



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 07:32 AM EDT

PDB ID : 6ORD / pdb_00006ord
Title : Crystal structure of tRNA^{Ala}(GGC) U32-A38 bound to cognate 70S A site
Authors : Nguyen, H.A.; Sunita, S.; Dunham, C.M.
Deposited on : 2019-04-30
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

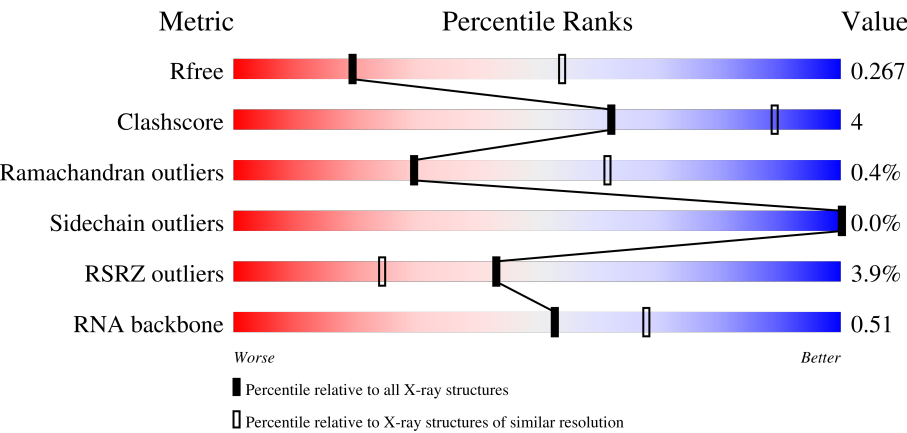
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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 $\leq 5\%$. 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	QA	1522	70%25% . .
1	XA	1522	70%26% . .
2	QB	256	5%68%20% . 10%
2	XB	256	3%73%17% . 10%

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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	

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Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	19	
23	XX	19	
24	QY	76	
24	XY	76	
25	R0	85	
25	Y0	85	
26	R1	98	
26	Y1	98	
27	R2	72	
27	Y2	72	

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Mol	Chain	Length	Quality of chain
28	R3	60	
28	Y3	60	
29	R4	71	
29	Y4	71	
30	R5	60	
30	Y5	60	
31	R6	54	
31	Y6	54	
32	R7	49	
32	Y7	49	
33	R8	65	
33	Y8	65	
34	R9	37	
34	Y9	37	
35	RA	2915	
35	YA	2915	
36	RB	122	
36	YB	122	
37	RD	276	
37	YD	276	
38	RE	206	
38	YE	206	
39	RF	210	
39	YF	210	
40	RG	182	

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Mol	Chain	Length	Quality of chain
40	YG	182	
41	RH	180	
41	YH	180	
42	RI	148	
42	YI	148	
43	RN	140	
43	YN	140	
44	RO	122	
44	YO	122	
45	RP	150	
45	YP	150	
46	RQ	141	
46	YQ	141	
47	RR	118	
47	YR	118	
48	RS	112	
48	YS	112	
49	RT	146	
49	YT	146	
50	RU	118	
50	YU	118	
51	RV	101	
51	YV	101	
52	RW	113	
52	YW	113	

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Mol	Chain	Length	Quality of chain
53	RX	96	
53	YX	96	
54	RY	110	
54	YY	110	
55	RZ	206	
55	YZ	206	

