%
52	1u	27	15% 85% 15%
52	2u	27	7% 85% 15%

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Mol	Chain	Length	Quality of chain
53	1v	24	12% 25% 71%
53	2v	24	4% 25% 75%
54	1w	4	50% 50%
54	2w	4	25% 75%
55	1x	77	% 83% 16%
55	2x	77	5% 78% 21%

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	17	101	-	-	-	X
56	MG	1A	3043	-	-	-	X
56	MG	1A	3058	-	-	-	X
56	MG	1A	3064	-	-	-	X
56	MG	1A	3075	-	-	-	X
56	MG	1A	3090	-	-	-	X
56	MG	1A	3093	-	-	-	X
56	MG	1A	3128	-	-	-	X
56	MG	1A	3130	-	-	-	X
56	MG	1A	3175	-	-	-	X
56	MG	1A	3182	-	-	-	X
56	MG	1A	3188	-	-	-	X
56	MG	1A	3189	-	-	-	X
56	MG	1A	3190	-	-	-	X
56	MG	1A	3191	-	-	-	X
56	MG	1A	3214	-	-	-	X
56	MG	1A	3218	-	-	-	X
56	MG	1A	3245	-	-	-	X
56	MG	1A	3259	-	-	-	X
56	MG	1A	3294	-	-	-	X
56	MG	1A	3299	-	-	-	X
56	MG	1A	3304	-	-	-	X
56	MG	1A	3346	-	-	-	X
56	MG	1A	3373	-	-	-	X
56	MG	1A	3376	-	-	-	X
56	MG	1A	3390	-	-	-	X
56	MG	1A	3409	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3410	-	-	-	X
56	MG	1A	3414	-	-	-	X
56	MG	1A	3422	-	-	-	X
56	MG	1A	3429	-	-	-	X
56	MG	1A	3431	-	-	-	X
56	MG	1A	3433	-	-	-	X
56	MG	1A	3437	-	-	-	X
56	MG	1A	3440	-	-	-	X
56	MG	1A	3456	-	-	-	X
56	MG	1A	3472	-	-	-	X
56	MG	1A	3474	-	-	-	X
56	MG	1A	3477	-	-	-	X
56	MG	1A	3491	-	-	-	X
56	MG	1A	3501	-	-	-	X
56	MG	1A	3511	-	-	-	X
56	MG	1A	3515	-	-	-	X
56	MG	1B	210	-	-	-	X
56	MG	1B	213	-	-	-	X
56	MG	1B	217	-	-	-	X
56	MG	1D	303	-	-	-	X
56	MG	1E	303	-	-	-	X
56	MG	1F	302	-	-	-	X
56	MG	1P	202	-	-	-	X
56	MG	1Q	202	-	-	-	X
56	MG	1T	202	-	-	-	X
56	MG	1V	202	-	-	-	X
56	MG	1V	203	-	-	-	X
56	MG	1W	201	-	-	-	X
56	MG	1X	101	-	-	-	X
56	MG	1a	1629	-	-	-	X
56	MG	1a	1633	-	-	-	X
56	MG	1a	1652	-	-	-	X
56	MG	1a	1674	-	-	-	X
56	MG	1v	101	-	-	-	X
56	MG	1x	109	-	-	-	X
56	MG	2A	3021	-	-	-	X
56	MG	2A	3022	-	-	-	X
56	MG	2A	3036	-	-	-	X
56	MG	2A	3043	-	-	-	X
56	MG	2A	3046	-	-	-	X
56	MG	2A	3058	-	-	-	X
56	MG	2A	3082	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3086	-	-	-	X
56	MG	2A	3087	-	-	-	X
56	MG	2A	3088	-	-	-	X
56	MG	2A	3095	-	-	-	X
56	MG	2A	3098	-	-	-	X
56	MG	2A	3101	-	-	-	X
56	MG	2A	3106	-	-	-	X
56	MG	2A	3122	-	-	-	X
56	MG	2A	3144	-	-	-	X
56	MG	2A	3170	-	-	-	X
56	MG	2A	3182	-	-	-	X
56	MG	2A	3191	-	-	-	X
56	MG	2A	3203	-	-	-	X
56	MG	2A	3205	-	-	-	X
56	MG	2A	3220	-	-	-	X
56	MG	2A	3240	-	-	-	X
56	MG	2A	3254	-	-	-	X
56	MG	2A	3306	-	-	-	X
56	MG	2A	3313	-	-	-	X
56	MG	2A	3327	-	-	-	X
56	MG	2A	3355	-	-	-	X
56	MG	2A	3364	-	-	-	X
56	MG	2A	3376	-	-	-	X
56	MG	2A	3381	-	-	-	X
56	MG	2A	3474	-	-	-	X
56	MG	2B	210	-	-	-	X
56	MG	2O	201	-	-	-	X
56	MG	2a	1601	-	-	-	X
56	MG	2a	1602	-	-	-	X
56	MG	2a	1606	-	-	-	X
56	MG	2a	1614	-	-	-	X
56	MG	2a	1630	-	-	-	X
56	MG	2a	1672	-	-	-	X
56	MG	2a	1703	-	-	-	X
56	MG	2l	201	-	-	-	X

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 288175 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1A	2871	61852	27531	11572	19878	2871	0	0	0
1	2A	2800	60322	26848	11284	19390	2800	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	1B	120	2577	1146	476	835	120	0	0	0
2	2B	120	2575	1146	476	833	120	0	0	0

- Molecule 3 is a protein called 50S Ribosomal Protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	1D	275	2136	1349	423	361	3	0	0	0
3	2D	275	2136	1349	423	361	3	0	0	0

- Molecule 4 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	1E	204	1559	985	298	270	6	0	0	0
4	2E	204	1559	985	298	270	6	0	0	0

- Molecule 5 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	1F	203	1584	1009	298	275	2	0	0	1
5	2F	203	1580	1007	297	274	2	0	0	1

- Molecule 6 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	1G	181	1423	913	253	253	4	0	0	0
6	2G	181	1428	913	258	253	4	0	0	0

- Molecule 7 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	1H	174	1330	845	248	236	1	0	0	0
7	2H	174	1330	845	248	236	1	0	0	0

- Molecule 8 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	1I	146	1097	701	191	204	1	0	0	0
8	2I	146	1064	681	186	196	1	0	0	0

- Molecule 9 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	1N	140	1117	719	207	187	4	0	0	0
9	2N	140	1117	719	207	187	4	0	0	0

- Molecule 10 is a protein called 50S Ribosomal Protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	1O	122	933	588	171	170	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	2O	122	933	588	171	170	4	0	0	0

- Molecule 11 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	1P	149	1135	706	230	196	3	0	0	0
			Total	C	N	O	S			
11	2P	149	1135	706	230	196	3	0	0	0

- Molecule 12 is a protein called 50S Ribosomal Protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	1Q	141	1122	715	212	188	7	0	0	0
			Total	C	N	O	S			
12	2Q	141	1122	715	212	188	7	0	0	0

- Molecule 13 is a protein called 50S Ribosomal Protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	1R	118	968	604	203	160	1	0	0	0
			Total	C	N	O	S			
13	2R	118	968	604	203	160	1	0	0	0

- Molecule 14 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	1S	110	873	550	174	149	0	0	0
			Total	C	N	O			
14	2S	110	870	549	173	148	0	0	0

- Molecule 15 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	1T	131	1091	680	225	185	1	0	0	0
			Total	C	N	O	S			
15	2T	131	1083	675	224	183	1	0	0	0

- Molecule 16 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	1U	116	959	608	201	149	1	0	0	0
16	2U	116	959	608	201	149	1	0	0	0

- Molecule 17 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	1V	101	771	495	140	135	1	0	0	0
17	2V	101	771	495	140	135	1	0	0	0

- Molecule 18 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	1W	112	886	557	174	153	2	0	0	0
18	2W	112	886	557	174	153	2	0	0	0

- Molecule 19 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	1X	95	750	488	135	126	1	0	0	0
19	2X	95	750	488	135	126	1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	1Y	107	806	517	152	131	6	0	0	0
20	2Y	107	806	517	152	131	6	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	1Z	154	1240	795	222	220	3	0	0	0
21	2Z	160	1271	814	228	227	2	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	10	83	653	404	139	109	1	0	0	0
22	20	83	653	404	139	109	1	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	11	97	755	475	148	131	1	0	0	0
23	21	97	755	475	148	131	1	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	12	70	588	365	118	103	2	0	0	0
24	22	70	588	365	118	103	2	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
25	13	59	469	298	90	81	0	0	0
25	23	59	464	296	90	78	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	14	69	552	349	99	99	5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	24	69	532	339	97	91	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	15	59	455	285	89	76	5	0	0	0
27	25	59	455	285	89	76	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	16	53	453	281	91	77	4	0	0	0
28	26	53	449	279	91	75	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	17	48	418	257	104	55	2	0	0	0
29	27	48	418	257	104	55	2	0	0	0

- Molecule 30 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	18	64	517	331	102	82	2	0	0	0
30	28	64	517	331	102	82	2	0	0	0

- Molecule 31 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	19	37	307	188	68	47	4	0	0	0
31	29	37	307	188	68	47	4	0	0	0

- Molecule 32 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
32	1a	1500	32246	14358	5975	10413	1500	0	0	0
32	2a	1503	32327	14396	5990	10438	1503	0	0	0

- Molecule 33 is a protein called 30S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	1b	231	1846	1179	331	331	5	0	0	0
33	2b	231	1825	1167	326	327	5	0	0	0

- Molecule 34 is a protein called 30S Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	1c	206	1548	973	301	273	1	0	0	0
34	2c	206	1542	968	300	273	1	0	0	0

- Molecule 35 is a protein called 30S Ribosomal Protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	1d	208	1655	1038	326	284	7	0	0	0
35	2d	208	1674	1050	333	284	7	0	0	0

- Molecule 36 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	1e	148	1129	714	213	198	4	0	0	0
36	2e	148	1133	716	214	199	4	0	0	0

- Molecule 37 is a protein called 30S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	1f	100	810	514	144	149	3	0	0	0
37	2f	100	816	516	146	151	3	0	0	0

- Molecule 38 is a protein called 30S Ribosomal Protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	1g	155	1231	766	243	216	6	0	0	0
38	2g	155	1235	769	244	216	6	0	0	0

- Molecule 39 is a protein called 30S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	1h	137	1088	689	206	191	2	0	0	0
39	2h	137	1088	689	206	191	2	0	0	0

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
40	1i	127	983	623	193	167	0	0	0
40	2i	127	978	619	190	169	0	0	0

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
41	1j	97	709	440	138	131	0	0	0
41	2j	96	714	445	138	131	0	0	0

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	1k	114	829	516	155	155	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	2k	114	833	519	156	155	3	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	1l	122	932	586	185	159	2	0	0	0
43	2l	122	932	586	185	159	2	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	1m	123	958	592	198	166	2	0	0	0
44	2m	122	950	586	197	165	2	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	1n	60	492	312	104	72	4	0	0	0
45	2n	60	492	312	104	72	4	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	1o	88	728	456	144	126	2	0	0	0
46	2o	88	728	456	144	126	2	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	1p	82	681	433	134	113	1	0	0	0
47	2p	82	677	430	133	113	1	0	0	0

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	1q	99	823	528	151	142	2	0	0	0
48	2q	99	823	528	151	142	2	0	0	0

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
49	1r	68	555	355	108	92	0	0	0
49	2r	68	555	355	108	92	0	0	0

- Molecule 50 is a protein called 30S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	1s	83	652	417	120	113	2	0	0	0
50	2s	83	646	412	119	113	2	0	0	0

- Molecule 51 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	1t	96	728	446	156	124	2	0	0	0
51	2t	96	727	446	155	124	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
52	1u	23	199	122	48	29	0	0	0
52	2u	23	199	122	48	29	0	0	0

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
53	1v	7	153	69	32	45	7	0	0	0
53	2v	6	113	49	22	36	6	0	0	0

- Molecule 54 is a RNA chain called ACCA-DPhe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
54	1w	4	75	38	13	21	3	0	0	1
54	2w	4	75	38	13	21	3	0	0	1

- Molecule 55 is a RNA chain called P-site tRNA, Deacylated Initiator Methionyl-tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
55	1x	76	1625	725	294	529	76	1	0	0	0
55	2x	76	1625	725	294	529	76	1	0	0	0

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	1A	548	548	548	0	0
56	1B	19	19	19	0	0
56	1D	4	4	4	0	0
56	1E	4	4	4	0	0
56	1F	2	2	2	0	0
56	1G	1	1	1	0	0
56	1H	1	1	1	0	0
56	1P	2	2	2	0	0
56	1Q	2	2	2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	1R	2	2	2	0	0
56	1T	3	3	3	0	0
56	1V	3	3	3	0	0
56	1W	1	1	1	0	0
56	1X	1	1	1	0	0
56	1Y	1	1	1	0	0
56	1Z	1	1	1	0	0
56	10	4	4	4	0	0
56	15	1	1	1	0	0
56	16	1	1	1	0	0
56	17	2	2	2	0	0
56	18	2	2	2	0	0
56	19	1	1	1	0	0
56	1a	89	89	89	0	0
56	1d	1	1	1	0	0
56	1e	1	1	1	0	0
56	1l	1	1	1	0	0
56	1r	1	1	1	0	0
56	1t	1	1	1	0	0
56	1v	1	1	1	0	0
56	1x	9	9	9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	2A	474	474	474	0	0
56	2B	10	10	10	0	0
56	2D	3	3	3	0	0
56	2E	5	5	5	0	0
56	2F	1	1	1	0	0
56	2O	1	1	1	0	0
56	2Q	1	1	1	0	0
56	2R	2	2	2	0	0
56	2W	1	1	1	0	0
56	2Z	1	1	1	0	0
56	20	1	1	1	0	0
56	21	1	1	1	0	0
56	23	1	1	1	0	0
56	25	1	1	1	0	0
56	27	1	1	1	0	0
56	28	2	2	2	0	0
56	2a	113	113	113	0	0
56	2c	1	1	1	0	0
56	2d	1	1	1	0	0
56	2f	2	2	2	0	0
56	2l	2	2	2	0	0

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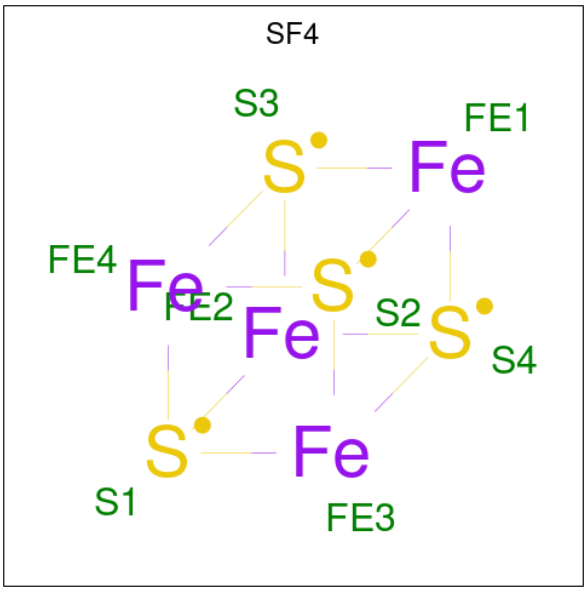
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2n	1	Total Mg 1 1	0	0
56	2q	1	Total Mg 1 1	0	0
56	2r	1	Total Mg 1 1	0	0
56	2x	1	Total Mg 1 1	0	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1Y	1	Total Zn 1 1	0	0
57	14	1	Total Zn 1 1	0	0
57	15	1	Total Zn 1 1	0	0
57	16	1	Total Zn 1 1	0	0
57	19	1	Total Zn 1 1	0	0
57	1n	1	Total Zn 1 1	0	0
57	2Y	1	Total Zn 1 1	0	0
57	24	1	Total Zn 1 1	0	0
57	25	1	Total Zn 1 1	0	0
57	26	1	Total Zn 1 1	0	0
57	29	1	Total Zn 1 1	0	0
57	2n	1	Total Zn 1 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
58	1d	1	8	4	4	0	0
			Total	Fe	S		
58	2d	1	8	4	4	0	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
59	1A	145	145	145	0	0
			Total	O		
59	1B	6	6	6	0	0
			Total	O		
59	1D	4	4	4	0	0
			Total	O		
59	1F	2	2	2	0	0
			Total	O		
59	1O	1	1	1	0	0
			Total	O		
59	1X	1	1	1	0	0
			Total	O		
59	10	1	1	1	0	0
			Total	O		
59	1a	12	12	12	0	0
			Total	O		
59	2A	44	44	44	0	0
			Total	O		
59	2E	1	1	1	0	0

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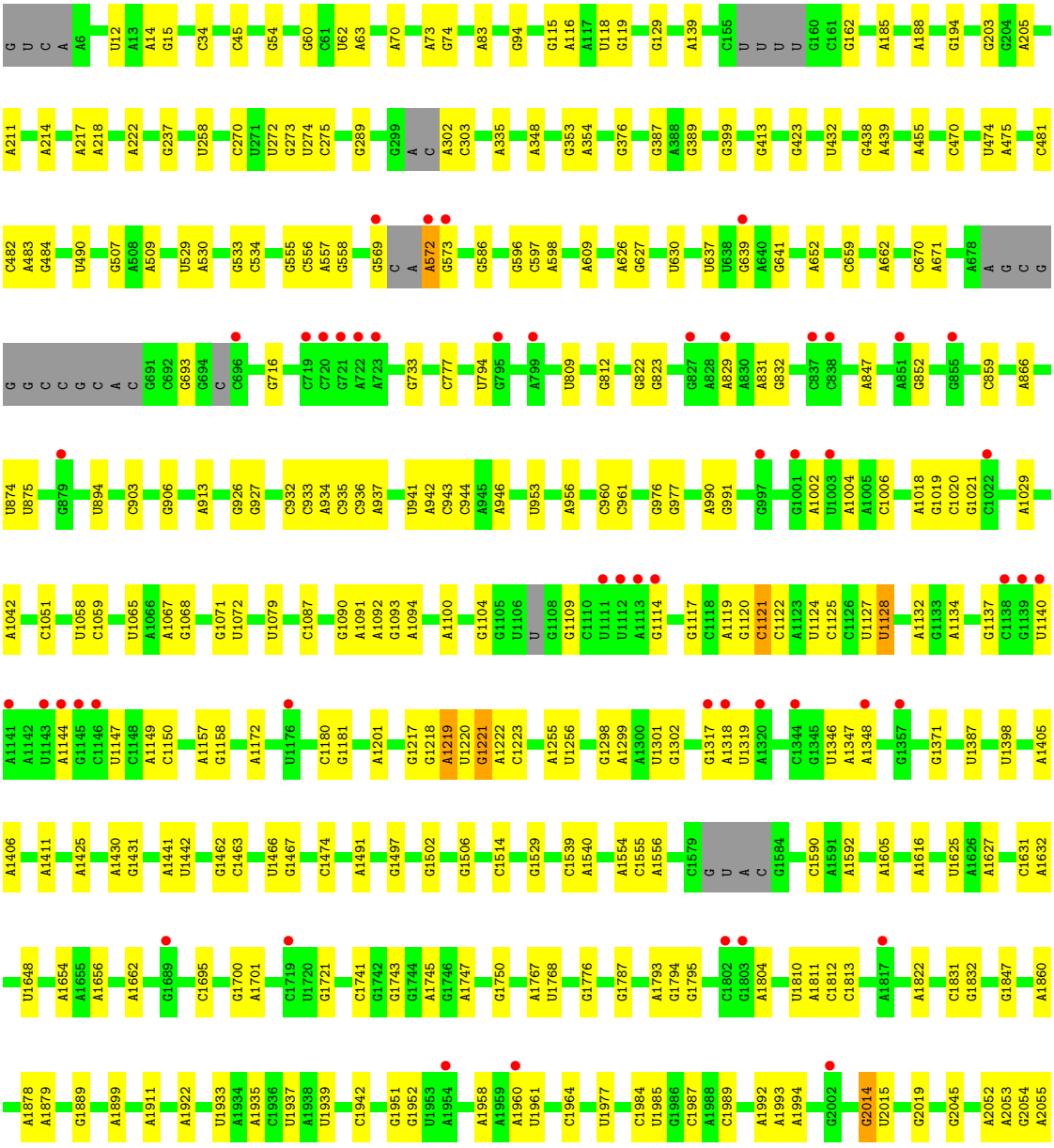
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
59	2a	30	30	30	0	0

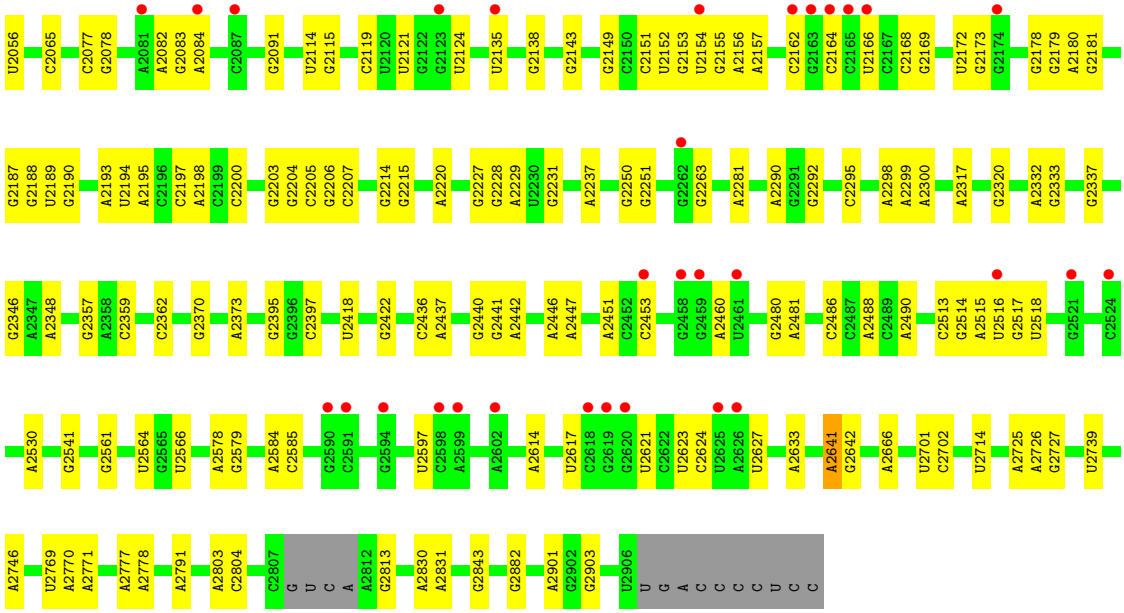
3 Residue-property plots (i)

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: 23S Ribosomal RNA

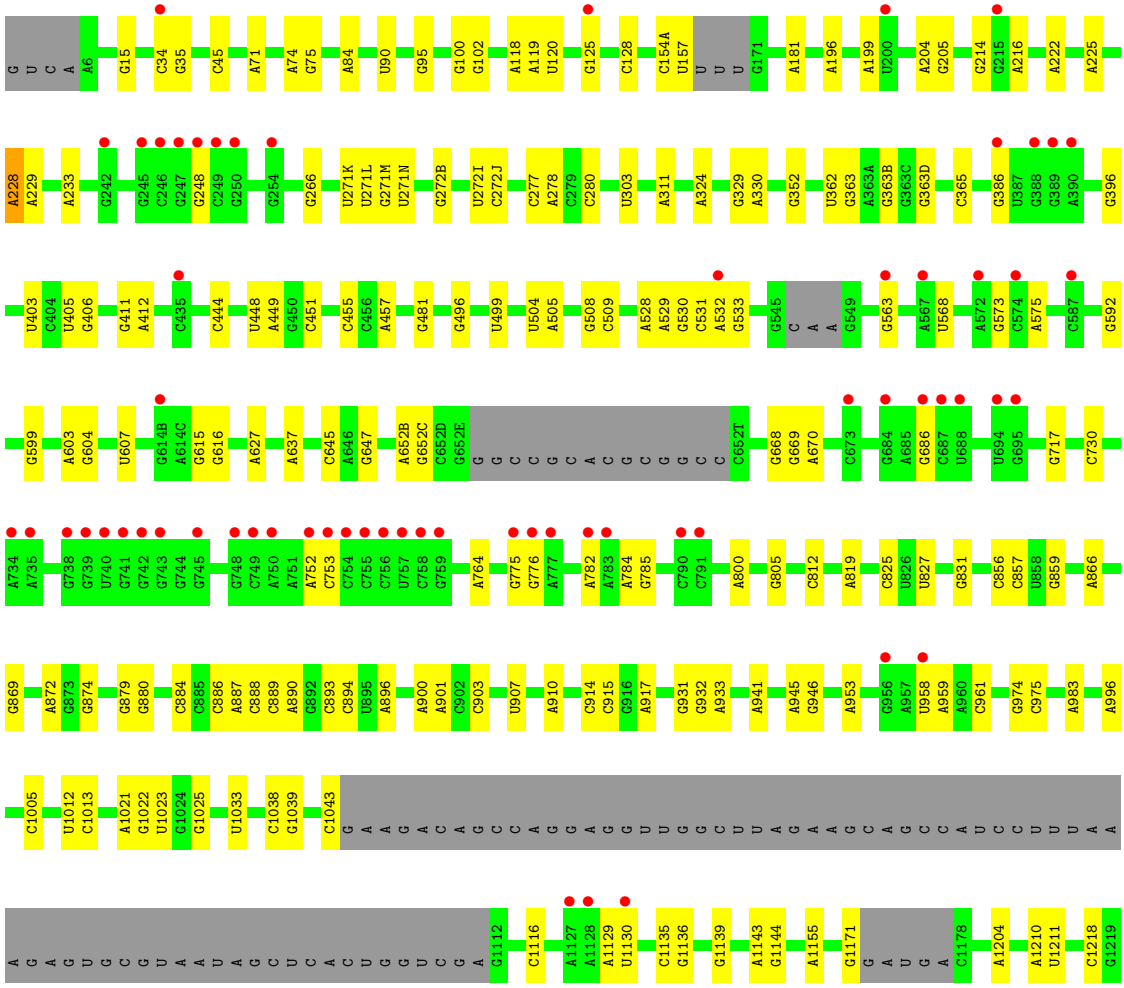
Chain 1A:

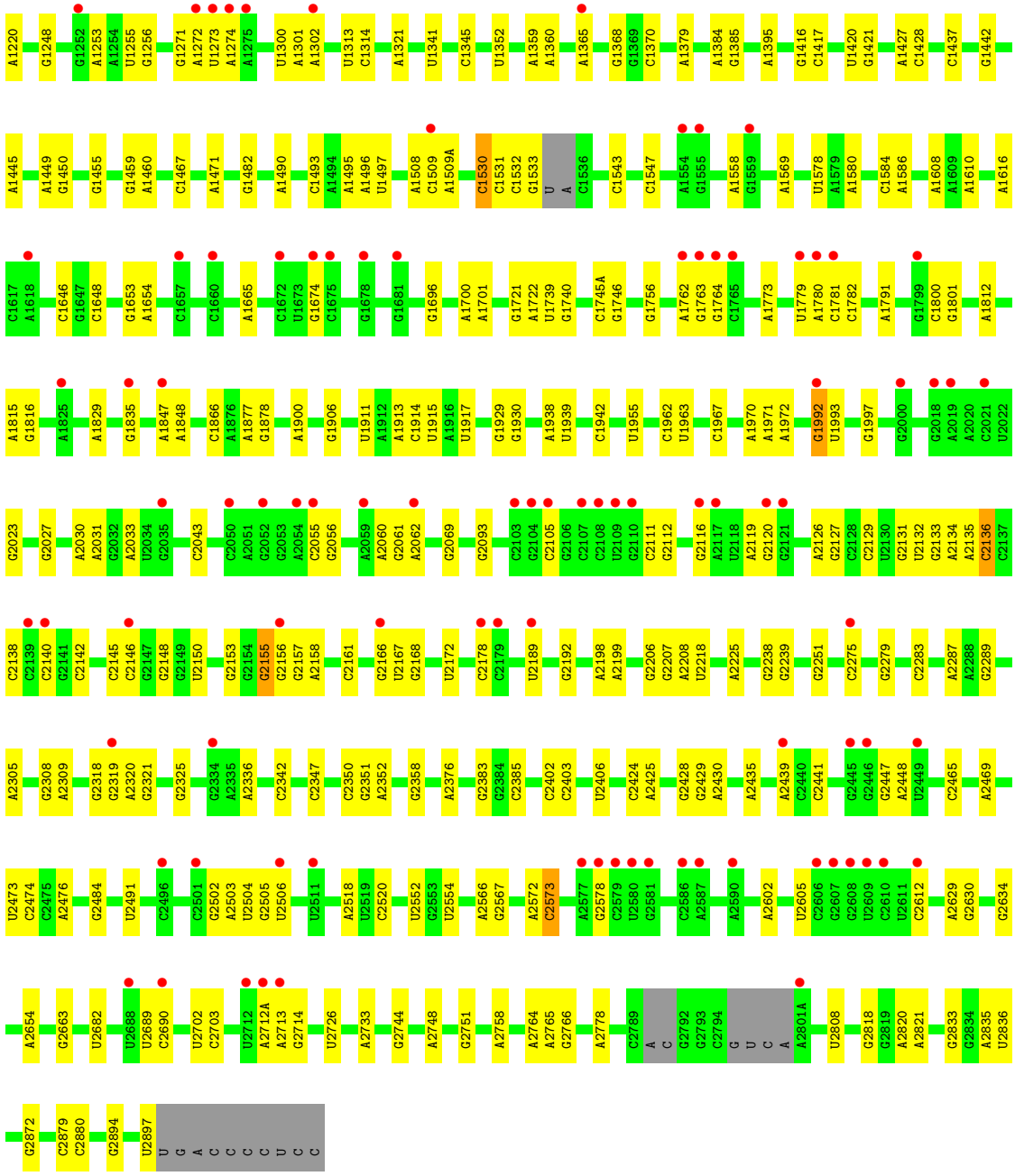




• Molecule 1: 23S Ribosomal RNA

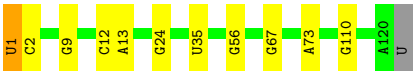
Chain 2A:





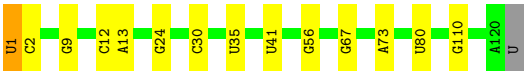
- Molecule 2: 5S Ribosomal RNA

Chain 1B:



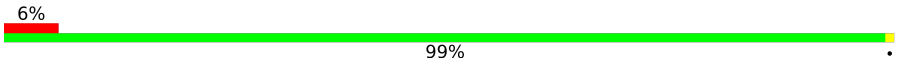
- Molecule 2: 5S Ribosomal RNA

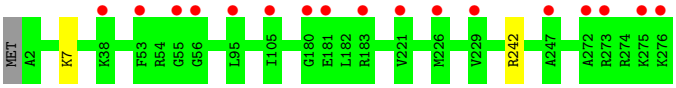
Chain 2B:



• Molecule 3: 50S Ribosomal Protein L2

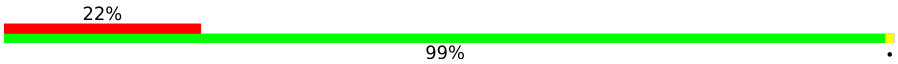
Chain 1D:

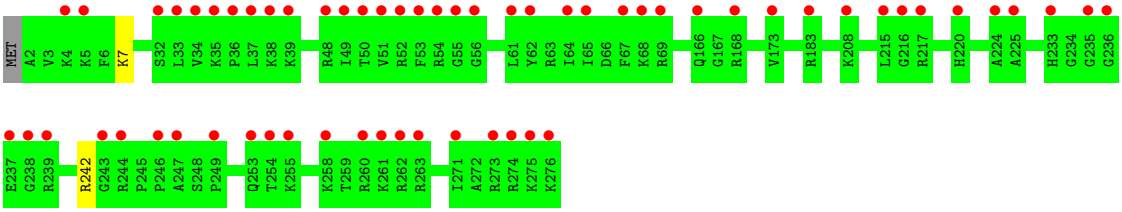




• Molecule 3: 50S Ribosomal Protein L2

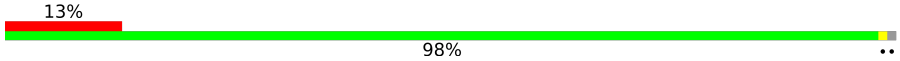
Chain 2D:

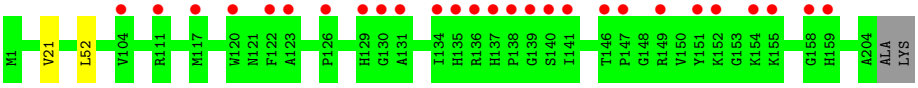




• Molecule 4: 50S Ribosomal Protein L3

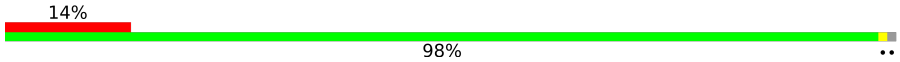
Chain 1E:

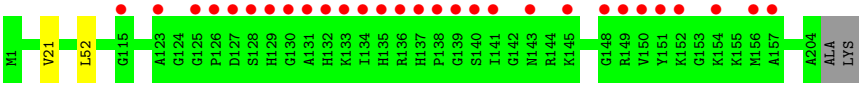




• Molecule 4: 50S Ribosomal Protein L3

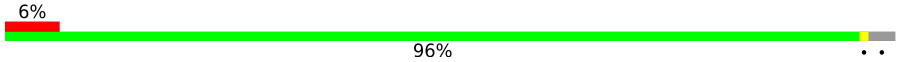
Chain 2E:

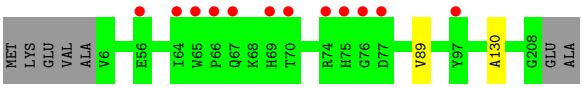




• Molecule 5: 50S Ribosomal Protein L4

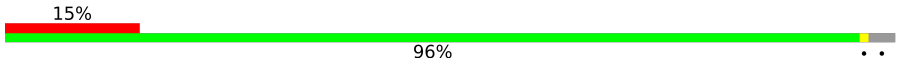
Chain 1F:

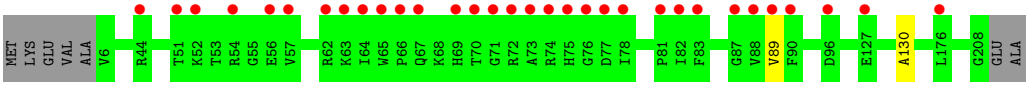




• Molecule 5: 50S Ribosomal Protein L4

Chain 2F:



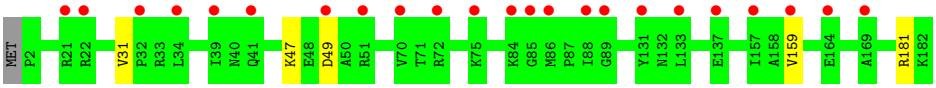


• Molecule 6: 50S Ribosomal Protein L5

Chain 1G: 98%

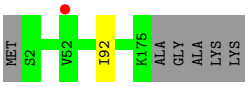
• Molecule 6: 50S Ribosomal Protein L5

Chain 2G: 13% 97%



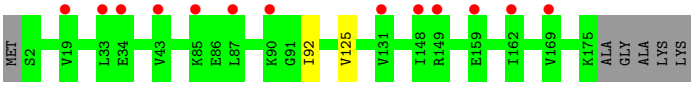
• Molecule 7: 50S Ribosomal Protein L6

Chain 1H: % 96%



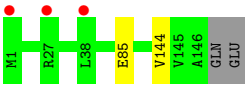
• Molecule 7: 50S Ribosomal Protein L6

Chain 2H: 7% 96%



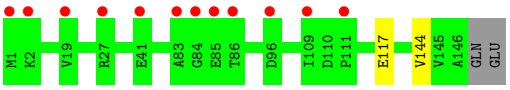
• Molecule 8: 50S Ribosomal Protein L9

Chain 1I: 2% 97%



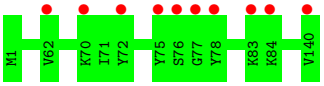
• Molecule 8: 50S Ribosomal Protein L9

Chain 2I: 8% 97%



• Molecule 9: 50S Ribosomal Protein L13

Chain 1N: 7% 100%



• Molecule 9: 50S Ribosomal Protein L13

Chain 2N: 15% 99%

M1 Q8 V9 L23 T43 A47 M48 V52 D58 R61 Y72 G77 L82 K83 K84 I85 K109 G110 P111 L112 R115 L116 R119 L120 V140

• Molecule 10: 50S Ribosomal Protein L14

Chain 1O: 30% 100%

M1 I2 Q3 P4 Q5 T6 Y7 L8 E9 V10 A11 R17 K18 I19 M20 C21 I22 R23 V24 L25 K26 G27 G36 I39 V40 A41 K44 E45 D56 V57 V58 V61 V62 V63 R64 I77 N82 A83 A84 V85 I86 P93 V98 F99 G100 L122

• Molecule 10: 50S Ribosomal Protein L14

Chain 2O: 16% 99%

M1 I2 Q3 P4 Q5 T6 Y7 L8 I19 M20 C21 I22 K31 Y32 A41 A46 K66 K67 I77 R78 N82 G100 L122

• Molecule 11: 50S Ribosomal Protein L15

Chain 1P: 5% 96%

M1 K17 R18 K29 H35 K36 G37 Q38 K39 L45 R49 L106 E119 E149 ALA

• Molecule 11: 50S Ribosomal Protein L15

Chain 2P: 22% 97%

M1 K17 R18 V19 P23 K29 H35 K36 L45 K46 D47 P48 R49 R50 G54 R55 S56 T57 T58 L59 M60 R61 L62 P63 K64 R65 Q68 G69 Q70 V71 P72 G73 E74 I75 K76 R77 P78 R79 L106 K107 K108 G109 E149 ALA

• Molecule 12: 50S Ribosomal Protein L16

Chain 1Q: 23% 99%

M1 L2 M3 P4 Y9 R10 K11 Q12 L17 A20 A40 W41 F65 I66 R67 I68 F69 P70 D71 K72 P73 Y74 T75 E80 K85 G86 K87 Y93 V96 P99 G100 M103 F104 E105 V106 T110 K130 I131 Q141

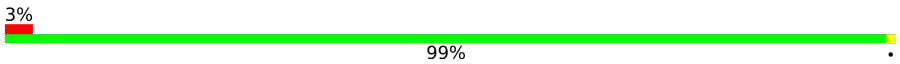
• Molecule 12: 50S Ribosomal Protein L16

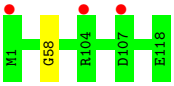
Chain 2Q: 11% 100%

M1 L34 L37 E38 P39 A40 W41 K77 P78 L79 E80 G84 K85 V97 K98 K128 Q141

• Molecule 13: 50S Ribosomal Protein L17

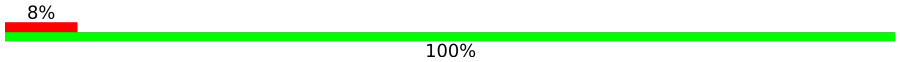
Chain 1R:

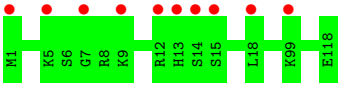




• Molecule 13: 50S Ribosomal Protein L17

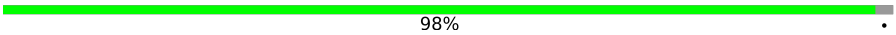
Chain 2R:





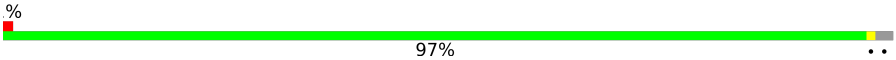
• Molecule 14: 50S Ribosomal Protein L18

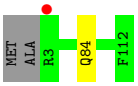
Chain 1S:



• Molecule 14: 50S Ribosomal Protein L18

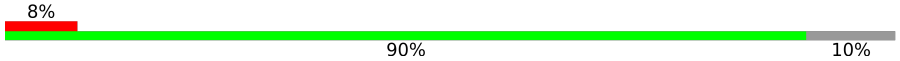
Chain 2S:

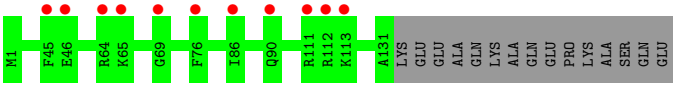




• Molecule 15: 50S Ribosomal Protein L19

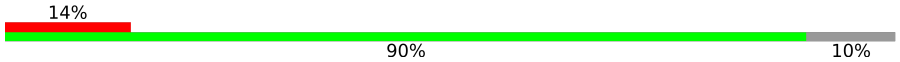
Chain 1T:

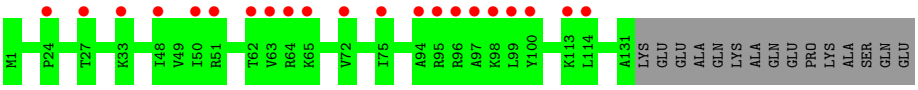




• Molecule 15: 50S Ribosomal Protein L19

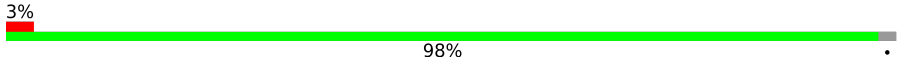
Chain 2T:

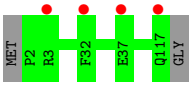




• Molecule 16: 50S Ribosomal Protein L20

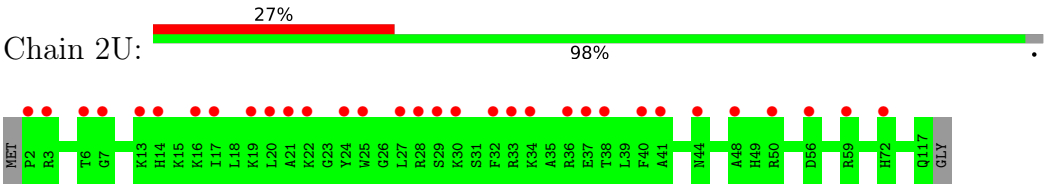
Chain 1U:





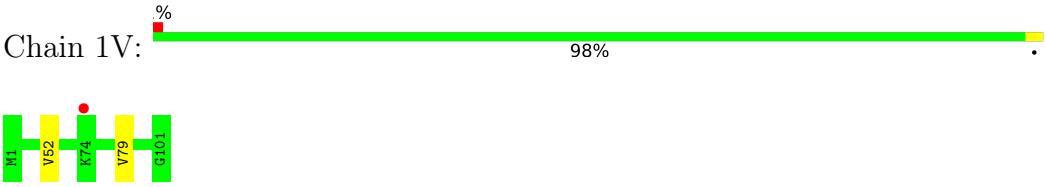
• Molecule 16: 50S Ribosomal Protein L20

Chain 2U:



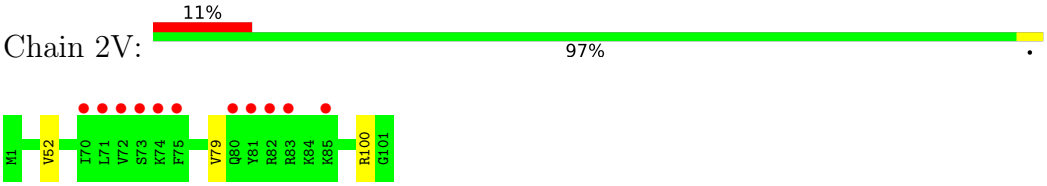
• Molecule 17: 50S Ribosomal Protein L21

Chain 1V:



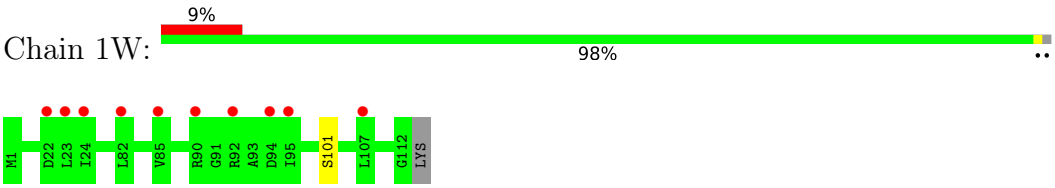
• Molecule 17: 50S Ribosomal Protein L21

Chain 2V:



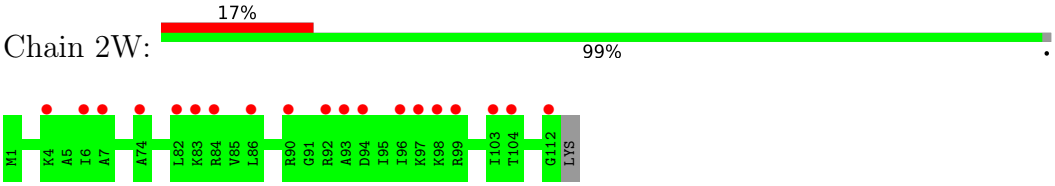
• Molecule 18: 50S Ribosomal Protein L22

Chain 1W:



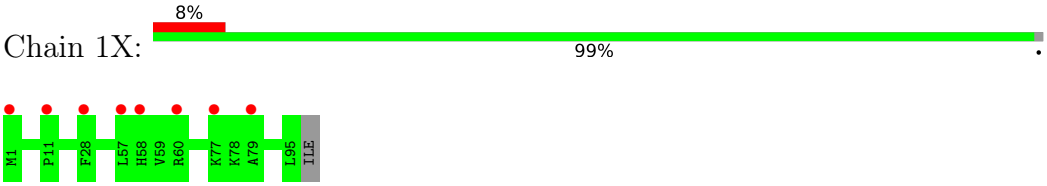
• Molecule 18: 50S Ribosomal Protein L22

Chain 2W:



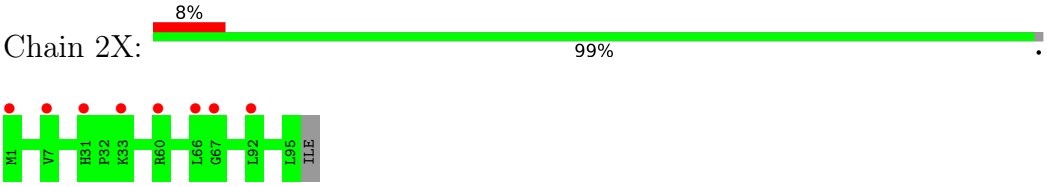
• Molecule 19: 50S Ribosomal Protein L23

Chain 1X:



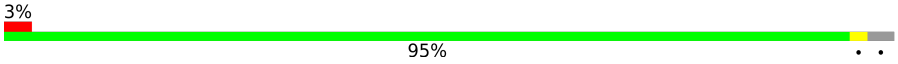
• Molecule 19: 50S Ribosomal Protein L23

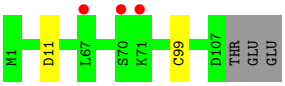
Chain 2X:



• Molecule 20: 50S ribosomal protein L24

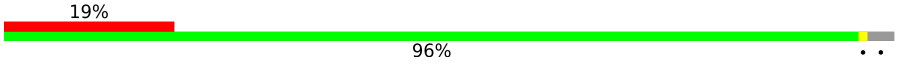
Chain 1Y:

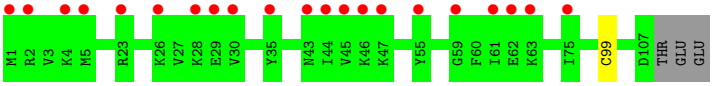




• Molecule 20: 50S ribosomal protein L24

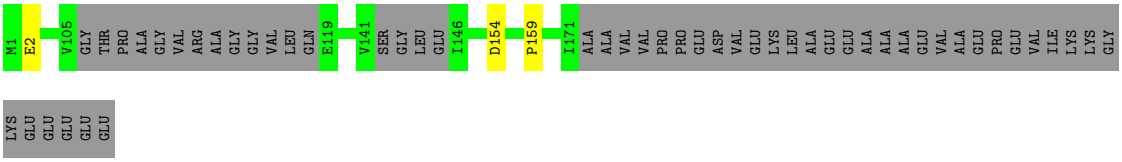
Chain 2Y:





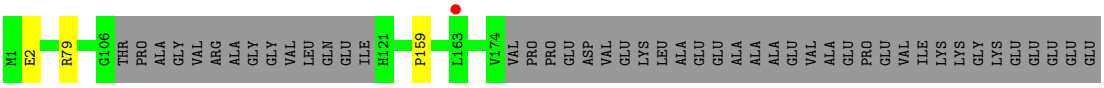
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



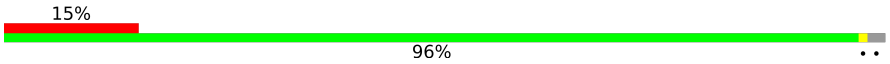
• Molecule 21: 50S ribosomal protein L25

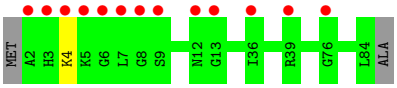
Chain 2Z:



• Molecule 22: 50S ribosomal protein L27

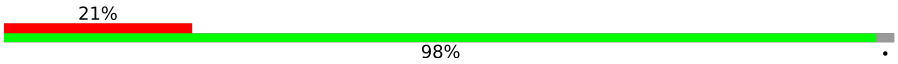
Chain 10:

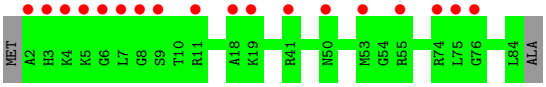




• Molecule 22: 50S ribosomal protein L27

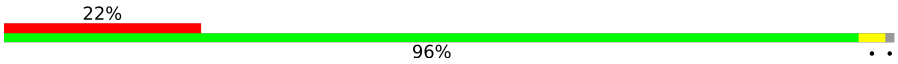
Chain 20:

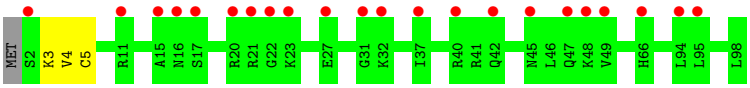




• Molecule 23: 50S ribosomal protein L28

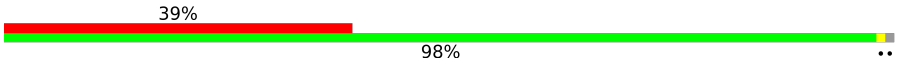
Chain 11:

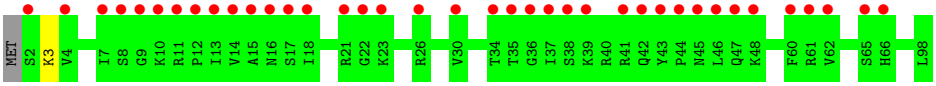




• Molecule 23: 50S ribosomal protein L28

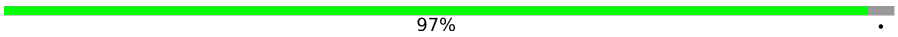
Chain 21:





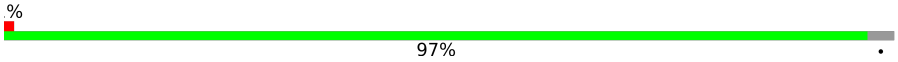
• Molecule 24: 50S ribosomal protein L29

Chain 12:



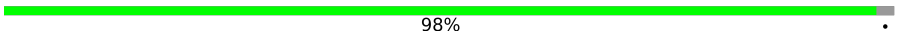
• Molecule 24: 50S ribosomal protein L29

Chain 22:



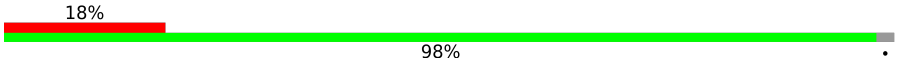
• Molecule 25: 50S ribosomal protein L30

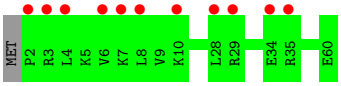
Chain 13:



• Molecule 25: 50S ribosomal protein L30

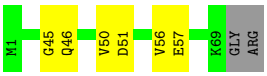
Chain 23:





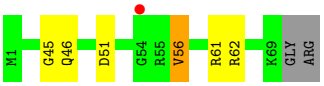
• Molecule 26: 50S ribosomal protein L31

Chain 14:



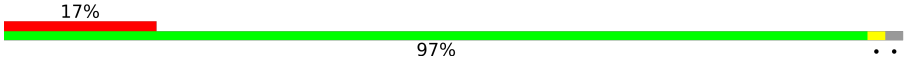
• Molecule 26: 50S ribosomal protein L31

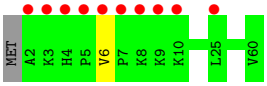
Chain 24:



• Molecule 27: 50S ribosomal protein L32

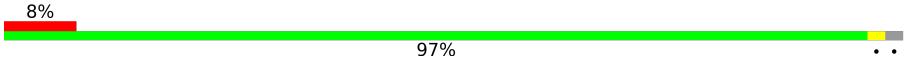
Chain 15:

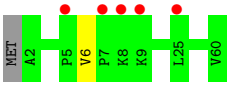




• Molecule 27: 50S ribosomal protein L32

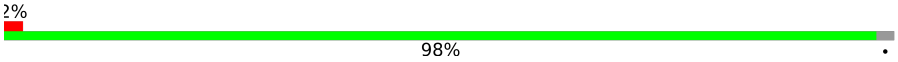
Chain 25:

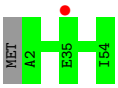




• Molecule 28: 50S ribosomal protein L33

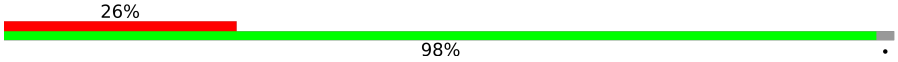
Chain 16:

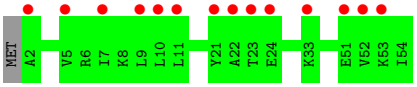




• Molecule 28: 50S ribosomal protein L33

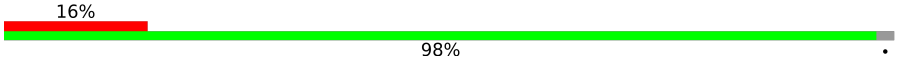
Chain 26:

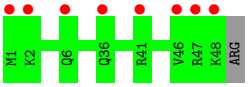




• Molecule 29: 50S ribosomal protein L34

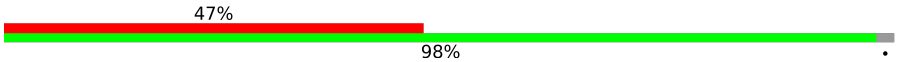
Chain 17:

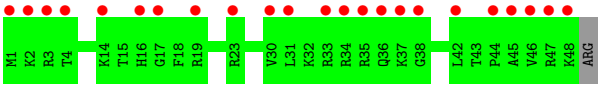




• Molecule 29: 50S ribosomal protein L34

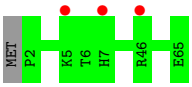
Chain 27:





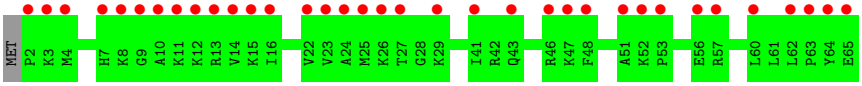
• Molecule 30: 50S Ribosomal Protein L35

Chain 18: 5% 98%



• Molecule 30: 50S Ribosomal Protein L35

Chain 28: 54% 98%



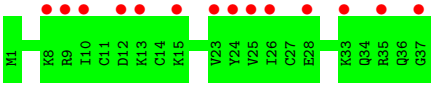
• Molecule 31: 50S Ribosomal Protein L36

Chain 19: 100%

There are no outlier residues recorded for this chain.

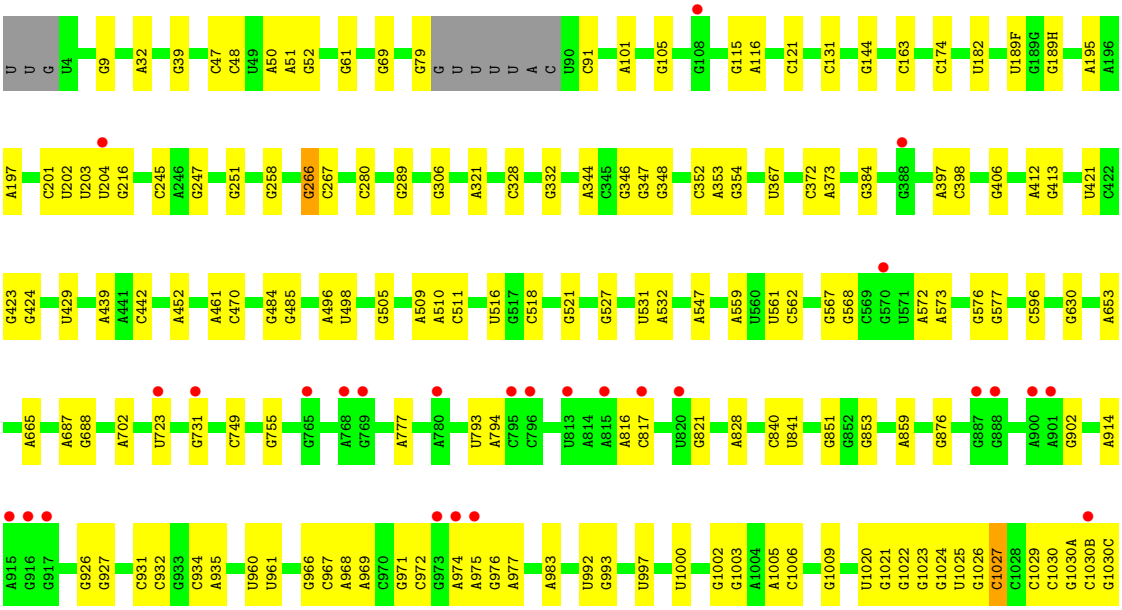
• Molecule 31: 50S Ribosomal Protein L36

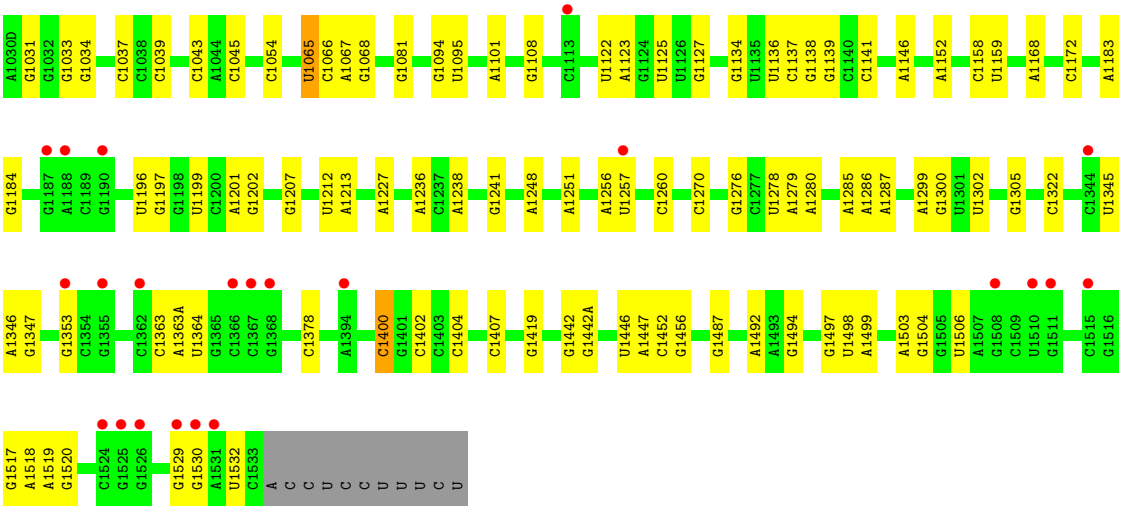
Chain 29: 38% 100%



• Molecule 32: 16S Ribosomal RNA

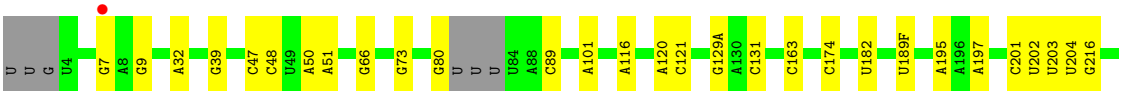
Chain 1a: 3% 82% 17%

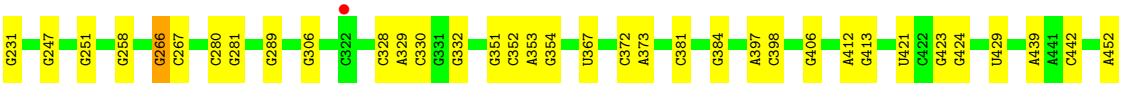


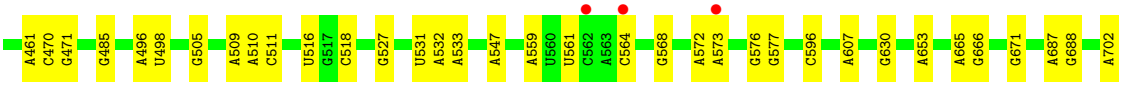


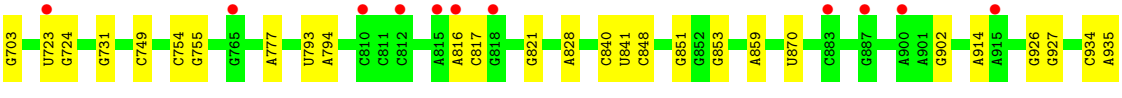
- Molecule 32: 16S Ribosomal RNA

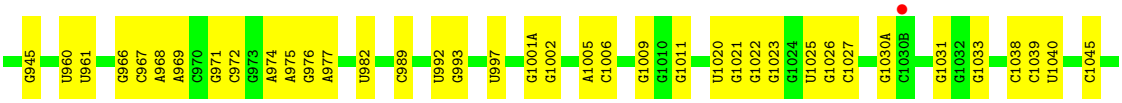
Chain 2a:

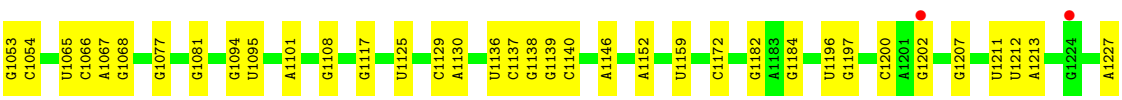


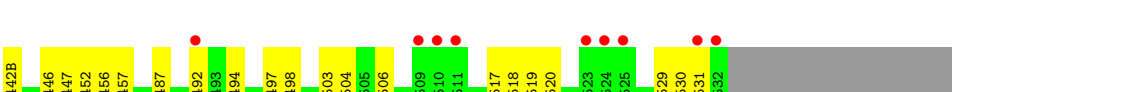






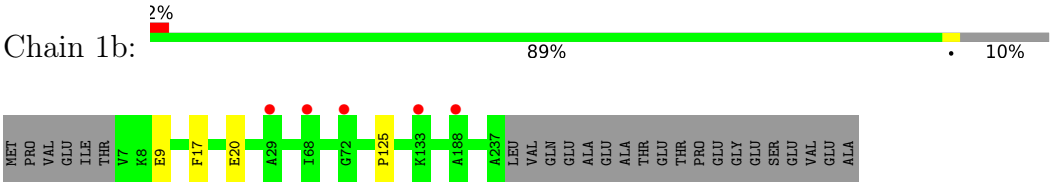






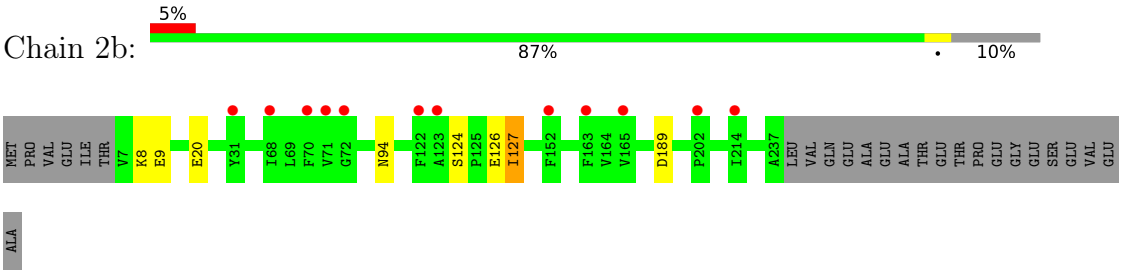
- Molecule 33: 30S Ribosomal Protein S2

Chain 1b:



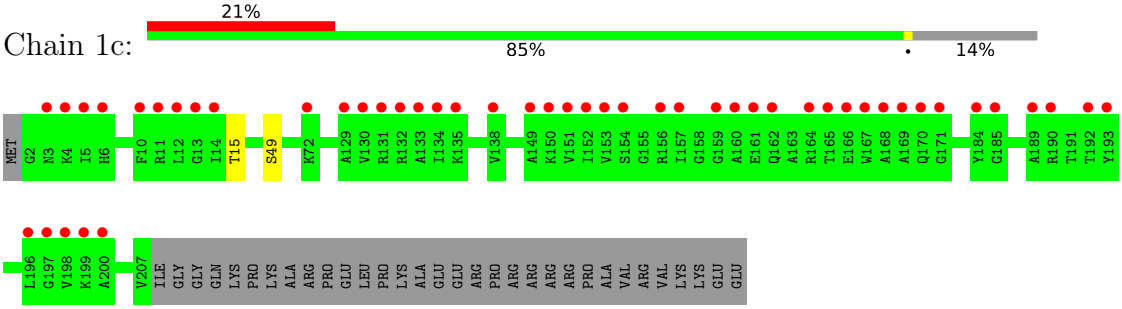
• Molecule 33: 30S Ribosomal Protein S2

Chain 2b:



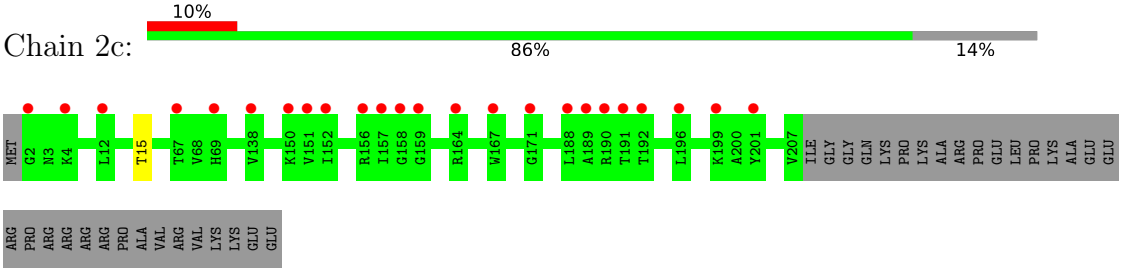
• Molecule 34: 30S Ribosomal Protein S3

Chain 1c:



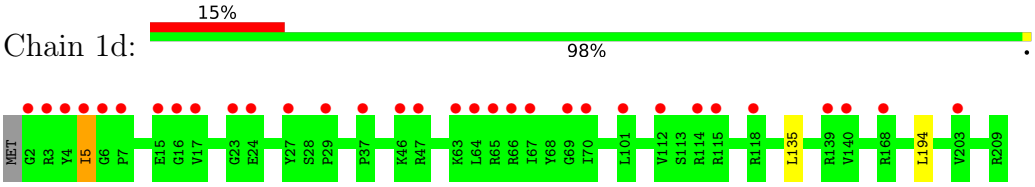
• Molecule 34: 30S Ribosomal Protein S3

Chain 2c:



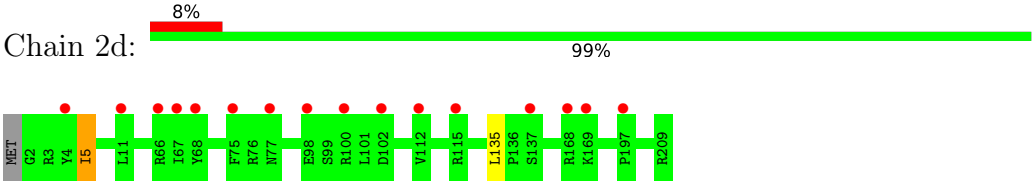
• Molecule 35: 30S Ribosomal Protein S4

Chain 1d:



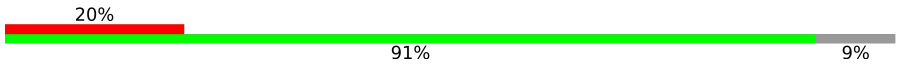
• Molecule 35: 30S Ribosomal Protein S4

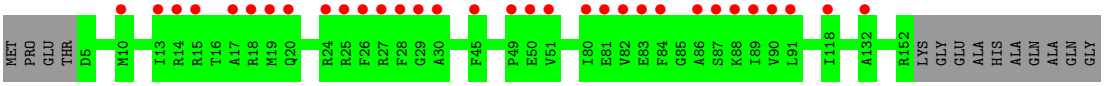
Chain 2d:



• Molecule 36: 30S Ribosomal Protein S5

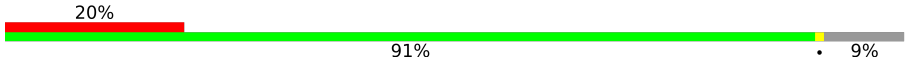
Chain 1e:

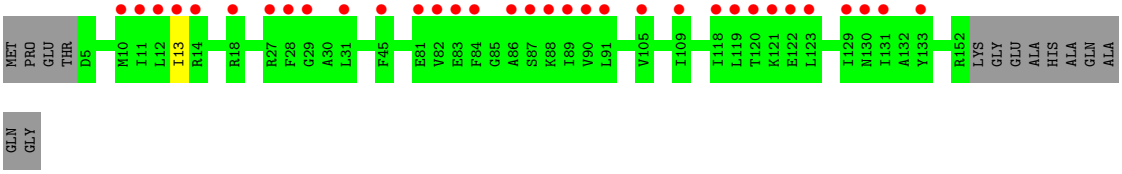




• Molecule 36: 30S Ribosomal Protein S5

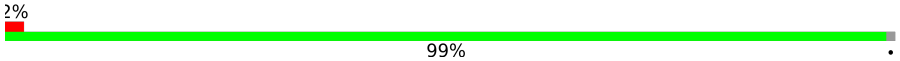
Chain 2e:

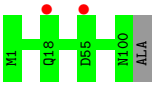




• Molecule 37: 30S Ribosomal Protein S6

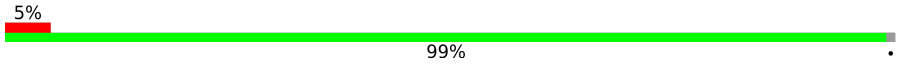
Chain 1f:

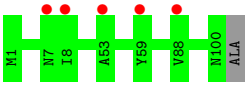




• Molecule 37: 30S Ribosomal Protein S6

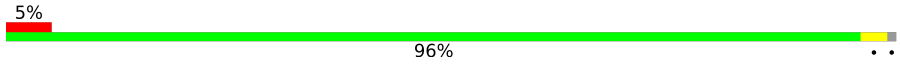
Chain 2f:

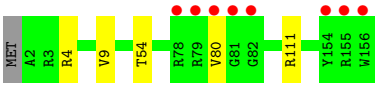




• Molecule 38: 30S Ribosomal Protein S7

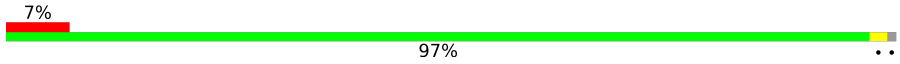
Chain 1g:

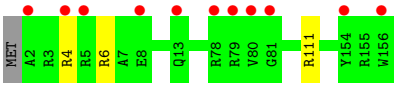




• Molecule 38: 30S Ribosomal Protein S7

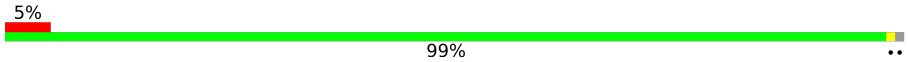
Chain 2g:

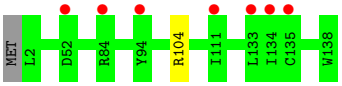




• Molecule 39: 30S Ribosomal Protein S8

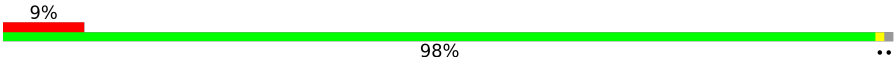
Chain 1h:

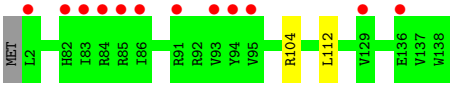




• Molecule 39: 30S Ribosomal Protein S8

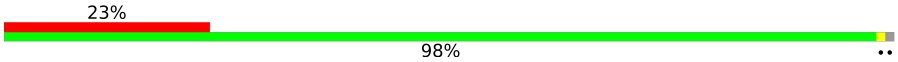
Chain 2h:

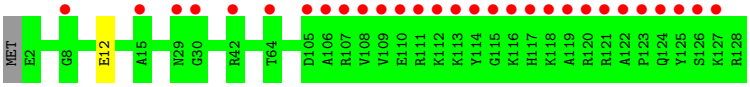




• Molecule 40: 30S ribosomal protein S9

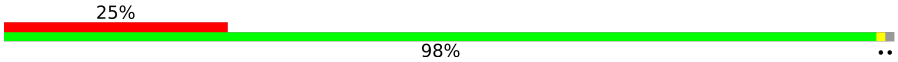
Chain 1i:

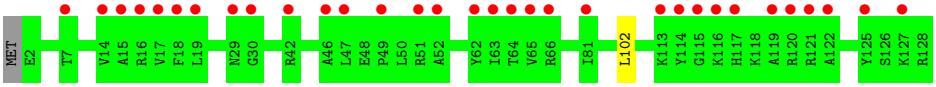




• Molecule 40: 30S ribosomal protein S9

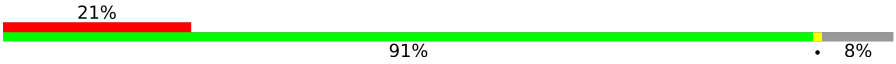
Chain 2i:

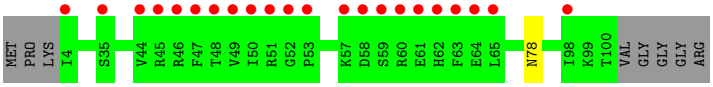




• Molecule 41: 30S ribosomal protein S10

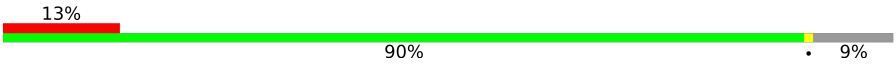
Chain 1j:

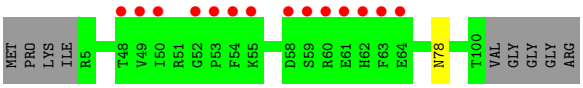




• Molecule 41: 30S ribosomal protein S10

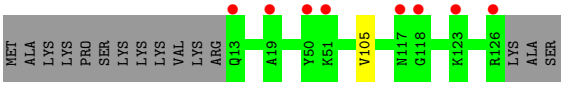
Chain 2j:





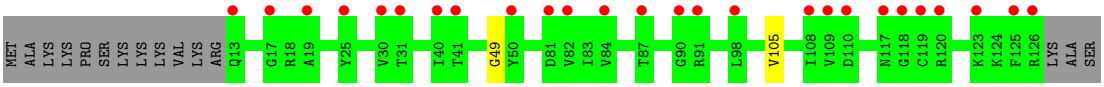
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



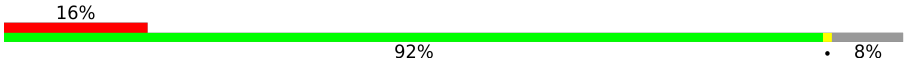
• Molecule 42: 30S ribosomal protein S11

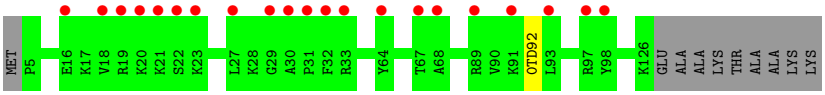
Chain 2k:



- Molecule 43: 30S ribosomal protein S12

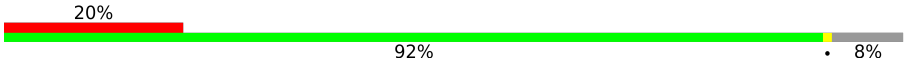
Chain 1l:

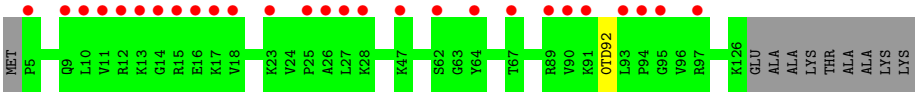




- Molecule 43: 30S ribosomal protein S12

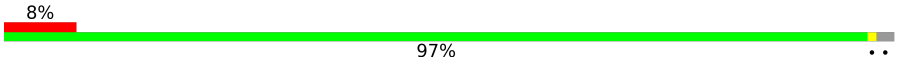
Chain 2l:

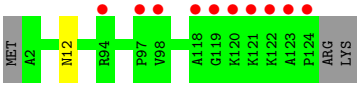




- Molecule 44: 30S ribosomal protein S13

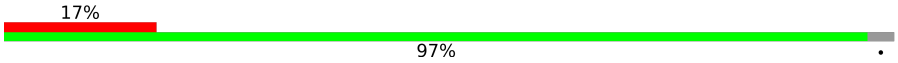
Chain 1m:

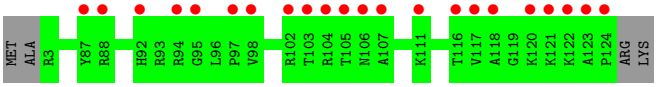




- Molecule 44: 30S ribosomal protein S13

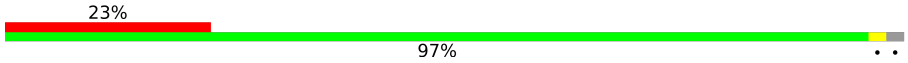
Chain 2m:

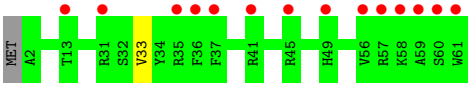




- Molecule 45: 30S ribosomal protein S14 type Z

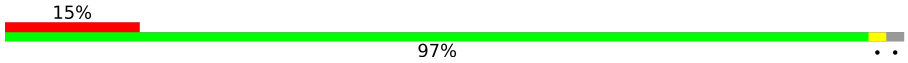
Chain 1n:

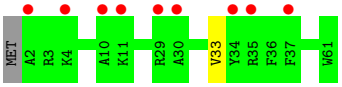




- Molecule 45: 30S ribosomal protein S14 type Z

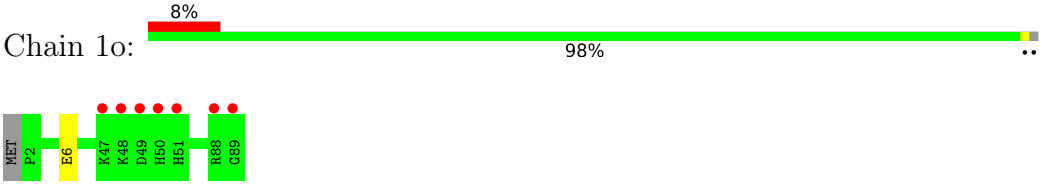
Chain 2n:





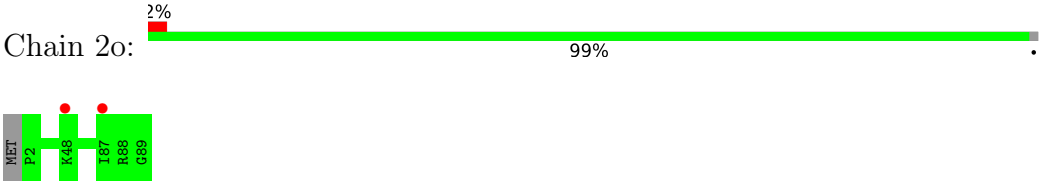
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



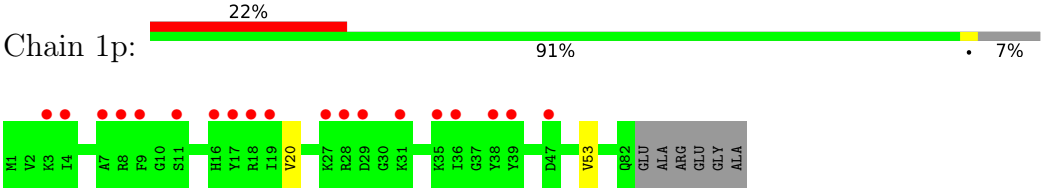
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



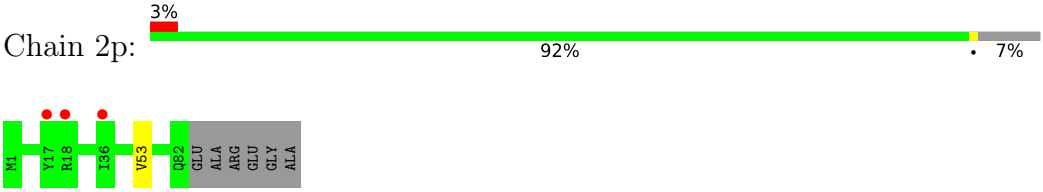
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



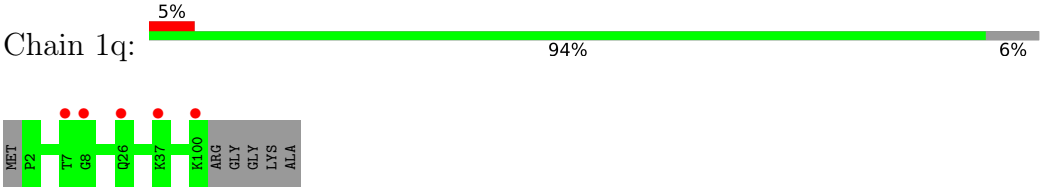
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



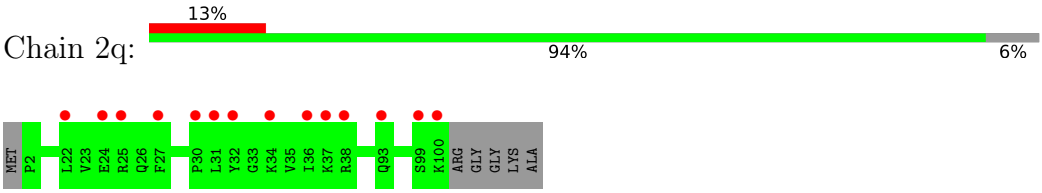
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



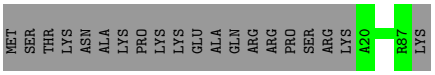
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



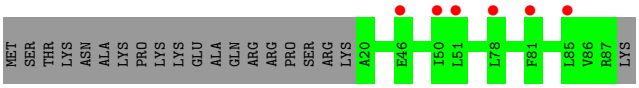
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



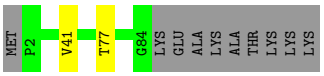
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



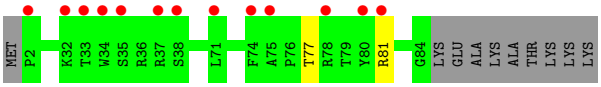
• Molecule 50: 30S Ribosomal Protein S19

Chain 1s:



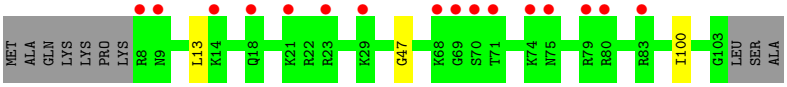
• Molecule 50: 30S Ribosomal Protein S19

Chain 2s:



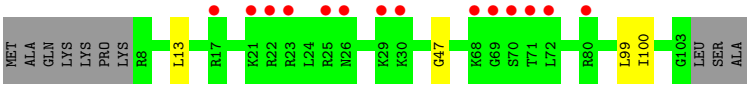
• Molecule 51: 30S Ribosomal Protein S20

Chain 1t:



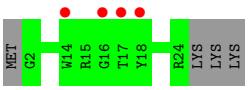
• Molecule 51: 30S Ribosomal Protein S20

Chain 2t:



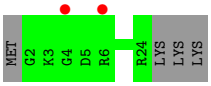
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



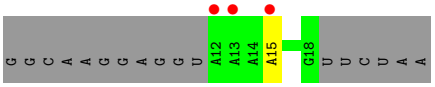
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



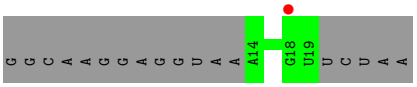
• Molecule 53: mRNA

Chain 1v:



• Molecule 53: mRNA

Chain 2v:



• Molecule 54: ACCA-DPhe

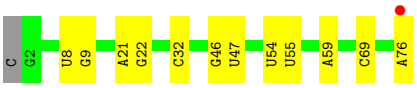
Chain 1w:

• Molecule 54: ACCA-DPhe

Chain 2w:

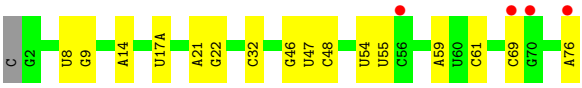
• Molecule 55: P-site tRNA, Deacylated Initiator Methionyl-tRNA

Chain 1x:



• Molecule 55: P-site tRNA, Deacylated Initiator Methionyl-tRNA

Chain 2x:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	211.39Å 452.15Å 617.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	255.01 – 3.70 255.01 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (255.01-3.70) 98.5 (255.01-3.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 3.68Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.236 , 0.279 0.236 , 0.279	Depositor DCC
R_{free} test set	30953 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	123.6	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	288175	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: ZN, 0TD, 2MA, MA6, 2MU, M2G, MG, SF4, OMG, 4OC, 4SU, 5MU, PSU, 7MG, KGV, 5MC, 2MG, UR3