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	QA	1703	-	-	-	X
56	MG	QA	1795	-	-	-	X
56	MG	QO	101	-	-	-	X
56	MG	RA	3011	-	-	-	X
56	MG	RA	3027	-	-	-	X
56	MG	RA	3053	-	-	-	X
56	MG	RA	3063	-	-	-	X
56	MG	RA	3069	-	-	-	X
56	MG	RA	3072	-	-	-	X
56	MG	RA	3080	-	-	-	X
56	MG	RA	3104	-	-	-	X
56	MG	RA	3152	-	-	-	X
56	MG	RA	3153	-	-	-	X
56	MG	RA	3159	-	-	-	X
56	MG	RA	3173	-	-	-	X
56	MG	RA	3175	-	-	-	X
56	MG	RA	3192	-	-	-	X
56	MG	RA	3201	-	-	-	X
56	MG	RA	3205	-	-	-	X
56	MG	RA	3221	-	-	-	X
56	MG	RA	3256	-	-	-	X
56	MG	RA	3269	-	-	-	X
56	MG	RA	3311	-	-	-	X
56	MG	RA	3322	-	-	-	X
56	MG	RA	3350	-	-	-	X
56	MG	RA	3363	-	-	-	X
56	MG	RA	3381	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3383	-	-	-	X
56	MG	RA	3395	-	-	-	X
56	MG	RA	3401	-	-	-	X
56	MG	RA	3416	-	-	-	X
56	MG	RA	3417	-	-	-	X
56	MG	RA	3424	-	-	-	X
56	MG	RA	3450	-	-	-	X
56	MG	RA	3460	-	-	-	X
56	MG	RA	3469	-	-	-	X
56	MG	RA	3482	-	-	-	X
56	MG	RA	3499	-	-	-	X
56	MG	RA	3511	-	-	-	X
56	MG	RA	3514	-	-	-	X
56	MG	RA	3526	-	-	-	X
56	MG	RA	3591	-	-	-	X
56	MG	RA	3641	-	-	-	X
56	MG	RA	3647	-	-	-	X
56	MG	RA	3654	-	-	-	X
56	MG	RA	3673	-	-	-	X
56	MG	XA	1718	-	-	-	X
56	MG	XA	1778	-	-	-	X
56	MG	YA	3066	-	-	-	X
56	MG	YA	3119	-	-	-	X
56	MG	YA	3201	-	-	-	X
56	MG	YA	3400	-	-	-	X
56	MG	YA	3412	-	-	-	X
56	MG	YA	3478	-	-	-	X
56	MG	YA	3499	-	-	-	X
56	MG	YA	3512	-	-	-	X
56	MG	YA	3547	-	-	-	X
56	MG	YA	3697	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 293819 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
1	XA	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
2	XB	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	QC	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
3	XC	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	QD	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
4	XD	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
5	XE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	QF	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
6	XF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	QG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
7	XG	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
8	XH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	QI	127	Total	C	N	O		0	0	0
			986	625	193	168				
9	XI	126	Total	C	N	O		0	0	0
			966	613	186	167				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	QJ	97	Total	C	N	O		0	0	0
			719	446	142	131				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	XJ	96	Total	C	N	O			
			710	442	137	131	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	QK	114	Total	C	N	O	S		
			834	520	156	155	3	0	0
11	XK	114	Total	C	N	O	S		
			833	519	156	155	3	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	QL	122	Total	C	N	O	S		
			932	586	185	159	2	0	0
12	XL	122	Total	C	N	O	S		
			932	586	185	159	2	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	QM	116	Total	C	N	O	S		
			914	564	189	159	2	0	0
13	XM	114	Total	C	N	O	S		
			895	550	186	157	2	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	QN	60	Total	C	N	O	S		
			492	312	104	72	4	0	0
14	XN	60	Total	C	N	O	S		
			492	312	104	72	4	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	QO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0
15	XO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	QP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
16	XP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	QQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	XQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	68	Total	C	N	O	0	0	0
			555	355	108	92			
18	XR	68	Total	C	N	O	0	0	0
			555	355	108	92			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
19	XS	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
20	XT	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	QU	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	XU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 22 is a RNA chain called P-site tRNA^{fMet}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	18	Total	C	N	O	P	0	0	0
			394	176	80	120	18			
23	XX	18	Total	C	N	O	P	0	0	0
			394	176	80	120	18			

- Molecule 24 is a RNA chain called A-site tRNA^{Ala}(GGC) U32-A38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	76	Total	C	N	O	P	0	0	0
			1625	724	293	532	76			
24	XY	76	Total	C	N	O	P	0	0	0
			1625	724	293	532	76			

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
25	Y0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R1	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y1	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
27	Y2	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R3	59	Total	C	N	O		0	0	0
			469	298	90	81				
28	Y3	59	Total	C	N	O		0	0	0
			464	296	90	78				

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	R4	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			
29	Y4	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
30	Y5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
31	Y6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	R7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
32	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	R8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
33	Y8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	R9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
34	Y9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 35 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RA	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			
35	YA	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

- Molecule 36 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RB	120	Total	C	N	O	P	0	0	0
			2572	1145	476	832	119			
36	YB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 37 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RD	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
37	YD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 38 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
38	YE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 39 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RF	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
39	YF	202	Total	C	N	O	S	0	0	0
			1579	1007	296	274	2			

- Molecule 40 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RG	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
40	YG	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	4			

- Molecule 41 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
41	YH	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

- Molecule 42 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RI	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	YI	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			

- Molecule 43 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RN	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
43	YN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 44 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
44	YO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 45 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
45	YP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 46 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	RQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
46	YQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 47 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	RR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
47	YR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 48 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	RS	110	Total	C	N	O	0	0	0
			877	553	175	149			
48	YS	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 49 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	RT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
49	YT	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	RU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
50	YU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 51 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	RV	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
51	YV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 52 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	RW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
52	YW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 53 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	RX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
53	YX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 54 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RY	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
54	YY	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

- Molecule 55 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	RZ	178	Total	C	N	O	S	0	0	0
			1406	898	253	253	2			
55	YZ	177	Total	C	N	O	S	0	0	0
			1381	885	246	248	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	221	Total	Mg	0	0
			221	221		
56	QB	1	Total	Mg	0	0
			1	1		
56	QD	4	Total	Mg	0	0
			4	4		
56	QE	4	Total	Mg	0	0
			4	4		
56	QF	2	Total	Mg	0	0
			2	2		
56	QG	2	Total	Mg	0	0
			2	2		
56	QH	2	Total	Mg	0	0
			2	2		
56	QI	1	Total	Mg	0	0
			1	1		
56	QK	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QL	3	Total 3	Mg 3	0	0
56	QN	1	Total 1	Mg 1	0	0
56	QO	2	Total 2	Mg 2	0	0
56	QP	1	Total 1	Mg 1	0	0
56	QT	1	Total 1	Mg 1	0	0
56	QV	5	Total 5	Mg 5	0	0
56	R0	3	Total 3	Mg 3	0	0
56	R1	1	Total 1	Mg 1	0	0
56	R3	3	Total 3	Mg 3	0	0
56	R5	2	Total 2	Mg 2	0	0
56	R6	1	Total 1	Mg 1	0	0
56	R7	3	Total 3	Mg 3	0	0
56	R9	1	Total 1	Mg 1	0	0
56	RA	709	Total 709	Mg 709	0	0
56	RB	17	Total 17	Mg 17	0	0
56	RD	8	Total 8	Mg 8	0	0
56	RE	4	Total 4	Mg 4	0	0
56	RF	4	Total 4	Mg 4	0	0
56	RG	4	Total 4	Mg 4	0	0
56	RH	2	Total 2	Mg 2	0	0
56	RN	2	Total 2	Mg 2	0	0

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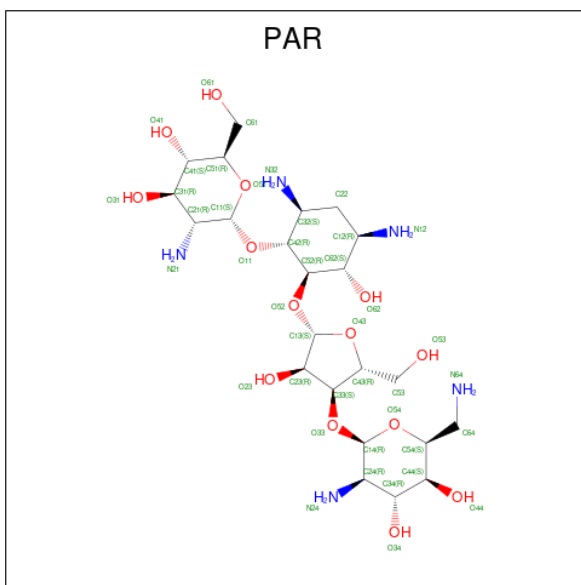
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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56	RP	3	Total 3	Mg 3	0	0
56	RQ	4	Total 4	Mg 4	0	0
56	RR	2	Total 2	Mg 2	0	0
56	RT	4	Total 4	Mg 4	0	0
56	RU	2	Total 2	Mg 2	0	0
56	RV	3	Total 3	Mg 3	0	0
56	RW	1	Total 1	Mg 1	0	0
56	RZ	1	Total 1	Mg 1	0	0
56	XA	193	Total 193	Mg 193	0	0
56	XE	2	Total 2	Mg 2	0	0
56	XF	2	Total 2	Mg 2	0	0
56	XJ	1	Total 1	Mg 1	0	0
56	XL	2	Total 2	Mg 2	0	0
56	XR	1	Total 1	Mg 1	0	0
56	XT	1	Total 1	Mg 1	0	0
56	XV	3	Total 3	Mg 3	0	0
56	XY	1	Total 1	Mg 1	0	0
56	Y0	1	Total 1	Mg 1	0	0
56	Y1	2	Total 2	Mg 2	0	0
56	Y3	1	Total 1	Mg 1	0	0