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	1A	0.38	0/69009	0.80	18/107712 (0.0%)
1	2A	0.33	0/67293	0.79	12/105034 (0.0%)
2	1B	0.34	1/2882 (0.0%)	0.76	0/4494
2	2B	0.34	1/2879 (0.0%)	0.76	1/4487 (0.0%)
3	1D	0.35	1/2186 (0.0%)	0.49	0/2944
3	2D	0.36	1/2186 (0.0%)	0.48	0/2944
4	1E	0.28	0/1592	0.47	0/2149
4	2E	0.29	0/1592	0.46	0/2149
5	1F	0.30	0/1619	0.46	0/2193
5	2F	0.29	0/1615	0.45	0/2188
6	1G	0.27	0/1448	0.46	0/1957
6	2G	0.28	0/1453	0.46	0/1963
7	1H	0.29	0/1356	0.44	0/1834
7	2H	0.28	0/1356	0.44	0/1834
8	1I	0.27	0/1112	0.44	0/1514
8	2I	0.27	0/1079	0.45	0/1475
9	1N	0.27	0/1144	0.44	0/1543
9	2N	0.27	0/1144	0.43	0/1543
10	1O	0.31	0/943	0.47	0/1269
10	2O	0.32	0/943	0.49	0/1269
11	1P	0.30	0/1152	0.50	0/1533
11	2P	0.29	0/1152	0.51	0/1533
12	1Q	0.30	0/1143	0.46	0/1527
12	2Q	0.27	0/1143	0.45	0/1527
13	1R	0.26	0/982	0.45	0/1312
13	2R	0.26	0/982	0.44	0/1312
14	1S	0.27	0/883	0.43	0/1176
14	2S	0.27	0/880	0.42	0/1172
15	1T	0.27	0/1105	0.44	0/1477
15	2T	0.30	0/1097	0.46	0/1468
16	1U	0.29	0/977	0.41	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.27	0/977	0.39	0/1301
17	1V	0.29	0/782	0.48	0/1049
17	2V	0.27	0/782	0.48	0/1049
18	1W	0.29	0/897	0.44	0/1205
18	2W	0.29	0/897	0.45	0/1205
19	1X	0.29	0/764	0.50	0/1025
19	2X	0.27	0/764	0.47	0/1025
20	1Y	0.31	0/819	0.46	0/1095
20	2Y	0.30	0/819	0.44	0/1095
21	1Z	0.27	0/1267	0.46	0/1717
21	2Z	0.27	0/1299	0.46	0/1763
22	10	0.27	0/662	0.45	0/881
22	20	0.27	0/662	0.45	0/881
23	11	0.31	0/762	0.47	0/1014
23	21	0.29	0/762	0.46	0/1014
24	12	0.29	0/590	0.41	0/781
24	22	0.27	0/590	0.38	0/781
25	13	0.29	0/474	0.45	0/635
25	23	0.26	0/469	0.45	0/630
26	14	0.32	0/565	0.54	0/761
26	24	0.30	0/545	0.48	0/737
27	15	0.31	0/469	0.44	0/635
27	25	0.30	0/469	0.44	0/635
28	16	0.28	0/460	0.46	0/613
28	26	0.28	0/456	0.45	0/608
29	17	0.30	0/426	0.45	0/561
29	27	0.27	0/426	0.44	0/561
30	18	0.29	0/525	0.46	0/691
30	28	0.27	0/525	0.46	0/691
31	19	0.31	0/310	0.50	0/407
31	29	0.32	0/310	0.46	0/407
32	1a	0.32	0/35795	0.82	18/55864 (0.0%)
32	2a	0.32	2/35886 (0.0%)	0.82	15/56005 (0.0%)
33	1b	0.28	0/1881	0.45	0/2542
33	2b	0.29	0/1860	0.44	0/2518
34	1c	0.27	0/1572	0.44	0/2126
34	2c	0.27	0/1566	0.43	0/2119
35	1d	0.27	0/1685	0.44	0/2262
35	2d	0.27	0/1704	0.44	0/2284
36	1e	0.27	0/1145	0.46	0/1543
36	2e	0.28	0/1149	0.47	0/1548
37	1f	0.27	0/823	0.46	0/1115
37	2f	0.26	0/829	0.46	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.29	0/1250	0.41	0/1679
38	2g	0.28	0/1254	0.40	0/1683
39	1h	0.27	0/1108	0.45	0/1494
39	2h	0.26	0/1108	0.44	0/1494
40	1i	0.30	0/1002	0.45	0/1346
40	2i	0.30	0/997	0.45	0/1343
41	1j	0.25	0/722	0.44	0/982
41	2j	0.26	0/727	0.45	0/988
42	1k	0.27	0/844	0.44	0/1145
42	2k	0.27	0/848	0.44	0/1149
43	1l	0.28	0/937	0.48	0/1260
43	2l	0.27	0/937	0.49	0/1260
44	1m	0.27	0/969	0.47	0/1302
44	2m	0.26	0/961	0.45	0/1291
45	1n	0.28	0/501	0.45	0/664
45	2n	0.27	0/501	0.44	0/664
46	1o	0.26	0/739	0.39	0/985
46	2o	0.27	0/739	0.40	0/985
47	1p	0.26	0/697	0.45	0/939
47	2p	0.29	0/693	0.47	0/935
48	1q	0.27	0/836	0.43	0/1117
48	2q	0.27	0/836	0.43	0/1117
49	1r	0.25	0/560	0.42	0/746
49	2r	0.27	0/560	0.42	0/746
50	1s	0.27	0/667	0.47	0/900
50	2s	0.27	0/661	0.48	0/893
51	1t	0.29	0/730	0.41	0/965
51	2t	0.29	0/729	0.40	0/965
52	1u	0.24	0/203	0.43	0/266
52	2u	0.26	0/203	0.42	0/266
53	1v	0.44	0/172	0.80	0/266
53	2v	0.30	0/126	0.72	0/195
54	1w	0.37	0/45	0.89	0/68
54	2w	0.33	0/45	1.08	0/68
55	1x	0.38	0/1725	0.95	2/2689 (0.1%)
55	2x	0.38	0/1725	0.96	3/2689 (0.1%)
All	All	0.33	6/310103 (0.0%)	0.73	69/463879 (0.0%)

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
21	1Z	0	1
21	2Z	0	1
33	2b	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1B	1	U	OP3-P	-10.32	1.48	1.61
2	2B	1	U	OP3-P	-10.23	1.48	1.61
3	2D	7	LYS	C-N	-9.93	1.15	1.34
32	2a	1272	G	C6-N1	-7.41	1.34	1.39
3	1D	7	LYS	C-N	-6.56	1.21	1.34
32	2a	1272	G	N1-C2	-6.01	1.32	1.37

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1272	G	C5-C6-O6	14.81	137.49	128.60
32	2a	1272	G	N3-C2-N2	14.25	129.87	119.90
32	2a	1272	G	N1-C2-N2	-12.32	105.11	116.20
32	2a	1272	G	N1-C6-O6	-11.36	113.09	119.90
32	1a	1030(B)	C	N1-C2-O2	9.18	124.41	118.90
32	2a	1263	C	N1-C2-O2	8.87	124.22	118.90
32	1a	1030(B)	C	C2-N1-C1'	8.72	128.39	118.80
1	1A	1109	G	C5-C6-O6	8.29	133.57	128.60
32	2a	1272	G	C4-N9-C1'	8.22	137.19	126.50
32	2a	1272	G	C8-N9-C1'	-7.67	117.03	127.00
1	1A	1121	C	C2-N3-C4	7.59	123.70	119.90
1	1A	1121	C	C5-C4-N4	7.36	125.35	120.20
32	1a	1030(B)	C	N3-C2-O2	-7.36	116.75	121.90
1	2A	2136	C	N1-C2-O2	7.22	123.23	118.90
2	2B	80	U	O4'-C1'-N1	7.14	113.91	108.20
32	1a	1158	C	C2-N1-C1'	6.97	126.47	118.80
32	1a	1027	C	N3-C4-C5	-6.91	119.13	121.90
32	1a	1158	C	N1-C2-O2	6.72	122.93	118.90
1	2A	2473	U	C2-N1-C1'	6.33	125.29	117.70
32	1a	1030(B)	C	C6-N1-C2	-6.30	117.78	120.30
32	2a	1263	C	N3-C2-O2	-6.27	117.51	121.90
32	2a	1272	G	C6-N1-C2	6.04	128.73	125.10
1	1A	1109	G	C6-N1-C2	5.97	128.68	125.10
1	2A	2473	U	N1-C2-O2	5.96	126.98	122.80
1	1A	1221	G	OP1-P-O3'	5.96	118.31	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1030(B)	C	C6-N1-C1'	-5.85	113.78	120.80
1	2A	1779	U	C2-N1-C1'	5.82	124.69	117.70
32	2a	1272	G	N3-C4-N9	5.79	129.48	126.00
1	1A	2641	A	P-O3'-C3'	5.67	126.50	119.70
32	1a	1034	G	C6-N1-C2	5.65	128.49	125.10
1	1A	894	U	C2-N1-C1'	5.63	124.46	117.70
55	1x	46	G	C6-N1-C2	-5.56	121.76	125.10
32	1a	1027	C	C4-C5-C6	5.56	120.18	117.40
1	1A	2014	G	P-O3'-C3'	5.55	126.37	119.70
32	2a	266	G	P-O3'-C3'	5.54	126.35	119.70
1	1A	1810	U	C2-N1-C1'	5.49	124.29	117.70
1	1A	2513	C	C6-N1-C2	5.46	122.49	120.30
55	2x	14	A	C5-N7-C8	5.46	106.63	103.90
1	1A	1128	U	C2-N1-C1'	5.44	124.23	117.70
1	1A	572	A	P-O3'-C3'	5.43	126.22	119.70
1	2A	228	A	OP1-P-O3'	5.43	117.15	105.20
32	2a	1263	C	C2-N3-C4	5.36	122.58	119.90
1	2A	2136	C	N3-C2-O2	-5.35	118.15	121.90
32	1a	1158	C	N3-C2-O2	-5.33	118.17	121.90
55	2x	22	G	N1-C6-O6	-5.33	116.70	119.90
32	2a	754	C	C2-N1-C1'	5.31	124.64	118.80
32	1a	1199	U	N1-C2-O2	5.30	126.51	122.80
55	2x	46	G	C6-N1-C2	-5.28	121.93	125.10
32	1a	1067	A	P-O3'-C3'	5.27	126.02	119.70
1	1A	1121	C	N3-C4-N4	-5.25	114.32	118.00
1	2A	1992	G	P-O3'-C3'	5.25	126.00	119.70
1	2A	1530	C	P-O3'-C3'	5.23	125.97	119.70
32	1a	266	G	P-O3'-C3'	5.21	125.95	119.70
1	2A	2573	C	N1-C2-O2	5.18	122.01	118.90
1	1A	2333	G	C4-N9-C1'	5.14	133.19	126.50
1	1A	1221	G	P-O3'-C3'	5.14	125.87	119.70
1	1A	637	U	N3-C2-O2	-5.13	118.61	122.20
32	1a	1201	A	P-O3'-C3'	5.11	125.84	119.70
1	2A	2318	G	C4-N9-C1'	5.09	133.12	126.50
1	1A	1219	A	P-O3'-C3'	5.09	125.81	119.70
32	1a	1065	U	P-O3'-C3'	5.08	125.80	119.70
55	1x	22	G	C8-N9-C1'	5.07	133.59	127.00
1	2A	2473	U	N3-C2-O2	-5.06	118.66	122.20
32	1a	1285	A	P-O3'-C3'	5.05	125.77	119.70
1	1A	1219	A	OP1-P-O3'	5.05	116.32	105.20
32	1a	115	G	P-O3'-C3'	5.05	125.76	119.70
1	2A	2155	G	C6-N1-C2	5.05	128.13	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1067	A	P-O3'-C3'	5.05	125.76	119.70
32	2a	1054	C	N1-C2-O2	5.01	121.91	118.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	1Z	159	PRO	Peptide
21	2Z	159	PRO	Peptide
33	2b	8	LYS	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	Percentiles	
3	1D	273/276 (99%)	262 (96%)	11 (4%)	0	100	100
3	2D	273/276 (99%)	265 (97%)	8 (3%)	0	100	100
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29	66
4	2E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	29	66
5	1F	201/210 (96%)	194 (96%)	5 (2%)	2 (1%)	15	51
5	2F	201/210 (96%)	194 (96%)	5 (2%)	2 (1%)	15	51
6	1G	179/182 (98%)	165 (92%)	13 (7%)	1 (1%)	25	62
6	2G	179/182 (98%)	170 (95%)	6 (3%)	3 (2%)	9	42
7	1H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	25	62
7	2H	172/180 (96%)	168 (98%)	3 (2%)	1 (1%)	25	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	1I	144/148 (97%)	130 (90%)	13 (9%)	1 (1%)	22	59
8	2I	144/148 (97%)	130 (90%)	13 (9%)	1 (1%)	22	59
9	1N	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
9	2N	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	22	59
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
11	1P	147/150 (98%)	137 (93%)	6 (4%)	4 (3%)	5	33
11	2P	147/150 (98%)	137 (93%)	8 (5%)	2 (1%)	11	45
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
13	1R	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	17	54
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	17	54
15	1T	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15	51
17	2V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	7	39
18	1W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	1Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
21	1Z	148/206 (72%)	134 (90%)	13 (9%)	1 (1%)	22	59
21	2Z	156/206 (76%)	142 (91%)	12 (8%)	2 (1%)	12	47
22	10	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	13	48
22	20	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	50
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	68 (100%)	0	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	51 (76%)	12 (18%)	4 (6%)	1	18
26	24	67/71 (94%)	51 (76%)	10 (15%)	6 (9%)	1	9
27	15	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
27	25	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	16	51/54 (94%)	46 (90%)	5 (10%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	204 (89%)	21 (9%)	4 (2%)	9	42
33	2b	229/256 (90%)	207 (90%)	18 (8%)	4 (2%)	9	42
34	1c	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
34	2c	204/239 (85%)	189 (93%)	15 (7%)	0	100	100
35	1d	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	29	66
35	2d	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	29	66
36	1e	146/162 (90%)	138 (94%)	8 (6%)	0	100	100
36	2e	146/162 (90%)	139 (95%)	7 (5%)	0	100	100
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	142 (93%)	8 (5%)	3 (2%)	7	39
38	2g	153/156 (98%)	141 (92%)	10 (6%)	2 (1%)	12	47
39	1h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
39	2h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	1i	125/128 (98%)	117 (94%)	7 (6%)	1 (1%)	19	56
40	2i	125/128 (98%)	116 (93%)	9 (7%)	0	100	100
41	1j	95/105 (90%)	87 (92%)	7 (7%)	1 (1%)	14	50
41	2j	94/105 (90%)	85 (90%)	8 (8%)	1 (1%)	14	50
42	1k	112/129 (87%)	104 (93%)	7 (6%)	1 (1%)	17	54
42	2k	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	8	41
43	1l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	114 (94%)	6 (5%)	1 (1%)	19	56
44	2m	120/126 (95%)	114 (95%)	6 (5%)	0	100	100
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	58 (100%)	0	0	100	100
46	1o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	13	48
46	2o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
47	1p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	12	47
47	2p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	12	47
48	1q	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
49	1r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
50	2s	81/93 (87%)	75 (93%)	5 (6%)	1 (1%)	13	48
51	1t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	7	38
51	2t	94/106 (89%)	83 (88%)	8 (8%)	3 (3%)	4	31
52	1u	21/27 (78%)	21 (100%)	0	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11370/12128 (94%)	10736 (94%)	561 (5%)	73 (1%)	25	62

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	47	LYS
21	1Z	2	GLU

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Mol	Chain	Res	Type
23	11	3	LYS
26	14	46	GLN
26	14	57	GLU
33	1b	9	GLU
35	1d	5	ILE
38	1g	4	ARG
5	2F	130	ALA
11	2P	45	LEU
21	2Z	2	GLU
23	21	3	LYS
33	2b	9	GLU
35	2d	5	ILE
5	1F	130	ALA
7	1H	92	ILE
11	1P	38	GLN
11	1P	45	LEU
17	1V	79	VAL
26	14	51	ASP
33	1b	20	GLU
47	1p	53	VAL
6	2G	47	LYS
6	2G	49	ASP
7	2H	92	ILE
9	2N	23	LEU
38	2g	4	ARG
38	2g	6	ARG
41	2j	78	ASN
47	2p	53	VAL
50	2s	81	ARG
8	1I	85	GLU
11	1P	39	LYS
33	1b	17	PHE
41	1j	78	ASN
14	2S	84	GLN
26	24	51	ASP
33	2b	20	GLU
33	2b	127	ILE
51	2t	47	GLY
22	10	4	LYS
44	1m	12	ASN
11	2P	29	LYS
26	24	61	ARG

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Mol	Chain	Res	Type
51	2t	99	LEU
11	1P	29	LYS
38	1g	54	THR
40	1i	12	GLU
46	1o	6	GLU
5	2F	89	VAL
6	2G	181	ARG
8	2I	117	GLU
17	2V	79	VAL
21	2Z	79	ARG
26	24	46	GLN
33	2b	126	GLU
17	2V	100	ARG
26	24	62	ARG
42	2k	49	GLY
51	2t	100	ILE
26	14	45	GLY
42	1k	105	VAL
51	1t	47	GLY
4	2E	52	LEU
42	2k	105	VAL
5	1F	89	VAL
13	1R	58	GLY
51	1t	100	ILE
38	1g	80	VAL
26	24	45	GLY
26	24	56	VAL
4	1E	52	LEU
33	1b	125	PRO

5.3.2 Protein 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
3	1D	215/218 (99%)	214 (100%)	1 (0%)	88 94
3	2D	215/218 (99%)	214 (100%)	1 (0%)	88 94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	1E	164/166 (99%)	163 (99%)	1 (1%)	86	93
4	2E	164/166 (99%)	163 (99%)	1 (1%)	86	93
5	1F	160/166 (96%)	160 (100%)	0	100	100
5	2F	159/166 (96%)	159 (100%)	0	100	100
6	1G	143/156 (92%)	142 (99%)	1 (1%)	84	91
6	2G	143/156 (92%)	141 (99%)	2 (1%)	67	82
7	1H	144/148 (97%)	144 (100%)	0	100	100
7	2H	144/148 (97%)	143 (99%)	1 (1%)	84	91
8	1I	113/124 (91%)	112 (99%)	1 (1%)	78	88
8	2I	105/124 (85%)	104 (99%)	1 (1%)	76	86
9	1N	118/119 (99%)	118 (100%)	0	100	100
9	2N	118/119 (99%)	117 (99%)	1 (1%)	81	89
10	1O	100/100 (100%)	100 (100%)	0	100	100
10	2O	100/100 (100%)	99 (99%)	1 (1%)	76	86
11	1P	115/116 (99%)	114 (99%)	1 (1%)	78	88
11	2P	115/116 (99%)	114 (99%)	1 (1%)	78	88
12	1Q	111/111 (100%)	110 (99%)	1 (1%)	78	88
12	2Q	111/111 (100%)	111 (100%)	0	100	100
13	1R	101/101 (100%)	101 (100%)	0	100	100
13	2R	101/101 (100%)	101 (100%)	0	100	100
14	1S	86/88 (98%)	86 (100%)	0	100	100
14	2S	85/88 (97%)	85 (100%)	0	100	100
15	1T	115/127 (91%)	115 (100%)	0	100	100
15	2T	113/127 (89%)	113 (100%)	0	100	100
16	1U	93/94 (99%)	93 (100%)	0	100	100
16	2U	93/94 (99%)	93 (100%)	0	100	100
17	1V	80/82 (98%)	79 (99%)	1 (1%)	69	83
17	2V	80/82 (98%)	79 (99%)	1 (1%)	69	83
18	1W	90/92 (98%)	89 (99%)	1 (1%)	73	85
18	2W	90/92 (98%)	90 (100%)	0	100	100
19	1X	77/78 (99%)	77 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	2X	77/78 (99%)	77 (100%)	0	100	100
20	1Y	85/91 (93%)	83 (98%)	2 (2%)	49	71
20	2Y	85/91 (93%)	84 (99%)	1 (1%)	71	84
21	1Z	135/179 (75%)	134 (99%)	1 (1%)	84	91
21	2Z	137/179 (76%)	137 (100%)	0	100	100
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	65 (100%)	0	100	100
23	11	80/83 (96%)	78 (98%)	2 (2%)	47	70
23	21	80/83 (96%)	80 (100%)	0	100	100
24	12	65/67 (97%)	65 (100%)	0	100	100
24	22	65/67 (97%)	65 (100%)	0	100	100
25	13	51/52 (98%)	51 (100%)	0	100	100
25	23	50/52 (96%)	50 (100%)	0	100	100
26	14	59/63 (94%)	57 (97%)	2 (3%)	37	64
26	24	53/63 (84%)	52 (98%)	1 (2%)	57	76
27	15	50/52 (96%)	49 (98%)	1 (2%)	55	74
27	25	50/52 (96%)	49 (98%)	1 (2%)	55	74
28	16	51/52 (98%)	51 (100%)	0	100	100
28	26	50/52 (96%)	50 (100%)	0	100	100
29	17	41/42 (98%)	41 (100%)	0	100	100
29	27	41/42 (98%)	41 (100%)	0	100	100
30	18	54/55 (98%)	54 (100%)	0	100	100
30	28	54/55 (98%)	54 (100%)	0	100	100
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	192/220 (87%)	192 (100%)	0	100	100
33	2b	187/220 (85%)	183 (98%)	4 (2%)	53	74
34	1c	142/188 (76%)	140 (99%)	2 (1%)	67	82
34	2c	140/188 (74%)	139 (99%)	1 (1%)	84	91
35	1d	169/181 (93%)	166 (98%)	3 (2%)	59	77
35	2d	173/181 (96%)	171 (99%)	2 (1%)	71	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	1e	113/123 (92%)	113 (100%)	0	100	100
36	2e	114/123 (93%)	113 (99%)	1 (1%)	78	88
37	1f	84/90 (93%)	84 (100%)	0	100	100
37	2f	85/90 (94%)	85 (100%)	0	100	100
38	1g	119/127 (94%)	117 (98%)	2 (2%)	60	79
38	2g	120/127 (94%)	119 (99%)	1 (1%)	81	89
39	1h	114/119 (96%)	113 (99%)	1 (1%)	78	88
39	2h	114/119 (96%)	112 (98%)	2 (2%)	59	77
40	1i	90/99 (91%)	90 (100%)	0	100	100
40	2i	89/99 (90%)	88 (99%)	1 (1%)	73	85
41	1j	66/92 (72%)	66 (100%)	0	100	100
41	2j	69/92 (75%)	69 (100%)	0	100	100
42	1k	82/99 (83%)	82 (100%)	0	100	100
42	2k	83/99 (84%)	83 (100%)	0	100	100
43	1l	96/108 (89%)	96 (100%)	0	100	100
43	2l	96/108 (89%)	96 (100%)	0	100	100
44	1m	93/101 (92%)	93 (100%)	0	100	100
44	2m	92/101 (91%)	92 (100%)	0	100	100
45	1n	49/50 (98%)	48 (98%)	1 (2%)	55	74
45	2n	49/50 (98%)	48 (98%)	1 (2%)	55	74
46	1o	78/80 (98%)	78 (100%)	0	100	100
46	2o	78/80 (98%)	78 (100%)	0	100	100
47	1p	69/74 (93%)	68 (99%)	1 (1%)	67	82
47	2p	68/74 (92%)	68 (100%)	0	100	100
48	1q	94/97 (97%)	94 (100%)	0	100	100
48	2q	94/97 (97%)	94 (100%)	0	100	100
49	1r	59/77 (77%)	59 (100%)	0	100	100
49	2r	59/77 (77%)	59 (100%)	0	100	100
50	1s	69/80 (86%)	67 (97%)	2 (3%)	42	66
50	2s	67/80 (84%)	66 (98%)	1 (2%)	65	81
51	1t	70/82 (85%)	69 (99%)	1 (1%)	67	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	2t	70/82 (85%)	69 (99%)	1 (1%)	67 82
52	1u	18/22 (82%)	18 (100%)	0	100 100
52	2u	18/22 (82%)	18 (100%)	0	100 100
All	All	9303/10064 (92%)	9246 (99%)	57 (1%)	86 93

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	242	ARG
4	1E	21	VAL
6	1G	31	VAL
8	1I	144	VAL
11	1P	106	LEU
12	1Q	110	THR
17	1V	52	VAL
18	1W	101	SER
20	1Y	11	ASP
20	1Y	99	CYS
21	1Z	154	ASP
23	11	4	VAL
23	11	5	CYS
26	14	50	VAL
26	14	56	VAL
27	15	6	VAL
34	1c	15	THR
34	1c	49	SER
35	1d	5	ILE
35	1d	135	LEU
35	1d	194	LEU
38	1g	9	VAL
38	1g	111	ARG
39	1h	104	ARG
45	1n	33	VAL
47	1p	20	VAL
50	1s	41	VAL
50	1s	77	THR
51	1t	13	LEU
3	2D	242	ARG
4	2E	21	VAL
6	2G	31	VAL
6	2G	159	VAL

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Mol	Chain	Res	Type
7	2H	125	VAL
8	2I	144	VAL
9	2N	58	ASP
10	2O	21	CYS
11	2P	106	LEU
17	2V	52	VAL
20	2Y	99	CYS
26	24	56	VAL
27	25	6	VAL
33	2b	94	ASN
33	2b	124	SER
33	2b	127	ILE
33	2b	189	ASP
34	2c	15	THR
35	2d	5	ILE
35	2d	135	LEU
36	2e	13	ILE
38	2g	111	ARG
39	2h	104	ARG
39	2h	112	LEU
40	2i	102	LEU
45	2n	33	VAL
50	2s	77	THR
51	2t	13	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
5	1F	69	HIS
5	1F	75	HIS
9	1N	38	HIS
10	1O	3	GLN
12	1Q	12	GLN
14	1S	38	GLN
19	1X	82	GLN
21	1Z	151	HIS
23	11	56	GLN
30	18	35	GLN
33	1b	78	GLN
33	1b	113	HIS
34	1c	37	GLN
34	1c	162	GLN

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Mol	Chain	Res	Type
34	1c	176	HIS
35	1d	125	HIS
36	1e	78	HIS
37	1f	100	ASN
39	1h	82	HIS
40	1i	58	HIS
44	1m	12	ASN
46	1o	62	GLN
47	1p	13	HIS
49	1r	63	GLN
50	1s	57	HIS
50	1s	83	HIS
3	2D	116	GLN
3	2D	166	GLN
4	2E	137	HIS
5	2F	69	HIS
5	2F	75	HIS
8	2I	11	ASN
10	2O	3	GLN
12	2Q	12	GLN
13	2R	3	HIS
14	2S	38	GLN
17	2V	64	HIS
21	2Z	55	HIS
21	2Z	151	HIS
23	21	56	GLN
33	2b	19	HIS
33	2b	78	GLN
33	2b	113	HIS
34	2c	37	GLN
34	2c	69	HIS
34	2c	176	HIS
35	2d	77	ASN
35	2d	201	GLN
36	2e	78	HIS
37	2f	100	ASN
40	2i	58	HIS
42	2k	22	HIS
43	2l	99	HIS
44	2m	12	ASN
47	2p	13	HIS
50	2s	57	HIS

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Mol	Chain	Res	Type
50	2s	83	HIS
51	2t	75	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	421 (14%)	24 (0%)
1	2A	2788/2915 (95%)	440 (15%)	19 (0%)
2	1B	120/121 (99%)	10 (8%)	1 (0%)
2	2B	119/121 (98%)	12 (10%)	1 (0%)
32	1a	1494/1521 (98%)	240 (16%)	0
32	2a	1498/1521 (98%)	243 (16%)	0
53	1v	6/24 (25%)	1 (16%)	0
53	2v	4/24 (16%)	0	0
54	1w	1/4 (25%)	1 (100%)	0
54	2w	2/4 (50%)	2 (100%)	0
55	1x	75/77 (97%)	6 (8%)	0
55	2x	75/77 (97%)	9 (12%)	0
All	All	9043/9324 (96%)	1385 (15%)	45 (0%)

All (1385) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	14	A
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	54	G
1	1A	60	G
1	1A	62	U
1	1A	63	A
1	1A	70	A
1	1A	73	A
1	1A	74	G
1	1A	83	A
1	1A	94	G
1	1A	116	A
1	1A	118	U
1	1A	119	G
1	1A	129	G

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Mol	Chain	Res	Type
1	1A	139	A
1	1A	162	G
1	1A	185	A
1	1A	188	A
1	1A	194	G
1	1A	203	G
1	1A	205	A
1	1A	211	A
1	1A	214	A
1	1A	217	A
1	1A	218	A
1	1A	222	A
1	1A	237	G
1	1A	258	U
1	1A	270	C
1	1A	272	U
1	1A	273	G
1	1A	274	U
1	1A	275	C
1	1A	289	G
1	1A	303	C
1	1A	335	A
1	1A	348	A
1	1A	353	G
1	1A	354	A
1	1A	376	G
1	1A	387	G
1	1A	389	G
1	1A	399	G
1	1A	413	G
1	1A	423	G
1	1A	432	U
1	1A	438	G
1	1A	439	A
1	1A	455	A
1	1A	470	C
1	1A	474	U
1	1A	475	A
1	1A	481	C
1	1A	482	C
1	1A	483	A
1	1A	484	G

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Mol	Chain	Res	Type
1	1A	490	U
1	1A	507	G
1	1A	529	U
1	1A	530	A
1	1A	533	G
1	1A	534	C
1	1A	555	G
1	1A	556	C
1	1A	557	A
1	1A	558	G
1	1A	569	G
1	1A	573	G
1	1A	586	G
1	1A	596	G
1	1A	597	C
1	1A	598	A
1	1A	609	A
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	639	G
1	1A	641	G
1	1A	652	A
1	1A	659	C
1	1A	662	A
1	1A	670	C
1	1A	671	A
1	1A	693	G
1	1A	716	G
1	1A	733	G
1	1A	777	C
1	1A	794	U
1	1A	809	U
1	1A	812	G
1	1A	822	G
1	1A	823	G
1	1A	829	A
1	1A	831	A
1	1A	832	G
1	1A	847	A
1	1A	852	G
1	1A	859	C

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Mol	Chain	Res	Type
1	1A	866	A
1	1A	874	U
1	1A	875	U
1	1A	903	C
1	1A	906	G
1	1A	926	G
1	1A	927	G
1	1A	932	C
1	1A	933	C
1	1A	934	A
1	1A	935	C
1	1A	936	C
1	1A	937	A
1	1A	941	U
1	1A	942	A
1	1A	943	C
1	1A	944	C
1	1A	946	A
1	1A	953	U
1	1A	956	A
1	1A	960	C
1	1A	961	C
1	1A	976	G
1	1A	977	G
1	1A	990	A
1	1A	991	G
1	1A	1002	A
1	1A	1004	A
1	1A	1006	C
1	1A	1018	A
1	1A	1019	G
1	1A	1020	C
1	1A	1021	G
1	1A	1029	A
1	1A	1042	A
1	1A	1051	C
1	1A	1058	U
1	1A	1059	C
1	1A	1068	G
1	1A	1071	G
1	1A	1072	U
1	1A	1079	U

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Mol	Chain	Res	Type
1	1A	1087	C
1	1A	1090	G
1	1A	1091	A
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1100	A
1	1A	1104	G
1	1A	1114	G
1	1A	1117	G
1	1A	1119	A
1	1A	1120	G
1	1A	1121	C
1	1A	1122	C
1	1A	1124	U
1	1A	1125	C
1	1A	1127	U
1	1A	1128	U
1	1A	1132	A
1	1A	1134	A
1	1A	1137	G
1	1A	1140	U
1	1A	1144	A
1	1A	1147	U
1	1A	1149	A
1	1A	1150	C
1	1A	1157	A
1	1A	1158	G
1	1A	1172	A
1	1A	1180	C
1	1A	1181	G
1	1A	1201	A
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1222	A
1	1A	1223	C
1	1A	1256	U
1	1A	1298	G
1	1A	1299	A

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Mol	Chain	Res	Type
1	1A	1301	U
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1319	U
1	1A	1346	U
1	1A	1347	A
1	1A	1348	A
1	1A	1371	G
1	1A	1387	U
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1425	A
1	1A	1430	A
1	1A	1431	G
1	1A	1441	A
1	1A	1442	U
1	1A	1462	G
1	1A	1463	C
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1491	A
1	1A	1497	G
1	1A	1502	G
1	1A	1506	G
1	1A	1514	C
1	1A	1529	G
1	1A	1539	C
1	1A	1540	A
1	1A	1554	A
1	1A	1555	C
1	1A	1556	A
1	1A	1590	C
1	1A	1592	A
1	1A	1605	A
1	1A	1616	A
1	1A	1625	U
1	1A	1627	A
1	1A	1631	C

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Mol	Chain	Res	Type
1	1A	1632	A
1	1A	1648	U
1	1A	1654	A
1	1A	1656	A
1	1A	1662	A
1	1A	1695	C
1	1A	1701	A
1	1A	1721	G
1	1A	1741	C
1	1A	1743	G
1	1A	1745	A
1	1A	1747	A
1	1A	1750	G
1	1A	1767	A
1	1A	1768	U
1	1A	1776	G
1	1A	1787	G
1	1A	1793	A
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A
1	1A	1811	A
1	1A	1812	C
1	1A	1813	C
1	1A	1822	A
1	1A	1831	C
1	1A	1832	G
1	1A	1847	G
1	1A	1860	A
1	1A	1878	A
1	1A	1879	A
1	1A	1889	G
1	1A	1899	A
1	1A	1911	A
1	1A	1922	A
1	1A	1935	A
1	1A	1951	G
1	1A	1952	G
1	1A	1958	A
1	1A	1960	A
1	1A	1977	U
1	1A	1985	U

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Mol	Chain	Res	Type
1	1A	1987	C
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2015	U
1	1A	2019	G
1	1A	2045	G
1	1A	2052	A
1	1A	2053	A
1	1A	2054	G
1	1A	2055	A
1	1A	2056	U
1	1A	2065	C
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2084	A
1	1A	2091	G
1	1A	2114	U
1	1A	2115	G
1	1A	2119	C
1	1A	2121	U
1	1A	2124	U
1	1A	2135	U
1	1A	2138	G
1	1A	2143	G
1	1A	2149	G
1	1A	2151	C
1	1A	2152	U
1	1A	2153	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2157	A
1	1A	2162	C
1	1A	2164	C
1	1A	2166	U
1	1A	2168	C
1	1A	2169	G
1	1A	2172	U

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Mol	Chain	Res	Type
1	1A	2173	G
1	1A	2178	G
1	1A	2179	G
1	1A	2180	A
1	1A	2181	G
1	1A	2187	G
1	1A	2188	G
1	1A	2189	U
1	1A	2190	G
1	1A	2193	A
1	1A	2194	U
1	1A	2195	A
1	1A	2197	C
1	1A	2198	A
1	1A	2200	C
1	1A	2204	G
1	1A	2206	G
1	1A	2207	C
1	1A	2214	G
1	1A	2215	G
1	1A	2220	A
1	1A	2227	G
1	1A	2228	G
1	1A	2229	A
1	1A	2231	G
1	1A	2237	A
1	1A	2250	G
1	1A	2251	G
1	1A	2281	A
1	1A	2290	A
1	1A	2292	G
1	1A	2295	C
1	1A	2298	A
1	1A	2299	A
1	1A	2300	A
1	1A	2317	A
1	1A	2320	G
1	1A	2332	A
1	1A	2337	G
1	1A	2346	G
1	1A	2348	A
1	1A	2357	G

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Mol	Chain	Res	Type
1	1A	2359	C
1	1A	2362	C
1	1A	2370	G
1	1A	2373	A
1	1A	2395	G
1	1A	2397	C
1	1A	2418	U
1	1A	2422	G
1	1A	2436	C
1	1A	2437	A
1	1A	2440	G
1	1A	2441	G
1	1A	2442	A
1	1A	2446	A
1	1A	2447	A
1	1A	2451	A
1	1A	2453	C
1	1A	2460	A
1	1A	2480	G
1	1A	2481	A
1	1A	2486	C
1	1A	2488	A
1	1A	2490	A
1	1A	2514	G
1	1A	2516	U
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2541	G
1	1A	2561	G
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2584	A
1	1A	2585	C
1	1A	2597	U
1	1A	2614	A
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2627	U
1	1A	2633	A

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Mol	Chain	Res	Type
1	1A	2641	A
1	1A	2642	G
1	1A	2666	A
1	1A	2701	U
1	1A	2702	C
1	1A	2714	U
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2746	A
1	1A	2770	A
1	1A	2771	A
1	1A	2777	A
1	1A	2778	A
1	1A	2791	A
1	1A	2803	A
1	1A	2804	C
1	1A	2813	G
1	1A	2830	A
1	1A	2831	A
1	1A	2843	G
1	1A	2882	G
1	1A	2901	A
1	1A	2903	G
2	1B	2	C
2	1B	9	G
2	1B	12	C
2	1B	13	A
2	1B	24	G
2	1B	35	U
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	110	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	50	A
32	1a	51	A

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Mol	Chain	Res	Type
32	1a	52	G
32	1a	61	G
32	1a	69	G
32	1a	79	G
32	1a	91	C
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	189(F)	U
32	1a	189(H)	G
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	245	C
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	280	C
32	1a	289	G
32	1a	306	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	344	A
32	1a	346	G
32	1a	347	G
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G

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Mol	Chain	Res	Type
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	421	U
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	484	G
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	562	C
32	1a	567	G
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	630	G

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Mol	Chain	Res	Type
32	1a	653	A
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	702	A
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	755	G
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	853	G
32	1a	859	A
32	1a	876	G
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	931	C
32	1a	932	C
32	1a	934	C
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	983	A
32	1a	992	U

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Mol	Chain	Res	Type
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1020	U
32	1a	1021	G
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1033	G
32	1a	1037	C
32	1a	1039	C
32	1a	1043	C
32	1a	1045	C
32	1a	1054	C
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1122	U
32	1a	1123	A
32	1a	1125	U
32	1a	1127	G
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C

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Mol	Chain	Res	Type
32	1a	1138	G
32	1a	1139	G
32	1a	1141	C
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1168	A
32	1a	1172	C
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1241	G
32	1a	1248	A
32	1a	1251	A
32	1a	1256	A
32	1a	1257	U
32	1a	1260	C
32	1a	1270	C
32	1a	1276	G
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1322	C
32	1a	1345	U
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A

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Mol	Chain	Res	Type
32	1a	1364	U
32	1a	1378	C
32	1a	1400	5MC
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1497	G
32	1a	1499	A
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	15	A
54	1w	75	C
55	1x	9	G
55	1x	21	A
55	1x	47	U
55	1x	59	A
55	1x	69	C
55	1x	76	A
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U
1	2A	95	G
1	2A	100	G

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Mol	Chain	Res	Type
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	125	G
1	2A	128	C
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	204	A
1	2A	205	G
1	2A	214	G
1	2A	216	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	233	A
1	2A	248	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(B)	G
1	2A	272(I)	U
1	2A	272(J)	C
1	2A	277	C
1	2A	278	A
1	2A	280	C
1	2A	303	U
1	2A	311	A
1	2A	324	A
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	363(D)	G
1	2A	365	C

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Mol	Chain	Res	Type
1	2A	386	G
1	2A	396	G
1	2A	403	U
1	2A	405	U
1	2A	406	G
1	2A	411	G
1	2A	412	A
1	2A	444	C
1	2A	448	U
1	2A	449	A
1	2A	451	C
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	496	G
1	2A	499	U
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	528	A
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	592	G
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	647	G
1	2A	652(B)	A

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Mol	Chain	Res	Type
1	2A	652(C)	G
1	2A	668	G
1	2A	669	G
1	2A	670	A
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	753	C
1	2A	764	A
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	800	A
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	825	C
1	2A	827	U
1	2A	831	G
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	872	A
1	2A	874	G
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	903	C
1	2A	907	U

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Mol	Chain	Res	Type
1	2A	910	A
1	2A	914	C
1	2A	915	C
1	2A	917	A
1	2A	931	G
1	2A	932	G
1	2A	933	A
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1021	A
1	2A	1022	G
1	2A	1023	U
1	2A	1025	G
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1043	C
1	2A	1116	C
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1143	A
1	2A	1144	G
1	2A	1155	A
1	2A	1171	G
1	2A	1204	A
1	2A	1211	U
1	2A	1218	C

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Mol	Chain	Res	Type
1	2A	1220	A
1	2A	1248	G
1	2A	1253	A
1	2A	1255	U
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1274	A
1	2A	1300	U
1	2A	1301	A
1	2A	1302	A
1	2A	1313	U
1	2A	1314	C
1	2A	1321	A
1	2A	1341	U
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1395	A
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1459	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A

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Mol	Chain	Res	Type
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1495	A
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1610	A
1	2A	1616	A
1	2A	1646	C
1	2A	1648	C
1	2A	1654	A
1	2A	1665	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1745(A)	C
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A

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Mol	Chain	Res	Type
1	2A	1780	A
1	2A	1781	C
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1815	A
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1866	C
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1997	G
1	2A	2023	G
1	2A	2027	G
1	2A	2030	A
1	2A	2031	A
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A

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Mol	Chain	Res	Type
1	2A	2069	G
1	2A	2093	G
1	2A	2105	C
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2119	A
1	2A	2120	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C
1	2A	2145	C
1	2A	2146	C
1	2A	2148	G
1	2A	2150	U
1	2A	2153	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2178	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2199	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A

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Mol	Chain	Res	Type
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A
1	2A	2319	G
1	2A	2320	A
1	2A	2321	G
1	2A	2325	G
1	2A	2336	A
1	2A	2342	C
1	2A	2347	C
1	2A	2350	C
1	2A	2352	A
1	2A	2358	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2402	C
1	2A	2403	C
1	2A	2406	U
1	2A	2424	C
1	2A	2425	A
1	2A	2428	G
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2447	G
1	2A	2448	A
1	2A	2465	C
1	2A	2469	A
1	2A	2474	C
1	2A	2476	A

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Mol	Chain	Res	Type
1	2A	2484	G
1	2A	2491	U
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2572	A
1	2A	2573	C
1	2A	2578	G
1	2A	2602	A
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A
1	2A	2663	G
1	2A	2682	U
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2744	G
1	2A	2748	A
1	2A	2751	G
1	2A	2758	A
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2808	U
1	2A	2818	G
1	2A	2820	A

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Mol	Chain	Res	Type
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2836	U
1	2A	2872	G
1	2A	2879	C
1	2A	2880	C
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	9	G
2	2B	12	C
2	2B	13	A
2	2B	24	G
2	2B	30	C
2	2B	35	U
2	2B	41	U
2	2B	56	G
2	2B	67	G
2	2B	73	A
2	2B	110	G
32	2a	7	G
32	2a	9	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	66	G
32	2a	73	G
32	2a	80	G
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	120	A
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C
32	2a	163	C
32	2a	174	C
32	2a	182	U

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Mol	Chain	Res	Type
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	231	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	280	C
32	2a	281	G
32	2a	289	G
32	2a	306	G
32	2a	328	C
32	2a	329	A
32	2a	330	C
32	2a	332	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	381	C
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	439	A
32	2a	442	C

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Mol	Chain	Res	Type
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	607	A
32	2a	630	G
32	2a	653	A
32	2a	665	A
32	2a	666	G
32	2a	671	G
32	2a	687	A
32	2a	688	G
32	2a	702	A
32	2a	703	G
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	749	C
32	2a	755	G
32	2a	777	A
32	2a	793	U

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Mol	Chain	Res	Type
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	848	C
32	2a	851	G
32	2a	853	G
32	2a	859	A
32	2a	870	U
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	945	G
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	997	U
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1020	U
32	2a	1021	G

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Mol	Chain	Res	Type
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1033	G
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1045	C
32	2a	1053	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1108	G
32	2a	1117	G
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1146	A
32	2a	1152	A
32	2a	1159	U
32	2a	1172	C
32	2a	1182	G
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1200	C
32	2a	1202	G
32	2a	1211	U