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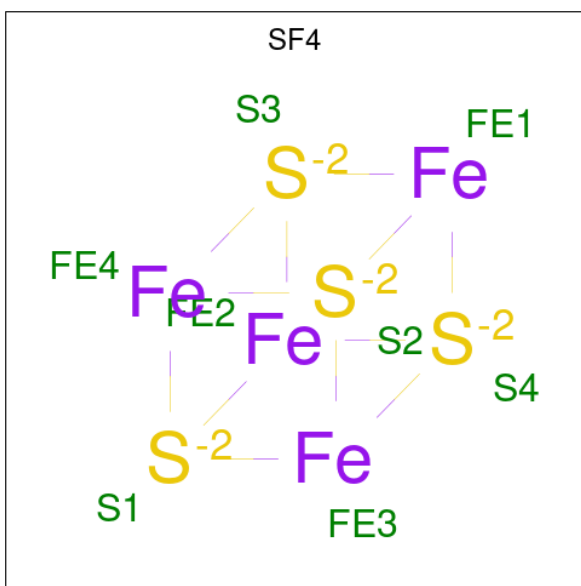
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	Y5	1	Total 1	Mg 1	0	0
56	Y6	1	Total 1	Mg 1	0	0
56	Y7	2	Total 2	Mg 2	0	0
56	Y8	1	Total 1	Mg 1	0	0
56	YA	707	Total 707	Mg 707	0	0
56	YB	20	Total 20	Mg 20	0	0
56	YD	7	Total 7	Mg 7	0	0
56	YE	5	Total 5	Mg 5	0	0
56	YF	3	Total 3	Mg 3	0	0
56	YG	3	Total 3	Mg 3	0	0
56	YI	1	Total 1	Mg 1	0	0
56	YN	1	Total 1	Mg 1	0	0
56	YO	1	Total 1	Mg 1	0	0
56	YP	2	Total 2	Mg 2	0	0
56	YQ	2	Total 2	Mg 2	0	0
56	YR	2	Total 2	Mg 2	0	0
56	YT	3	Total 3	Mg 3	0	0
56	YV	1	Total 1	Mg 1	0	0
56	YW	2	Total 2	Mg 2	0	0

- Molecule 57 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	QA	1	Total 42	C 23	N 5	O 14	0	0
57	XA	1	Total 42	C 23	N 5	O 14	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	QD	1	Total 8	Fe 4	S 4	0	0
58	XD	1	Total 8	Fe 4	S 4	0	0

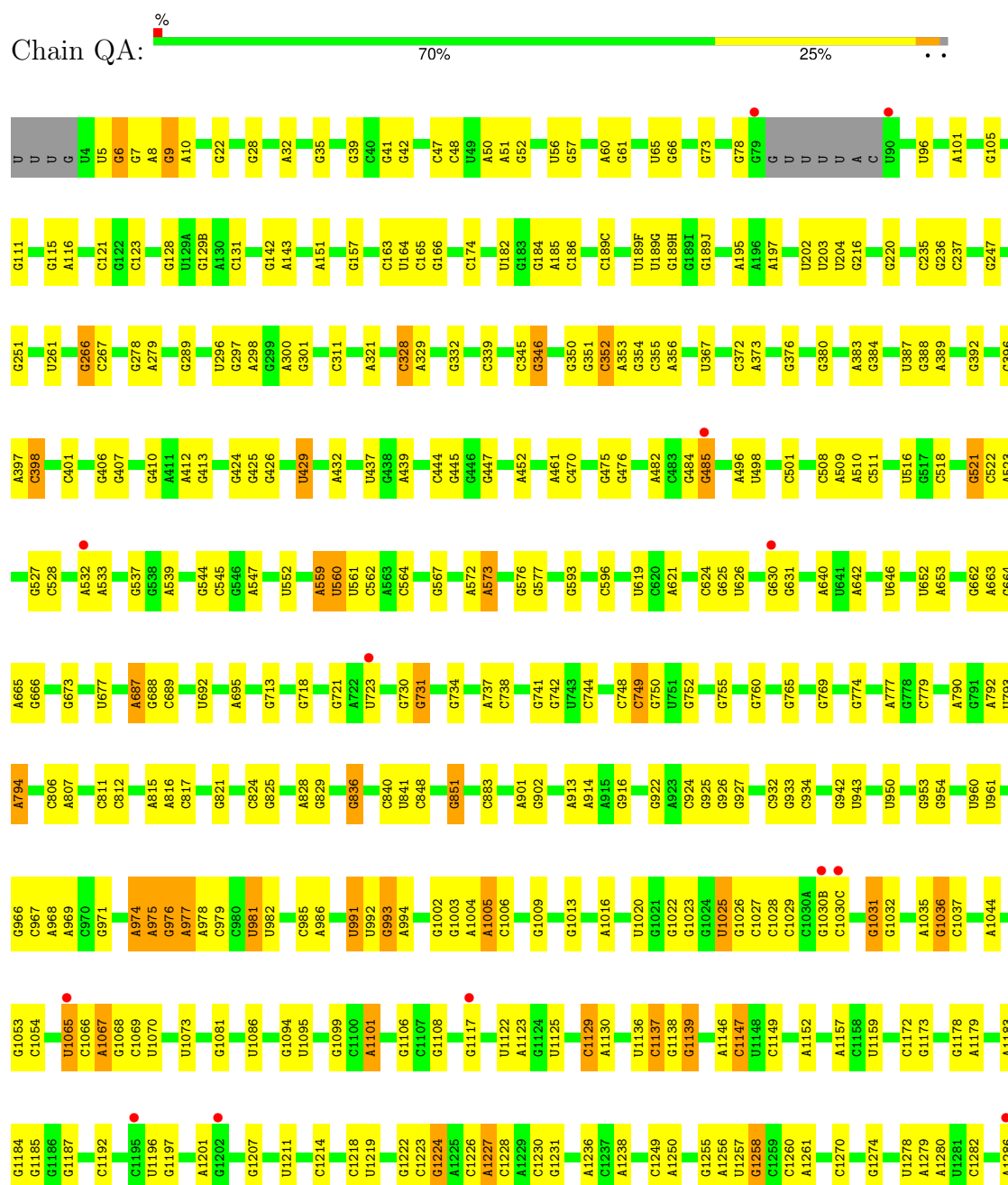
- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