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Mol	Chain	Res	Type
32	2a	1212	U
32	2a	1213	A
32	2a	1227	A
32	2a	1236	A
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1264	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1276	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1301	U
32	2a	1302	U
32	2a	1305	G
32	2a	1322	C
32	2a	1345	U
32	2a	1346	A
32	2a	1347	G
32	2a	1359	C
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1368	G
32	2a	1370	G
32	2a	1398	A
32	2a	1400	5MC
32	2a	1401	G
32	2a	1403	C
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1442(B)	A
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1457	G

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Mol	Chain	Res	Type
32	2a	1487	G
32	2a	1492	A
32	2a	1494	G
32	2a	1497	G
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
54	2w	74	C
54	2w	75	C
55	2x	9	G
55	2x	17(A)	U
55	2x	21	A
55	2x	47	U
55	2x	48	C
55	2x	59	A
55	2x	61	C
55	2x	69	C
55	2x	76	A

All (45) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	115	G
1	1A	302	A
1	1A	509	A
1	1A	572	A
1	1A	913	A
1	1A	941	U
1	1A	1065	U
1	1A	1067	A
1	1A	1093	G
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1255	A
1	1A	1466	U

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Mol	Chain	Res	Type
1	1A	1554	A
1	1A	1700	G
1	1A	2014	G
1	1A	2156	A
1	1A	2203	G
1	1A	2205	C
1	1A	2641	A
1	1A	2701	U
1	1A	2769	U
2	1B	1	U
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2351	G
1	2A	2689	U
2	2B	1	U

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

58 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
43	0TD	1l	92	43	7,9,10	4.63	1 (14%)	6,11,13	7.99	2 (33%)
1	OMG	1A	2263	55,1	18,26,27	0.96	1 (5%)	19,38,41	1.17	4 (21%)
32	4OC	1a	1402	32	20,23,24	0.76	0	26,32,35	0.87	1 (3%)
55	PSU	2x	55	55	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	2A	2251	55,1	18,26,27	1.01	1 (5%)	19,38,41	1.12	3 (15%)
1	4OC	1A	1942	1	19,22,24	0.84	0	26,31,35	0.98	1 (3%)
32	4OC	2a	1402	32	20,23,24	0.80	0	26,32,35	0.93	1 (3%)
32	2MG	1a	1207	32	18,26,27	0.88	1 (5%)	16,38,41	1.07	2 (12%)
55	4SU	2x	8	55	18,21,22	1.90	6 (33%)	26,30,33	1.59	7 (26%)
55	5MU	1x	54	55	19,22,23	1.44	6 (31%)	28,32,35	1.87	8 (28%)
32	UR3	1a	1498	32	19,22,23	1.03	1 (5%)	26,32,35	1.45	2 (7%)
1	5MU	2A	1939	1	19,22,23	1.37	4 (21%)	28,32,35	2.11	6 (21%)
1	5MC	1A	1984	1	18,22,23	0.94	2 (11%)	26,32,35	1.23	4 (15%)
1	5MC	2A	1942	1	18,22,23	0.99	2 (11%)	26,32,35	1.21	3 (11%)
32	M2G	1a	966	32	20,27,28	1.49	3 (15%)	22,40,43	0.92	2 (9%)
32	5MC	1a	1404	32	18,22,23	0.99	2 (11%)	26,32,35	1.14	2 (7%)
1	PSU	1A	1933	1	18,21,22	1.37	2 (11%)	22,30,33	1.81	3 (13%)
32	M2G	2a	966	32	20,27,28	1.46	3 (15%)	22,40,43	0.90	1 (4%)
32	MA6	2a	1519	32	19,26,27	1.02	1 (5%)	18,38,41	1.75	5 (27%)
1	5MU	1A	1961	1	19,22,23	1.41	5 (26%)	28,32,35	2.25	6 (21%)
1	5MC	1A	1964	1	18,22,23	0.98	2 (11%)	26,32,35	1.15	3 (11%)
32	5MC	1a	1400	32	18,22,23	0.96	2 (11%)	26,32,35	1.14	2 (7%)
55	5MC	2x	32	55	18,22,23	1.00	2 (11%)	26,32,35	1.18	3 (11%)
1	5MU	1A	1937	1	19,22,23	1.46	4 (21%)	28,32,35	2.17	7 (25%)
32	PSU	1a	516	32	18,21,22	1.38	2 (11%)	22,30,33	1.78	4 (18%)
55	5MU	2x	54	55	19,22,23	1.44	6 (31%)	28,32,35	2.05	8 (28%)
32	MA6	1a	1519	32	19,26,27	0.98	1 (5%)	18,38,41	1.65	5 (27%)
55	PSU	1x	55	55	18,21,22	1.34	2 (11%)	22,30,33	1.90	4 (18%)
32	5MC	1a	1407	32	18,22,23	0.99	1 (5%)	26,32,35	1.15	3 (11%)
1	5MC	2A	1962	1	18,22,23	0.95	2 (11%)	26,32,35	1.23	2 (7%)
32	7MG	2a	527	32	22,26,27	1.36	3 (13%)	29,39,42	2.52	7 (24%)
32	2MG	2a	1207	32	18,26,27	0.84	0	16,38,41	1.19	4 (25%)
32	5MC	2a	1407	32	18,22,23	1.01	2 (11%)	26,32,35	1.15	2 (7%)
54	KGV	1w	76	54	30,36,37	0.93	1 (3%)	29,51,54	1.16	4 (13%)
54	KGV	2w	76	56,54	30,36,37	0.93	1 (3%)	29,51,54	1.19	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
55	5MC	1x	32	55	18,22,23	0.97	2 (11%)	26,32,35	1.20	3 (11%)
1	2MU	2A	2552	1	19,22,24	1.24	3 (15%)	26,31,36	1.86	6 (23%)
1	2MA	2A	2503	1	17,25,26	1.04	1 (5%)	17,37,40	0.94	2 (11%)
1	PSU	1A	2617	1	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
32	MA6	2a	1518	32	19,26,27	0.97	1 (5%)	18,38,41	1.78	6 (33%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
32	UR3	2a	1498	32	19,22,23	1.04	2 (10%)	26,32,35	1.40	2 (7%)
1	4OC	2A	1920	1	19,22,24	0.82	0	26,31,35	0.81	0
32	MA6	1a	1518	32	19,26,27	0.94	1 (5%)	18,38,41	1.67	5 (27%)
1	PSU	2A	2605	1	18,21,22	1.34	2 (11%)	22,30,33	1.79	3 (13%)
32	5MC	2a	1404	32	18,22,23	0.95	2 (11%)	26,32,35	1.15	3 (11%)
1	2MU	1A	2564	1	19,22,24	1.28	3 (15%)	26,31,36	1.69	5 (19%)
32	5MC	2a	967	32	18,22,23	0.98	2 (11%)	26,32,35	1.07	2 (7%)
55	4SU	1x	8	55	18,21,22	1.88	5 (27%)	26,30,33	1.80	8 (30%)
32	5MC	2a	1400	32	18,22,23	0.94	2 (11%)	26,32,35	1.14	3 (11%)
43	0TD	2l	92	43	7,9,10	4.67	1 (14%)	6,11,13	6.18	2 (33%)
32	PSU	2a	516	32	18,21,22	1.33	2 (11%)	22,30,33	1.77	3 (13%)
1	5MU	2A	1915	1	19,22,23	1.42	5 (26%)	28,32,35	2.00	6 (21%)
1	PSU	1A	1939	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
32	7MG	1a	527	32	22,26,27	1.35	3 (13%)	29,39,42	2.48	6 (20%)
32	5MC	1a	967	32	18,22,23	1.01	1 (5%)	26,32,35	1.19	3 (11%)
1	PSU	2A	1917	1	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
1	2MA	1A	2515	56,1	17,25,26	1.00	2 (11%)	17,37,40	0.98	2 (11%)

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
43	0TD	1l	92	43	-	2/7/12/14	-
1	OMG	1A	2263	55,1	-	0/5/27/28	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/5/27/28	0/3/3/3
1	4OC	1A	1942	1	-	1/9/27/30	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1984	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	3/7/29/30	0/3/3/3
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3
1	5MU	1A	1961	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1964	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	2/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32	-	0/7/37/38	0/3/3/3
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
54	KGV	1w	76	54	-	6/15/37/38	0/4/4/4
54	KGV	2w	76	56,54	-	6/15/37/38	0/4/4/4
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1	-	0/9/27/28	0/2/2/2
1	2MA	2A	2503	1	-	1/3/25/26	0/3/3/3
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	1/7/29/30	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
32	MA6	1a	1518	32	-	2/7/29/30	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	2MU	1A	2564	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32	-	2/7/37/38	0/3/3/3
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2515	56,1	-	1/3/25/26	0/3/3/3

All (122) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.01	1.70	1.82
43	1l	92	0TD	CB-SB	-11.96	1.70	1.82
32	1a	966	M2G	C2-N3	4.85	1.36	1.30
32	2a	966	M2G	C2-N3	4.66	1.36	1.30
55	1x	8	4SU	C4-S4	-4.47	1.59	1.68
55	2x	8	4SU	C4-S4	-4.14	1.60	1.68
55	2x	8	4SU	C4-N3	-3.97	1.33	1.37
32	1a	516	PSU	C6-C5	3.57	1.39	1.35
55	1x	8	4SU	C4-N3	-3.56	1.33	1.37
55	2x	55	PSU	C6-C5	3.42	1.39	1.35
1	2A	1911	PSU	C6-C5	3.37	1.39	1.35
1	2A	1917	PSU	C6-C5	3.37	1.39	1.35
55	1x	55	PSU	C6-C5	3.36	1.39	1.35
32	2a	516	PSU	C6-C5	3.29	1.39	1.35
55	1x	8	4SU	C5-C4	-3.24	1.38	1.42
32	2a	527	7MG	C4-N9	-3.23	1.34	1.37
1	1A	1933	PSU	C6-C5	3.15	1.39	1.35
1	1A	1939	PSU	C6-C5	3.14	1.39	1.35
32	2a	1407	5MC	C6-C5	3.12	1.39	1.34
32	1a	527	7MG	C4-N9	-3.06	1.34	1.37
55	2x	8	4SU	C2-N3	-3.06	1.32	1.38
1	2A	2605	PSU	C6-C5	3.03	1.38	1.35
32	1a	1407	5MC	C6-C5	3.02	1.39	1.34
32	1a	967	5MC	C6-C5	3.01	1.39	1.34
1	1A	2617	PSU	C6-C5	3.00	1.38	1.35
32	1a	527	7MG	C5-C4	2.96	1.47	1.38
55	2x	32	5MC	C6-C5	2.96	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	527	7MG	C5-C4	2.95	1.47	1.38
1	1A	1937	5MU	C2-N1	2.94	1.43	1.38
32	1a	966	M2G	C2-N2	2.92	1.40	1.35
55	1x	32	5MC	C6-C5	2.92	1.39	1.34
1	1A	1964	5MC	C6-C5	2.92	1.39	1.34
32	2a	967	5MC	C6-C5	2.90	1.39	1.34
32	1a	1404	5MC	C6-C5	2.88	1.39	1.34
1	2A	1915	5MU	C6-C5	2.88	1.39	1.34
1	2A	1942	5MC	C6-C5	2.85	1.39	1.34
1	2A	2552	2MU	C4-N3	-2.81	1.33	1.38
1	1A	1937	5MU	C6-C5	2.80	1.39	1.34
32	2a	966	M2G	C2-N2	2.80	1.40	1.35
55	2x	8	4SU	C5-C4	-2.74	1.39	1.42
32	2a	1404	5MC	C6-C5	2.73	1.39	1.34
1	2A	2605	PSU	C4-N3	-2.72	1.33	1.38
55	1x	54	5MU	C6-C5	2.71	1.39	1.34
1	1A	1961	5MU	C4-N3	-2.69	1.33	1.38
32	1a	1400	5MC	C6-C5	2.68	1.39	1.34
55	1x	55	PSU	C4-N3	-2.67	1.33	1.38
1	1A	2263	OMG	C6-N1	-2.66	1.33	1.37
32	2a	1519	MA6	C5-C4	2.66	1.48	1.40
1	1A	1939	PSU	C4-N3	-2.66	1.33	1.38
55	2x	54	5MU	C6-C5	2.65	1.39	1.34
1	2A	2251	OMG	C6-N1	-2.65	1.33	1.37
55	2x	54	5MU	C4-C5	2.65	1.49	1.44
55	1x	54	5MU	C4-N3	-2.65	1.33	1.38
1	1A	2617	PSU	C4-N3	-2.64	1.33	1.38
1	1A	1961	5MU	C6-C5	2.63	1.38	1.34
1	2A	1939	5MU	C4-N3	-2.61	1.34	1.38
1	2A	1939	5MU	C6-C5	2.60	1.38	1.34
1	2A	1917	PSU	C4-N3	-2.60	1.34	1.38
32	2a	1400	5MC	C6-C5	2.59	1.38	1.34
55	1x	54	5MU	C4-C5	2.59	1.49	1.44
55	2x	55	PSU	C4-N3	-2.57	1.34	1.38
1	1A	1984	5MC	C6-N1	-2.56	1.33	1.38
1	1A	1933	PSU	C4-N3	-2.55	1.34	1.38
1	1A	1937	5MU	C4-C5	2.55	1.49	1.44
55	2x	54	5MU	C4-N3	-2.54	1.34	1.38
55	1x	8	4SU	C2-N3	-2.53	1.33	1.38
1	2A	1911	PSU	C4-N3	-2.53	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.52	1.34	1.38
1	1A	2564	2MU	C4-N3	-2.52	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	527	7MG	C6-N1	-2.51	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.49	1.33	1.38
32	2a	966	M2G	C6-N1	-2.48	1.34	1.37
1	1A	1961	5MU	C6-N1	-2.47	1.33	1.38
1	1A	1984	5MC	C6-C5	2.46	1.38	1.34
1	1A	1937	5MU	C4-N3	-2.45	1.34	1.38
32	1a	1519	MA6	C5-C4	2.45	1.47	1.40
54	2w	76	KGV	C5-C4	2.44	1.47	1.40
1	2A	1962	5MC	C6-C5	2.43	1.38	1.34
1	2A	1915	5MU	C4-C5	2.43	1.48	1.44
1	2A	1939	5MU	C6-N1	-2.43	1.33	1.38
1	2A	1915	5MU	C2-N1	2.41	1.42	1.38
32	2a	1518	MA6	C5-C4	2.41	1.47	1.40
1	1A	1961	5MU	C4-C5	2.40	1.48	1.44
54	1w	76	KGV	C5-C4	2.40	1.47	1.40
32	1a	1518	MA6	C5-C4	2.38	1.47	1.40
32	2a	516	PSU	C4-N3	-2.36	1.34	1.38
32	2a	527	7MG	C6-N1	-2.36	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.35	1.34	1.38
1	1A	2564	2MU	C2-N1	2.33	1.42	1.38
55	2x	8	4SU	C2-N1	2.33	1.42	1.38
55	2x	54	5MU	C2-N1	2.31	1.42	1.38
32	1a	1207	2MG	C6-N1	-2.30	1.34	1.37
32	1a	516	PSU	C4-N3	-2.29	1.34	1.38
1	2A	2503	2MA	C2-N3	2.27	1.36	1.31
32	2a	1404	5MC	C6-N1	-2.25	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.25	1.34	1.38
1	1A	2564	2MU	C5-C4	2.25	1.48	1.43
55	1x	54	5MU	C6-N1	-2.22	1.34	1.38
1	1A	1961	5MU	C2-N3	-2.21	1.34	1.38
55	1x	8	4SU	C2-N1	2.20	1.42	1.38
32	1a	966	M2G	C6-N1	-2.20	1.34	1.37
55	1x	54	5MU	C2-N3	-2.19	1.34	1.38
32	2a	1498	UR3	C2-N1	2.18	1.41	1.38
55	2x	54	5MU	C6-N1	-2.18	1.34	1.38
55	1x	32	5MC	C6-N1	-2.17	1.34	1.38
1	1A	1964	5MC	C6-N1	-2.15	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.12	1.34	1.38
1	2A	1939	5MU	C4-C5	2.12	1.48	1.44
32	1a	1404	5MC	C6-N1	-2.11	1.34	1.38
55	2x	32	5MC	C6-N1	-2.09	1.34	1.38
1	1A	2515	2MA	C2-N3	2.07	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1498	UR3	C6-C5	2.07	1.39	1.35
55	2x	54	5MU	C2-N3	-2.06	1.34	1.38
1	2A	2552	2MU	C2-N3	-2.06	1.34	1.38
1	2A	2552	2MU	C5-C4	2.06	1.48	1.43
55	1x	54	5MU	C2-N1	2.02	1.41	1.38
1	2A	1915	5MU	C6-N1	-2.02	1.34	1.38
55	2x	8	4SU	C6-C5	2.02	1.39	1.35
32	2a	967	5MC	C6-N1	-2.01	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.01	1.34	1.38
1	1A	2515	2MA	C6-N1	-2.01	1.33	1.38
32	1a	1498	UR3	C2-N1	2.01	1.41	1.38

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	-19.27	67.58	102.44
43	2l	92	0TD	CSB-SB-CB	-14.76	75.73	102.44
32	2a	527	7MG	N9-C4-N3	8.82	138.67	125.47
32	1a	527	7MG	N9-C4-N3	8.79	138.62	125.47
1	2A	1911	PSU	N1-C2-N3	6.15	122.10	115.13
1	1A	1939	PSU	N1-C2-N3	6.01	121.94	115.13
55	2x	55	PSU	N1-C2-N3	6.01	121.94	115.13
55	1x	55	PSU	N1-C2-N3	5.90	121.82	115.13
1	2A	1917	PSU	N1-C2-N3	5.90	121.82	115.13
32	1a	1498	UR3	C4-N3-C2	-5.89	119.01	124.56
1	1A	1961	5MU	C4-N3-C2	-5.75	119.91	127.35
1	1A	1933	PSU	N1-C2-N3	5.74	121.63	115.13
32	2a	1498	UR3	C4-N3-C2	-5.68	119.21	124.56
1	1A	2617	PSU	N1-C2-N3	5.62	121.50	115.13
32	2a	516	PSU	N1-C2-N3	5.46	121.31	115.13
32	1a	527	7MG	C5-C4-N3	-5.40	117.83	128.13
32	1a	516	PSU	N1-C2-N3	5.37	121.21	115.13
1	2A	2605	PSU	N1-C2-N3	5.36	121.21	115.13
32	2a	527	7MG	C5-C4-N3	-5.36	117.92	128.13
32	1a	527	7MG	N9-C8-N7	-5.31	95.79	103.38
1	1A	1937	5MU	C4-N3-C2	-5.28	120.52	127.35
32	2a	527	7MG	N9-C8-N7	-5.27	95.83	103.38
1	2A	1939	5MU	C4-N3-C2	-5.20	120.62	127.35
1	2A	2552	2MU	N3-C2-N1	5.12	121.68	114.89
1	1A	1937	5MU	C5-C4-N3	5.09	119.66	115.31
55	2x	54	5MU	C4-N3-C2	-5.04	120.83	127.35
1	1A	1961	5MU	C5-C4-N3	5.03	119.60	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	8	4SU	C5-C4-N3	4.97	119.30	114.69
1	1A	1961	5MU	N3-C2-N1	4.96	121.47	114.89
1	1A	2564	2MU	N3-C2-N1	4.94	121.44	114.89
1	2A	1915	5MU	C4-N3-C2	-4.93	120.97	127.35
1	2A	1915	5MU	N3-C2-N1	4.83	121.30	114.89
1	1A	1937	5MU	N3-C2-N1	4.81	121.27	114.89
1	1A	1961	5MU	C5-C6-N1	-4.76	118.44	123.34
1	2A	1939	5MU	N3-C2-N1	4.72	121.15	114.89
55	2x	54	5MU	N3-C2-N1	4.67	121.09	114.89
55	1x	54	5MU	N3-C2-N1	4.67	121.09	114.89
55	1x	54	5MU	C4-N3-C2	-4.50	121.52	127.35
1	2A	2552	2MU	C4-N3-C2	-4.48	120.67	126.58
1	2A	1915	5MU	C5-C4-N3	4.42	119.09	115.31
55	2x	54	5MU	C5-C4-N3	4.41	119.08	115.31
32	2a	527	7MG	C2-N3-C4	4.35	120.05	112.30
1	2A	1939	5MU	C5-C4-N3	4.34	119.01	115.31
32	2a	1519	MA6	N1-C6-N6	4.32	121.60	117.06
1	2A	1939	5MU	O4-C4-C5	-4.30	119.92	124.90
1	1A	1937	5MU	O4-C4-C5	-4.24	119.98	124.90
55	1x	55	PSU	C4-N3-C2	-4.13	120.39	126.34
32	1a	527	7MG	C2-N3-C4	4.12	119.65	112.30
1	2A	1962	5MC	C5-C6-N1	-4.11	119.11	123.34
1	1A	2564	2MU	C4-N3-C2	-4.10	121.17	126.58
1	2A	1939	5MU	C5-C6-N1	-4.01	119.22	123.34
32	1a	1400	5MC	C5-C6-N1	-3.96	119.26	123.34
1	1A	1984	5MC	C5-C6-N1	-3.96	119.27	123.34
1	1A	2617	PSU	C4-N3-C2	-3.94	120.67	126.34
1	2A	1942	5MC	C5-C6-N1	-3.92	119.31	123.34
1	2A	2605	PSU	C4-N3-C2	-3.92	120.69	126.34
1	1A	1939	PSU	C4-N3-C2	-3.91	120.71	126.34
55	2x	55	PSU	C4-N3-C2	-3.90	120.72	126.34
1	2A	1915	5MU	O4-C4-C5	-3.89	120.39	124.90
1	2A	1917	PSU	C4-N3-C2	-3.86	120.78	126.34
1	2A	1911	PSU	O2-C2-N1	-3.85	118.55	122.79
55	2x	54	5MU	C5-C6-N1	-3.85	119.38	123.34
1	2A	1911	PSU	C4-N3-C2	-3.82	120.84	126.34
32	2a	1400	5MC	C5-C6-N1	-3.81	119.42	123.34
55	1x	32	5MC	C5-C6-N1	-3.80	119.43	123.34
1	1A	1964	5MC	C5-C6-N1	-3.74	119.49	123.34
55	2x	8	4SU	C5-C4-N3	3.72	118.14	114.69
1	1A	1933	PSU	O2-C2-N1	-3.71	118.70	122.79
32	1a	1404	5MC	C5-C6-N1	-3.69	119.54	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	54	5MU	C5-C4-N3	3.65	118.43	115.31
32	2a	1407	5MC	C5-C6-N1	-3.63	119.60	123.34
55	1x	8	4SU	C1'-N1-C2	3.61	124.11	117.57
32	1a	1518	MA6	C9-N6-C6	-3.60	108.61	119.51
1	1A	1961	5MU	O4-C4-C5	-3.57	120.76	124.90
1	1A	1933	PSU	C4-N3-C2	-3.50	121.29	126.34
32	2a	516	PSU	C4-N3-C2	-3.50	121.29	126.34
32	2a	967	5MC	C5-C6-N1	-3.50	119.74	123.34
55	1x	54	5MU	C5-C6-N1	-3.49	119.75	123.34
55	2x	8	4SU	C1'-N1-C2	3.48	123.88	117.57
32	2a	1404	5MC	C5-C6-N1	-3.47	119.77	123.34
32	2a	516	PSU	O2-C2-N1	-3.46	118.98	122.79
55	2x	54	5MU	O4-C4-C5	-3.43	120.93	124.90
32	1a	1407	5MC	C5-C6-N1	-3.37	119.88	123.34
55	2x	32	5MC	C5-C6-N1	-3.36	119.89	123.34
32	1a	1518	MA6	N3-C2-N1	-3.35	123.44	128.68
32	2a	1518	MA6	N3-C2-N1	-3.35	123.45	128.68
32	1a	1518	MA6	C4-C5-N7	-3.34	105.92	109.40
32	1a	1519	MA6	C4-C5-N7	-3.34	105.92	109.40
55	2x	55	PSU	O2-C2-N1	-3.33	119.13	122.79
32	1a	516	PSU	C4-N3-C2	-3.32	121.56	126.34
1	1A	1937	5MU	C5-C6-N1	-3.31	119.93	123.34
1	1A	1939	PSU	O2-C2-N1	-3.31	119.15	122.79
32	2a	1518	MA6	C9-N6-C6	-3.28	109.58	119.51
1	2A	1915	5MU	C5-C6-N1	-3.26	119.98	123.34
1	1A	1961	5MU	O2-C2-N1	-3.23	118.49	122.79
32	1a	1519	MA6	C9-N6-C6	-3.22	109.75	119.51
32	1a	516	PSU	O2-C2-N1	-3.17	119.30	122.79
1	2A	1917	PSU	O2-C2-N1	-3.16	119.31	122.79
32	2a	1518	MA6	C4-C5-N7	-3.15	106.12	109.40
1	1A	2617	PSU	O2-C2-N1	-3.13	119.35	122.79
32	1a	516	PSU	C6-C5-C4	-3.12	116.02	118.20
32	1a	967	5MC	C5-C6-N1	-3.10	120.15	123.34
55	1x	8	4SU	C5-C4-S4	-3.08	120.50	124.47
1	2A	1939	5MU	O2-C2-N1	-3.05	118.73	122.79
32	1a	1519	MA6	N3-C2-N1	-3.04	123.92	128.68
55	1x	55	PSU	O2-C2-N1	-3.04	119.45	122.79
54	1w	76	KGV	N3-C2-N1	-3.02	123.95	128.68
55	2x	8	4SU	O2-C2-N3	-2.98	115.95	121.50
55	1x	8	4SU	C4-N3-C2	-2.96	124.46	127.34
55	1x	8	4SU	C6-C5-C4	-2.94	117.41	119.95
32	2a	1519	MA6	C4-C5-N7	-2.93	106.34	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2552	2MU	O4-C4-C5	-2.88	120.09	125.16
32	2a	1519	MA6	C9-N6-C6	-2.87	110.82	119.51
32	1a	1404	5MC	C5-C4-N3	-2.86	118.59	121.67
54	2w	76	KGV	C3'-N3'-C	-2.85	118.91	123.21
1	2A	2552	2MU	C5-C4-N3	2.81	119.04	114.84
32	2a	1518	MA6	N1-C6-N6	2.80	120.00	117.06
1	2A	2605	PSU	O2-C2-N1	-2.78	119.73	122.79
54	2w	76	KGV	N3-C2-N1	-2.78	124.34	128.68
1	2A	2552	2MU	O2-C2-N1	-2.76	119.12	122.79
32	2a	527	7MG	C5-C6-N1	2.75	115.84	110.99
55	1x	54	5MU	O4-C4-C5	-2.74	121.72	124.90
32	1a	967	5MC	C5-C4-N3	-2.72	118.73	121.67
32	2a	1519	MA6	N3-C2-N1	-2.71	124.45	128.68
55	1x	32	5MC	C5-C4-N3	-2.68	118.79	121.67
32	2a	1407	5MC	C5-C4-N3	-2.67	118.80	121.67
1	1A	2515	2MA	C5-C6-N1	2.66	118.61	114.02
1	1A	2564	2MU	O4-C4-C5	-2.66	120.49	125.16
55	2x	8	4SU	O2-C2-N1	2.65	126.31	122.79
55	2x	32	5MC	C5-C4-N3	-2.62	118.85	121.67
54	2w	76	KGV	C4-C5-N7	-2.62	106.67	109.40
32	1a	1407	5MC	C5-C4-N3	-2.60	118.87	121.67
32	2a	1518	MA6	C10-N6-C9	-2.59	107.76	116.12
55	2x	54	5MU	C5M-C5-C4	2.56	121.58	118.77
32	1a	967	5MC	O2-C2-N3	-2.56	118.17	122.33
1	1A	2263	OMG	C5-C6-N1	2.54	118.43	113.95
54	1w	76	KGV	C3'-N3'-C	-2.52	119.41	123.21
1	1A	2564	2MU	C5-C4-N3	2.52	118.61	114.84
1	2A	1942	5MC	C5-C4-N3	-2.51	118.97	121.67
1	1A	1942	4OC	O2-C2-N3	-2.49	118.28	122.33
32	1a	1519	MA6	N1-C6-N6	2.49	119.68	117.06
55	2x	32	5MC	O2-C2-N3	-2.48	118.29	122.33
32	1a	527	7MG	C5-C6-N1	2.48	115.36	110.99
32	2a	967	5MC	C5-C4-N3	-2.47	119.01	121.67
43	1l	92	0TD	OD2-CG-CB	2.47	118.49	113.15
43	2l	92	0TD	OD2-CG-CB	2.47	118.48	113.15
1	2A	2251	OMG	C5-C6-N1	2.46	118.30	113.95
55	1x	32	5MC	O2-C2-N3	-2.46	118.33	122.33
55	1x	54	5MU	C5M-C5-C4	2.44	121.46	118.77
32	2a	1207	2MG	C8-N7-C5	2.44	107.64	102.99
1	1A	1964	5MC	C5-C4-N3	-2.42	119.07	121.67
32	1a	1519	MA6	C10-N6-C6	-2.37	112.35	119.51
32	2a	1518	MA6	C10-N6-C6	-2.36	112.38	119.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1207	2MG	C8-N7-C5	2.35	107.46	102.99
54	1w	76	KGV	C4-C5-N7	-2.35	106.95	109.40
1	1A	2263	OMG	C8-N7-C5	2.31	107.40	102.99
32	2a	1519	MA6	C10-N6-C6	-2.29	112.58	119.51
32	2a	1404	5MC	C5-C4-N3	-2.29	119.21	121.67
1	2A	2251	OMG	O6-C6-C5	-2.27	119.93	124.37
32	2a	527	7MG	C5-C4-N9	-2.27	103.40	106.35
1	1A	1937	5MU	C1'-N1-C2	2.26	121.66	117.57
32	1a	1400	5MC	C5-C4-N3	-2.25	119.24	121.67
1	2A	2503	2MA	C5-C6-N1	2.24	117.89	114.02
54	2w	76	KGV	CG-CB-CA	-2.23	109.49	114.13
1	2A	1962	5MC	C5-C4-N3	-2.23	119.27	121.67
55	2x	54	5MU	C5M-C5-C6	-2.23	119.87	122.85
1	1A	1937	5MU	C5M-C5-C4	2.22	121.21	118.77
32	2a	966	M2G	C8-N7-C5	2.22	107.22	102.99
32	1a	1407	5MC	O2-C2-N3	-2.20	118.75	122.33
32	2a	1404	5MC	O2-C2-N3	-2.19	118.77	122.33
1	1A	1984	5MC	C5-C4-N3	-2.19	119.31	121.67
32	2a	1207	2MG	C5-C6-N1	2.18	117.81	113.95
1	2A	2503	2MA	C8-N7-C5	2.18	107.14	102.99
32	1a	1498	UR3	C3U-N3-C2	2.18	121.13	117.31
32	2a	1400	5MC	C5-C4-N3	-2.17	119.33	121.67
32	1a	527	7MG	C5-C4-N9	-2.16	103.54	106.35
32	1a	1518	MA6	C10-N6-C6	-2.16	112.97	119.51
55	2x	8	4SU	N3-C2-N1	2.15	117.75	114.89
32	1a	966	M2G	C5-C6-N1	2.15	117.75	113.95
1	1A	2515	2MA	C8-N7-C5	2.15	107.09	102.99
55	2x	8	4SU	C6-N1-C2	-2.15	118.24	120.99
55	1x	54	5MU	C5M-C5-C6	-2.14	119.98	122.85
54	1w	76	KGV	O4'-C4'-C3'	2.14	107.12	104.06
32	2a	527	7MG	CM7-N7-C5	2.13	131.91	126.40
55	2x	8	4SU	C6-C5-C4	-2.13	118.11	119.95
55	1x	8	4SU	N3-C2-N1	2.12	117.70	114.89
55	2x	54	5MU	O2-C2-N1	-2.12	119.97	122.79
1	2A	1942	5MC	O2-C2-N3	-2.10	118.92	122.33
55	1x	8	4SU	C6-N1-C2	-2.09	118.33	120.99
1	1A	2564	2MU	O2-C2-N1	-2.08	120.02	122.79
32	1a	1518	MA6	C10-N6-C9	-2.08	109.43	116.12
1	1A	1984	5MC	O2-C2-N3	-2.07	118.96	122.33
1	2A	2552	2MU	C2'-C1'-N1	-2.07	110.21	114.22
1	1A	2263	OMG	C2-N1-C6	-2.07	121.29	125.10
32	1a	966	M2G	O6-C6-C5	-2.06	120.34	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1402	4OC	C6-C5-C4	2.06	119.49	116.96
32	2a	1207	2MG	CM2-N2-C2	-2.06	119.31	123.86
55	1x	55	PSU	C5-C6-N1	-2.06	119.03	122.11
1	2A	1915	5MU	O2-C2-N1	-2.05	120.06	122.79
1	1A	2263	OMG	O6-C6-C5	-2.04	120.38	124.37
55	1x	54	5MU	O2-C2-N1	-2.04	120.08	122.79
1	1A	1964	5MC	O2-C2-N3	-2.04	119.02	122.33
32	2a	1498	UR3	C3U-N3-C4	2.04	120.80	117.89
32	2a	1402	4OC	C5-C4-N4	-2.02	118.49	122.61
1	2A	2251	OMG	C8-N7-C5	2.02	106.84	102.99
55	1x	8	4SU	O2-C2-N3	-2.02	117.74	121.50
1	1A	1984	5MC	CM5-C5-C6	-2.02	120.15	122.85
32	2a	1207	2MG	O6-C6-C5	-2.01	120.44	124.37
32	2a	1400	5MC	CM5-C5-C6	-2.01	120.16	122.85
32	1a	1207	2MG	C5-C6-N1	2.01	117.50	113.95

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	516	PSU	C2'-C1'-C5-C4
32	1a	516	PSU	C2'-C1'-C5-C6
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C10
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
54	1w	76	KGV	N3'-C-CA-CB
54	1w	76	KGV	N3'-C-CA-N
54	1w	76	KGV	C3'-C4'-C5'-O5'
54	2w	76	KGV	N3'-C-CA-CB
54	2w	76	KGV	N3'-C-CA-N
54	2w	76	KGV	C3'-C4'-C5'-O5'
54	2w	76	KGV	O4'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
54	1w	76	KGV	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	967	5MC	C3'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C9
32	2a	1518	MA6	C5-C6-N6-C10
54	1w	76	KGV	O-C-CA-CB
54	2w	76	KGV	O-C-CA-CB
32	2a	1519	MA6	C4'-C5'-O5'-P
43	1l	92	0TD	SB-CB-CG-OD1
32	1a	527	7MG	C3'-C4'-C5'-O5'
54	1w	76	KGV	O-C-CA-N
54	2w	76	KGV	O-C-CA-N
32	1a	1519	MA6	C5-C6-N6-C10
32	2a	1519	MA6	C5-C6-N6-C10
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	966	M2G	N3-C2-N2-CM2
32	2a	966	M2G	N1-C2-N2-CM1
32	2a	966	M2G	N1-C2-N2-CM2
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
32	1a	527	7MG	O4'-C4'-C5'-O5'
1	1A	1942	4OC	C2'-C1'-N1-C2
1	1A	2515	2MA	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1353 ligands modelled in this entry, 1351 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	SF4	1d	302	35	0,12,12	-	-	-		
58	SF4	2d	302	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	1d	302	35	-	-	0/6/5/5
58	SF4	2d	302	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	2D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2D	7:LYS	C	8:PRO	N	1.15

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	1A	2860/2915 (98%)	0.27	81 (2%)	53	40	74, 93, 132, 148	0
1	2A	2789/2915 (95%)	0.26	155 (5%)	24	17	81, 97, 127, 148	0
2	1B	120/121 (99%)	-0.45	0	100	100	93, 111, 121, 125	0
2	2B	120/121 (99%)	-0.56	0	100	100	102, 115, 123, 137	0
3	1D	275/276 (99%)	0.82	17 (6%)	20	14	76, 86, 97, 117	0
3	2D	275/276 (99%)	1.17	61 (22%)	0	0	79, 93, 105, 120	0
4	1E	204/206 (99%)	0.59	27 (13%)	3	3	78, 97, 111, 119	0
4	2E	204/206 (99%)	0.47	29 (14%)	2	2	80, 96, 107, 115	0
5	1F	203/210 (96%)	0.30	12 (5%)	22	15	72, 92, 109, 120	0
5	2F	203/210 (96%)	0.63	32 (15%)	2	1	85, 99, 114, 123	0
6	1G	181/182 (99%)	-0.31	0	100	100	100, 112, 122, 126	0
6	2G	181/182 (99%)	0.65	23 (12%)	3	4	102, 115, 125, 135	0
7	1H	174/180 (96%)	-0.08	1 (0%)	89	83	91, 103, 113, 124	0
7	2H	174/180 (96%)	0.54	13 (7%)	14	10	97, 114, 123, 132	0
8	1I	146/148 (98%)	-0.33	3 (2%)	63	52	89, 105, 115, 125	0
8	2I	146/148 (98%)	0.26	12 (8%)	11	9	97, 118, 130, 135	0
9	1N	140/140 (100%)	0.44	10 (7%)	16	11	85, 96, 109, 118	0
9	2N	140/140 (100%)	0.99	21 (15%)	2	2	91, 102, 115, 122	0
10	1O	122/122 (100%)	1.46	37 (30%)	0	0	83, 96, 109, 117	0
10	2O	122/122 (100%)	0.86	20 (16%)	1	1	82, 93, 101, 112	0
11	1P	149/150 (99%)	0.40	7 (4%)	31	23	80, 98, 116, 126	0
11	2P	149/150 (99%)	0.86	33 (22%)	0	0	86, 103, 115, 124	0
12	1Q	141/141 (100%)	1.06	32 (22%)	0	0	82, 98, 110, 117	0
12	2Q	141/141 (100%)	0.74	16 (11%)	5	4	88, 101, 113, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	0.46	3 (2%) 57 45	86, 95, 107, 114	0
13	2R	118/118 (100%)	0.50	10 (8%) 10 8	83, 94, 102, 110	0
14	1S	110/112 (98%)	-0.35	0 100 100	94, 109, 118, 123	0
14	2S	110/112 (98%)	-0.06	1 (0%) 84 76	98, 111, 118, 126	0
15	1T	131/146 (89%)	0.44	11 (8%) 11 8	88, 101, 116, 125	0
15	2T	131/146 (89%)	0.75	21 (16%) 1 1	85, 96, 110, 121	0
16	1U	116/118 (98%)	0.44	4 (3%) 45 34	76, 95, 107, 114	0
16	2U	116/118 (98%)	1.20	32 (27%) 0 0	88, 100, 109, 118	0
17	1V	101/101 (100%)	-0.00	1 (0%) 82 73	79, 97, 110, 115	0
17	2V	101/101 (100%)	0.51	11 (10%) 5 4	87, 103, 116, 122	0
18	1W	112/113 (99%)	0.76	10 (8%) 9 7	81, 91, 109, 124	0
18	2W	112/113 (99%)	1.07	19 (16%) 1 1	81, 93, 107, 119	0
19	1X	95/96 (98%)	0.74	8 (8%) 11 8	82, 91, 106, 117	0
19	2X	95/96 (98%)	0.73	8 (8%) 11 8	86, 98, 113, 121	0
20	1Y	107/110 (97%)	0.38	3 (2%) 53 40	83, 96, 109, 114	0
20	2Y	107/110 (97%)	1.21	21 (19%) 1 1	90, 105, 118, 123	0
21	1Z	154/206 (74%)	-0.29	0 100 100	96, 111, 120, 128	0
21	2Z	160/206 (77%)	-0.14	1 (0%) 89 83	101, 113, 123, 130	0
22	10	83/85 (97%)	0.94	13 (15%) 2 1	90, 101, 110, 116	0
22	20	83/85 (97%)	1.22	18 (21%) 0 0	92, 104, 111, 113	0
23	11	97/98 (98%)	1.26	22 (22%) 0 0	82, 92, 107, 114	0
23	21	97/98 (98%)	1.62	38 (39%) 0 0	86, 98, 110, 119	0
24	12	70/72 (97%)	-0.14	0 100 100	81, 92, 103, 122	0
24	22	70/72 (97%)	0.19	1 (1%) 75 64	93, 106, 116, 121	0
25	13	59/60 (98%)	0.06	0 100 100	78, 97, 116, 134	0
25	23	59/60 (98%)	1.20	11 (18%) 1 1	88, 99, 118, 130	0
26	14	69/71 (97%)	-0.71	0 100 100	107, 122, 134, 137	0
26	24	69/71 (97%)	-0.23	1 (1%) 75 64	106, 118, 131, 135	0
27	15	59/60 (98%)	0.66	10 (16%) 1 1	82, 93, 107, 111	0
27	25	59/60 (98%)	0.35	5 (8%) 10 8	84, 92, 109, 112	0
28	16	53/54 (98%)	0.22	1 (1%) 66 55	86, 98, 110, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.96	14 (26%)	0	0	94, 104, 115, 123	0
29	17	48/49 (97%)	1.21	8 (16%)	1	1	72, 82, 99, 113	0
29	27	48/49 (97%)	2.19	23 (47%)	0	0	83, 91, 105, 117	0
30	18	64/65 (98%)	0.73	3 (4%)	31	23	82, 90, 99, 112	0
30	28	64/65 (98%)	2.17	35 (54%)	0	0	89, 97, 106, 112	0
31	19	37/37 (100%)	0.17	0	100	100	91, 98, 106, 107	0
31	29	37/37 (100%)	1.66	14 (37%)	0	0	97, 106, 115, 118	0
32	1a	1488/1521 (97%)	-0.08	50 (3%)	45	34	85, 114, 131, 153	0
32	2a	1491/1521 (98%)	-0.11	29 (1%)	66	55	87, 108, 129, 149	0
33	1b	231/256 (90%)	-0.16	5 (2%)	62	50	104, 117, 126, 132	0
33	2b	231/256 (90%)	0.27	12 (5%)	27	20	101, 117, 127, 136	0
34	1c	206/239 (86%)	1.06	49 (23%)	0	0	104, 119, 128, 133	0
34	2c	206/239 (86%)	0.32	24 (11%)	4	4	104, 116, 124, 131	0
35	1d	208/209 (99%)	0.70	32 (15%)	2	1	97, 112, 122, 130	0
35	2d	208/209 (99%)	0.57	16 (7%)	13	10	91, 105, 114, 121	0
36	1e	148/162 (91%)	0.96	32 (21%)	0	0	96, 110, 119, 124	0
36	2e	148/162 (91%)	0.92	33 (22%)	0	0	93, 107, 118, 126	0
37	1f	100/101 (99%)	-0.14	2 (2%)	65	53	86, 105, 115, 117	0
37	2f	100/101 (99%)	-0.07	5 (5%)	28	21	95, 108, 117, 123	0
38	1g	155/156 (99%)	-0.12	8 (5%)	27	20	101, 115, 126, 132	0
38	2g	155/156 (99%)	0.14	11 (7%)	16	11	102, 114, 124, 129	0
39	1h	137/138 (99%)	0.27	7 (5%)	28	21	100, 110, 119, 129	0
39	2h	137/138 (99%)	0.28	12 (8%)	10	7	94, 106, 116, 126	0
40	1i	127/128 (99%)	0.70	29 (22%)	0	0	109, 120, 126, 130	0
40	2i	127/128 (99%)	0.99	32 (25%)	0	0	103, 118, 126, 129	0
41	1j	97/105 (92%)	0.96	22 (22%)	0	0	111, 122, 130, 135	0
41	2j	96/105 (91%)	0.37	14 (14%)	2	2	111, 122, 129, 137	0
42	1k	114/129 (88%)	0.45	8 (7%)	16	11	94, 105, 115, 122	0
42	2k	114/129 (88%)	1.08	26 (22%)	0	0	96, 110, 119, 122	0
43	1l	121/132 (91%)	0.82	21 (17%)	1	1	92, 105, 114, 116	0
43	2l	121/132 (91%)	0.82	27 (22%)	0	0	89, 102, 112, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.16	10 (8%)	12	9	104, 116, 125, 136	0
44	2m	122/126 (96%)	0.23	22 (18%)	1	1	106, 117, 124, 130	0
45	1n	60/61 (98%)	1.29	14 (23%)	0	0	105, 117, 126, 134	0
45	2n	60/61 (98%)	0.87	9 (15%)	2	2	107, 117, 125, 128	0
46	1o	88/89 (98%)	0.40	7 (7%)	12	9	93, 105, 114, 118	0
46	2o	88/89 (98%)	-0.06	2 (2%)	60	48	89, 106, 115, 123	0
47	1p	82/88 (93%)	1.24	19 (23%)	0	0	106, 114, 122, 129	0
47	2p	82/88 (93%)	0.26	3 (3%)	41	30	85, 100, 109, 114	0
48	1q	99/105 (94%)	0.33	5 (5%)	28	21	92, 107, 116, 122	0
48	2q	99/105 (94%)	0.68	14 (14%)	2	2	92, 104, 113, 120	0
49	1r	68/88 (77%)	-0.06	0	100	100	94, 105, 113, 124	0
49	2r	68/88 (77%)	0.51	6 (8%)	10	7	97, 107, 119, 122	0
50	1s	83/93 (89%)	-0.46	0	100	100	108, 119, 128, 133	0
50	2s	83/93 (89%)	0.55	13 (15%)	2	1	103, 118, 125, 128	0
51	1t	96/106 (90%)	0.61	16 (16%)	1	1	103, 111, 120, 122	0
51	2t	96/106 (90%)	0.58	14 (14%)	2	2	92, 104, 115, 121	0
52	1u	23/27 (85%)	0.92	4 (17%)	1	1	112, 118, 121, 125	0
52	2u	23/27 (85%)	0.44	2 (8%)	10	7	112, 118, 123, 127	0
53	1v	7/24 (29%)	2.46	3 (42%)	0	0	105, 107, 133, 138	0
53	2v	6/24 (25%)	1.40	1 (16%)	1	1	106, 113, 119, 134	0
54	1w	3/4 (75%)	0.47	0	100	100	88, 88, 101, 110	0
54	2w	3/4 (75%)	-0.07	0	100	100	93, 93, 104, 105	0
55	1x	72/77 (93%)	-0.16	1 (1%)	75	64	85, 111, 123, 134	0
55	2x	72/77 (93%)	0.05	4 (5%)	24	17	92, 113, 121, 132	0
All	All	20603/21452 (96%)	0.35	1698 (8%)	11	9	72, 104, 125, 153	0