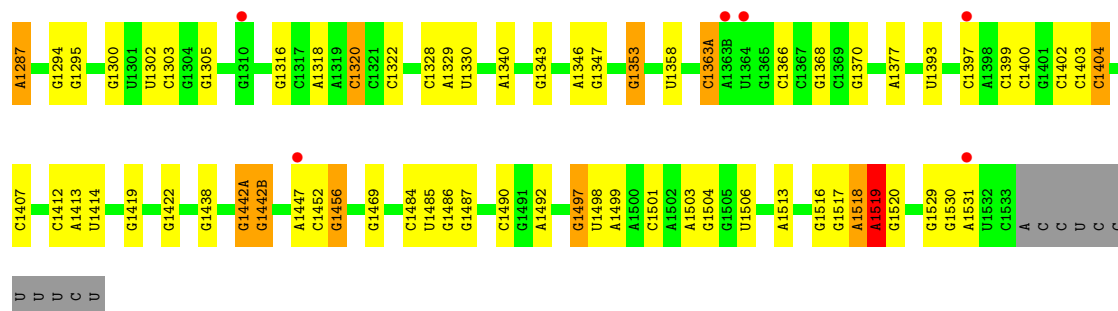
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	QN	1	Total 1	Zn 1	0	0
59	R4	1	Total 1	Zn 1	0	0
59	R5	1	Total 1	Zn 1	0	0
59	R6	1	Total 1	Zn 1	0	0
59	R9	1	Total 1	Zn 1	0	0
59	RY	1	Total 1	Zn 1	0	0
59	XN	1	Total 1	Zn 1	0	0
59	Y4	1	Total 1	Zn 1	0	0
59	Y5	1	Total 1	Zn 1	0	0
59	Y6	1	Total 1	Zn 1	0	0
59	Y9	1	Total 1	Zn 1	0	0
59	YY	1	Total 1	Zn 1	0	0

3 Residue-property plots

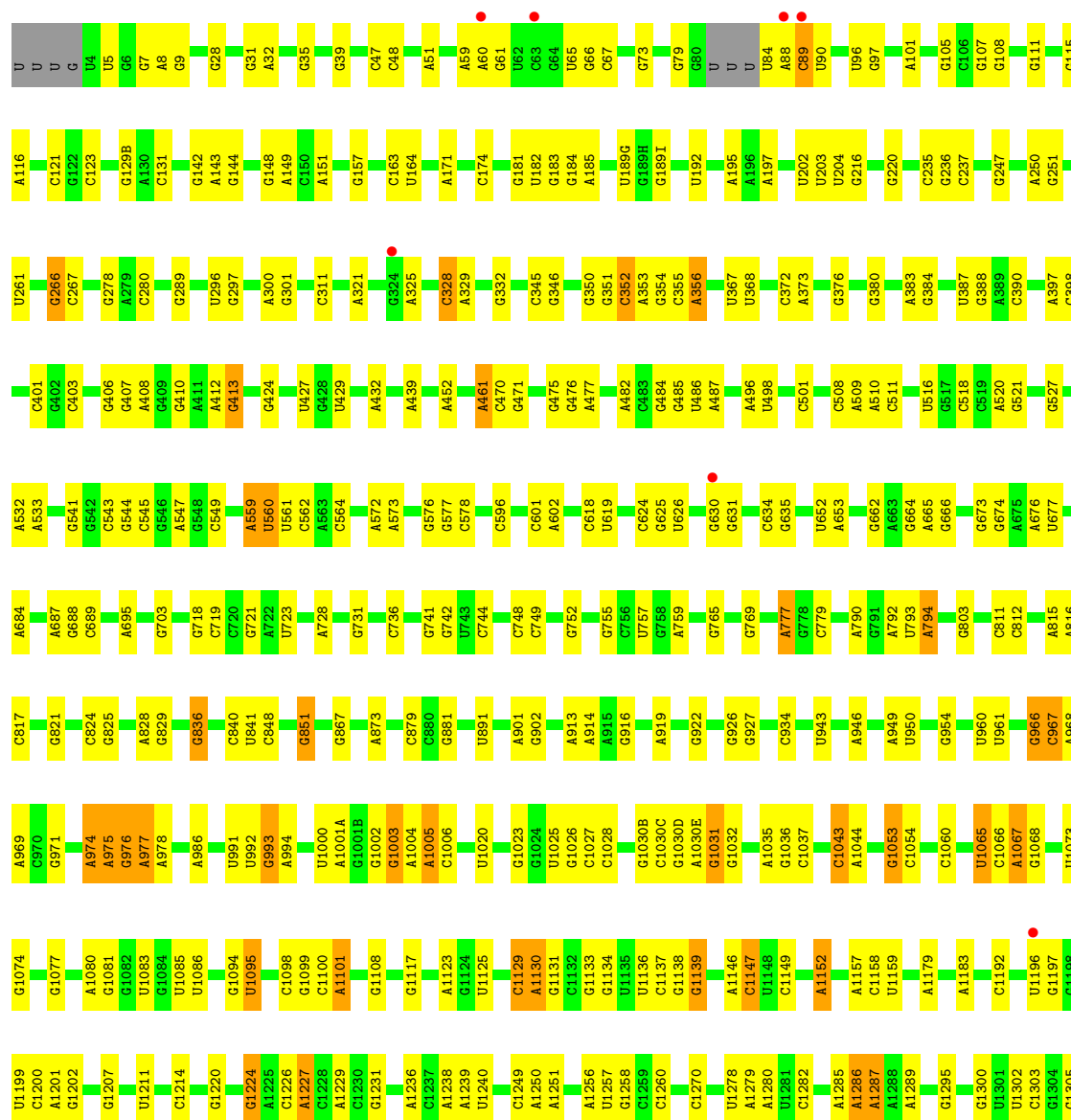
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