All (1698) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	2D	276	LYS	8.8
44	2m	124	PRO	8.4
41	1j	61	GLU	8.2
34	1c	169	ALA	8.1
32	1a	1030(B)	C	7.8

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Mol	Chain	Res	Type	RSRZ
34	1c	168	ALA	7.7
44	1m	124	PRO	7.4
41	1j	58	ASP	7.4
28	26	2	ALA	7.3
34	1c	12	LEU	7.2
41	1j	47	PHE	6.8
41	1j	63	PHE	6.7
40	1i	117	HIS	6.5
34	1c	160	ALA	6.5
41	1j	60	ARG	6.4
40	1i	118	LYS	6.4
30	28	65	GLU	6.2
29	27	48	LYS	6.2
40	1i	121	ARG	6.1
44	1m	123	ALA	6.1
34	1c	149	ALA	6.0
41	1j	64	GLU	5.9
8	2I	84	GLY	5.9
40	1i	124	GLN	5.8
40	1i	113	LYS	5.8
32	2a	1532	U	5.8
45	1n	49	HIS	5.8
53	1v	13	A	5.7
38	1g	82	GLY	5.7
35	1d	24	GLU	5.7
44	1m	122	LYS	5.7
40	1i	115	GLY	5.6
23	11	2	SER	5.6
32	1a	975	A	5.6
34	1c	166	GLU	5.6
41	1j	62	HIS	5.6
47	1p	18	ARG	5.5
23	21	2	SER	5.5
20	2Y	1	MET	5.5
43	2l	91	LYS	5.5
45	1n	58	LYS	5.5
45	2n	2	ALA	5.5
29	17	48	LYS	5.5
40	1i	120	ARG	5.5
3	2D	261	LYS	5.4
40	1i	116	LYS	5.4
23	21	16	ASN	5.3

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Mol	Chain	Res	Type	RSRZ
41	1j	65	LEU	5.3
1	2A	2178	C	5.3
47	1p	8	ARG	5.3
40	1i	119	ALA	5.3
1	1A	1141	A	5.2
34	1c	11	ARG	5.2
38	2g	80	VAL	5.1
34	1c	4	LYS	5.1
40	1i	114	TYR	5.1
22	20	76	GLY	5.0
9	2N	8	GLN	5.0
23	21	4	VAL	5.0
32	1a	1531	A	5.0
3	2D	275	LYS	5.0
34	1c	167	TRP	4.9
29	27	46	VAL	4.9
34	1c	165	THR	4.9
40	1i	112	LYS	4.9
1	2A	2179	C	4.9
41	1j	48	THR	4.9
20	2Y	62	GLU	4.9
41	1j	59	SER	4.9
34	1c	152	ILE	4.9
43	2l	16	GLU	4.8
23	21	10	LYS	4.8
29	17	47	ARG	4.8
11	2P	70	GLN	4.8
40	1i	30	GLY	4.8
45	1n	61	TRP	4.8
28	26	10	LEU	4.8
34	1c	13	GLY	4.8
3	1D	276	LYS	4.8
18	2W	94	ASP	4.7
1	1A	1113	A	4.7
5	2F	87	GLY	4.7
45	1n	57	ARG	4.7
36	2e	88	LYS	4.7
43	2l	89	ARG	4.6
22	20	75	LEU	4.6
11	2P	63	PRO	4.6
36	2e	29	GLY	4.6
47	1p	19	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
40	1i	110	GLU	4.6
29	27	1	MET	4.6
34	2c	157	ILE	4.6
34	1c	159	GLY	4.6
39	2h	84	ARG	4.6
29	27	47	ARG	4.6
23	21	48	LYS	4.5
6	2G	49	ASP	4.5
40	2i	46	ALA	4.5
9	2N	140	VAL	4.5
1	2A	247	G	4.5
23	21	61	ARG	4.5
33	2b	122	PHE	4.5
36	1e	81	GLU	4.5
34	2c	190	ARG	4.5
1	2A	389	G	4.4
38	1g	80	VAL	4.4
34	1c	170	GLN	4.4
16	2U	28	ARG	4.4
5	2F	51	THR	4.4
34	1c	164	ARG	4.4
1	2A	125	G	4.4
16	2U	22	LYS	4.4
7	2H	159	GLU	4.4
44	2m	94	ARG	4.4
48	1q	37	LYS	4.4
42	2k	126	ARG	4.4
45	1n	59	ALA	4.4
10	2O	1	MET	4.4
22	20	74	ARG	4.3
43	1l	89	ARG	4.3
30	28	8	LYS	4.3
3	2D	53	PHE	4.3
20	2Y	4	LYS	4.3
38	1g	154	TYR	4.3
1	1A	2163	G	4.3
41	1j	45	ARG	4.2
51	1t	9	ASN	4.2
1	1A	1140	U	4.2
34	2c	189	ALA	4.2
47	1p	17	TYR	4.2
53	1v	15	A	4.2

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Mol	Chain	Res	Type	RSRZ
44	2m	120	LYS	4.2
8	2I	86	THR	4.2
44	2m	123	ALA	4.1
16	2U	36	ARG	4.1
31	29	37	GLY	4.1
23	21	39	LYS	4.1
35	2d	67	ILE	4.1
23	21	66	HIS	4.1
3	2D	52	ARG	4.1
17	2V	74	LYS	4.1
40	2i	64	THR	4.1
11	2P	65	ARG	4.1
3	2D	273	ARG	4.1
44	2m	102	ARG	4.1
34	1c	153	VAL	4.0
29	27	36	GLN	4.0
47	1p	35	LYS	4.0
42	2k	119	CYS	4.0
38	1g	79	ARG	4.0
23	11	48	LYS	4.0
43	2l	94	PRO	4.0
16	2U	25	TRP	4.0
4	2E	134	ILE	4.0
47	1p	31	LYS	4.0
45	1n	13	THR	4.0
4	2E	125	GLY	4.0
44	2m	92	HIS	4.0
1	2A	753	C	4.0
5	2F	75	HIS	3.9
20	2Y	2	ARG	3.9
11	2P	71	VAL	3.9
17	2V	73	SER	3.9
10	1O	26	LYS	3.9
34	2c	158	GLY	3.9
23	21	13	ILE	3.9
12	2Q	40	ALA	3.9
3	2D	5	LYS	3.9
30	28	11	LYS	3.9
51	1t	70	SER	3.9
32	1a	1190	G	3.9
18	2W	83	LYS	3.9
48	1q	26	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
12	1Q	68	ILE	3.9
10	1O	11	ALA	3.9
42	1k	50	TYR	3.9
24	22	1	MET	3.9
12	1Q	80	GLU	3.9
1	1A	2084	A	3.9
15	2T	97	ALA	3.9
34	1c	162	GLN	3.9
1	1A	696	C	3.9
34	1c	131	ARG	3.9
34	1c	150	LYS	3.9
42	2k	109	VAL	3.9
40	1i	123	PRO	3.9
36	1e	50	GLU	3.8
16	2U	29	SER	3.8
36	2e	130	ASN	3.8
36	1e	27	ARG	3.8
12	1Q	11	LYS	3.8
33	2b	71	VAL	3.8
3	2D	236	GLY	3.8
30	28	14	VAL	3.8
32	1a	916	G	3.8
23	21	44	PRO	3.8
18	2W	90	ARG	3.8
22	10	2	ALA	3.8
31	29	13	LYS	3.8
36	2e	121	LYS	3.8
20	2Y	29	GLU	3.8
4	1E	138	PRO	3.8
6	2G	157	ILE	3.8
41	2j	53	PRO	3.7
36	1e	18	ARG	3.7
28	26	22	ALA	3.7
46	1o	89	GLY	3.7
11	2P	64	LYS	3.7
1	2A	2062	A	3.7
20	2Y	46	LYS	3.7
47	1p	7	ALA	3.7
48	2q	30	PRO	3.7
18	2W	84	ARG	3.7
3	2D	37	LEU	3.7
34	1c	190	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
36	1e	29	GLY	3.7
41	1j	46	ARG	3.7
10	1O	99	PHE	3.7
40	1i	109	VAL	3.7
30	28	64	TYR	3.7
41	2j	54	PHE	3.7
3	2D	55	GLY	3.7
34	1c	199	LYS	3.7
32	1a	1525	G	3.7
4	2E	157	ALA	3.7
51	2t	23	ARG	3.7
3	2D	38	LYS	3.6
11	2P	72	PRO	3.6
16	2U	37	GLU	3.6
16	2U	21	ALA	3.6
22	20	7	LEU	3.6
15	2T	51	ARG	3.6
32	1a	974	A	3.6
36	1e	28	PHE	3.6
40	1i	127	LYS	3.6
1	2A	2035	G	3.6
41	2j	63	PHE	3.6
3	2D	271	ILE	3.6
18	2W	103	ILE	3.6
22	10	7	LEU	3.6
42	1k	51	LYS	3.6
8	2I	83	ALA	3.6
1	2A	2446	G	3.6
42	2k	120	ARG	3.6
35	1d	112	VAL	3.6
40	2i	115	GLY	3.6
11	2P	68	GLN	3.6
43	2l	15	ARG	3.6
4	2E	127	ASP	3.6
23	21	11	ARG	3.6
29	17	46	VAL	3.6
10	1O	1	MET	3.6
23	21	9	GLY	3.6
6	2G	75	LYS	3.5
48	2q	99	SER	3.5
44	1m	118	ALA	3.5
32	2a	1492	A	3.5

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Mol	Chain	Res	Type	RSRZ
3	2D	253	GLN	3.5
40	2i	7	THR	3.5
43	2l	5	PRO	3.5
45	2n	11	LYS	3.5
36	1e	51	VAL	3.5
5	2F	81	PRO	3.5
3	2D	35	LYS	3.5
11	2P	79	ARG	3.5
42	2k	118	GLY	3.5
42	2k	82	VAL	3.5
10	1O	84	ALA	3.5
51	1t	71	THR	3.5
1	2A	739	G	3.5
27	25	8	LYS	3.5
32	1a	1367	C	3.5
11	2P	76	LYS	3.5
36	1e	26	PHE	3.5
15	2T	94	ALA	3.5
48	2q	24	GLU	3.5
22	1O	4	LYS	3.5
34	1c	134	ILE	3.5
3	2D	39	LYS	3.5
35	1d	168	ARG	3.4
4	2E	151	TYR	3.4
46	1o	51	HIS	3.4
23	21	47	GLN	3.4
48	2q	38	ARG	3.4
25	23	2	PRO	3.4
29	27	23	ARG	3.4
36	2e	12	LEU	3.4
51	1t	8	ARG	3.4
47	1p	36	ILE	3.4
1	2A	2121	G	3.4
17	2V	75	PHE	3.4
4	2E	135	HIS	3.4
10	2O	82	ASN	3.4
23	21	12	PRO	3.4
36	2e	13	ILE	3.4
36	1e	88	LYS	3.4
32	2a	723	U	3.4
47	1p	9	PHE	3.4
6	2G	32	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
22	20	8	GLY	3.4
23	11	27	GLU	3.4
42	2k	90	GLY	3.4
17	2V	72	VAL	3.4
16	2U	27	LEU	3.4
51	2t	29	LYS	3.4
3	2D	260	ARG	3.4
6	2G	51	ARG	3.4
13	1R	104	ARG	3.4
1	1A	2590	G	3.4
12	2Q	85	LYS	3.4
12	1Q	10	ARG	3.4
4	2E	145	LYS	3.4
5	2F	52	LYS	3.4
29	27	2	LYS	3.4
49	2r	46	GLU	3.4
48	1q	100	LYS	3.4
5	2F	56	GLU	3.4
34	1c	161	GLU	3.4
30	28	46	ARG	3.4
40	1i	126	SER	3.4
43	1l	22	SER	3.4
31	29	9	ARG	3.4
9	2N	109	LYS	3.4
23	21	36	GLY	3.4
34	2c	67	THR	3.4
18	2W	97	LYS	3.4
4	1E	135	HIS	3.4
18	1W	23	LEU	3.3
3	2D	262	ARG	3.3
27	15	2	ALA	3.3
6	2G	41	GLN	3.3
34	1c	193	TYR	3.3
30	28	13	ARG	3.3
35	1d	69	GLY	3.3
51	2t	70	SER	3.3
16	2U	19	LYS	3.3
30	28	3	LYS	3.3
35	1d	101	LEU	3.3
35	1d	70	ILE	3.3
36	1e	14	ARG	3.3
4	2E	126	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	1A	2594	G	3.3
36	2e	86	ALA	3.3
38	1g	156	TRP	3.3
4	2E	150	VAL	3.3
29	27	37	LYS	3.3
1	2A	758	C	3.3
23	11	42	GLN	3.3
4	1E	141	ILE	3.3
16	2U	30	LYS	3.3
5	2F	73	ALA	3.3
40	1i	108	VAL	3.3
6	2G	39	ILE	3.3
20	2Y	26	LYS	3.3
36	2e	45	PHE	3.3
4	1E	123	ALA	3.3
32	2a	1510	U	3.3
32	2a	1511	G	3.3
4	1E	155	LYS	3.3
40	1i	111	ARG	3.3
3	1D	273	ARG	3.3
35	1d	115	ARG	3.3
43	1l	20	LYS	3.3
5	2F	70	THR	3.3
12	1Q	1	MET	3.3
42	2k	84	VAL	3.3
34	2c	188	LEU	3.3
22	10	39	ARG	3.3
36	1e	24	ARG	3.3
52	1u	17	THR	3.3
1	1A	1144	A	3.3
43	1l	68	ALA	3.3
23	21	23	LYS	3.3
22	10	9	SER	3.3
44	2m	116	THR	3.3
3	1D	275	LYS	3.2
23	21	14	VAL	3.2
22	10	3	HIS	3.2
22	10	8	GLY	3.2
40	2i	49	PRO	3.2
5	2F	88	VAL	3.2
32	1a	1257	U	3.2
4	2E	149	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
27	15	4	HIS	3.2
30	28	12	LYS	3.2
12	1Q	41	TRP	3.2
1	1A	1003	U	3.2
40	2i	63	ILE	3.2
9	1N	83	LYS	3.2
34	1c	196	LEU	3.2
10	1O	58	VAL	3.2
1	1A	1145	G	3.2
1	2A	2052	G	3.2
9	1N	72	TYR	3.2
4	2E	138	PRO	3.2
34	2c	167	TRP	3.2
5	2F	127	GLU	3.2
15	2T	96	ARG	3.2
40	2i	117	HIS	3.2
28	26	51	GLU	3.2
30	28	25	MET	3.2
43	1l	23	LYS	3.2
5	2F	69	HIS	3.2
36	1e	118	ILE	3.2
1	2A	2116	G	3.2
1	2A	2120	G	3.2
40	2i	119	ALA	3.2
6	2G	89	GLY	3.2
36	2e	81	GLU	3.2
10	1O	27	GLY	3.2
35	1d	4	TYR	3.2
40	2i	127	LYS	3.2
5	2F	72	ARG	3.2
29	27	38	GLY	3.2
32	1a	1524	C	3.2
46	1o	88	ARG	3.2
40	1i	122	ALA	3.2
52	1u	14	TRP	3.2
34	1c	72	LYS	3.2
36	2e	122	GLU	3.2
1	2A	2713	A	3.1
13	1R	107	ASP	3.1
30	28	53	PRO	3.1
35	1d	16	GLY	3.1
1	1A	2458	G	3.1

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Mol	Chain	Res	Type	RSRZ
32	2a	1030(B)	C	3.1
34	1c	151	VAL	3.1
41	2j	48	THR	3.1
17	2V	81	TYR	3.1
22	20	2	ALA	3.1
43	1l	64	TYR	3.1
41	2j	59	SER	3.1
12	2Q	80	GLU	3.1
32	1a	1394	A	3.1
11	2P	77	ARG	3.1
38	1g	155	ARG	3.1
16	2U	20	LEU	3.1
1	2A	245	G	3.1
7	2H	85	LYS	3.1
29	17	1	MET	3.1
17	2V	82	ARG	3.1
7	2H	19	VAL	3.1
11	2P	50	ARG	3.1
16	2U	41	ALA	3.1
32	1a	1366	C	3.1
32	1a	1368	G	3.1
36	1e	17	ALA	3.1
18	1W	90	ARG	3.1
18	2W	92	ARG	3.1
40	2i	120	ARG	3.1
42	2k	123	LYS	3.1
52	1u	18	TYR	3.1
29	27	16	HIS	3.1
19	2X	1	MET	3.1
5	1F	66	PRO	3.1
15	2T	64	ARG	3.1
43	2l	18	VAL	3.1
23	11	45	ASN	3.1
10	2O	19	ILE	3.1
15	2T	48	ILE	3.1
35	1d	66	ARG	3.1
36	1e	91	LEU	3.1
20	2Y	5	MET	3.1
20	2Y	23	ARG	3.1
25	23	4	LEU	3.1
1	1A	2618	C	3.1
1	2A	2146	C	3.1

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Mol	Chain	Res	Type	RSRZ
51	2t	71	THR	3.1
40	2i	121	ARG	3.1
44	1m	121	LYS	3.1
49	2r	51	LEU	3.1
1	2A	2579	C	3.1
8	2I	19	VAL	3.1
34	1c	138	VAL	3.1
12	2Q	38	GLU	3.1
1	2A	752	A	3.1
4	1E	149	ARG	3.1
6	2G	21	ARG	3.1
1	2A	34	C	3.1
3	1D	55	GLY	3.1
51	2t	26	ASN	3.1
4	1E	139	GLY	3.0
23	21	17	SER	3.0
36	2e	84	PHE	3.0
18	1W	94	ASP	3.0
43	1l	21	LYS	3.0
43	1l	97	ARG	3.0
31	29	15	LYS	3.0
3	2D	237	GLU	3.0
4	1E	137	HIS	3.0
50	2s	34	TRP	3.0
1	2A	1847	A	3.0
11	2P	56	SER	3.0
11	2P	54	GLY	3.0
1	1A	1139	G	3.0
1	1A	2521	G	3.0
1	2A	614(B)	G	3.0
23	21	38	SER	3.0
9	2N	115	ARG	3.0
9	2N	119	ARG	3.0
11	2P	59	LEU	3.0
22	20	9	SER	3.0
44	2m	105	THR	3.0
34	1c	157	ILE	3.0
46	1o	48	LYS	3.0
28	26	23	THR	3.0
35	2d	169	LYS	3.0
20	1Y	67	LEU	3.0
22	20	55	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
15	2T	50	ILE	3.0
28	16	35	GLU	3.0
39	2h	94	TYR	3.0
42	1k	118	GLY	3.0
5	2F	64	ILE	3.0
51	1t	18	GLN	3.0
1	1A	2162	C	3.0
30	28	10	ALA	3.0
32	1a	1511	G	3.0
8	2I	27	ARG	3.0
34	2c	196	LEU	3.0
4	1E	117	MET	3.0
1	2A	1678	G	3.0
18	2W	82	LEU	3.0
3	2D	168	ARG	3.0
41	1j	53	PRO	3.0
42	2k	91	ARG	3.0
43	2l	64	TYR	3.0
11	2P	74	GLU	3.0
50	2s	71	LEU	3.0
1	1A	2591	C	3.0
1	2A	757	U	3.0
5	1F	69	HIS	3.0
15	2T	98	LYS	3.0
10	1O	39	ILE	3.0
32	2a	1531	A	3.0
10	1O	64	ARG	3.0
1	2A	2139	C	2.9
3	2D	238	GLY	2.9
5	2F	57	VAL	2.9
48	2q	37	LYS	2.9
50	2s	74	PHE	2.9
23	21	15	ALA	2.9
30	28	43	GLN	2.9
47	1p	47	ASP	2.9
48	1q	8	GLY	2.9
5	2F	62	ARG	2.9
36	2e	11	ILE	2.9
3	2D	4	LYS	2.9
40	2i	16	ARG	2.9
3	2D	225	ALA	2.9
40	2i	15	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
42	1k	117	ASN	2.9
50	2s	75	ALA	2.9
34	2c	69	HIS	2.9
30	28	2	PRO	2.9
34	1c	10	PHE	2.9
41	2j	49	VAL	2.9
42	2k	25	TYR	2.9
44	1m	98	VAL	2.9
4	1E	120	TRP	2.9
34	1c	3	ASN	2.9
9	1N	76	SER	2.9
12	1Q	2	LEU	2.9
42	1k	126	ARG	2.9
43	2l	12	ARG	2.9
9	2N	84	LYS	2.9
11	2P	58	THR	2.9
16	2U	38	THR	2.9
20	2Y	28	LYS	2.9
39	2h	82	HIS	2.9
34	2c	192	THR	2.9
41	1j	51	ARG	2.9
12	2Q	39	PRO	2.9
15	2T	65	LYS	2.9
25	23	29	ARG	2.9
30	28	9	GLY	2.9
34	1c	5	ILE	2.9
1	2A	563	G	2.9
49	2r	85	LEU	2.9
16	2U	32	PHE	2.9
10	1O	62	VAL	2.9
10	1O	98	VAL	2.9
52	1u	16	GLY	2.9
36	1e	45	PHE	2.9
7	2H	34	GLU	2.9
10	2O	20	MET	2.9
13	2R	1	MET	2.9
18	2W	104	THR	2.9
28	26	52	VAL	2.9
4	1E	134	ILE	2.9
34	1c	135	LYS	2.9
48	2q	100	LYS	2.9
34	2c	152	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
35	2d	168	ARG	2.9
40	1i	8	GLY	2.9
40	2i	19	LEU	2.9
12	2Q	77	LYS	2.9
35	1d	15	GLU	2.9
12	1Q	12	GLN	2.9
1	2A	2334	G	2.9
42	2k	108	ILE	2.9
1	1A	838	C	2.9
11	2P	35	HIS	2.9
30	28	22	VAL	2.9
42	2k	110	ASP	2.9
10	2O	32	TYR	2.9
35	1d	23	GLY	2.9
38	2g	81	GLY	2.9
50	2s	2	PRO	2.9
11	2P	61	ARG	2.9
18	2W	86	LEU	2.9
18	2W	98	LYS	2.8
4	1E	136	ARG	2.8
8	1I	27	ARG	2.8
32	1a	815	A	2.8
4	1E	151	TYR	2.8
23	21	37	ILE	2.8
30	28	52	LYS	2.8
43	2l	23	LYS	2.8
44	2m	107	ALA	2.8
43	1l	18	VAL	2.8
51	1t	69	GLY	2.8
3	2D	48	ARG	2.8
27	25	7	PRO	2.8
1	2A	1252	G	2.8
1	2A	1681	G	2.8
11	2P	62	LEU	2.8
29	27	31	LEU	2.8
31	29	26	ILE	2.8
4	2E	143	ASN	2.8
36	2e	83	GLU	2.8
3	2D	61	LEU	2.8
1	2A	1273	U	2.8
5	2F	71	GLY	2.8
1	2A	755	C	2.8

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Mol	Chain	Res	Type	RSRZ
1	2A	756	C	2.8
30	18	46	ARG	2.8
1	2A	2578	G	2.8
1	2A	2581	G	2.8
4	1E	147	PRO	2.8
16	2U	16	LYS	2.8
27	15	5	PRO	2.8
43	2l	93	LEU	2.8
1	2A	1128	A	2.8
15	2T	63	VAL	2.8
33	2b	165	VAL	2.8
55	2x	76	A	2.8
4	2E	141	ILE	2.8
6	2G	34	LEU	2.8
22	10	6	GLY	2.8
32	2a	322	C	2.8
23	11	23	LYS	2.8
27	15	7	PRO	2.8
3	2D	224	ALA	2.8
10	1O	41	ALA	2.8
10	1O	63	VAL	2.8
30	28	23	VAL	2.8
36	2e	82	VAL	2.8
51	1t	83	ARG	2.8
31	29	28	GLU	2.8
36	1e	89	ILE	2.8
36	2e	118	ILE	2.8
9	1N	77	GLY	2.8
30	28	27	THR	2.8
1	2A	2506	U	2.8
8	2I	85	GLU	2.8
13	2R	18	LEU	2.8
30	28	26	LYS	2.8
17	2V	70	ILE	2.8
34	1c	14	ILE	2.8
41	2j	50	ILE	2.8
16	2U	24	TYR	2.8
47	1p	39	TYR	2.8
34	2c	156	ARG	2.8
40	1i	64	THR	2.8
1	2A	673	C	2.8
5	2F	83	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
10	1O	23	ARG	2.8
19	2X	60	ARG	2.8
41	1j	49	VAL	2.8
1	2A	2109	U	2.8
10	2O	41	ALA	2.8
12	1Q	100	GLY	2.8
30	28	15	LYS	2.8
9	2N	43	THR	2.8
11	2P	49	ARG	2.8
19	2X	31	HIS	2.8
35	1d	3	ARG	2.8
36	2e	87	SER	2.8
51	2t	25	ARG	2.8
3	2D	235	GLY	2.8
9	2N	120	LEU	2.8
15	2T	114	LEU	2.8
10	1O	17	ARG	2.8
45	2n	29	ARG	2.8
27	15	25	LEU	2.8
43	1l	32	PHE	2.8
23	21	21	ARG	2.8
10	1O	8	LEU	2.8
13	2R	9	LYS	2.8
1	2A	2319	G	2.8
6	2G	133	LEU	2.8
5	2F	74	ARG	2.8
7	2H	162	ILE	2.8
15	1T	111	ARG	2.8
1	2A	735	A	2.8
17	2V	71	LEU	2.8
3	2D	244	ARG	2.7
10	2O	22	ILE	2.7
34	1c	132	ARG	2.7
1	1A	795	G	2.7
12	2Q	41	TRP	2.7
32	2a	765	G	2.7
42	1k	123	LYS	2.7
43	1l	33	ARG	2.7
3	2D	36	PRO	2.7
1	2A	2019	A	2.7
3	2D	216	GLY	2.7
11	2P	47	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
35	2d	11	LEU	2.7
4	1E	111	ARG	2.7
39	2h	86	ILE	2.7
11	1P	119	GLU	2.7
13	1R	1	MET	2.7
21	2Z	163	LEU	2.7
32	1a	888	G	2.7
1	2A	791	C	2.7
44	1m	119	GLY	2.7
22	10	5	LYS	2.7
27	15	3	LYS	2.7
35	1d	27	TYR	2.7
39	1h	94	TYR	2.7
23	11	31	GLY	2.7
25	23	7	LYS	2.7
35	1d	139	ARG	2.7
43	1l	29	GLY	2.7
48	2q	25	ARG	2.7
49	2r	50	ILE	2.7
1	2A	742	G	2.7
10	1O	82	ASN	2.7
6	2G	159	VAL	2.7
29	27	17	GLY	2.7
40	2i	65	VAL	2.7
43	2l	17	LYS	2.7
4	1E	122	PHE	2.7
5	1F	75	HIS	2.7
23	21	8	SER	2.7
6	2G	22	ARG	2.7
10	1O	24	VAL	2.7
22	20	4	LYS	2.7
23	21	45	ASN	2.7
37	2f	8	ILE	2.7
42	2k	13	GLN	2.7
10	1O	7	TYR	2.7
1	2A	2587	A	2.7
3	2D	217	ARG	2.7
9	1N	84	LYS	2.7
33	2b	123	ALA	2.7
38	1g	81	GLY	2.7
36	1e	83	GLU	2.7
30	28	62	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
51	1t	79	ARG	2.7
1	2A	754	C	2.7
1	2A	250	G	2.7
3	2D	258	LYS	2.7
5	1F	74	ARG	2.7
1	2A	2609	U	2.7
9	2N	9	VAL	2.7
36	2e	89	ILE	2.7
35	2d	75	PHE	2.7
34	1c	156	ARG	2.7
1	2A	246	C	2.7
32	2a	812	C	2.7
35	1d	5	ILE	2.7
1	2A	1127	A	2.7
13	2R	15	SER	2.7
35	1d	7	PRO	2.7
11	2P	46	LYS	2.7
12	2Q	79	LEU	2.7
25	23	8	LEU	2.7
32	1a	108	G	2.7
34	1c	130	VAL	2.7
35	1d	17	VAL	2.7
39	1h	111	ILE	2.7
43	2l	95	GLY	2.7
4	2E	133	LYS	2.7
1	2A	2586	C	2.7
1	1A	2602	A	2.7
1	2A	2054	A	2.7
16	2U	7	GLY	2.7
47	1p	29	ASP	2.7
3	2D	243	GLY	2.7
34	2c	2	GLY	2.7
4	2E	152	LYS	2.7
1	2A	1765	C	2.7
1	1A	1176	U	2.7
6	2G	137	GLU	2.7
8	2I	41	GLU	2.7
1	1A	721	G	2.7
1	2A	248	G	2.7
36	2e	133	TYR	2.6
1	2A	2606	C	2.6
9	2N	82	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
22	20	18	ALA	2.6
23	11	32	LYS	2.6
3	2D	220	HIS	2.6
15	2T	95	ARG	2.6
42	2k	98	LEU	2.6
46	1o	50	HIS	2.6
22	20	50	ASN	2.6
36	1e	90	VAL	2.6
1	1A	2453	C	2.6
3	2D	208	LYS	2.6
30	28	63	PRO	2.6
10	1O	100	GLY	2.6
32	1a	795	C	2.6
32	2a	883	C	2.6
28	26	9	LEU	2.6
43	1l	30	ALA	2.6
1	2A	532	A	2.6
10	2O	5	GLN	2.6
23	21	42	GLN	2.6
29	27	35	ARG	2.6
40	1i	106	ALA	2.6
43	2l	9	GLN	2.6
53	2v	18	G	2.6
43	2l	13	LYS	2.6
43	2l	28	LYS	2.6
45	2n	34	TYR	2.6
35	1d	65	ARG	2.6
6	2G	169	ALA	2.6
12	1Q	106	VAL	2.6
18	1W	22	ASP	2.6
42	2k	81	ASP	2.6
3	2D	254	THR	2.6
1	1A	2166	U	2.6
1	2A	2607	G	2.6
3	2D	67	PHE	2.6
5	2F	66	PRO	2.6
19	1X	60	ARG	2.6
10	1O	83	ALA	2.6
1	2A	2801(A)	A	2.6
12	2Q	37	LEU	2.6
1	1A	569	G	2.6
1	1A	2619	G	2.6

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Mol	Chain	Res	Type	RSRZ
1	2A	1764	G	2.6
1	2A	1992	G	2.6
15	1T	64	ARG	2.6
16	2U	40	PHE	2.6
16	2U	72	HIS	2.6
32	1a	1526	G	2.6
32	2a	1525	G	2.6
35	2d	66	ARG	2.6
35	2d	115	ARG	2.6
1	2A	2103	C	2.6
12	1Q	40	ALA	2.6
5	2F	67	GLN	2.6
5	2F	82	ILE	2.6
33	2b	163	PHE	2.6
4	2E	148	GLY	2.6
10	1O	122	LEU	2.6
4	1E	152	LYS	2.6
43	1l	91	LYS	2.6
7	2H	149	ARG	2.6
1	2A	2055	C	2.6
20	1Y	70	SER	2.6
1	1A	829	A	2.6
1	2A	2439	A	2.6
9	2N	116	LEU	2.6
25	23	3	ARG	2.6
29	17	41	ARG	2.6
33	2b	202	PRO	2.6
1	1A	1001	G	2.6
1	2A	242	G	2.6
1	2A	687	C	2.6
32	1a	1362	C	2.6
42	2k	87	THR	2.6
1	2A	1618	A	2.6
1	2A	2590	A	2.6
5	2F	65	TRP	2.6
5	2F	176	LEU	2.6
7	2H	87	LEU	2.6
8	1I	38	LEU	2.6
30	28	29	LYS	2.6
32	1a	900	A	2.6
3	2D	233	HIS	2.6
10	1O	21	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
39	1h	135	CYS	2.6
10	1O	18	LYS	2.6
10	2O	8	LEU	2.6
47	1p	11	SER	2.6
1	2A	759	G	2.6
1	2A	2104	G	2.6
1	2A	2110	G	2.6
1	2A	2577	A	2.6
16	2U	14	HIS	2.6
23	21	60	PHE	2.6
23	21	35	THR	2.6
47	2p	17	TYR	2.6
36	1e	82	VAL	2.6
20	2Y	59	GLY	2.6
35	1d	2	GLY	2.6
3	2D	54	ARG	2.6
7	2H	90	LYS	2.5
11	2P	29	LYS	2.5
20	2Y	63	LYS	2.5
25	23	34	GLU	2.5
28	26	53	LYS	2.5
37	2f	59	TYR	2.5
39	1h	52	ASP	2.5
1	1A	1112	U	2.5
1	1A	2087	C	2.5
1	1A	2516	U	2.5
18	2W	93	ALA	2.5
34	1c	129	ALA	2.5
1	1A	1357	G	2.5
1	2A	254	G	2.5
41	1j	4	ILE	2.5
3	2D	51	VAL	2.5
45	1n	56	VAL	2.5
4	1E	131	ALA	2.5
39	2h	91	ARG	2.5
30	28	48	PHE	2.5
3	2D	32	SER	2.5
11	2P	75	ILE	2.5
33	2b	68	ILE	2.5
1	1A	2598	C	2.5
32	1a	1515	C	2.5
35	2d	68	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
12	2Q	1	MET	2.5
32	2a	816	A	2.5
37	1f	18	GLN	2.5
1	2A	741	G	2.5
48	2q	22	LEU	2.5
39	1h	84	ARG	2.5
30	18	7	HIS	2.5
22	20	5	LYS	2.5
36	1e	80	ILE	2.5
1	1A	1318	A	2.5
1	2A	2712(A)	A	2.5
32	1a	768	A	2.5
40	2i	42	ARG	2.5
8	2I	111	PRO	2.5
12	1Q	99	PRO	2.5
40	2i	47	LEU	2.5
29	27	4	THR	2.5
32	1a	723	U	2.5
33	2b	72	GLY	2.5
40	2i	18	PHE	2.5
43	2l	25	PRO	2.5
1	2A	1780	A	2.5
1	2A	2117	A	2.5
30	28	7	HIS	2.5
30	28	60	LEU	2.5
22	10	12	ASN	2.5
33	2b	214	ILE	2.5
1	1A	1114	G	2.5
4	1E	158	GLY	2.5
32	1a	973	G	2.5
32	2a	818	G	2.5
35	1d	29	PRO	2.5
35	2d	197	PRO	2.5
20	2Y	61	ILE	2.5
48	2q	36	ILE	2.5
22	20	11	ARG	2.5
1	1A	720	C	2.5
27	25	9	LYS	2.5
32	1a	1344	C	2.5
35	1d	64	LEU	2.5
37	2f	88	VAL	2.5
44	1m	97	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
51	1t	80	ARG	2.5
1	2A	2449	U	2.5
19	2X	33	LYS	2.5
6	2G	85	GLY	2.5
42	2k	31	THR	2.5
23	21	65	SER	2.5
44	2m	117	VAL	2.5
10	1O	5	GLN	2.5
45	1n	41	ARG	2.5
1	1A	719	C	2.5
30	18	5	LYS	2.5
40	2i	114	TYR	2.5
4	1E	146	THR	2.5
4	2E	130	GLY	2.5
25	23	28	LEU	2.5
43	2l	14	GLY	2.5
5	1F	64	ILE	2.5
1	1A	1143	U	2.5
23	11	20	ARG	2.5
42	2k	50	TYR	2.5
47	1p	27	LYS	2.5
32	1a	765	G	2.5
4	2E	139	GLY	2.5
36	2e	10	MET	2.5
10	1O	77	ILE	2.5
18	1W	24	ILE	2.5
23	21	41	ARG	2.5
29	27	30	VAL	2.5
39	2h	93	VAL	2.5
1	2A	2610	C	2.5
27	15	10	LYS	2.5
51	2t	30	LYS	2.5
33	2b	152	PHE	2.5
34	1c	184	TYR	2.5
43	1l	98	TYR	2.5
7	2H	169	VAL	2.5
33	1b	133	LYS	2.5
44	1m	94	ARG	2.5
50	2s	37	ARG	2.5
1	2A	215	G	2.5
1	2A	956	G	2.5
48	2q	27	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	1A	799	A	2.5
1	2A	2059	A	2.5
16	2U	34	LYS	2.5
38	2g	79	ARG	2.5
50	2s	81	ARG	2.5
5	1F	67	GLN	2.5
48	2q	32	TYR	2.5
34	2c	151	VAL	2.5
1	2A	745	G	2.4
16	2U	56	ASP	2.4
1	2A	2140	C	2.4
32	1a	780	A	2.4
6	2G	84	LYS	2.4
16	2U	33	ARG	2.4
30	28	47	LYS	2.4
34	1c	185	GLY	2.4
44	2m	121	LYS	2.4
3	1D	272	ALA	2.4
4	1E	140	SER	2.4
5	1F	76	GLY	2.4
8	1I	1	MET	2.4
9	1N	140	VAL	2.4
12	1Q	75	THR	2.4
38	2g	13	GLN	2.4
10	1O	19	ILE	2.4
43	2l	90	VAL	2.4
51	2t	17	ARG	2.4
5	2F	90	PHE	2.4
1	1A	837	C	2.4
1	1A	2620	G	2.4
1	2A	1365	A	2.4
32	2a	562	C	2.4
32	2a	815	A	2.4
32	2a	887	G	2.4
11	1P	36	LYS	2.4
3	2D	247	ALA	2.4
44	2m	103	THR	2.4
12	1Q	65	PHE	2.4
33	2b	70	PHE	2.4
12	2Q	97	VAL	2.4
20	1Y	71	LYS	2.4
22	20	3	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
51	1t	74	LYS	2.4
1	2A	1274	A	2.4
1	2A	1302	A	2.4
1	2A	1554	A	2.4
1	2A	1763	G	2.4
4	2E	128	SER	2.4
32	1a	817	C	2.4
32	1a	820	U	2.4
32	2a	915	A	2.4
42	2k	117	ASN	2.4
55	2x	70	G	2.4
4	1E	154	LYS	2.4
12	1Q	74	TYR	2.4
36	2e	129	ILE	2.4
41	2j	62	HIS	2.4
4	2E	136	ARG	2.4
27	15	9	LYS	2.4
35	2d	77	ASN	2.4
51	1t	68	LYS	2.4
1	1A	1817	A	2.4
1	1A	2164	C	2.4
39	2h	83	ILE	2.4
51	2t	69	GLY	2.4
19	1X	11	PRO	2.4
29	27	19	ARG	2.4
36	2e	14	ARG	2.4
40	1i	42	ARG	2.4
16	2U	17	ILE	2.4
23	11	15	ALA	2.4
10	2O	31	LYS	2.4
18	1W	107	LEU	2.4
23	21	46	LEU	2.4
40	2i	51	ARG	2.4
41	2j	55	LYS	2.4
50	2s	32	LYS	2.4
1	1A	1960	A	2.4
3	2D	50	THR	2.4
32	1a	901	A	2.4
1	2A	748	G	2.4
1	2A	1674	G	2.4
4	1E	130	GLY	2.4
35	1d	37	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
51	2t	68	LYS	2.4
12	1Q	9	TYR	2.4
4	2E	156	MET	2.4
36	2e	109	ILE	2.4
34	1c	133	ALA	2.4
40	1i	29	ASN	2.4
1	2A	1275	A	2.4
3	2D	34	VAL	2.4
1	2A	686	G	2.4
1	2A	2445	G	2.4
9	2N	1	MET	2.4
23	1l	22	GLY	2.4
31	29	12	ASP	2.4
41	2j	52	GLY	2.4
1	1A	2154	U	2.4
1	2A	2580	U	2.4
36	2e	91	LEU	2.4
36	2e	123	LEU	2.4
50	2s	78	ARG	2.4
29	17	36	GLN	2.4
36	1e	49	PRO	2.4
8	2I	109	ILE	2.4
10	1O	44	LYS	2.4
43	2l	11	VAL	2.4
17	2V	80	GLN	2.4
18	1W	95	ILE	2.4
8	2I	1	MET	2.4
10	1O	20	MET	2.4
18	2W	4	LYS	2.4
20	2Y	47	LYS	2.4
3	2D	274	ARG	2.4
42	2k	17	GLY	2.4
9	2N	112	LEU	2.4
50	2s	38	SER	2.4
43	1l	67	THR	2.4
1	2A	1781	C	2.4
15	1T	65	LYS	2.4
19	1X	28	PHE	2.4
45	2n	4	LYS	2.4
35	1d	114	ARG	2.4
39	2h	129	VAL	2.4
1	1A	1111	U	2.4

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Mol	Chain	Res	Type	RSRZ
1	2A	2712	U	2.4
9	1N	75	TYR	2.4
1	2A	386	G	2.4
1	2A	2156	G	2.4
29	17	2	LYS	2.4
30	28	56	GLU	2.4
32	1a	570	G	2.4
36	1e	19	MET	2.4
36	2e	18	ARG	2.4
28	26	5	VAL	2.4
32	2a	1398	A	2.4
1	2A	587	C	2.4
12	1Q	72	LYS	2.4
9	2N	77	GLY	2.3
43	2l	27	LEU	2.3
20	2Y	75	ILE	2.3
32	1a	1508	G	2.3
16	2U	3	ARG	2.3
1	2A	734	A	2.3
1	2A	783	A	2.3
6	2G	70	VAL	2.3
31	29	23	VAL	2.3
33	1b	29	ALA	2.3
40	1i	15	ALA	2.3
1	2A	790	C	2.3
1	2A	2050	C	2.3
1	2A	2496	C	2.3
1	2A	694	U	2.3
5	1F	97	TYR	2.3
42	2k	40	ILE	2.3
41	2j	58	ASP	2.3
41	2j	60	ARG	2.3
51	1t	23	ARG	2.3
30	28	24	ALA	2.3
35	1d	140	VAL	2.3
11	2P	17	LYS	2.3
29	27	14	LYS	2.3
44	2m	122	LYS	2.3
45	1n	36	PHE	2.3
51	2t	21	LYS	2.3
20	2Y	44	ILE	2.3
32	1a	1529	G	2.3

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Mol	Chain	Res	Type	RSRZ
36	1e	25	ARG	2.3
1	1A	2081	A	2.3
1	2A	390	A	2.3
5	1F	65	TRP	2.3
10	2O	2	ILE	2.3
20	2Y	55	TYR	2.3
39	1h	134	ILE	2.3
40	2i	125	TYR	2.3
50	2s	80	TYR	2.3
3	1D	226	MET	2.3
10	1O	93	PRO	2.3
17	2V	85	LYS	2.3
15	1T	76	PHE	2.3
1	1A	1146	C	2.3
5	1F	56	GLU	2.3
34	1c	197	GLY	2.3
4	2E	131	ALA	2.3
10	2O	46	ALA	2.3
15	2T	24	PRO	2.3
39	1h	133	LEU	2.3
3	1D	38	LYS	2.3
12	2Q	98	LYS	2.3
42	2k	30	VAL	2.3
1	2A	1779	U	2.3
43	2l	62	SER	2.3
1	2A	1509	C	2.3
15	1T	112	ARG	2.3
32	1a	769	G	2.3
12	2Q	128	LYS	2.3
15	2T	113	LYS	2.3
19	1X	77	LYS	2.3
29	27	42	LEU	2.3
36	2e	119	LEU	2.3
3	1D	247	ALA	2.3
6	2G	86	MET	2.3
41	1j	52	GLY	2.3
37	2f	7	ASN	2.3
47	2p	18	ARG	2.3
3	2D	215	LEU	2.3
23	21	34	THR	2.3
35	2d	4	TYR	2.3
25	23	10	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
43	1l	93	LEU	2.3
1	1A	722	A	2.3
1	2A	1272	A	2.3
4	1E	159	HIS	2.3
25	23	35	ARG	2.3
32	1a	1530	G	2.3
51	2t	80	ARG	2.3
19	2X	92	LEU	2.3
12	1Q	105	GLU	2.3
20	2Y	30	VAL	2.3
20	2Y	45	VAL	2.3
35	1d	203	VAL	2.3
39	2h	95	VAL	2.3
41	2j	61	GLU	2.3
1	1A	2135	U	2.3
4	2E	132	HIS	2.3
6	2G	72	ARG	2.3
30	28	4	MET	2.3
1	1A	572	A	2.3
15	2T	99	LEU	2.3
16	2U	2	PRO	2.3
38	2g	154	TYR	2.3
40	2i	14	VAL	2.3
43	1l	31	PRO	2.3
1	1A	2524	C	2.3
1	1A	2002	G	2.3
1	2A	743	G	2.3
3	2D	239	ARG	2.3
9	2N	61	ARG	2.3
44	2m	88	ARG	2.3
44	2m	118	ALA	2.3
23	21	18	ILE	2.3
33	2b	31	TYR	2.3
1	2A	2688	U	2.3
15	1T	46	GLU	2.3
8	2I	96	ASP	2.3
28	26	7	ILE	2.3
40	2i	122	ALA	2.3
10	2O	67	LYS	2.3
32	1a	1188	A	2.3
41	1j	50	ILE	2.3
48	2q	34	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
40	2i	17	VAL	2.3
1	2A	684	G	2.3
3	2D	65	ILE	2.3
30	28	41	ILE	2.3
33	1b	68	ILE	2.3
34	2c	4	LYS	2.3
37	1f	55	ASP	2.3
11	2P	19	VAL	2.3
34	2c	138	VAL	2.3
22	20	6	GLY	2.3
51	1t	29	LYS	2.3
55	1x	76	A	2.3
1	2A	2612	C	2.3
19	1X	57	LEU	2.3
22	10	36	ILE	2.3
27	25	25	LEU	2.3
9	1N	78	TYR	2.3
12	1Q	93	TYR	2.3
1	1A	573	G	2.2
1	2A	738	G	2.2
6	2G	164	GLU	2.2
28	26	24	GLU	2.2
32	1a	731	G	2.2
31	29	8	LYS	2.2
34	2c	199	LYS	2.2
1	2A	777	A	2.2
38	2g	78	ARG	2.2
1	2A	2275	C	2.2
34	1c	171	GLY	2.2
35	2d	137	SER	2.2
7	2H	43	VAL	2.2
38	2g	156	TRP	2.2
51	2t	72	LEU	2.2
1	2A	200	U	2.2
1	1A	2174	G	2.2
5	2F	77	ASP	2.2
10	2O	78	ARG	2.2
47	1p	38	TYR	2.2
15	2T	27	THR	2.2
39	2h	136	GLU	2.2
19	2X	67	GLY	2.2
23	11	49	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
35	1d	67	ILE	2.2
45	2n	35	ARG	2.2
32	1a	796	C	2.2
11	1P	37	GLY	2.2
40	1i	105	ASP	2.2
12	1Q	3	MET	2.2
23	21	62	VAL	2.2
46	2o	87	ILE	2.2
16	1U	3	ARG	2.2
52	2u	6	ARG	2.2
1	2A	775	G	2.2
32	2a	1523	G	2.2
1	1A	1954	A	2.2
16	2U	48	ALA	2.2
18	2W	96	ILE	2.2
42	2k	41	THR	2.2
47	2p	36	ILE	2.2
19	1X	58	HIS	2.2
23	21	43	TYR	2.2
36	1e	15	ARG	2.2
28	26	33	LYS	2.2
31	29	24	TYR	2.2
10	1O	9	GLU	2.2
12	2Q	84	GLY	2.2
19	2X	7	VAL	2.2
14	2S	3	ARG	2.2
29	27	44	PRO	2.2
35	2d	102	ASP	2.2
8	2I	2	LYS	2.2
44	2m	87	TYR	2.2
1	1A	2626	A	2.2
1	2A	782	A	2.2
40	2i	81	ILE	2.2
1	1A	1344	C	2.2
5	2F	54	ARG	2.2
45	2n	30	ALA	2.2
3	2D	249	PRO	2.2
49	2r	81	PHE	2.2
11	1P	35	HIS	2.2
34	1c	6	HIS	2.2
47	1p	16	HIS	2.2
7	1H	52	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
12	1Q	96	VAL	2.2
36	2e	131	ILE	2.2
10	1O	3	GLN	2.2
22	20	41	ARG	2.2
29	27	3	ARG	2.2
35	1d	46	LYS	2.2
47	1p	28	ARG	2.2
1	1A	855	G	2.2
32	2a	1202	G	2.2
1	1A	1348	A	2.2
1	2A	2511	U	2.2
53	1v	12	A	2.2
3	2D	173	VAL	2.2
13	2R	7	GLY	2.2
28	26	11	LEU	2.2
35	2d	98	GLU	2.2
41	1j	98	ILE	2.2
36	1e	20	GLN	2.2
48	2q	93	GLN	2.2
5	2F	89	VAL	2.2
46	1o	49	ASP	2.2
31	29	10	ILE	2.2
35	1d	118	ARG	2.2
40	2i	66	ARG	2.2
1	1A	879	G	2.2
1	2A	1675	C	2.2
1	2A	2690	C	2.2
3	1D	95	LEU	2.2
10	1O	36	GLY	2.2
12	1Q	66	ILE	2.2
12	1Q	131	ILE	2.2
23	21	7	ILE	2.2
30	28	16	ILE	2.2
34	1c	198	VAL	2.2
44	2m	95	GLY	2.2
1	2A	688	U	2.2
3	1D	181	GLU	2.2
5	2F	78	ILE	2.2
6	2G	88	ILE	2.2
10	2O	66	LYS	2.2
13	2R	13	HIS	2.2
1	2A	2108	C	2.2

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Mol	Chain	Res	Type	RSRZ
3	2D	246	PRO	2.2
9	1N	70	LYS	2.2
18	1W	92	ARG	2.2
31	29	25	VAL	2.2
36	2e	31	LEU	2.2
39	2h	2	LEU	2.2
27	25	5	PRO	2.2
34	2c	171	GLY	2.2
47	1p	4	ILE	2.2
12	1Q	20	ALA	2.2
32	1a	204	U	2.2
22	20	19	LYS	2.2
23	11	47	GLN	2.2
46	2o	48	LYS	2.2
1	1A	639	G	2.2
32	1a	1355	G	2.2
4	1E	104	VAL	2.2
11	2P	36	LYS	2.2
12	1Q	87	LYS	2.2
35	1d	63	LYS	2.2
40	2i	116	LYS	2.2
1	2A	958	U	2.2
1	2A	2189	U	2.2
32	1a	1510	U	2.2
36	2e	28	PHE	2.2
42	1k	19	ALA	2.1
3	2D	183	ARG	2.1
3	2D	255	LYS	2.1
10	1O	56	ASP	2.1
10	1O	61	VAL	2.1
12	1Q	130	LYS	2.1
17	1V	74	LYS	2.1
23	11	11	ARG	2.1
35	2d	112	VAL	2.1
40	2i	29	ASN	2.1
43	2l	67	THR	2.1
44	2m	111	LYS	2.1
50	2s	33	THR	2.1
1	1A	1719	C	2.1
1	1A	1803	G	2.1
1	2A	388	G	2.1
1	2A	1799	G	2.1

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Mol	Chain	Res	Type	RSRZ
32	2a	1524	C	2.1
3	2D	68	LYS	2.1
4	2E	129	HIS	2.1
9	1N	62	VAL	2.1
23	11	21	ARG	2.1
31	29	35	ARG	2.1
34	2c	12	LEU	2.1
34	2c	201	TYR	2.1
36	2e	105	VAL	2.1
41	1j	57	LYS	2.1
4	2E	140	SER	2.1
10	2O	77	ILE	2.1
15	1T	45	PHE	2.1
16	2U	44	ASN	2.1
11	2P	109	GLY	2.1
33	1b	72	GLY	2.1
34	2c	159	GLY	2.1
35	1d	6	GLY	2.1
41	2j	64	GLU	2.1
9	2N	111	PRO	2.1
3	2D	33	LEU	2.1
13	2R	99	LYS	2.1
34	1c	189	ALA	2.1
36	1e	10	MET	2.1
37	2f	53	ALA	2.1
38	2g	2	ALA	2.1
23	21	26	ARG	2.1
4	2E	137	HIS	2.1
1	1A	827	G	2.1
1	2A	2000	G	2.1
4	2E	115	GLY	2.1
32	2a	1224	G	2.1
50	2s	35	SER	2.1
11	2P	48	PRO	2.1
16	2U	50	ARG	2.1
18	2W	99	ARG	2.1
43	1l	27	LEU	2.1
36	1e	84	PHE	2.1
1	1A	851	A	2.1
1	2A	1762	A	2.1
1	2A	1825	A	2.1
4	1E	129	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
16	1U	37	GLU	2.1
16	2U	6	THR	2.1
38	2g	8	GLU	2.1
41	1j	35	SER	2.1
43	1l	16	GLU	2.1
11	1P	17	LYS	2.1
1	2A	574	C	2.1
1	2A	749	C	2.1
1	2A	1672	C	2.1
5	2F	44	ARG	2.1
7	2H	131	VAL	2.1
18	1W	85	VAL	2.1
19	1X	1	MET	2.1
48	2q	31	LEU	2.1
1	1A	2625	U	2.1
3	2D	49	ILE	2.1
10	1O	86	ILE	2.1
42	2k	125	PHE	2.1
1	1A	1317	G	2.1
1	2A	2166	G	2.1
32	1a	1187	G	2.1
32	1a	1353	G	2.1
32	2a	7	G	2.1
12	1Q	103	MET	2.1
30	28	51	ALA	2.1
40	2i	52	ALA	2.1
4	1E	126	PRO	2.1
6	2G	131	TYR	2.1
9	2N	85	ILE	2.1
10	1O	45	GLU	2.1
1	1A	2165	C	2.1
1	2A	740	U	2.1
22	10	13	GLY	2.1
32	1a	1113	C	2.1
55	2x	56	C	2.1
5	1F	77	ASP	2.1
13	2R	14	SER	2.1
16	1U	117	GLN	2.1
18	2W	7	ALA	2.1
36	1e	30	ALA	2.1
45	1n	60	SER	2.1
10	2O	21	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	2D	263	ARG	2.1
35	2d	100	ARG	2.1
40	1i	107	ARG	2.1
40	2i	30	GLY	2.1
45	1n	45	ARG	2.1
22	20	53	MET	2.1
5	2F	96	ASP	2.1
12	1Q	4	PRO	2.1
15	2T	75	ILE	2.1
15	2T	100	TYR	2.1
34	2c	191	THR	2.1
1	2A	1660	C	2.1
1	2A	2107	C	2.1
16	2U	13	LYS	2.1
40	2i	113	LYS	2.1
46	1o	47	LYS	2.1
55	2x	69	C	2.1
9	2N	48	MET	2.1
11	2P	45	LEU	2.1
16	1U	32	PHE	2.1
18	2W	74	ALA	2.1
23	11	94	LEU	2.1
33	1b	188	ALA	2.1
34	1c	200	ALA	2.1
36	1e	86	ALA	2.1
36	2e	90	VAL	2.1
45	1n	31	ARG	2.1
23	11	66	HIS	2.1
1	1A	1689	G	2.1
1	2A	1559	G	2.1
1	2A	2018	G	2.1
36	1e	87	SER	2.1
15	2T	33	LYS	2.1
44	1m	120	LYS	2.1
3	1D	56	GLY	2.1
3	1D	183	ARG	2.1
1	1A	2461	U	2.1
7	2H	33	LEU	2.1
44	2m	98	VAL	2.1
52	2u	4	GLY	2.1
12	1Q	69	PHE	2.1
19	1X	79	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	1A	1802	C	2.1
15	1T	113	LYS	2.1
18	2W	6	ILE	2.1
34	2c	150	LYS	2.1
40	1i	125	TYR	2.1
9	2N	52	VAL	2.1
15	2T	72	VAL	2.1
18	2W	112	GLY	2.1
22	10	76	GLY	2.1
25	23	6	VAL	2.1
35	1d	47	ARG	2.1
43	2l	97	ARG	2.1
1	1A	2262	G	2.1
1	2A	776	G	2.1
3	1D	105	ILE	2.1
3	2D	62	TYR	2.1
1	2A	1130	U	2.1
17	2V	83	ARG	2.1
23	11	40	ARG	2.1
32	2a	900	A	2.1
38	1g	78	ARG	2.1
10	2O	100	GLY	2.1
19	2X	66	LEU	2.1
1	2A	1657	C	2.1
32	2a	564	C	2.1
51	1t	14	LYS	2.1
29	27	33	ARG	2.1
38	2g	4	ARG	2.1
3	1D	221	VAL	2.1
3	1D	229	VAL	2.1
23	21	30	VAL	2.1
41	1j	44	VAL	2.1
15	2T	62	THR	2.1
1	2A	1555	G	2.1
11	2P	107	LYS	2.1
32	1a	813	U	2.1
15	1T	86	ILE	2.1
40	2i	62	TYR	2.1
44	2m	106	ASN	2.1
13	2R	12	ARG	2.1
1	2A	435	C	2.1
1	2A	2021	C	2.1

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Mol	Chain	Res	Type	RSRZ
1	2A	2501	C	2.1
12	2Q	78	PRO	2.1
26	24	54	GLY	2.1
49	2r	78	LEU	2.1
4	2E	154	LYS	2.1
5	2F	63	LYS	2.1
9	2N	47	ALA	2.1
3	2D	69	ARG	2.1
34	2c	164	ARG	2.1
23	11	95	LEU	2.1
1	1A	723	A	2.0
3	1D	53	PHE	2.1
12	1Q	85	LYS	2.0
1	1A	2123	G	2.0
1	2A	2608	G	2.0
38	2g	5	ARG	2.0
44	2m	104	ARG	2.0
1	1A	1138	C	2.0
1	2A	249	C	2.0
1	2A	2105	C	2.0
42	1k	13	GLN	2.0
3	2D	56	GLY	2.0
5	2F	76	GLY	2.0
13	2R	5	LYS	2.0
15	1T	69	GLY	2.0
43	2l	47	LYS	2.0
45	1n	37	PHE	2.0
3	2D	64	ILE	2.0
11	1P	18	ARG	2.0
16	2U	59	ARG	2.0
23	11	37	ILE	2.0
43	2l	26	ALA	2.0
43	1l	19	ARG	2.0
1	1A	1320	A	2.0
1	2A	567	A	2.0
1	2A	572	A	2.0
1	2A	750	A	2.0
18	1W	82	LEU	2.0
3	2D	166	GLN	2.0
47	1p	3	LYS	2.0
1	2A	695	G	2.0
32	1a	388	G	2.0