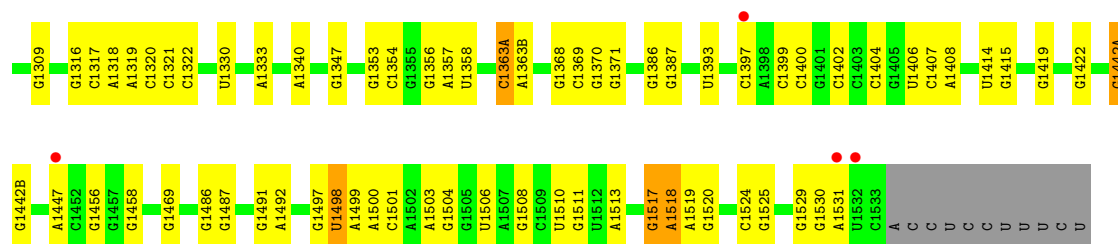
• Molecule 1: 16S rRNA



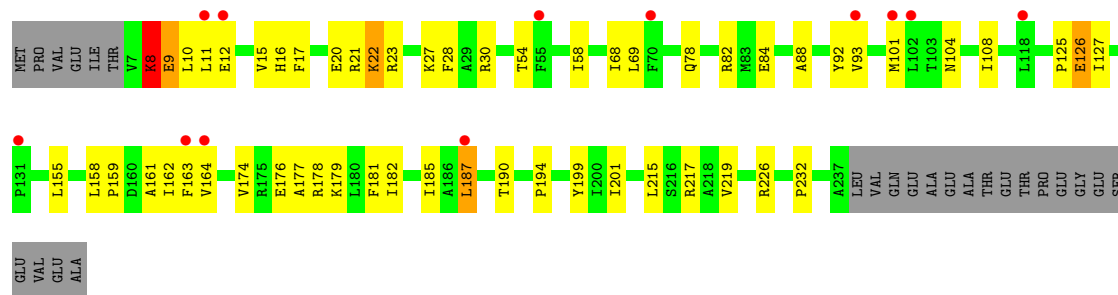


- Molecule 1: 16S rRNA

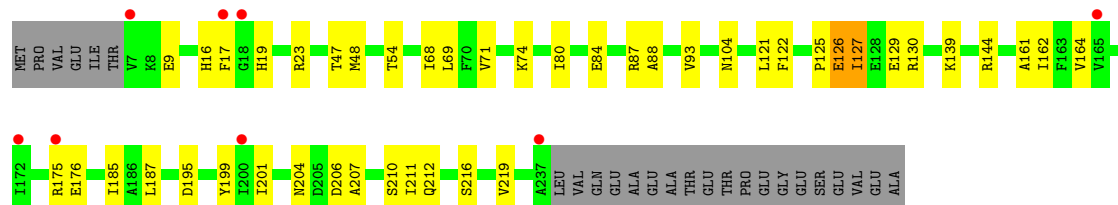
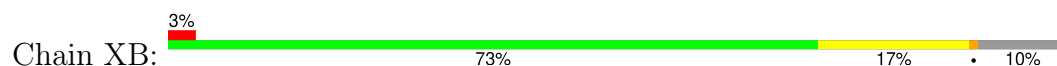