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Mol	Chain	Res	Type	RSRZ
32	1a	917	G	2.0
12	1Q	70	PRO	2.0
20	2Y	35	TYR	2.0
23	11	17	SER	2.0
29	27	34	ARG	2.0
36	1e	13	ILE	2.0
44	2m	97	PRO	2.0
45	1n	35	ARG	2.0
51	2t	22	ARG	2.0
5	1F	70	THR	2.0
15	1T	90	GLN	2.0
1	1A	2599	A	2.0
32	1a	915	A	2.0
34	1c	154	SER	2.0
11	2P	57	THR	2.0
36	2e	120	THR	2.0
48	1q	7	THR	2.0
1	1A	2459	G	2.0
1	2A	1835	G	2.0
32	2a	810	C	2.0
32	2a	1509	C	2.0
23	11	16	ASN	2.0
36	2e	27	ARG	2.0
45	2n	10	ALA	2.0
28	26	21	TYR	2.0
51	1t	75	ASN	2.0
12	2Q	34	LEU	2.0
51	1t	21	LYS	2.0
3	1D	180	GLY	2.0
34	1c	192	THR	2.0
4	2E	123	ALA	2.0
7	2H	148	ILE	2.0
29	17	6	GLN	2.0
30	28	57	ARG	2.0
42	2k	19	ALA	2.0
11	2P	23	PRO	2.0
27	15	6	VAL	2.0
27	15	8	LYS	2.0
31	29	33	LYS	2.0
1	1A	997	G	2.0
1	1A	1022	C	2.0
23	21	22	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
32	1a	887	G	2.0
10	2O	3	GLN	2.0
29	27	45	ALA	2.0
36	1e	132	ALA	2.0
9	2N	72	TYR	2.0
10	2O	7	TYR	2.0
12	1Q	17	LEU	2.0
43	2l	10	LEU	2.0
20	2Y	43	ASN	2.0
45	2n	37	PHE	2.0
11	1P	49	ARG	2.0
32	2a	573	A	2.0
39	2h	85	ARG	2.0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	4SU	2x	8	20/21	0.83	0.15	106,121,131,139	0
55	PSU	2x	55	20/21	0.85	0.26	105,119,134,136	0
32	PSU	1a	516	20/21	0.86	0.15	105,119,129,131	0
1	5MU	1A	1937	21/22	0.88	0.14	102,113,123,145	0
55	4SU	1x	8	20/21	0.89	0.15	106,116,122,129	0
32	4OC	2a	1402	22/23	0.90	0.28	94,104,112,115	0
1	4OC	1A	1942	21/23	0.91	0.20	86,99,108,110	0
32	5MC	1a	1407	21/22	0.91	0.21	96,103,114,123	0
32	7MG	2a	527	24/25	0.91	0.19	97,107,113,115	0
32	2MG	1a	1207	24/25	0.91	0.18	105,114,134,137	0
55	PSU	1x	55	20/21	0.91	0.14	99,110,130,130	0
32	4OC	1a	1402	22/23	0.91	0.29	87,102,109,116	0
32	2MG	2a	1207	24/25	0.92	0.19	102,116,123,129	0
32	PSU	2a	516	20/21	0.92	0.12	93,110,115,116	0
32	5MC	1a	967	21/22	0.92	0.39	108,116,125,130	0
32	7MG	1a	527	24/25	0.92	0.21	100,108,119,126	0
1	5MU	2A	1915	21/22	0.93	0.10	103,108,119,134	0
1	PSU	2A	1917	20/21	0.93	0.15	96,99,107,111	0
43	0TD	2l	92	10/11	0.93	0.58	101,110,117,134	0
1	5MC	1A	1964	21/22	0.93	0.19	81,91,96,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	KGV	2w	76	33/34	0.93	0.50	75,89,98,102	0
32	M2G	1a	966	25/26	0.93	0.28	102,108,121,122	0
1	2MA	2A	2503	23/24	0.93	0.32	80,86,93,105	0
55	5MU	1x	54	21/22	0.93	0.12	108,113,121,124	0
32	5MC	2a	967	21/22	0.93	0.21	93,101,111,116	0
1	2MU	1A	2564	21/23	0.93	0.40	83,90,99,103	0
32	M2G	2a	966	25/26	0.94	0.29	94,103,117,121	0
32	5MC	1a	1404	21/22	0.94	0.28	89,96,99,110	0
32	5MC	2a	1404	21/22	0.94	0.30	91,98,104,109	0
1	PSU	2A	1911	20/21	0.94	0.14	89,100,112,117	0
1	OMG	2A	2251	24/25	0.94	0.35	77,93,100,104	0
1	4OC	2A	1920	21/23	0.94	0.22	93,100,108,109	0
1	5MU	2A	1939	21/22	0.94	0.27	77,88,97,102	0
55	5MC	2x	32	21/22	0.94	0.21	106,110,114,119	0
32	5MC	1a	1400	21/22	0.94	0.27	96,105,118,123	0
32	5MC	2a	1400	21/22	0.94	0.23	99,109,117,118	0
1	PSU	1A	2617	20/21	0.94	0.39	71,82,92,95	0
32	UR3	2a	1498	21/22	0.95	0.42	92,102,109,111	0
54	KGV	1w	76	33/34	0.95	0.45	80,87,97,101	0
43	0TD	1l	92	10/11	0.95	0.39	102,110,112,117	0
1	2MU	2A	2552	21/23	0.95	0.24	77,85,90,96	0
1	5MC	2A	1942	21/22	0.95	0.18	78,92,102,106	0
55	5MC	1x	32	21/22	0.95	0.21	98,107,111,124	0
1	PSU	1A	1939	20/21	0.95	0.16	86,100,107,115	0
1	PSU	1A	1933	20/21	0.95	0.17	84,98,106,107	0
55	5MU	2x	54	21/22	0.95	0.24	104,110,120,126	0
32	5MC	2a	1407	21/22	0.95	0.25	81,93,102,104	0
32	UR3	1a	1498	21/22	0.95	0.27	86,95,101,105	0
32	MA6	2a	1518	24/25	0.96	0.28	90,100,106,108	0
32	MA6	2a	1519	24/25	0.96	0.34	80,100,106,109	0
1	PSU	2A	2605	20/21	0.96	0.34	70,86,90,91	0
1	5MC	2A	1962	21/22	0.96	0.19	66,90,94,99	0
1	5MU	1A	1961	21/22	0.96	0.33	66,83,90,94	0
32	MA6	1a	1518	24/25	0.96	0.21	87,93,98,101	0
32	MA6	1a	1519	24/25	0.97	0.30	82,94,101,105	0
1	OMG	1A	2263	24/25	0.97	0.37	70,82,95,97	0
1	5MC	1A	1984	21/22	0.97	0.18	80,89,92,99	0
1	2MA	1A	2515	23/24	0.97	0.30	69,78,88,94	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1616	1/1	0.28	0.32	87,87,87,87	0
56	MG	1a	1663	1/1	0.31	0.34	97,97,97,97	0
56	MG	2A	3098	1/1	0.33	0.51	81,81,81,81	0
56	MG	1B	213	1/1	0.34	0.42	74,74,74,74	0
56	MG	2A	3377	1/1	0.39	0.24	71,71,71,71	0
56	MG	1A	3182	1/1	0.39	0.85	100,100,100,100	0
56	MG	2a	1632	1/1	0.39	0.28	82,82,82,82	0
56	MG	2A	3220	1/1	0.41	0.51	78,78,78,78	0
56	MG	1A	3226	1/1	0.42	0.34	68,68,68,68	0
56	MG	2A	3225	1/1	0.45	0.37	83,83,83,83	0
56	MG	1F	302	1/1	0.45	0.81	68,68,68,68	0
56	MG	2A	3393	1/1	0.47	0.35	84,84,84,84	0
56	MG	2a	1668	1/1	0.48	0.24	79,79,79,79	0
56	MG	2d	301	1/1	0.48	0.28	68,68,68,68	0
56	MG	1x	105	1/1	0.49	0.28	109,109,109,109	0
56	MG	1A	3515	1/1	0.50	0.65	60,60,60,60	0
56	MG	1A	3189	1/1	0.50	0.47	83,83,83,83	0
56	MG	1A	3214	1/1	0.51	0.47	74,74,74,74	0
56	MG	1A	3130	1/1	0.52	0.51	73,73,73,73	0
56	MG	2A	3013	1/1	0.53	0.23	97,97,97,97	0
56	MG	2A	3021	1/1	0.53	0.48	87,87,87,87	0
56	MG	2A	3036	1/1	0.53	0.91	92,92,92,92	0
56	MG	1A	3429	1/1	0.53	0.54	80,80,80,80	0
56	MG	1B	219	1/1	0.54	0.09	116,116,116,116	0
56	MG	1a	1628	1/1	0.55	0.28	82,82,82,82	0
56	MG	2B	203	1/1	0.55	0.32	79,79,79,79	0
56	MG	1A	3433	1/1	0.56	0.42	67,67,67,67	0
56	MG	2A	3467	1/1	0.57	0.22	86,86,86,86	0
56	MG	1A	3299	1/1	0.57	0.81	71,71,71,71	0
56	MG	2E	302	1/1	0.57	0.28	69,69,69,69	0
56	MG	2A	3092	1/1	0.57	0.31	76,76,76,76	0
56	MG	2A	3249	1/1	0.57	0.32	75,75,75,75	0
56	MG	1A	3245	1/1	0.57	0.51	74,74,74,74	0
56	MG	2A	3210	1/1	0.57	0.20	71,71,71,71	0
56	MG	1A	3298	1/1	0.58	0.38	71,71,71,71	0
56	MG	2A	3115	1/1	0.58	0.30	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3364	1/1	0.58	1.96	65,65,65,65	0
56	MG	1A	3128	1/1	0.59	0.51	70,70,70,70	0
56	MG	1A	3362	1/1	0.59	0.28	82,82,82,82	0
56	MG	1A	3373	1/1	0.59	0.47	71,71,71,71	0
56	MG	2A	3186	1/1	0.59	0.19	64,64,64,64	0
56	MG	1A	3294	1/1	0.59	0.48	75,75,75,75	0
56	MG	1A	3232	1/1	0.59	0.34	59,59,59,59	0
56	MG	1a	1607	1/1	0.60	0.33	81,81,81,81	0
56	MG	2A	3321	1/1	0.60	0.38	67,67,67,67	0
56	MG	1A	3529	1/1	0.61	0.22	73,73,73,73	0
56	MG	2A	3100	1/1	0.61	0.20	68,68,68,68	0
56	MG	1A	3477	1/1	0.61	0.45	61,61,61,61	0
56	MG	1A	3360	1/1	0.61	0.30	84,84,84,84	0
56	MG	2A	3208	1/1	0.61	0.20	95,95,95,95	0
56	MG	2A	3200	1/1	0.62	0.37	81,81,81,81	0
56	MG	2A	3356	1/1	0.62	0.22	77,77,77,77	0
56	MG	2a	1703	1/1	0.62	0.51	88,88,88,88	0
56	MG	1A	3422	1/1	0.62	0.64	70,70,70,70	0
56	MG	2a	1634	1/1	0.63	0.28	81,81,81,81	0
56	MG	1A	3093	1/1	0.63	0.77	82,82,82,82	0
56	MG	1A	3440	1/1	0.63	0.45	81,81,81,81	0
56	MG	1A	3199	1/1	0.63	0.34	61,61,61,61	0
56	MG	2A	3218	1/1	0.64	0.19	77,77,77,77	0
56	MG	2a	1602	1/1	0.64	0.87	78,78,78,78	0
56	MG	2A	3087	1/1	0.64	0.51	96,96,96,96	0
56	MG	2A	3122	1/1	0.64	0.52	66,66,66,66	0
56	MG	2A	3140	1/1	0.64	0.24	81,81,81,81	0
56	MG	2A	3461	1/1	0.64	0.28	67,67,67,67	0
56	MG	2A	3308	1/1	0.64	0.28	63,63,63,63	0
56	MG	2A	3151	1/1	0.64	0.22	77,77,77,77	0
56	MG	2A	3201	1/1	0.65	0.25	81,81,81,81	0
56	MG	1W	201	1/1	0.65	1.02	69,69,69,69	0
56	MG	1A	3188	1/1	0.65	0.64	86,86,86,86	0
56	MG	2A	3164	1/1	0.65	0.17	78,78,78,78	0
56	MG	2A	3003	1/1	0.65	0.21	72,72,72,72	0
56	MG	1A	3285	1/1	0.65	0.34	76,76,76,76	0
56	MG	1D	303	1/1	0.66	1.15	70,70,70,70	0
56	MG	1A	3472	1/1	0.66	1.50	70,70,70,70	0
56	MG	2A	3342	1/1	0.66	0.26	61,61,61,61	0
56	MG	2A	3022	1/1	0.66	0.77	87,87,87,87	0
56	MG	1a	1679	1/1	0.66	0.26	76,76,76,76	0
56	MG	2A	3058	1/1	0.66	0.91	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3086	1/1	0.66	0.82	79,79,79,79	0
56	MG	1A	3075	1/1	0.66	0.49	83,83,83,83	0
56	MG	1A	3223	1/1	0.66	0.36	84,84,84,84	0
56	MG	1A	3473	1/1	0.67	0.37	68,68,68,68	0
56	MG	2A	3179	1/1	0.67	0.18	75,75,75,75	0
56	MG	2A	3266	1/1	0.67	0.23	59,59,59,59	0
56	MG	2a	1614	1/1	0.67	0.80	76,76,76,76	0
56	MG	2A	3043	1/1	0.67	0.40	78,78,78,78	0
56	MG	2A	3240	1/1	0.68	0.76	75,75,75,75	0
56	MG	2A	3144	1/1	0.68	0.40	88,88,88,88	0
56	MG	2A	3219	1/1	0.68	0.23	90,90,90,90	0
56	MG	2A	3097	1/1	0.68	0.19	77,77,77,77	0
56	MG	2W	201	1/1	0.68	0.27	64,64,64,64	0
56	MG	2Z	301	1/1	0.68	0.25	54,54,54,54	0
56	MG	1a	1652	1/1	0.68	0.43	68,68,68,68	0
56	MG	1Q	202	1/1	0.69	0.42	56,56,56,56	0
56	MG	1A	3058	1/1	0.69	0.59	71,71,71,71	0
56	MG	1A	3376	1/1	0.69	0.54	92,92,92,92	0
56	MG	2A	3474	1/1	0.69	0.71	84,84,84,84	0
56	MG	1x	108	1/1	0.69	0.21	103,103,103,103	0
56	MG	2a	1639	1/1	0.69	0.30	64,64,64,64	0
56	MG	1A	3395	1/1	0.69	0.18	96,96,96,96	0
56	MG	2a	1676	1/1	0.69	0.24	82,82,82,82	0
56	MG	2A	3371	1/1	0.69	0.22	86,86,86,86	0
56	MG	1A	3190	1/1	0.69	0.48	78,78,78,78	0
56	MG	2A	3327	1/1	0.70	0.51	73,73,73,73	0
56	MG	2A	3039	1/1	0.70	0.23	88,88,88,88	0
56	MG	1a	1633	1/1	0.70	0.56	73,73,73,73	0
56	MG	2A	3357	1/1	0.70	0.30	67,67,67,67	0
56	MG	1A	3449	1/1	0.70	0.28	66,66,66,66	0
56	MG	1a	1660	1/1	0.70	0.24	62,62,62,62	0
56	MG	2A	3234	1/1	0.70	0.30	60,60,60,60	0
56	MG	1E	303	1/1	0.70	0.77	77,77,77,77	0
56	MG	2A	3459	1/1	0.70	0.28	69,69,69,69	0
56	MG	2a	1644	1/1	0.70	0.38	63,63,63,63	0
56	MG	2A	3202	1/1	0.70	0.30	86,86,86,86	0
56	MG	2a	1675	1/1	0.70	0.20	85,85,85,85	0
56	MG	2A	3204	1/1	0.70	0.32	68,68,68,68	0
56	MG	1E	304	1/1	0.70	0.35	69,69,69,69	0
56	MG	1A	3427	1/1	0.70	0.29	56,56,56,56	0
56	MG	2l	201	1/1	0.70	1.61	68,68,68,68	0
56	MG	2A	3376	1/1	0.71	0.48	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3203	1/1	0.71	0.83	66,66,66,66	0
56	MG	2A	3384	1/1	0.71	0.26	77,77,77,77	0
56	MG	1A	3259	1/1	0.71	0.48	73,73,73,73	0
56	MG	2A	3442	1/1	0.71	0.21	76,76,76,76	0
56	MG	2A	3023	1/1	0.71	0.24	74,74,74,74	0
56	MG	1A	3096	1/1	0.71	0.24	95,95,95,95	0
56	MG	2a	1664	1/1	0.71	0.25	77,77,77,77	0
56	MG	1A	3012	1/1	0.71	0.30	70,70,70,70	0
56	MG	1A	3183	1/1	0.71	0.38	59,59,59,59	0
56	MG	1a	1683	1/1	0.71	0.15	84,84,84,84	0
56	MG	2A	3065	1/1	0.71	0.38	101,101,101,101	0
56	MG	2A	3077	1/1	0.71	0.26	58,58,58,58	0
56	MG	2A	3138	1/1	0.71	0.30	90,90,90,90	0
56	MG	1a	1623	1/1	0.72	0.26	87,87,87,87	0
56	MG	1a	1627	1/1	0.72	0.32	67,67,67,67	0
56	MG	2a	1603	1/1	0.72	0.26	70,70,70,70	0
56	MG	1A	3511	1/1	0.72	0.50	76,76,76,76	0
56	MG	2A	3191	1/1	0.72	0.58	78,78,78,78	0
56	MG	1A	3390	1/1	0.72	0.48	67,67,67,67	0
56	MG	2A	3399	1/1	0.72	0.17	80,80,80,80	0
56	MG	1A	3386	1/1	0.72	0.36	55,55,55,55	0
56	MG	1A	3474	1/1	0.72	0.63	50,50,50,50	0
56	MG	2a	1657	1/1	0.72	0.23	50,50,50,50	0
56	MG	1A	3410	1/1	0.72	0.43	82,82,82,82	0
56	MG	17	101	1/1	0.72	0.69	77,77,77,77	0
56	MG	2a	1672	1/1	0.72	0.43	89,89,89,89	0
56	MG	17	102	1/1	0.72	0.39	54,54,54,54	0
56	MG	1e	201	1/1	0.72	0.30	80,80,80,80	0
56	MG	2a	1699	1/1	0.72	0.37	61,61,61,61	0
56	MG	1x	104	1/1	0.72	0.13	107,107,107,107	0
56	MG	2O	201	1/1	0.72	1.56	73,73,73,73	0
56	MG	1A	3501	1/1	0.72	0.50	66,66,66,66	0
56	MG	1A	3333	1/1	0.73	0.34	73,73,73,73	0
56	MG	2a	1606	1/1	0.73	0.47	65,65,65,65	0
56	MG	2A	3143	1/1	0.73	0.32	60,60,60,60	0
56	MG	2A	3095	1/1	0.73	0.54	70,70,70,70	0
56	MG	2A	3011	1/1	0.73	0.17	84,84,84,84	0
56	MG	2A	3406	1/1	0.73	0.29	72,72,72,72	0
56	MG	2A	3435	1/1	0.73	0.29	71,71,71,71	0
56	MG	2A	3320	1/1	0.73	0.39	76,76,76,76	0
56	MG	2A	3206	1/1	0.73	0.31	78,78,78,78	0
56	MG	1A	3070	1/1	0.73	0.15	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3333	1/1	0.73	0.23	51,51,51,51	0
56	MG	2A	3337	1/1	0.73	0.24	59,59,59,59	0
56	MG	2A	3177	1/1	0.73	0.30	71,71,71,71	0
56	MG	1A	3385	1/1	0.73	0.20	79,79,79,79	0
56	MG	2a	1684	1/1	0.73	0.28	61,61,61,61	0
56	MG	2A	3182	1/1	0.73	0.99	66,66,66,66	0
56	MG	1A	3048	1/1	0.73	0.36	65,65,65,65	0
56	MG	1a	1615	1/1	0.73	0.10	80,80,80,80	0
56	MG	1V	203	1/1	0.73	0.54	75,75,75,75	0
56	MG	1A	3064	1/1	0.74	0.43	77,77,77,77	0
56	MG	2A	3075	1/1	0.74	0.23	75,75,75,75	0
56	MG	1A	3431	1/1	0.74	0.64	61,61,61,61	0
56	MG	2A	3156	1/1	0.74	0.31	75,75,75,75	0
56	MG	2a	1630	1/1	0.74	0.48	65,65,65,65	0
56	MG	1x	109	1/1	0.74	0.69	88,88,88,88	0
56	MG	1A	3060	1/1	0.74	0.27	55,55,55,55	0
56	MG	2a	1638	1/1	0.74	0.20	68,68,68,68	0
56	MG	2A	3088	1/1	0.74	0.48	61,61,61,61	0
56	MG	1A	3191	1/1	0.74	1.18	51,51,51,51	0
56	MG	1A	3409	1/1	0.74	0.52	71,71,71,71	0
56	MG	1A	3532	1/1	0.74	0.21	113,113,113,113	0
56	MG	1A	3547	1/1	0.74	0.37	78,78,78,78	0
56	MG	1a	1674	1/1	0.74	0.59	89,89,89,89	0
56	MG	2A	3107	1/1	0.74	0.21	91,91,91,91	0
56	MG	1A	3346	1/1	0.74	0.48	73,73,73,73	0
56	MG	2A	3338	1/1	0.74	0.38	68,68,68,68	0
56	MG	2a	1689	1/1	0.74	0.15	91,91,91,91	0
56	MG	2A	3120	1/1	0.74	0.36	66,66,66,66	0
56	MG	1A	3381	1/1	0.74	0.33	67,67,67,67	0
56	MG	1a	1609	1/1	0.74	0.33	106,106,106,106	0
56	MG	1A	3350	1/1	0.74	0.33	72,72,72,72	0
56	MG	2A	3425	1/1	0.75	0.23	72,72,72,72	0
56	MG	1A	3445	1/1	0.75	0.38	70,70,70,70	0
56	MG	2A	3214	1/1	0.75	0.26	77,77,77,77	0
56	MG	2A	3101	1/1	0.75	1.12	75,75,75,75	0
56	MG	2A	3104	1/1	0.75	0.28	64,64,64,64	0
56	MG	2A	3350	1/1	0.75	0.23	69,69,69,69	0
56	MG	1A	3300	1/1	0.75	0.34	70,70,70,70	0
56	MG	1A	3531	1/1	0.75	0.23	71,71,71,71	0
56	MG	2A	3358	1/1	0.75	0.23	62,62,62,62	0
56	MG	1A	3100	1/1	0.75	0.39	74,74,74,74	0
56	MG	1A	3137	1/1	0.75	0.33	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1B	205	1/1	0.75	0.37	73,73,73,73	0
56	MG	27	101	1/1	0.75	0.27	60,60,60,60	0
56	MG	1A	3218	1/1	0.75	0.58	73,73,73,73	0
56	MG	1A	3150	1/1	0.75	0.25	93,93,93,93	0
56	MG	1A	3491	1/1	0.75	0.41	73,73,73,73	0
56	MG	1A	3161	1/1	0.75	0.25	69,69,69,69	0
56	MG	1A	3053	1/1	0.75	0.28	80,80,80,80	0
56	MG	2a	1612	1/1	0.76	0.34	74,74,74,74	0
56	MG	1A	3494	1/1	0.76	0.31	50,50,50,50	0
56	MG	2A	3312	1/1	0.76	0.37	72,72,72,72	0
56	MG	2A	3313	1/1	0.76	0.42	75,75,75,75	0
56	MG	1B	201	1/1	0.76	0.33	67,67,67,67	0
56	MG	1A	3464	1/1	0.76	0.39	55,55,55,55	0
56	MG	2A	3205	1/1	0.76	0.52	68,68,68,68	0
56	MG	1A	3231	1/1	0.76	0.26	65,65,65,65	0
56	MG	1A	3090	1/1	0.76	0.63	75,75,75,75	0
56	MG	2A	3161	1/1	0.76	0.21	66,66,66,66	0
56	MG	2A	3162	1/1	0.76	0.17	64,64,64,64	0
56	MG	1a	1644	1/1	0.76	0.30	89,89,89,89	0
56	MG	1A	3367	1/1	0.76	0.30	65,65,65,65	0
56	MG	2F	301	1/1	0.76	0.14	79,79,79,79	0
56	MG	1A	3167	1/1	0.76	0.35	61,61,61,61	0
56	MG	1A	3216	1/1	0.76	0.28	69,69,69,69	0
56	MG	1a	1668	1/1	0.76	0.39	63,63,63,63	0
56	MG	2A	3082	1/1	0.76	0.55	71,71,71,71	0
56	MG	1a	1671	1/1	0.76	0.38	71,71,71,71	0
56	MG	2A	3262	1/1	0.76	0.27	50,50,50,50	0
56	MG	2A	3018	1/1	0.76	0.22	60,60,60,60	0
56	MG	2n	101	1/1	0.76	0.39	77,77,77,77	0
56	MG	2A	3345	1/1	0.77	0.31	58,58,58,58	0
56	MG	2A	3290	1/1	0.77	0.18	67,67,67,67	0
56	MG	1T	202	1/1	0.77	0.41	58,58,58,58	0
56	MG	2a	1658	1/1	0.77	0.37	60,60,60,60	0
56	MG	2a	1601	1/1	0.77	0.97	63,63,63,63	0
56	MG	19	101	1/1	0.77	0.37	72,72,72,72	0
56	MG	2A	3160	1/1	0.77	0.26	78,78,78,78	0
56	MG	1A	3175	1/1	0.77	0.45	57,57,57,57	0
56	MG	1a	1635	1/1	0.77	0.22	76,76,76,76	0
56	MG	2A	3472	1/1	0.77	0.13	107,107,107,107	0
56	MG	1A	3414	1/1	0.77	0.60	77,77,77,77	0
56	MG	2a	1696	1/1	0.77	0.23	52,52,52,52	0
56	MG	2a	1629	1/1	0.77	0.31	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1647	1/1	0.77	0.20	58,58,58,58	0
56	MG	10	102	1/1	0.77	0.37	84,84,84,84	0
56	MG	1v	101	1/1	0.77	0.88	67,67,67,67	0
56	MG	1A	3085	1/1	0.77	0.33	77,77,77,77	0
56	MG	1A	3086	1/1	0.78	0.34	63,63,63,63	0
56	MG	1A	3456	1/1	0.78	0.44	75,75,75,75	0
56	MG	2A	3381	1/1	0.78	0.43	58,58,58,58	0
56	MG	1V	202	1/1	0.78	0.91	68,68,68,68	0
56	MG	1a	1614	1/1	0.78	0.17	74,74,74,74	0
56	MG	1A	3310	1/1	0.78	0.39	54,54,54,54	0
56	MG	2A	3106	1/1	0.78	0.84	70,70,70,70	0
56	MG	1A	3008	1/1	0.78	0.20	100,100,100,100	0
56	MG	2A	3254	1/1	0.78	0.45	66,66,66,66	0
56	MG	2A	3438	1/1	0.78	0.24	64,64,64,64	0
56	MG	2A	3031	1/1	0.78	0.12	89,89,89,89	0
56	MG	2A	3355	1/1	0.78	0.54	69,69,69,69	0
56	MG	1A	3224	1/1	0.78	0.29	81,81,81,81	0
56	MG	2A	3170	1/1	0.78	0.43	58,58,58,58	0
56	MG	1A	3043	1/1	0.78	0.46	79,79,79,79	0
56	MG	2A	3178	1/1	0.78	0.24	76,76,76,76	0
56	MG	2a	1633	1/1	0.78	0.14	74,74,74,74	0
56	MG	1P	202	1/1	0.78	0.70	84,84,84,84	0
56	MG	1A	3114	1/1	0.79	0.29	72,72,72,72	0
56	MG	1A	3171	1/1	0.79	0.25	71,71,71,71	0
56	MG	1A	3437	1/1	0.79	0.64	83,83,83,83	0
56	MG	1X	101	1/1	0.79	1.15	85,85,85,85	0
56	MG	1A	3478	1/1	0.79	0.32	50,50,50,50	0
56	MG	1B	210	1/1	0.79	0.43	69,69,69,69	0
56	MG	1A	3489	1/1	0.79	0.25	85,85,85,85	0
56	MG	1B	217	1/1	0.79	0.49	92,92,92,92	0
56	MG	2A	3103	1/1	0.79	0.36	61,61,61,61	0
56	MG	2a	1649	1/1	0.79	0.29	66,66,66,66	0
56	MG	1A	3083	1/1	0.79	0.34	55,55,55,55	0
56	MG	2B	204	1/1	0.79	0.30	91,91,91,91	0
56	MG	2B	210	1/1	0.79	0.47	80,80,80,80	0
56	MG	2A	3105	1/1	0.79	0.28	75,75,75,75	0
56	MG	1A	3344	1/1	0.79	0.23	57,57,57,57	0
56	MG	1A	3236	1/1	0.79	0.32	61,61,61,61	0
56	MG	1A	3451	1/1	0.79	0.22	52,52,52,52	0
56	MG	2a	1682	1/1	0.79	0.15	56,56,56,56	0
56	MG	2A	3192	1/1	0.79	0.21	50,50,50,50	0
56	MG	1A	3348	1/1	0.79	0.29	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3306	1/1	0.79	0.63	56,56,56,56	0
56	MG	1A	3524	1/1	0.79	0.09	93,93,93,93	0
56	MG	1A	3179	1/1	0.79	0.26	69,69,69,69	0
56	MG	1a	1629	1/1	0.79	1.22	85,85,85,85	0
56	MG	1A	3352	1/1	0.79	0.39	50,50,50,50	0
56	MG	2A	3414	1/1	0.79	0.37	76,76,76,76	0
56	MG	1A	3077	1/1	0.80	0.37	72,72,72,72	0
56	MG	2a	1608	1/1	0.80	0.23	58,58,58,58	0
56	MG	2A	3260	1/1	0.80	0.24	62,62,62,62	0
56	MG	1a	1676	1/1	0.80	0.32	67,67,67,67	0
56	MG	1A	3127	1/1	0.80	0.49	73,73,73,73	0
56	MG	2A	3009	1/1	0.80	0.29	67,67,67,67	0
56	MG	1B	214	1/1	0.80	0.30	85,85,85,85	0
56	MG	2A	3046	1/1	0.80	0.47	74,74,74,74	0
56	MG	2a	1685	1/1	0.80	0.27	67,67,67,67	0
56	MG	1A	3027	1/1	0.80	0.15	81,81,81,81	0
56	MG	1A	3206	1/1	0.80	0.42	59,59,59,59	0
56	MG	2A	3226	1/1	0.80	1.90	82,82,82,82	0
56	MG	2A	3456	1/1	0.80	0.22	52,52,52,52	0
56	MG	2A	3125	1/1	0.80	0.23	67,67,67,67	0
56	MG	1A	3304	1/1	0.80	0.43	63,63,63,63	0
56	MG	1a	1636	1/1	0.80	0.39	55,55,55,55	0
57	ZN	24	501	1/1	0.80	0.05	171,171,171,171	0
56	MG	1a	1675	1/1	0.81	0.28	60,60,60,60	0
56	MG	1A	3460	1/1	0.81	0.38	64,64,64,64	0
56	MG	2A	3117	1/1	0.81	0.23	64,64,64,64	0
56	MG	2a	1619	1/1	0.81	0.28	62,62,62,62	0
56	MG	2A	3431	1/1	0.81	0.24	65,65,65,65	0
56	MG	1A	3026	1/1	0.81	0.93	73,73,73,73	0
56	MG	1A	3467	1/1	0.81	0.47	82,82,82,82	0
56	MG	1a	1626	1/1	0.81	0.10	82,82,82,82	0
56	MG	2A	3451	1/1	0.81	0.24	62,62,62,62	0
56	MG	2a	1637	1/1	0.81	0.18	75,75,75,75	0
56	MG	2A	3072	1/1	0.81	0.25	77,77,77,77	0
56	MG	1A	3103	1/1	0.81	0.20	73,73,73,73	0
56	MG	1A	3309	1/1	0.81	0.36	62,62,62,62	0
56	MG	1A	3548	1/1	0.81	0.83	60,60,60,60	0
56	MG	1a	1632	1/1	0.81	0.19	68,68,68,68	0
56	MG	2A	3215	1/1	0.81	1.06	57,57,57,57	0
56	MG	2A	3155	1/1	0.81	0.15	93,93,93,93	0
56	MG	1A	3374	1/1	0.81	0.36	68,68,68,68	0
56	MG	1A	3237	1/1	0.81	0.80	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3028	1/1	0.81	0.27	63,63,63,63	0
56	MG	2E	305	1/1	0.81	0.21	71,71,71,71	0
56	MG	1A	3159	1/1	0.81	0.27	68,68,68,68	0
56	MG	1A	3119	1/1	0.81	0.26	78,78,78,78	0
56	MG	1A	3292	1/1	0.81	0.78	53,53,53,53	0
56	MG	18	101	1/1	0.81	0.24	68,68,68,68	0
56	MG	1A	3121	1/1	0.81	0.46	75,75,75,75	0
56	MG	1A	3094	1/1	0.81	0.40	67,67,67,67	0
56	MG	1A	3037	1/1	0.81	0.59	53,53,53,53	0
56	MG	1a	1612	1/1	0.81	0.32	91,91,91,91	0
56	MG	2A	3394	1/1	0.81	0.23	67,67,67,67	0
56	MG	2a	1607	1/1	0.81	0.34	70,70,70,70	0
56	MG	2q	201	1/1	0.81	0.11	96,96,96,96	0
56	MG	2A	3038	1/1	0.81	0.11	87,87,87,87	0
56	MG	1A	3072	1/1	0.82	0.27	73,73,73,73	0
56	MG	1R	202	1/1	0.82	0.32	59,59,59,59	0
56	MG	1A	3145	1/1	0.82	0.45	84,84,84,84	0
56	MG	2a	1636	1/1	0.82	0.29	79,79,79,79	0
56	MG	1T	203	1/1	0.82	1.14	78,78,78,78	0
56	MG	2B	206	1/1	0.82	0.18	71,71,71,71	0
56	MG	1A	3404	1/1	0.82	0.59	50,50,50,50	0
56	MG	2D	303	1/1	0.82	0.57	61,61,61,61	0
56	MG	1a	1611	1/1	0.82	0.18	78,78,78,78	0
56	MG	2A	3146	1/1	0.82	0.28	79,79,79,79	0
56	MG	2A	3149	1/1	0.82	0.24	64,64,64,64	0
56	MG	2A	3402	1/1	0.82	0.16	73,73,73,73	0
56	MG	2a	1667	1/1	0.82	0.53	83,83,83,83	0
56	MG	1A	3450	1/1	0.82	1.34	66,66,66,66	0
56	MG	1A	3366	1/1	0.82	0.31	57,57,57,57	0
56	MG	2A	3424	1/1	0.82	0.88	81,81,81,81	0
56	MG	28	102	1/1	0.82	0.29	74,74,74,74	0
56	MG	2A	3252	1/1	0.82	0.19	79,79,79,79	0
56	MG	2A	3347	1/1	0.82	0.54	75,75,75,75	0
56	MG	1a	1685	1/1	0.82	0.34	73,73,73,73	0
56	MG	2A	3080	1/1	0.82	0.49	87,87,87,87	0
56	MG	1A	3078	1/1	0.82	0.37	64,64,64,64	0
56	MG	2a	1698	1/1	0.82	0.21	57,57,57,57	0
56	MG	2A	3450	1/1	0.82	0.25	64,64,64,64	0
56	MG	1A	3124	1/1	0.82	0.41	51,51,51,51	0
56	MG	1x	101	1/1	0.82	0.38	50,50,50,50	0
56	MG	1A	3479	1/1	0.82	0.31	62,62,62,62	0
56	MG	2A	3365	1/1	0.82	0.70	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3366	1/1	0.82	0.15	68,68,68,68	0
56	MG	2x	101	1/1	0.82	0.47	56,56,56,56	0
56	MG	2A	3470	1/1	0.82	0.13	83,83,83,83	0
56	MG	1A	3262	1/1	0.83	0.25	59,59,59,59	0
56	MG	1A	3469	1/1	0.83	0.40	61,61,61,61	0
56	MG	2A	3207	1/1	0.83	0.40	63,63,63,63	0
56	MG	2A	3158	1/1	0.83	0.21	68,68,68,68	0
56	MG	2B	207	1/1	0.83	0.31	91,91,91,91	0
56	MG	2A	3315	1/1	0.83	0.21	52,52,52,52	0
56	MG	2D	301	1/1	0.83	1.05	63,63,63,63	0
56	MG	2A	3319	1/1	0.83	0.17	61,61,61,61	0
56	MG	2E	301	1/1	0.83	0.93	69,69,69,69	0
56	MG	1a	1602	1/1	0.83	0.26	70,70,70,70	0
56	MG	1A	3134	1/1	0.83	0.25	76,76,76,76	0
56	MG	1A	3286	1/1	0.83	0.29	54,54,54,54	0
56	MG	2A	3410	1/1	0.83	0.19	78,78,78,78	0
56	MG	2R	202	1/1	0.83	0.34	54,54,54,54	0
56	MG	2A	3068	1/1	0.83	0.34	79,79,79,79	0
56	MG	2A	3418	1/1	0.83	0.35	77,77,77,77	0
56	MG	25	101	1/1	0.83	0.27	65,65,65,65	0
56	MG	1a	1654	1/1	0.83	0.20	82,82,82,82	0
56	MG	1A	3050	1/1	0.83	0.52	50,50,50,50	0
56	MG	1A	3011	1/1	0.83	0.62	84,84,84,84	0
56	MG	1A	3173	1/1	0.83	0.17	66,66,66,66	0
56	MG	1A	3359	1/1	0.83	0.31	57,57,57,57	0
56	MG	1A	3146	1/1	0.83	0.28	65,65,65,65	0
56	MG	1B	211	1/1	0.83	0.50	74,74,74,74	0
56	MG	1A	3098	1/1	0.83	0.59	77,77,77,77	0
56	MG	2c	301	1/1	0.83	0.16	94,94,94,94	0
56	MG	1A	3152	1/1	0.83	0.18	100,100,100,100	0
56	MG	1A	3049	1/1	0.83	0.33	60,60,60,60	0
56	MG	2A	3096	1/1	0.83	0.32	63,63,63,63	0
56	MG	1A	3184	1/1	0.83	0.44	54,54,54,54	0
56	MG	1A	3425	1/1	0.83	0.25	73,73,73,73	0
56	MG	2A	3302	1/1	0.83	0.43	81,81,81,81	0
56	MG	2A	3171	1/1	0.84	0.79	77,77,77,77	0
56	MG	2A	3173	1/1	0.84	0.39	70,70,70,70	0
56	MG	1A	3430	1/1	0.84	0.34	108,108,108,108	0
56	MG	1A	3143	1/1	0.84	0.22	76,76,76,76	0
56	MG	2A	3062	1/1	0.84	0.27	72,72,72,72	0
56	MG	2A	3372	1/1	0.84	0.35	73,73,73,73	0
56	MG	2A	3110	1/1	0.84	0.81	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3044	1/1	0.84	0.89	59,59,59,59	0
56	MG	1A	3030	1/1	0.84	0.45	84,84,84,84	0
56	MG	2D	302	1/1	0.84	1.20	62,62,62,62	0
56	MG	2a	1650	1/1	0.84	0.22	66,66,66,66	0
56	MG	1B	209	1/1	0.84	0.29	57,57,57,57	0
56	MG	2A	3199	1/1	0.84	0.61	72,72,72,72	0
56	MG	1A	3438	1/1	0.84	0.44	50,50,50,50	0
56	MG	2a	1666	1/1	0.84	0.53	73,73,73,73	0
56	MG	1A	3059	1/1	0.84	0.41	69,69,69,69	0
56	MG	1A	3210	1/1	0.84	0.30	54,54,54,54	0
56	MG	1a	1646	1/1	0.84	0.25	72,72,72,72	0
56	MG	2A	3407	1/1	0.84	0.23	75,75,75,75	0
56	MG	1A	3405	1/1	0.84	0.35	74,74,74,74	0
56	MG	1A	3023	1/1	0.84	0.43	57,57,57,57	0
56	MG	1A	3254	1/1	0.84	0.26	69,69,69,69	0
56	MG	2A	3423	1/1	0.84	0.24	88,88,88,88	0
56	MG	1A	3507	1/1	0.84	0.37	64,64,64,64	0
56	MG	2A	3093	1/1	0.84	0.34	71,71,71,71	0
56	MG	1A	3113	1/1	0.84	0.22	75,75,75,75	0
56	MG	1A	3320	1/1	0.84	0.44	71,71,71,71	0
56	MG	1A	3461	1/1	0.84	0.33	71,71,71,71	0
56	MG	2A	3216	1/1	0.84	0.22	64,64,64,64	0
56	MG	1A	3528	1/1	0.84	0.13	101,101,101,101	0
56	MG	1A	3020	1/1	0.84	0.21	69,69,69,69	0
56	MG	1a	1620	1/1	0.84	0.19	95,95,95,95	0
56	MG	2A	3224	1/1	0.84	0.31	74,74,74,74	0
56	MG	1A	3163	1/1	0.84	0.44	65,65,65,65	0
56	MG	1A	3079	1/1	0.84	0.63	73,73,73,73	0
56	MG	1A	3455	1/1	0.85	0.27	78,78,78,78	0
56	MG	1A	3213	1/1	0.85	0.47	71,71,71,71	0
56	MG	1A	3139	1/1	0.85	0.41	50,50,50,50	0
56	MG	2A	3090	1/1	0.85	0.40	82,82,82,82	0
56	MG	1A	3508	1/1	0.85	0.40	72,72,72,72	0
56	MG	1A	3019	1/1	0.85	0.39	81,81,81,81	0
56	MG	1A	3003	1/1	0.85	0.27	95,95,95,95	0
56	MG	2a	1640	1/1	0.85	0.43	67,67,67,67	0
56	MG	2a	1643	1/1	0.85	0.19	77,77,77,77	0
56	MG	2A	3382	1/1	0.85	0.16	70,70,70,70	0
56	MG	2A	3153	1/1	0.85	0.17	81,81,81,81	0
56	MG	1A	3194	1/1	0.85	0.45	71,71,71,71	0
56	MG	1A	3195	1/1	0.85	0.29	50,50,50,50	0
56	MG	2A	3314	1/1	0.85	0.24	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1661	1/1	0.85	0.24	67,67,67,67	0
56	MG	1A	3015	1/1	0.85	0.63	54,54,54,54	0
56	MG	2A	3040	1/1	0.85	0.24	56,56,56,56	0
56	MG	1a	1640	1/1	0.85	0.32	84,84,84,84	0
56	MG	1A	3402	1/1	0.85	0.27	53,53,53,53	0
56	MG	2A	3411	1/1	0.85	0.18	62,62,62,62	0
56	MG	1x	103	1/1	0.85	0.23	95,95,95,95	0
56	MG	2A	3417	1/1	0.85	0.17	52,52,52,52	0
56	MG	2A	3169	1/1	0.85	0.22	56,56,56,56	0
56	MG	2A	3061	1/1	0.85	0.15	87,87,87,87	0
56	MG	1A	3365	1/1	0.85	0.43	70,70,70,70	0
56	MG	2a	1688	1/1	0.85	0.24	59,59,59,59	0
56	MG	1A	3069	1/1	0.85	0.46	65,65,65,65	0
56	MG	2A	3343	1/1	0.85	0.17	67,67,67,67	0
56	MG	1A	3406	1/1	0.85	0.25	59,59,59,59	0
56	MG	1A	3290	1/1	0.85	0.39	50,50,50,50	0
56	MG	2A	3348	1/1	0.85	0.26	53,53,53,53	0
56	MG	2A	3230	1/1	0.85	0.25	56,56,56,56	0
56	MG	2A	3232	1/1	0.85	0.24	81,81,81,81	0
56	MG	1A	3370	1/1	0.85	0.38	52,52,52,52	0
56	MG	2A	3458	1/1	0.85	0.53	67,67,67,67	0
56	MG	2A	3006	1/1	0.85	0.15	86,86,86,86	0
56	MG	1a	1662	1/1	0.85	0.30	89,89,89,89	0
56	MG	1A	3024	1/1	0.85	0.44	75,75,75,75	0
56	MG	2A	3403	1/1	0.86	0.87	81,81,81,81	0
56	MG	1A	3361	1/1	0.86	0.29	70,70,70,70	0
56	MG	2A	3121	1/1	0.86	0.26	54,54,54,54	0
56	MG	2A	3408	1/1	0.86	0.20	65,65,65,65	0
56	MG	2A	3409	1/1	0.86	0.23	69,69,69,69	0
56	MG	2A	3310	1/1	0.86	0.24	50,50,50,50	0
56	MG	1A	3133	1/1	0.86	0.29	74,74,74,74	0
56	MG	1A	3287	1/1	0.86	0.19	51,51,51,51	0
56	MG	2A	3002	1/1	0.86	0.34	61,61,61,61	0
56	MG	1a	1649	1/1	0.86	0.20	66,66,66,66	0
56	MG	2A	3419	1/1	0.86	0.18	72,72,72,72	0
56	MG	1A	3466	1/1	0.86	0.28	79,79,79,79	0
56	MG	1A	3153	1/1	0.86	0.22	61,61,61,61	0
56	MG	1E	301	1/1	0.86	0.52	76,76,76,76	0
56	MG	2A	3089	1/1	0.86	0.68	78,78,78,78	0
56	MG	2A	3432	1/1	0.86	0.39	74,74,74,74	0
56	MG	1A	3435	1/1	0.86	0.31	75,75,75,75	0
56	MG	2A	3091	1/1	0.86	0.35	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3203	1/1	0.86	0.54	50,50,50,50	0
56	MG	1A	3368	1/1	0.86	0.22	76,76,76,76	0
56	MG	1A	3250	1/1	0.86	0.41	68,68,68,68	0
56	MG	2A	3159	1/1	0.86	0.15	76,76,76,76	0
56	MG	1A	3372	1/1	0.86	1.00	51,51,51,51	0
56	MG	2a	1653	1/1	0.86	0.47	51,51,51,51	0
56	MG	2A	3223	1/1	0.86	1.12	55,55,55,55	0
56	MG	1A	3148	1/1	0.86	0.29	51,51,51,51	0
56	MG	2A	3353	1/1	0.86	0.25	65,65,65,65	0
56	MG	2A	3354	1/1	0.86	0.32	82,82,82,82	0
56	MG	1A	3172	1/1	0.86	0.23	51,51,51,51	0
56	MG	1A	3481	1/1	0.86	0.48	50,50,50,50	0
56	MG	2A	3229	1/1	0.86	0.99	52,52,52,52	0
56	MG	2a	1669	1/1	0.86	0.53	74,74,74,74	0
56	MG	1a	1681	1/1	0.86	0.13	69,69,69,69	0
56	MG	2A	3359	1/1	0.86	0.23	59,59,59,59	0
56	MG	2A	3361	1/1	0.86	0.21	54,54,54,54	0
56	MG	1B	204	1/1	0.86	0.27	70,70,70,70	0
56	MG	1A	3487	1/1	0.86	0.47	69,69,69,69	0
56	MG	1d	301	1/1	0.86	0.11	96,96,96,96	0
56	MG	2A	3369	1/1	0.86	0.21	78,78,78,78	0
56	MG	2A	3241	1/1	0.86	0.31	68,68,68,68	0
56	MG	1B	208	1/1	0.86	0.43	73,73,73,73	0
56	MG	2A	3373	1/1	0.86	0.28	73,73,73,73	0
56	MG	1A	3192	1/1	0.86	0.25	64,64,64,64	0
56	MG	2A	3109	1/1	0.86	1.06	76,76,76,76	0
56	MG	2a	1705	1/1	0.86	0.26	70,70,70,70	0
56	MG	1Y	201	1/1	0.86	0.96	77,77,77,77	0
56	MG	2A	3183	1/1	0.86	0.83	53,53,53,53	0
56	MG	1A	3280	1/1	0.86	0.24	53,53,53,53	0
56	MG	2A	3272	1/1	0.86	0.29	78,78,78,78	0
56	MG	2A	3116	1/1	0.86	0.53	59,59,59,59	0
56	MG	2A	3296	1/1	0.86	0.42	89,89,89,89	0
56	MG	1A	3006	1/1	0.86	0.16	80,80,80,80	0
56	MG	1a	1616	1/1	0.87	0.14	75,75,75,75	0
56	MG	1F	301	1/1	0.87	0.21	65,65,65,65	0
56	MG	1A	3301	1/1	0.87	0.22	57,57,57,57	0
56	MG	1H	201	1/1	0.87	0.27	68,68,68,68	0
56	MG	1A	3009	1/1	0.87	0.10	85,85,85,85	0
56	MG	1A	3066	1/1	0.87	0.43	63,63,63,63	0
56	MG	2A	3217	1/1	0.87	0.34	71,71,71,71	0
56	MG	1R	201	1/1	0.87	0.49	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3078	1/1	0.87	0.11	82,82,82,82	0
56	MG	2A	3079	1/1	0.87	0.16	86,86,86,86	0
56	MG	1a	1631	1/1	0.87	0.22	70,70,70,70	0
56	MG	1A	3475	1/1	0.87	0.27	60,60,60,60	0
56	MG	1A	3537	1/1	0.87	0.10	93,93,93,93	0
56	MG	1x	106	1/1	0.87	0.18	79,79,79,79	0
56	MG	1A	3068	1/1	0.87	0.73	67,67,67,67	0
56	MG	1A	3412	1/1	0.87	0.24	75,75,75,75	0
56	MG	1a	1639	1/1	0.87	0.18	92,92,92,92	0
56	MG	1A	3447	1/1	0.87	0.75	72,72,72,72	0
56	MG	2A	3004	1/1	0.87	1.02	67,67,67,67	0
56	MG	2A	3005	1/1	0.87	0.13	68,68,68,68	0
56	MG	1A	3054	1/1	0.87	0.20	71,71,71,71	0
56	MG	1A	3484	1/1	0.87	0.24	63,63,63,63	0
56	MG	1A	3486	1/1	0.87	0.27	66,66,66,66	0
56	MG	2A	3255	1/1	0.87	0.16	62,62,62,62	0
56	MG	2A	3375	1/1	0.87	0.18	62,62,62,62	0
56	MG	2A	3175	1/1	0.87	0.42	71,71,71,71	0
56	MG	1A	3416	1/1	0.87	0.35	75,75,75,75	0
56	MG	2A	3265	1/1	0.87	0.26	51,51,51,51	0
56	MG	1A	3420	1/1	0.87	0.29	58,58,58,58	0
56	MG	1A	3057	1/1	0.87	0.25	61,61,61,61	0
56	MG	2A	3102	1/1	0.87	0.15	90,90,90,90	0
56	MG	1A	3493	1/1	0.87	0.35	50,50,50,50	0
56	MG	2R	201	1/1	0.87	0.46	55,55,55,55	0
56	MG	1A	3111	1/1	0.87	0.36	51,51,51,51	0
56	MG	2A	3188	1/1	0.87	0.23	50,50,50,50	0
56	MG	1A	3388	1/1	0.87	0.43	50,50,50,50	0
56	MG	2A	3033	1/1	0.87	0.18	63,63,63,63	0
56	MG	1a	1667	1/1	0.87	0.19	97,97,97,97	0
56	MG	1A	3428	1/1	0.87	0.60	75,75,75,75	0
56	MG	1D	302	1/1	0.87	0.39	78,78,78,78	0
56	MG	1A	3142	1/1	0.87	0.34	67,67,67,67	0
56	MG	1A	3156	1/1	0.87	0.34	51,51,51,51	0
56	MG	1A	3281	1/1	0.87	0.33	50,50,50,50	0
56	MG	2A	3415	1/1	0.87	0.21	74,74,74,74	0
56	MG	2A	3050	1/1	0.87	0.18	87,87,87,87	0
56	MG	1A	3371	1/1	0.87	0.26	55,55,55,55	0
56	MG	1A	3221	1/1	0.88	0.41	50,50,50,50	0
56	MG	1r	101	1/1	0.88	0.32	74,74,74,74	0
56	MG	1A	3108	1/1	0.88	0.30	76,76,76,76	0
56	MG	1B	206	1/1	0.88	0.29	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	1x	102	1/1	0.88	0.24	71,71,71,71	0
56	MG	1A	3122	1/1	0.88	0.22	60,60,60,60	0
56	MG	1A	3087	1/1	0.88	0.26	56,56,56,56	0
56	MG	1A	3140	1/1	0.88	0.17	67,67,67,67	0
56	MG	1A	3074	1/1	0.88	0.21	71,71,71,71	0
56	MG	1A	3353	1/1	0.88	0.19	72,72,72,72	0
56	MG	2A	3168	1/1	0.88	0.19	82,82,82,82	0
56	MG	2A	3386	1/1	0.88	0.27	66,66,66,66	0
56	MG	2A	3391	1/1	0.88	0.34	70,70,70,70	0
56	MG	1A	3092	1/1	0.88	0.31	66,66,66,66	0
56	MG	2a	1655	1/1	0.88	0.44	70,70,70,70	0
56	MG	2A	3317	1/1	0.88	0.25	57,57,57,57	0
56	MG	1a	1664	1/1	0.88	0.19	92,92,92,92	0
56	MG	1A	3116	1/1	0.88	0.89	65,65,65,65	0
56	MG	1A	3384	1/1	0.88	0.32	55,55,55,55	0
56	MG	1A	3240	1/1	0.88	0.24	60,60,60,60	0
56	MG	1a	1673	1/1	0.88	0.36	75,75,75,75	0
56	MG	1A	3314	1/1	0.88	0.51	59,59,59,59	0
56	MG	10	103	1/1	0.88	0.26	69,69,69,69	0
56	MG	1A	3533	1/1	0.88	0.18	104,104,104,104	0
56	MG	2A	3231	1/1	0.88	0.49	75,75,75,75	0
56	MG	2A	3017	1/1	0.88	0.53	80,80,80,80	0
56	MG	1A	3363	1/1	0.88	0.23	51,51,51,51	0
56	MG	20	101	1/1	0.88	0.18	64,64,64,64	0
56	MG	2A	3235	1/1	0.88	0.23	66,66,66,66	0
56	MG	1A	3317	1/1	0.88	0.37	89,89,89,89	0
56	MG	2A	3190	1/1	0.88	0.43	53,53,53,53	0
56	MG	2a	1690	1/1	0.88	0.09	84,84,84,84	0
56	MG	1a	1682	1/1	0.88	0.25	69,69,69,69	0
56	MG	18	102	1/1	0.88	0.29	56,56,56,56	0
56	MG	2A	3193	1/1	0.88	0.23	56,56,56,56	0
56	MG	2A	3427	1/1	0.88	0.29	102,102,102,102	0
56	MG	1A	3105	1/1	0.88	0.26	65,65,65,65	0
56	MG	2a	1711	1/1	0.88	0.10	87,87,87,87	0
56	MG	1A	3399	1/1	0.88	0.23	62,62,62,62	0
56	MG	2A	3147	1/1	0.88	0.64	61,61,61,61	0
56	MG	2a	1613	1/1	0.88	0.19	90,90,90,90	0
56	MG	2A	3263	1/1	0.88	0.23	54,54,54,54	0
56	MG	2A	3264	1/1	0.88	0.39	76,76,76,76	0
56	MG	2A	3445	1/1	0.88	0.23	51,51,51,51	0
56	MG	2A	3034	1/1	0.88	0.16	102,102,102,102	0
56	MG	1A	3536	1/1	0.89	0.10	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3073	1/1	0.89	0.52	50,50,50,50	0
56	MG	2A	3440	1/1	0.89	0.29	50,50,50,50	0
56	MG	2A	3074	1/1	0.89	0.43	63,63,63,63	0
56	MG	1A	3005	1/1	0.89	0.19	91,91,91,91	0
56	MG	1a	1617	1/1	0.89	0.24	87,87,87,87	0
56	MG	1A	3051	1/1	0.89	0.23	73,73,73,73	0
56	MG	2A	3195	1/1	0.89	0.85	65,65,65,65	0
56	MG	2A	3196	1/1	0.89	0.19	50,50,50,50	0
56	MG	2A	3197	1/1	0.89	1.20	87,87,87,87	0
56	MG	1A	3446	1/1	0.89	0.23	75,75,75,75	0
56	MG	2a	1641	1/1	0.89	0.28	63,63,63,63	0
56	MG	1A	3106	1/1	0.89	0.30	90,90,90,90	0
56	MG	2A	3142	1/1	0.89	0.52	65,65,65,65	0
56	MG	1A	3375	1/1	0.89	0.28	58,58,58,58	0
56	MG	2A	3015	1/1	0.89	0.15	63,63,63,63	0
56	MG	2B	201	1/1	0.89	0.14	70,70,70,70	0
56	MG	2A	3016	1/1	0.89	0.17	70,70,70,70	0
56	MG	1A	3263	1/1	0.89	0.24	64,64,64,64	0
56	MG	1A	3378	1/1	0.89	0.22	71,71,71,71	0
56	MG	1A	3052	1/1	0.89	0.53	71,71,71,71	0
56	MG	1A	3492	1/1	0.89	0.18	66,66,66,66	0
56	MG	1A	3421	1/1	0.89	0.48	67,67,67,67	0
56	MG	2A	3397	1/1	0.89	0.18	73,73,73,73	0
56	MG	1a	1634	1/1	0.89	0.29	86,86,86,86	0
56	MG	2A	3400	1/1	0.89	0.34	55,55,55,55	0
56	MG	2A	3401	1/1	0.89	0.14	87,87,87,87	0
56	MG	1A	3305	1/1	0.89	0.39	50,50,50,50	0
56	MG	1A	3084	1/1	0.89	0.18	77,77,77,77	0
56	MG	1A	3208	1/1	0.89	0.32	50,50,50,50	0
56	MG	1A	3465	1/1	0.89	0.34	63,63,63,63	0
56	MG	1A	3312	1/1	0.89	0.48	62,62,62,62	0
56	MG	1A	3513	1/1	0.89	0.33	63,63,63,63	0
56	MG	2A	3222	1/1	0.89	1.63	72,72,72,72	0
56	MG	2A	3041	1/1	0.89	0.16	76,76,76,76	0
56	MG	2a	1693	1/1	0.89	0.26	67,67,67,67	0
56	MG	2A	3412	1/1	0.89	0.45	68,68,68,68	0
56	MG	1A	3389	1/1	0.89	0.26	60,60,60,60	0
56	MG	1A	3021	1/1	0.89	0.25	81,81,81,81	0
56	MG	1A	3036	1/1	0.89	0.25	96,96,96,96	0
56	MG	1A	3013	1/1	0.89	0.26	70,70,70,70	0
56	MG	2A	3174	1/1	0.89	0.16	52,52,52,52	0
56	MG	1x	107	1/1	0.89	0.29	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3149	1/1	0.89	0.55	78,78,78,78	0
56	MG	1A	3118	1/1	0.89	0.21	63,63,63,63	0
56	MG	2A	3111	1/1	0.89	0.55	77,77,77,77	0
56	MG	2A	3428	1/1	0.89	0.23	85,85,85,85	0
56	MG	2A	3113	1/1	0.89	0.17	70,70,70,70	0
56	MG	1A	3296	1/1	0.89	0.49	80,80,80,80	0
56	MG	1Q	201	1/1	0.90	0.11	78,78,78,78	0
56	MG	1A	3526	1/1	0.90	0.16	88,88,88,88	0
56	MG	1a	1638	1/1	0.90	0.22	67,67,67,67	0
56	MG	1A	3031	1/1	0.90	0.25	81,81,81,81	0
56	MG	1A	3383	1/1	0.90	0.24	62,62,62,62	0
56	MG	2a	1620	1/1	0.90	0.14	72,72,72,72	0
56	MG	2a	1625	1/1	0.90	0.21	74,74,74,74	0
56	MG	2A	3434	1/1	0.90	0.32	79,79,79,79	0
56	MG	2A	3187	1/1	0.90	0.47	80,80,80,80	0
56	MG	2A	3436	1/1	0.90	0.19	76,76,76,76	0
56	MG	2A	3124	1/1	0.90	0.33	77,77,77,77	0
56	MG	2A	3084	1/1	0.90	0.19	56,56,56,56	0
56	MG	2a	1635	1/1	0.90	0.48	90,90,90,90	0
56	MG	2A	3129	1/1	0.90	0.12	67,67,67,67	0
56	MG	2A	3137	1/1	0.90	0.23	64,64,64,64	0
56	MG	2A	3085	1/1	0.90	0.85	73,73,73,73	0
56	MG	1a	1687	1/1	0.90	0.17	90,90,90,90	0
56	MG	1A	3109	1/1	0.90	0.23	52,52,52,52	0
56	MG	1a	1645	1/1	0.90	0.34	75,75,75,75	0
56	MG	2A	3198	1/1	0.90	0.24	75,75,75,75	0
56	MG	1A	3302	1/1	0.90	0.35	64,64,64,64	0
56	MG	1V	201	1/1	0.90	0.29	55,55,55,55	0
56	MG	1A	3303	1/1	0.90	0.40	53,53,53,53	0
56	MG	1a	1650	1/1	0.90	0.26	62,62,62,62	0
56	MG	2A	3275	1/1	0.90	0.17	61,61,61,61	0
56	MG	2A	3278	1/1	0.90	0.31	50,50,50,50	0
56	MG	2A	3282	1/1	0.90	0.20	71,71,71,71	0
56	MG	1A	3535	1/1	0.90	0.13	91,91,91,91	0
56	MG	2a	1663	1/1	0.90	0.31	50,50,50,50	0
56	MG	2A	3294	1/1	0.90	0.19	67,67,67,67	0
56	MG	2a	1665	1/1	0.90	0.42	54,54,54,54	0
56	MG	1a	1619	1/1	0.90	0.26	63,63,63,63	0
56	MG	1A	3387	1/1	0.90	0.36	65,65,65,65	0
56	MG	2A	3042	1/1	0.90	0.24	72,72,72,72	0
56	MG	1A	3110	1/1	0.90	0.26	75,75,75,75	0
56	MG	1a	1625	1/1	0.90	0.28	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1673	1/1	0.90	0.35	53,53,53,53	0
56	MG	1D	304	1/1	0.90	1.02	68,68,68,68	0
56	MG	2A	3212	1/1	0.90	0.63	64,64,64,64	0
56	MG	2a	1678	1/1	0.90	0.37	59,59,59,59	0
56	MG	2A	3053	1/1	0.90	0.60	59,59,59,59	0
56	MG	1A	3506	1/1	0.90	0.30	50,50,50,50	0
56	MG	2A	3163	1/1	0.90	0.14	66,66,66,66	0
56	MG	2Q	201	1/1	0.90	0.32	50,50,50,50	0
56	MG	1A	3081	1/1	0.90	0.25	54,54,54,54	0
56	MG	1a	1669	1/1	0.90	0.17	69,69,69,69	0
56	MG	1A	3120	1/1	0.90	0.15	88,88,88,88	0
56	MG	2a	1695	1/1	0.90	0.28	53,53,53,53	0
56	MG	2A	3325	1/1	0.90	0.43	73,73,73,73	0
56	MG	1a	1672	1/1	0.90	0.26	51,51,51,51	0
56	MG	2A	3330	1/1	0.90	0.16	80,80,80,80	0
56	MG	2a	1701	1/1	0.90	0.25	65,65,65,65	0
56	MG	2A	3071	1/1	0.90	0.30	72,72,72,72	0
56	MG	28	101	1/1	0.90	0.27	53,53,53,53	0
56	MG	2a	1709	1/1	0.90	0.10	110,110,110,110	0
56	MG	2A	3335	1/1	0.90	0.18	70,70,70,70	0
56	MG	2a	1712	1/1	0.90	0.12	100,100,100,100	0
56	MG	1A	3417	1/1	0.90	0.40	50,50,50,50	0
56	MG	1A	3463	1/1	0.90	0.47	60,60,60,60	0
56	MG	2A	3341	1/1	0.90	0.22	51,51,51,51	0
56	MG	2l	202	1/1	0.90	0.14	53,53,53,53	0
56	MG	1A	3252	1/1	0.90	0.17	71,71,71,71	0
56	MG	1A	3082	1/1	0.90	0.31	56,56,56,56	0
56	MG	2A	3227	1/1	0.90	0.38	54,54,54,54	0
56	MG	2a	1611	1/1	0.90	0.33	97,97,97,97	0
56	MG	1A	3517	1/1	0.91	0.17	72,72,72,72	0
56	MG	1A	3522	1/1	0.91	0.42	86,86,86,86	0
56	MG	2a	1626	1/1	0.91	0.24	67,67,67,67	0
56	MG	2A	3099	1/1	0.91	0.12	54,54,54,54	0
56	MG	1A	3470	1/1	0.91	0.42	53,53,53,53	0
56	MG	1A	3177	1/1	0.91	0.32	61,61,61,61	0
56	MG	1A	3398	1/1	0.91	0.18	57,57,57,57	0
56	MG	1A	3129	1/1	0.91	0.23	85,85,85,85	0
56	MG	1A	3530	1/1	0.91	0.10	98,98,98,98	0
56	MG	1A	3400	1/1	0.91	0.26	75,75,75,75	0
56	MG	1A	3180	1/1	0.91	0.13	66,66,66,66	0
56	MG	1A	3091	1/1	0.91	0.16	58,58,58,58	0
56	MG	2A	3454	1/1	0.91	0.25	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3250	1/1	0.91	0.14	88,88,88,88	0
56	MG	2A	3457	1/1	0.91	0.41	51,51,51,51	0
56	MG	1A	3288	1/1	0.91	0.25	56,56,56,56	0
56	MG	2A	3184	1/1	0.91	0.93	53,53,53,53	0
56	MG	2A	3460	1/1	0.91	0.27	59,59,59,59	0
56	MG	1a	1630	1/1	0.91	0.12	73,73,73,73	0
56	MG	1A	3480	1/1	0.91	0.32	61,61,61,61	0
56	MG	2A	3054	1/1	0.91	0.14	50,50,50,50	0
56	MG	1A	3239	1/1	0.91	0.25	65,65,65,65	0
56	MG	1A	3337	1/1	0.91	0.24	58,58,58,58	0
56	MG	1A	3164	1/1	0.91	0.47	74,74,74,74	0
56	MG	2A	3374	1/1	0.91	0.50	50,50,50,50	0
56	MG	1A	3165	1/1	0.91	0.31	52,52,52,52	0
56	MG	2A	3194	1/1	0.91	0.67	71,71,71,71	0
56	MG	1B	202	1/1	0.91	0.26	114,114,114,114	0
56	MG	2A	3070	1/1	0.91	0.21	64,64,64,64	0
56	MG	2A	3281	1/1	0.91	0.23	57,57,57,57	0
56	MG	1A	3151	1/1	0.91	0.30	84,84,84,84	0
56	MG	1A	3490	1/1	0.91	0.20	53,53,53,53	0
56	MG	2A	3390	1/1	0.91	0.14	65,65,65,65	0
56	MG	1Z	301	1/1	0.91	0.18	69,69,69,69	0
56	MG	1A	3251	1/1	0.91	0.31	53,53,53,53	0
56	MG	1A	3168	1/1	0.91	0.33	81,81,81,81	0
56	MG	2a	1679	1/1	0.91	0.38	67,67,67,67	0
56	MG	2A	3001	1/1	0.91	0.26	61,61,61,61	0
56	MG	2a	1683	1/1	0.91	0.29	53,53,53,53	0
56	MG	2A	3307	1/1	0.91	0.19	73,73,73,73	0
56	MG	10	104	1/1	0.91	0.17	99,99,99,99	0
56	MG	2a	1687	1/1	0.91	0.21	65,65,65,65	0
56	MG	2A	3309	1/1	0.91	0.30	50,50,50,50	0
56	MG	15	101	1/1	0.91	0.24	53,53,53,53	0
56	MG	16	101	1/1	0.91	0.22	83,83,83,83	0
56	MG	2a	1691	1/1	0.91	0.44	62,62,62,62	0
56	MG	1A	3457	1/1	0.91	0.24	58,58,58,58	0
56	MG	2a	1694	1/1	0.91	0.21	73,73,73,73	0
56	MG	1A	3170	1/1	0.91	0.27	73,73,73,73	0
56	MG	1A	3354	1/1	0.91	0.23	51,51,51,51	0
56	MG	2a	1697	1/1	0.91	0.20	83,83,83,83	0
56	MG	2A	3010	1/1	0.91	0.17	72,72,72,72	0
56	MG	1A	3504	1/1	0.91	0.96	54,54,54,54	0
56	MG	1A	3257	1/1	0.91	0.24	51,51,51,51	0
56	MG	2a	1702	1/1	0.91	0.28	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3095	1/1	0.91	0.94	54,54,54,54	0
56	MG	1a	1604	1/1	0.91	0.23	88,88,88,88	0
56	MG	2a	1605	1/1	0.91	0.16	86,86,86,86	0
56	MG	2a	1710	1/1	0.91	0.13	114,114,114,114	0
56	MG	2A	3326	1/1	0.91	0.24	76,76,76,76	0
56	MG	1A	3104	1/1	0.91	0.29	56,56,56,56	0
56	MG	1D	301	1/1	0.91	0.21	72,72,72,72	0
56	MG	1A	3089	1/1	0.91	0.17	53,53,53,53	0
56	MG	2f	202	1/1	0.91	0.11	84,84,84,84	0
56	MG	2A	3094	1/1	0.91	1.14	74,74,74,74	0
56	MG	1A	3265	1/1	0.91	0.13	53,53,53,53	0
56	MG	1A	3018	1/1	0.91	0.35	50,50,50,50	0
56	MG	2a	1615	1/1	0.91	0.21	71,71,71,71	0
56	MG	2A	3165	1/1	0.91	0.68	65,65,65,65	0
56	MG	2A	3166	1/1	0.91	0.19	58,58,58,58	0
56	MG	2A	3473	1/1	0.92	0.34	95,95,95,95	0
56	MG	1a	1648	1/1	0.92	0.25	54,54,54,54	0
56	MG	1A	3488	1/1	0.92	0.33	50,50,50,50	0
56	MG	1A	3016	1/1	0.92	0.30	79,79,79,79	0
56	MG	1A	3022	1/1	0.92	0.16	82,82,82,82	0
56	MG	2A	3066	1/1	0.92	0.13	76,76,76,76	0
56	MG	1a	1613	1/1	0.92	0.24	72,72,72,72	0
56	MG	2B	209	1/1	0.92	0.29	75,75,75,75	0
56	MG	1A	3230	1/1	0.92	0.16	73,73,73,73	0
56	MG	2a	1659	1/1	0.92	0.16	53,53,53,53	0
56	MG	1A	3040	1/1	0.92	0.19	68,68,68,68	0
56	MG	2a	1662	1/1	0.92	0.31	52,52,52,52	0
56	MG	2A	3176	1/1	0.92	0.14	75,75,75,75	0
56	MG	1A	3002	1/1	0.92	0.19	67,67,67,67	0
56	MG	1A	3323	1/1	0.92	0.31	54,54,54,54	0
56	MG	1A	3499	1/1	0.92	0.32	52,52,52,52	0
56	MG	2A	3180	1/1	0.92	0.14	79,79,79,79	0
56	MG	1A	3233	1/1	0.92	0.44	50,50,50,50	0
56	MG	2A	3076	1/1	0.92	0.38	67,67,67,67	0
56	MG	1A	3369	1/1	0.92	0.28	51,51,51,51	0
56	MG	2A	3336	1/1	0.92	0.37	55,55,55,55	0
56	MG	2a	1674	1/1	0.92	0.10	67,67,67,67	0
56	MG	2A	3123	1/1	0.92	0.34	83,83,83,83	0
56	MG	1a	1624	1/1	0.92	0.63	68,68,68,68	0
56	MG	1A	3234	1/1	0.92	0.31	52,52,52,52	0
56	MG	2A	3244	1/1	0.92	0.19	74,74,74,74	0
56	MG	2a	1681	1/1	0.92	0.12	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3247	1/1	0.92	0.32	50,50,50,50	0
56	MG	1A	3343	1/1	0.92	0.29	68,68,68,68	0
56	MG	2A	3421	1/1	0.92	0.38	83,83,83,83	0
56	MG	2A	3131	1/1	0.92	0.28	51,51,51,51	0
56	MG	1A	3215	1/1	0.92	0.28	65,65,65,65	0
56	MG	1A	3035	1/1	0.92	0.25	55,55,55,55	0
56	MG	2A	3019	1/1	0.92	0.30	102,102,102,102	0
56	MG	1A	3439	1/1	0.92	0.42	70,70,70,70	0
56	MG	2A	3261	1/1	0.92	0.25	50,50,50,50	0
56	MG	2a	1692	1/1	0.92	0.18	59,59,59,59	0
56	MG	1A	3266	1/1	0.92	0.22	59,59,59,59	0
56	MG	1A	3441	1/1	0.92	0.32	57,57,57,57	0
56	MG	1B	218	1/1	0.92	0.45	78,78,78,78	0
56	MG	1A	3476	1/1	0.92	0.58	54,54,54,54	0
56	MG	1A	3523	1/1	0.92	0.27	89,89,89,89	0
56	MG	1A	3274	1/1	0.92	0.19	55,55,55,55	0
56	MG	2A	3441	1/1	0.92	0.21	57,57,57,57	0
56	MG	1A	3238	1/1	0.92	0.19	80,80,80,80	0
56	MG	1A	3117	1/1	0.92	0.39	50,50,50,50	0
56	MG	1A	3448	1/1	0.92	0.43	63,63,63,63	0
56	MG	2a	1621	1/1	0.92	0.28	89,89,89,89	0
56	MG	1A	3204	1/1	0.92	0.29	50,50,50,50	0
56	MG	2A	3453	1/1	0.92	0.20	52,52,52,52	0
56	MG	2A	3284	1/1	0.92	0.16	58,58,58,58	0
56	MG	1a	1642	1/1	0.92	0.22	70,70,70,70	0
56	MG	2a	1713	1/1	0.92	0.12	64,64,64,64	0
56	MG	1a	1643	1/1	0.92	0.52	87,87,87,87	0
56	MG	2A	3045	1/1	0.92	1.12	78,78,78,78	0
56	MG	2A	3299	1/1	0.92	0.16	75,75,75,75	0
56	MG	1a	1601	1/1	0.92	0.22	56,56,56,56	0
56	MG	2A	3378	1/1	0.92	0.18	63,63,63,63	0
56	MG	1A	3356	1/1	0.92	0.27	79,79,79,79	0
56	MG	2A	3469	1/1	0.92	0.22	78,78,78,78	0
56	MG	2r	101	1/1	0.92	0.11	84,84,84,84	0
56	MG	1A	3308	1/1	0.92	0.41	82,82,82,82	0
56	MG	1A	3136	1/1	0.92	0.25	63,63,63,63	0
56	MG	1A	3436	1/1	0.93	0.23	75,75,75,75	0
56	MG	1A	3351	1/1	0.93	0.27	50,50,50,50	0
56	MG	2A	3213	1/1	0.93	0.62	83,83,83,83	0
56	MG	1A	3123	1/1	0.93	0.60	72,72,72,72	0
56	MG	2A	3148	1/1	0.93	0.22	70,70,70,70	0
56	MG	1A	3004	1/1	0.93	0.21	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3150	1/1	0.93	0.18	79,79,79,79	0
56	MG	1A	3539	1/1	0.93	0.15	77,77,77,77	0
56	MG	1A	3545	1/1	0.93	0.23	99,99,99,99	0
56	MG	1A	3001	1/1	0.93	0.09	79,79,79,79	0
56	MG	1A	3270	1/1	0.93	0.31	53,53,53,53	0
56	MG	2A	3083	1/1	0.93	0.53	57,57,57,57	0
56	MG	1A	3393	1/1	0.93	0.34	50,50,50,50	0
56	MG	1A	3358	1/1	0.93	0.30	60,60,60,60	0
56	MG	1B	203	1/1	0.93	0.35	75,75,75,75	0
56	MG	1A	3045	1/1	0.93	0.08	74,74,74,74	0
56	MG	2a	1647	1/1	0.93	0.27	81,81,81,81	0
56	MG	1A	3279	1/1	0.93	0.13	83,83,83,83	0
56	MG	1A	3307	1/1	0.93	0.29	88,88,88,88	0
56	MG	1A	3056	1/1	0.93	0.17	82,82,82,82	0
56	MG	1A	3158	1/1	0.93	0.41	69,69,69,69	0
56	MG	2A	3233	1/1	0.93	0.23	54,54,54,54	0
56	MG	1A	3364	1/1	0.93	0.20	77,77,77,77	0
56	MG	1A	3282	1/1	0.93	0.26	94,94,94,94	0
56	MG	1a	1661	1/1	0.93	0.25	74,74,74,74	0
56	MG	1B	212	1/1	0.93	0.37	79,79,79,79	0
56	MG	1A	3311	1/1	0.93	0.55	77,77,77,77	0
56	MG	2A	3468	1/1	0.93	0.23	75,75,75,75	0
56	MG	1A	3505	1/1	0.93	0.33	54,54,54,54	0
56	MG	2A	3248	1/1	0.93	0.23	71,71,71,71	0
56	MG	1a	1665	1/1	0.93	0.20	93,93,93,93	0
56	MG	2A	3362	1/1	0.93	0.10	77,77,77,77	0
56	MG	1a	1666	1/1	0.93	0.25	83,83,83,83	0
56	MG	2A	3251	1/1	0.93	0.12	85,85,85,85	0
56	MG	2A	3029	1/1	0.93	1.26	73,73,73,73	0
56	MG	2A	3368	1/1	0.93	0.21	93,93,93,93	0
56	MG	1A	3242	1/1	0.93	0.29	64,64,64,64	0
56	MG	1A	3112	1/1	0.93	0.24	65,65,65,65	0
56	MG	2a	1677	1/1	0.93	0.26	81,81,81,81	0
56	MG	2B	208	1/1	0.93	0.30	83,83,83,83	0
56	MG	2A	3258	1/1	0.93	0.16	52,52,52,52	0
56	MG	1A	3316	1/1	0.93	0.28	58,58,58,58	0
56	MG	1A	3509	1/1	0.93	0.35	56,56,56,56	0
56	MG	1A	3510	1/1	0.93	0.94	66,66,66,66	0
56	MG	1A	3131	1/1	0.93	0.42	53,53,53,53	0
56	MG	1A	3196	1/1	0.93	0.33	70,70,70,70	0
56	MG	1A	3514	1/1	0.93	0.31	68,68,68,68	0
56	MG	1E	302	1/1	0.93	0.26	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3322	1/1	0.93	0.17	71,71,71,71	0
56	MG	1A	3178	1/1	0.93	0.21	57,57,57,57	0
56	MG	2A	3277	1/1	0.93	0.12	72,72,72,72	0
56	MG	1A	3132	1/1	0.93	0.34	59,59,59,59	0
56	MG	1A	3293	1/1	0.93	0.30	71,71,71,71	0
56	MG	2A	3392	1/1	0.93	0.26	73,73,73,73	0
56	MG	2A	3051	1/1	0.93	0.14	73,73,73,73	0
56	MG	1G	201	1/1	0.93	0.09	90,90,90,90	0
56	MG	23	101	1/1	0.93	0.29	65,65,65,65	0
56	MG	1A	3338	1/1	0.93	0.54	58,58,58,58	0
56	MG	1a	1688	1/1	0.93	0.11	93,93,93,93	0
56	MG	2A	3060	1/1	0.93	0.24	71,71,71,71	0
56	MG	2A	3297	1/1	0.93	0.18	63,63,63,63	0
56	MG	1P	201	1/1	0.93	0.56	80,80,80,80	0
56	MG	2A	3301	1/1	0.93	0.31	83,83,83,83	0
56	MG	2A	3404	1/1	0.93	0.22	74,74,74,74	0
56	MG	1A	3065	1/1	0.93	0.39	75,75,75,75	0
56	MG	2A	3303	1/1	0.93	0.25	69,69,69,69	0
56	MG	2A	3304	1/1	0.93	0.22	73,73,73,73	0
56	MG	2A	3305	1/1	0.93	0.22	85,85,85,85	0
56	MG	2A	3126	1/1	0.93	0.42	80,80,80,80	0
56	MG	1l	201	1/1	0.93	0.20	64,64,64,64	0
56	MG	1A	3258	1/1	0.93	0.33	68,68,68,68	0
56	MG	1t	201	1/1	0.93	0.53	89,89,89,89	0
56	MG	1A	3382	1/1	0.93	0.14	70,70,70,70	0
56	MG	2A	3311	1/1	0.93	0.31	50,50,50,50	0
56	MG	1A	3297	1/1	0.93	0.20	62,62,62,62	0
56	MG	1A	3047	1/1	0.93	0.18	79,79,79,79	0
56	MG	1A	3166	1/1	0.93	0.14	66,66,66,66	0
57	ZN	1Y	202	1/1	0.93	0.13	138,138,138,138	0
56	MG	2a	1624	1/1	0.93	0.11	74,74,74,74	0
56	MG	1A	3380	1/1	0.94	0.28	55,55,55,55	0
56	MG	2A	3340	1/1	0.94	0.23	53,53,53,53	0
56	MG	1a	1608	1/1	0.94	0.15	78,78,78,78	0
56	MG	2a	1628	1/1	0.94	0.28	75,75,75,75	0
56	MG	1A	3244	1/1	0.94	0.27	50,50,50,50	0
56	MG	2A	3067	1/1	0.94	0.86	84,84,84,84	0
56	MG	1a	1659	1/1	0.94	0.30	68,68,68,68	0
56	MG	2A	3069	1/1	0.94	0.19	82,82,82,82	0
56	MG	1A	3155	1/1	0.94	0.49	66,66,66,66	0
56	MG	2A	3256	1/1	0.94	0.18	52,52,52,52	0
56	MG	1A	3283	1/1	0.94	0.44	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3446	1/1	0.94	0.24	59,59,59,59	0
56	MG	2A	3449	1/1	0.94	0.36	50,50,50,50	0
56	MG	1A	3541	1/1	0.94	0.15	116,116,116,116	0
56	MG	1A	3249	1/1	0.94	0.21	50,50,50,50	0
56	MG	2A	3452	1/1	0.94	0.72	103,103,103,103	0
56	MG	1A	3502	1/1	0.94	0.67	79,79,79,79	0
56	MG	1A	3071	1/1	0.94	0.24	54,54,54,54	0
56	MG	2a	1645	1/1	0.94	0.20	66,66,66,66	0
56	MG	2A	3455	1/1	0.94	0.24	61,61,61,61	0
56	MG	2a	1648	1/1	0.94	0.23	69,69,69,69	0
56	MG	1A	3062	1/1	0.94	0.27	56,56,56,56	0
56	MG	1a	1618	1/1	0.94	0.17	70,70,70,70	0
56	MG	2A	3360	1/1	0.94	0.44	76,76,76,76	0
56	MG	1A	3174	1/1	0.94	0.62	77,77,77,77	0
56	MG	2A	3267	1/1	0.94	0.25	53,53,53,53	0
56	MG	2A	3141	1/1	0.94	0.21	57,57,57,57	0
56	MG	2A	3462	1/1	0.94	0.52	66,66,66,66	0
56	MG	2a	1660	1/1	0.94	0.13	72,72,72,72	0
56	MG	1A	3253	1/1	0.94	0.21	51,51,51,51	0
56	MG	1a	1621	1/1	0.94	0.33	83,83,83,83	0
56	MG	2A	3081	1/1	0.94	0.87	54,54,54,54	0
56	MG	1A	3432	1/1	0.94	0.24	61,61,61,61	0
56	MG	1A	3315	1/1	0.94	0.27	50,50,50,50	0
56	MG	1A	3097	1/1	0.94	0.15	61,61,61,61	0
56	MG	2A	3285	1/1	0.94	0.19	55,55,55,55	0
56	MG	2A	3289	1/1	0.94	0.18	51,51,51,51	0
56	MG	2B	202	1/1	0.94	0.07	89,89,89,89	0
56	MG	2a	1670	1/1	0.94	0.19	62,62,62,62	0
56	MG	1A	3176	1/1	0.94	0.36	63,63,63,63	0
56	MG	1A	3147	1/1	0.94	0.24	50,50,50,50	0
56	MG	2A	3024	1/1	0.94	0.10	84,84,84,84	0
56	MG	2A	3152	1/1	0.94	0.19	74,74,74,74	0
56	MG	2A	3298	1/1	0.94	0.33	56,56,56,56	0
56	MG	1A	3295	1/1	0.94	0.37	59,59,59,59	0
56	MG	2A	3300	1/1	0.94	0.10	60,60,60,60	0
56	MG	1A	3063	1/1	0.94	0.26	71,71,71,71	0
56	MG	2a	1680	1/1	0.94	0.27	53,53,53,53	0
56	MG	1A	3017	1/1	0.94	0.36	77,77,77,77	0
56	MG	1A	3138	1/1	0.94	0.24	68,68,68,68	0
56	MG	1A	3181	1/1	0.94	0.36	50,50,50,50	0
56	MG	1B	215	1/1	0.94	0.36	87,87,87,87	0
56	MG	1B	216	1/1	0.94	0.37	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3395	1/1	0.94	0.10	81,81,81,81	0
56	MG	1A	3339	1/1	0.94	0.19	66,66,66,66	0
56	MG	1A	3525	1/1	0.94	0.11	81,81,81,81	0
56	MG	1A	3101	1/1	0.94	0.23	95,95,95,95	0
56	MG	1A	3527	1/1	0.94	0.14	52,52,52,52	0
56	MG	2A	3044	1/1	0.94	0.45	77,77,77,77	0
56	MG	1A	3102	1/1	0.94	0.21	56,56,56,56	0
56	MG	1A	3041	1/1	0.94	0.31	66,66,66,66	0
56	MG	2A	3405	1/1	0.94	1.22	71,71,71,71	0
56	MG	2A	3047	1/1	0.94	0.42	63,63,63,63	0
56	MG	2A	3048	1/1	0.94	0.21	85,85,85,85	0
56	MG	2A	3316	1/1	0.94	0.15	50,50,50,50	0
56	MG	1A	3347	1/1	0.94	0.33	57,57,57,57	0
56	MG	2a	1700	1/1	0.94	0.19	50,50,50,50	0
56	MG	2A	3318	1/1	0.94	0.18	50,50,50,50	0
56	MG	1A	3169	1/1	0.94	0.47	64,64,64,64	0
56	MG	1A	3349	1/1	0.94	0.22	65,65,65,65	0
56	MG	1a	1603	1/1	0.94	0.12	110,110,110,110	0
56	MG	2a	1707	1/1	0.94	0.09	114,114,114,114	0
56	MG	2A	3323	1/1	0.94	0.47	64,64,64,64	0
56	MG	2A	3108	1/1	0.94	0.28	107,107,107,107	0
56	MG	2A	3236	1/1	0.94	0.18	55,55,55,55	0
56	MG	2a	1609	1/1	0.94	0.23	74,74,74,74	0
56	MG	2a	1610	1/1	0.94	0.14	82,82,82,82	0
56	MG	1A	3154	1/1	0.94	0.18	58,58,58,58	0
56	MG	2A	3059	1/1	0.94	0.28	62,62,62,62	0
56	MG	2A	3422	1/1	0.94	0.36	51,51,51,51	0
56	MG	2A	3332	1/1	0.94	0.20	50,50,50,50	0
56	MG	1a	1605	1/1	0.94	0.07	117,117,117,117	0
56	MG	2A	3245	1/1	0.94	0.40	50,50,50,50	0
56	MG	2a	1618	1/1	0.94	0.06	89,89,89,89	0
56	MG	2A	3426	1/1	0.94	0.53	88,88,88,88	0
56	MG	2A	3246	1/1	0.94	0.30	69,69,69,69	0
56	MG	1a	1606	1/1	0.94	0.20	81,81,81,81	0
57	ZN	14	501	1/1	0.94	0.10	157,157,157,157	0
56	MG	2a	1623	1/1	0.94	0.37	84,84,84,84	0
56	MG	1A	3444	1/1	0.95	0.22	51,51,51,51	0
56	MG	1a	1678	1/1	0.95	0.15	109,109,109,109	0
56	MG	1A	3408	1/1	0.95	0.32	72,72,72,72	0
56	MG	2a	1646	1/1	0.95	0.22	79,79,79,79	0
56	MG	2A	3389	1/1	0.95	0.13	71,71,71,71	0
56	MG	1A	3209	1/1	0.95	0.20	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3538	1/1	0.95	0.36	73,73,73,73	0
56	MG	1T	201	1/1	0.95	0.15	99,99,99,99	0
56	MG	2a	1651	1/1	0.95	0.16	83,83,83,83	0
56	MG	1A	3241	1/1	0.95	0.28	52,52,52,52	0
56	MG	2a	1654	1/1	0.95	0.43	53,53,53,53	0
56	MG	1A	3061	1/1	0.95	0.37	57,57,57,57	0
56	MG	1A	3542	1/1	0.95	0.11	98,98,98,98	0
56	MG	2B	205	1/1	0.95	0.39	50,50,50,50	0
56	MG	1a	1689	1/1	0.95	0.07	109,109,109,109	0
56	MG	2A	3398	1/1	0.95	0.12	66,66,66,66	0
56	MG	1A	3291	1/1	0.95	0.18	50,50,50,50	0
56	MG	1A	3415	1/1	0.95	0.21	71,71,71,71	0
56	MG	1A	3227	1/1	0.95	0.60	51,51,51,51	0
56	MG	1A	3453	1/1	0.95	0.30	60,60,60,60	0
56	MG	2A	3243	1/1	0.95	0.25	62,62,62,62	0
56	MG	1A	3496	1/1	0.95	0.38	51,51,51,51	0
56	MG	1A	3212	1/1	0.95	0.23	50,50,50,50	0
56	MG	1A	3500	1/1	0.95	0.21	50,50,50,50	0
56	MG	2E	304	1/1	0.95	0.13	61,61,61,61	0
56	MG	2A	3112	1/1	0.95	0.29	84,84,84,84	0
56	MG	1A	3418	1/1	0.95	0.29	57,57,57,57	0
56	MG	1A	3419	1/1	0.95	0.26	62,62,62,62	0
56	MG	1a	1641	1/1	0.95	0.29	67,67,67,67	0
56	MG	2A	3063	1/1	0.95	0.11	61,61,61,61	0
56	MG	2A	3118	1/1	0.95	0.20	66,66,66,66	0
56	MG	2A	3334	1/1	0.95	0.51	71,71,71,71	0
56	MG	2A	3253	1/1	0.95	0.25	54,54,54,54	0
56	MG	2A	3416	1/1	0.95	0.40	100,100,100,100	0
56	MG	1B	207	1/1	0.95	0.38	77,77,77,77	0
56	MG	1A	3459	1/1	0.95	0.28	50,50,50,50	0
56	MG	1A	3269	1/1	0.95	0.30	89,89,89,89	0
56	MG	1A	3246	1/1	0.95	0.41	50,50,50,50	0
56	MG	1A	3272	1/1	0.95	0.33	50,50,50,50	0
56	MG	1A	3273	1/1	0.95	0.17	53,53,53,53	0
56	MG	1A	3014	1/1	0.95	0.25	52,52,52,52	0
56	MG	1A	3277	1/1	0.95	0.27	83,83,83,83	0
56	MG	2a	1604	1/1	0.95	0.12	83,83,83,83	0
56	MG	1A	3327	1/1	0.95	0.14	56,56,56,56	0
56	MG	2A	3136	1/1	0.95	0.26	50,50,50,50	0
56	MG	1a	1651	1/1	0.95	0.19	50,50,50,50	0
56	MG	1A	3468	1/1	0.95	0.27	69,69,69,69	0
56	MG	2A	3268	1/1	0.95	0.41	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3332	1/1	0.95	0.18	55,55,55,55	0
56	MG	2A	3274	1/1	0.95	0.20	57,57,57,57	0
56	MG	1a	1658	1/1	0.95	0.21	92,92,92,92	0
56	MG	1A	3067	1/1	0.95	0.27	65,65,65,65	0
56	MG	2A	3439	1/1	0.95	0.25	56,56,56,56	0
56	MG	1A	3336	1/1	0.95	0.41	50,50,50,50	0
56	MG	1A	3519	1/1	0.95	0.16	73,73,73,73	0
56	MG	1A	3520	1/1	0.95	0.21	63,63,63,63	0
56	MG	1A	3073	1/1	0.95	0.55	60,60,60,60	0
56	MG	2a	1704	1/1	0.95	0.23	65,65,65,65	0
56	MG	2A	3209	1/1	0.95	0.97	62,62,62,62	0
56	MG	2A	3286	1/1	0.95	0.54	51,51,51,51	0
56	MG	2a	1708	1/1	0.95	0.24	110,110,110,110	0
56	MG	1A	3434	1/1	0.95	0.26	54,54,54,54	0
56	MG	1A	3007	1/1	0.95	0.20	65,65,65,65	0
56	MG	1A	3032	1/1	0.95	0.11	69,69,69,69	0
56	MG	2A	3370	1/1	0.95	0.23	89,89,89,89	0
56	MG	1A	3341	1/1	0.95	0.23	50,50,50,50	0
56	MG	1A	3219	1/1	0.95	0.33	64,64,64,64	0
56	MG	1A	3160	1/1	0.95	0.23	56,56,56,56	0
56	MG	2f	201	1/1	0.95	0.21	75,75,75,75	0
56	MG	2A	3027	1/1	0.95	0.11	82,82,82,82	0
56	MG	1A	3306	1/1	0.95	0.19	50,50,50,50	0
56	MG	1A	3193	1/1	0.95	0.18	64,64,64,64	0
56	MG	1A	3482	1/1	0.95	0.33	55,55,55,55	0
56	MG	1A	3483	1/1	0.95	0.22	50,50,50,50	0
56	MG	2A	3379	1/1	0.95	0.32	78,78,78,78	0
56	MG	2A	3463	1/1	0.95	0.04	115,115,115,115	0
56	MG	2A	3464	1/1	0.95	0.12	81,81,81,81	0
56	MG	2A	3465	1/1	0.95	0.12	81,81,81,81	0
57	ZN	1n	501	1/1	0.95	0.11	140,140,140,140	0
56	MG	1A	3442	1/1	0.95	0.35	56,56,56,56	0
56	MG	2A	3032	1/1	0.96	0.12	75,75,75,75	0
56	MG	2A	3383	1/1	0.96	0.08	64,64,64,64	0
56	MG	2A	3471	1/1	0.96	0.18	75,75,75,75	0
56	MG	1A	3200	1/1	0.96	0.32	51,51,51,51	0
56	MG	2A	3221	1/1	0.96	0.19	73,73,73,73	0
56	MG	2A	3157	1/1	0.96	0.19	65,65,65,65	0
56	MG	1A	3544	1/1	0.96	0.17	62,62,62,62	0
56	MG	1A	3497	1/1	0.96	0.28	58,58,58,58	0
56	MG	2A	3037	1/1	0.96	0.18	79,79,79,79	0
56	MG	1A	3498	1/1	0.96	0.38	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1656	1/1	0.96	0.16	81,81,81,81	0
56	MG	1A	3379	1/1	0.96	0.19	59,59,59,59	0
56	MG	1A	3458	1/1	0.96	0.24	59,59,59,59	0
56	MG	1a	1686	1/1	0.96	0.42	50,50,50,50	0
56	MG	1A	3201	1/1	0.96	0.28	50,50,50,50	0
56	MG	1A	3284	1/1	0.96	0.20	73,73,73,73	0
56	MG	1A	3225	1/1	0.96	0.28	80,80,80,80	0
56	MG	1A	3423	1/1	0.96	0.22	50,50,50,50	0
56	MG	1a	1637	1/1	0.96	0.19	71,71,71,71	0
56	MG	1A	3126	1/1	0.96	0.29	55,55,55,55	0
56	MG	2A	3238	1/1	0.96	0.13	77,77,77,77	0
56	MG	2A	3172	1/1	0.96	0.22	72,72,72,72	0
56	MG	1A	3426	1/1	0.96	0.19	90,90,90,90	0
56	MG	1A	3010	1/1	0.96	0.21	88,88,88,88	0
56	MG	2A	3324	1/1	0.96	0.18	73,73,73,73	0
56	MG	1A	3256	1/1	0.96	0.28	50,50,50,50	0
56	MG	1A	3355	1/1	0.96	0.29	53,53,53,53	0
56	MG	1A	3289	1/1	0.96	0.40	50,50,50,50	0
56	MG	2A	3328	1/1	0.96	0.15	52,52,52,52	0
56	MG	1A	3357	1/1	0.96	0.07	112,112,112,112	0
56	MG	1A	3187	1/1	0.96	0.34	80,80,80,80	0
56	MG	1A	3207	1/1	0.96	0.26	51,51,51,51	0
56	MG	21	101	1/1	0.96	0.20	56,56,56,56	0
56	MG	2A	3114	1/1	0.96	0.09	77,77,77,77	0
56	MG	1A	3516	1/1	0.96	0.18	79,79,79,79	0
56	MG	1A	3392	1/1	0.96	0.22	54,54,54,54	0
56	MG	2A	3185	1/1	0.96	0.15	72,72,72,72	0
56	MG	1A	3518	1/1	0.96	0.16	71,71,71,71	0
56	MG	1A	3318	1/1	0.96	0.27	50,50,50,50	0
56	MG	2a	1686	1/1	0.96	0.20	70,70,70,70	0
56	MG	1A	3080	1/1	0.96	0.14	76,76,76,76	0
56	MG	1A	3162	1/1	0.96	0.21	55,55,55,55	0
56	MG	1A	3033	1/1	0.96	0.25	84,84,84,84	0
56	MG	2A	3344	1/1	0.96	0.21	64,64,64,64	0
56	MG	1a	1657	1/1	0.96	0.19	72,72,72,72	0
56	MG	1A	3211	1/1	0.96	0.27	50,50,50,50	0
56	MG	1A	3038	1/1	0.96	0.29	80,80,80,80	0
56	MG	1a	1610	1/1	0.96	0.20	68,68,68,68	0
56	MG	2A	3351	1/1	0.96	0.26	73,73,73,73	0
56	MG	2A	3128	1/1	0.96	0.19	88,88,88,88	0
56	MG	2A	3437	1/1	0.96	0.19	51,51,51,51	0
56	MG	1A	3268	1/1	0.96	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3141	1/1	0.96	1.08	89,89,89,89	0
56	MG	2A	3135	1/1	0.96	0.17	92,92,92,92	0
56	MG	2A	3012	1/1	0.96	0.20	72,72,72,72	0
56	MG	2a	1617	1/1	0.96	0.12	81,81,81,81	0
56	MG	1A	3076	1/1	0.96	0.13	75,75,75,75	0
56	MG	2A	3444	1/1	0.96	0.27	50,50,50,50	0
56	MG	1A	3029	1/1	0.96	0.09	94,94,94,94	0
56	MG	2a	1706	1/1	0.96	0.25	62,62,62,62	0
56	MG	1A	3144	1/1	0.96	0.30	84,84,84,84	0
56	MG	1A	3217	1/1	0.96	0.34	98,98,98,98	0
56	MG	1A	3342	1/1	0.96	0.21	58,58,58,58	0
56	MG	1A	3413	1/1	0.96	0.12	79,79,79,79	0
56	MG	2A	3283	1/1	0.96	0.14	50,50,50,50	0
56	MG	1A	3046	1/1	0.96	0.19	56,56,56,56	0
56	MG	2A	3367	1/1	0.96	0.19	68,68,68,68	0
56	MG	2A	3145	1/1	0.96	0.14	82,82,82,82	0
56	MG	1A	3198	1/1	0.96	0.21	50,50,50,50	0
56	MG	1A	3125	1/1	0.96	0.30	51,51,51,51	0
56	MG	2A	3211	1/1	0.96	0.22	60,60,60,60	0
56	MG	2A	3291	1/1	0.96	0.15	50,50,50,50	0
56	MG	2A	3293	1/1	0.96	0.16	51,51,51,51	0
56	MG	1A	3454	1/1	0.96	0.26	50,50,50,50	0
56	MG	2A	3025	1/1	0.96	0.17	92,92,92,92	0
56	MG	1A	3222	1/1	0.96	0.17	68,68,68,68	0
56	MG	2A	3028	1/1	0.96	0.13	86,86,86,86	0
56	MG	1A	3540	1/1	0.96	0.17	91,91,91,91	0
56	MG	2a	1642	1/1	0.96	0.30	68,68,68,68	0
57	ZN	16	102	1/1	0.96	0.16	91,91,91,91	0
56	MG	1A	3495	1/1	0.96	0.33	50,50,50,50	0
57	ZN	2Y	501	1/1	0.96	0.10	166,166,166,166	0
56	MG	2A	3154	1/1	0.96	0.11	76,76,76,76	0
57	ZN	29	501	1/1	0.96	0.09	96,96,96,96	0
56	MG	1A	3534	1/1	0.97	0.07	89,89,89,89	0
56	MG	2A	3270	1/1	0.97	0.27	66,66,66,66	0
56	MG	2A	3271	1/1	0.97	0.14	58,58,58,58	0
56	MG	1A	3326	1/1	0.97	0.30	54,54,54,54	0
56	MG	2A	3413	1/1	0.97	0.25	50,50,50,50	0
56	MG	2A	3273	1/1	0.97	0.14	56,56,56,56	0
56	MG	2E	303	1/1	0.97	0.14	50,50,50,50	0
56	MG	1A	3275	1/1	0.97	0.29	54,54,54,54	0
56	MG	2A	3064	1/1	0.97	0.10	78,78,78,78	0
56	MG	2A	3276	1/1	0.97	0.15	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3346	1/1	0.97	0.15	50,50,50,50	0
56	MG	2A	3014	1/1	0.97	0.19	107,107,107,107	0
56	MG	1A	3328	1/1	0.97	0.28	81,81,81,81	0
56	MG	1A	3443	1/1	0.97	0.12	65,65,65,65	0
56	MG	1A	3330	1/1	0.97	0.29	65,65,65,65	0
56	MG	2A	3352	1/1	0.97	0.29	67,67,67,67	0
56	MG	1a	1680	1/1	0.97	0.18	62,62,62,62	0
56	MG	2A	3167	1/1	0.97	0.14	77,77,77,77	0
56	MG	1A	3331	1/1	0.97	0.19	54,54,54,54	0
56	MG	2A	3020	1/1	0.97	0.09	93,93,93,93	0
56	MG	2A	3429	1/1	0.97	0.20	60,60,60,60	0
56	MG	2A	3430	1/1	0.97	0.34	59,59,59,59	0
56	MG	1A	3088	1/1	0.97	0.28	96,96,96,96	0
56	MG	1A	3278	1/1	0.97	0.23	66,66,66,66	0
56	MG	2A	3433	1/1	0.97	0.22	66,66,66,66	0
56	MG	2A	3119	1/1	0.97	0.13	86,86,86,86	0
56	MG	2A	3292	1/1	0.97	0.16	52,52,52,52	0
56	MG	1a	1684	1/1	0.97	0.16	82,82,82,82	0
56	MG	1A	3543	1/1	0.97	0.20	75,75,75,75	0
56	MG	1A	3334	1/1	0.97	0.13	77,77,77,77	0
56	MG	2A	3228	1/1	0.97	0.13	78,78,78,78	0
56	MG	1A	3055	1/1	0.97	0.27	86,86,86,86	0
56	MG	1A	3546	1/1	0.97	0.17	54,54,54,54	0
56	MG	1A	3512	1/1	0.97	0.27	60,60,60,60	0
56	MG	1A	3247	1/1	0.97	0.19	62,62,62,62	0
56	MG	2A	3127	1/1	0.97	0.19	68,68,68,68	0
56	MG	2A	3181	1/1	0.97	0.20	65,65,65,65	0
56	MG	2A	3447	1/1	0.97	0.16	53,53,53,53	0
56	MG	1A	3186	1/1	0.97	0.34	50,50,50,50	0
56	MG	1A	3264	1/1	0.97	0.19	58,58,58,58	0
56	MG	2A	3130	1/1	0.97	0.14	76,76,76,76	0
56	MG	2A	3239	1/1	0.97	0.12	64,64,64,64	0
56	MG	1A	3391	1/1	0.97	0.18	62,62,62,62	0
56	MG	2A	3133	1/1	0.97	0.12	76,76,76,76	0
56	MG	1A	3485	1/1	0.97	0.32	50,50,50,50	0
56	MG	1A	3313	1/1	0.97	0.33	68,68,68,68	0
56	MG	2A	3189	1/1	0.97	0.81	50,50,50,50	0
56	MG	1a	1653	1/1	0.97	0.30	61,61,61,61	0
56	MG	2a	1627	1/1	0.97	0.31	82,82,82,82	0
56	MG	1A	3157	1/1	0.97	0.16	77,77,77,77	0
56	MG	1A	3394	1/1	0.97	0.40	50,50,50,50	0
56	MG	2A	3385	1/1	0.97	0.16	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3039	1/1	0.97	0.12	82,82,82,82	0
56	MG	2A	3387	1/1	0.97	0.21	50,50,50,50	0
56	MG	1A	3197	1/1	0.97	0.21	53,53,53,53	0
56	MG	1A	3228	1/1	0.97	0.17	54,54,54,54	0
56	MG	2A	3466	1/1	0.97	0.21	71,71,71,71	0
56	MG	1a	1622	1/1	0.97	0.09	99,99,99,99	0
56	MG	1A	3115	1/1	0.97	0.56	51,51,51,51	0
56	MG	1A	3462	1/1	0.97	0.42	50,50,50,50	0
56	MG	2A	3322	1/1	0.97	0.17	50,50,50,50	0
56	MG	1A	3319	1/1	0.97	0.31	50,50,50,50	0
56	MG	10	101	1/1	0.97	0.23	51,51,51,51	0
56	MG	2A	3257	1/1	0.97	0.32	50,50,50,50	0
56	MG	1A	3255	1/1	0.97	0.33	50,50,50,50	0
56	MG	1A	3321	1/1	0.97	0.27	87,87,87,87	0
56	MG	2A	3052	1/1	0.97	0.14	80,80,80,80	0
56	MG	2A	3329	1/1	0.97	0.13	61,61,61,61	0
56	MG	1A	3099	1/1	0.97	0.15	64,64,64,64	0
56	MG	1A	3042	1/1	0.97	0.50	80,80,80,80	0
56	MG	2A	3057	1/1	0.97	0.20	90,90,90,90	0
56	MG	2A	3007	1/1	0.97	0.12	82,82,82,82	0
56	MG	2a	1652	1/1	0.97	0.08	69,69,69,69	0
56	MG	1A	3377	1/1	0.97	0.17	50,50,50,50	0
57	ZN	25	102	1/1	0.97	0.20	81,81,81,81	0
57	ZN	26	501	1/1	0.97	0.13	111,111,111,111	0
56	MG	1A	3325	1/1	0.97	0.27	63,63,63,63	0
57	ZN	2n	102	1/1	0.97	0.13	120,120,120,120	0
58	SF4	1d	302	8/8	0.97	0.15	107,123,153,161	0
56	MG	1a	1656	1/1	0.98	0.21	68,68,68,68	0
56	MG	2A	3134	1/1	0.98	0.15	58,58,58,58	0
56	MG	2A	3331	1/1	0.98	0.14	54,54,54,54	0
56	MG	2a	1631	1/1	0.98	0.13	81,81,81,81	0
56	MG	2A	3287	1/1	0.98	0.27	51,51,51,51	0
56	MG	2A	3288	1/1	0.98	0.26	55,55,55,55	0
56	MG	1A	3107	1/1	0.98	0.17	69,69,69,69	0
56	MG	2A	3035	1/1	0.98	0.27	92,92,92,92	0
56	MG	1A	3329	1/1	0.98	0.49	52,52,52,52	0
56	MG	1A	3401	1/1	0.98	0.35	79,79,79,79	0
56	MG	2A	3139	1/1	0.98	0.13	51,51,51,51	0
56	MG	2A	3388	1/1	0.98	0.24	50,50,50,50	0
56	MG	2A	3339	1/1	0.98	0.15	52,52,52,52	0
56	MG	2A	3008	1/1	0.98	0.25	71,71,71,71	0
56	MG	2A	3295	1/1	0.98	0.25	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3503	1/1	0.98	0.12	71,71,71,71	0
56	MG	1A	3267	1/1	0.98	0.28	54,54,54,54	0
56	MG	1A	3403	1/1	0.98	0.50	50,50,50,50	0
56	MG	1A	3424	1/1	0.98	0.26	58,58,58,58	0
56	MG	2A	3396	1/1	0.98	0.05	96,96,96,96	0
56	MG	1A	3202	1/1	0.98	0.35	52,52,52,52	0
56	MG	1A	3345	1/1	0.98	0.25	52,52,52,52	0
56	MG	1A	3260	1/1	0.98	0.30	50,50,50,50	0
56	MG	2A	3349	1/1	0.98	0.19	55,55,55,55	0
56	MG	1A	3261	1/1	0.98	0.17	60,60,60,60	0
56	MG	2A	3259	1/1	0.98	0.14	50,50,50,50	0
56	MG	1A	3248	1/1	0.98	0.43	52,52,52,52	0
56	MG	1A	3335	1/1	0.98	0.14	55,55,55,55	0
56	MG	2A	3049	1/1	0.98	0.17	90,90,90,90	0
56	MG	1a	1670	1/1	0.98	0.13	73,73,73,73	0
56	MG	1A	3243	1/1	0.98	0.27	50,50,50,50	0
56	MG	1A	3471	1/1	0.98	0.31	98,98,98,98	0
56	MG	1A	3235	1/1	0.98	0.16	60,60,60,60	0
56	MG	1A	3452	1/1	0.98	0.42	51,51,51,51	0
56	MG	2A	3055	1/1	0.98	0.14	67,67,67,67	0
56	MG	2A	3269	1/1	0.98	0.26	73,73,73,73	0
56	MG	2A	3056	1/1	0.98	0.17	88,88,88,88	0
56	MG	2A	3363	1/1	0.98	0.13	66,66,66,66	0
56	MG	1A	3229	1/1	0.98	0.16	62,62,62,62	0
56	MG	1A	3276	1/1	0.98	0.20	51,51,51,51	0
56	MG	2A	3026	1/1	0.98	0.30	69,69,69,69	0
56	MG	1a	1677	1/1	0.98	0.19	108,108,108,108	0
56	MG	1A	3396	1/1	0.98	0.21	64,64,64,64	0
56	MG	2A	3420	1/1	0.98	0.14	50,50,50,50	0
56	MG	1A	3397	1/1	0.98	0.20	67,67,67,67	0
56	MG	2A	3237	1/1	0.98	0.19	67,67,67,67	0
56	MG	2A	3030	1/1	0.98	0.10	92,92,92,92	0
56	MG	2a	1622	1/1	0.98	0.15	79,79,79,79	0
56	MG	2A	3280	1/1	0.98	0.22	50,50,50,50	0
56	MG	1A	3521	1/1	0.98	0.19	63,63,63,63	0
56	MG	1A	3340	1/1	0.98	0.26	50,50,50,50	0
56	MG	2A	3132	1/1	0.98	0.13	80,80,80,80	0
56	MG	2A	3242	1/1	0.98	0.11	63,63,63,63	0
56	MG	2a	1671	1/1	0.99	0.11	64,64,64,64	0
56	MG	1A	3034	1/1	0.99	0.14	90,90,90,90	0
56	MG	2A	3443	1/1	0.99	0.24	50,50,50,50	0
56	MG	1a	1655	1/1	0.99	0.22	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3411	1/1	0.99	0.26	57,57,57,57	0
56	MG	2A	3380	1/1	0.99	0.19	61,61,61,61	0
56	MG	1A	3135	1/1	0.99	0.14	100,100,100,100	0
57	ZN	15	102	1/1	0.99	0.18	91,91,91,91	0
56	MG	2A	3448	1/1	0.99	0.27	59,59,59,59	0
57	ZN	19	102	1/1	0.99	0.20	98,98,98,98	0
56	MG	1A	3025	1/1	0.99	0.20	70,70,70,70	0
56	MG	1A	3324	1/1	0.99	0.24	54,54,54,54	0
56	MG	1A	3220	1/1	0.99	0.24	51,51,51,51	0
56	MG	1A	3205	1/1	0.99	0.19	69,69,69,69	0
56	MG	1A	3407	1/1	0.99	0.32	61,61,61,61	0
56	MG	1A	3185	1/1	0.99	0.20	51,51,51,51	0
56	MG	2A	3279	1/1	0.99	0.14	63,63,63,63	0
56	MG	1A	3271	1/1	0.99	0.16	78,78,78,78	0
58	SF4	2d	302	8/8	0.99	0.16	90,106,116,116	0

6.5 Other polymers (i)

There are no such residues in this entry.