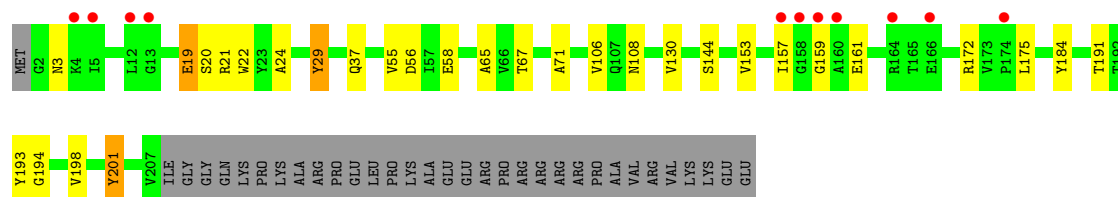
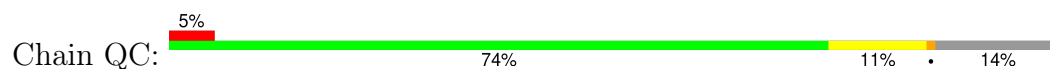
• Molecule 2: 30S ribosomal protein S2



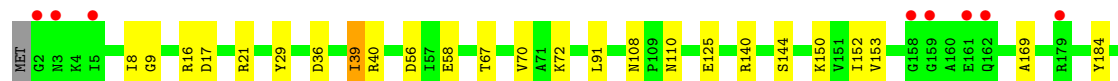
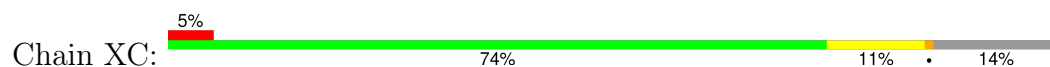
• Molecule 2: 30S ribosomal protein S2

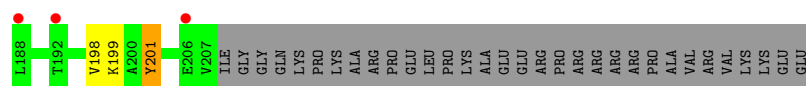


• Molecule 3: 30S ribosomal protein S3

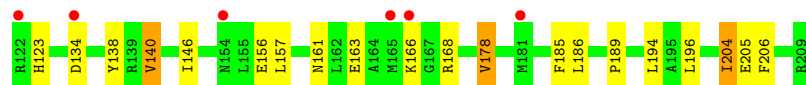
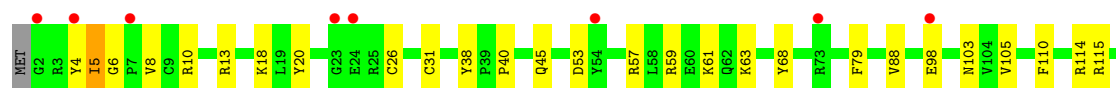
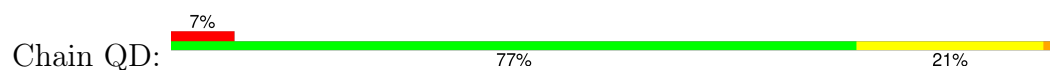


• Molecule 3: 30S ribosomal protein S3

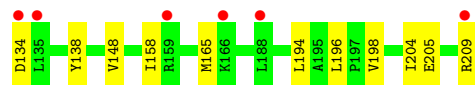
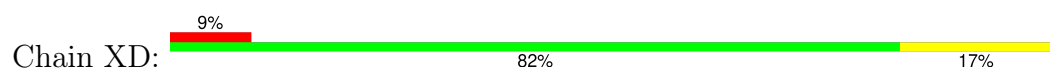




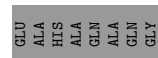
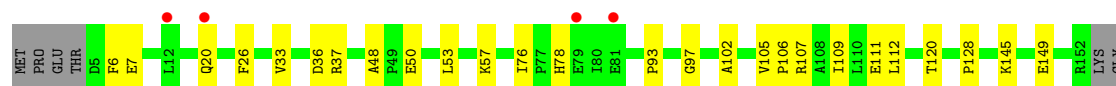
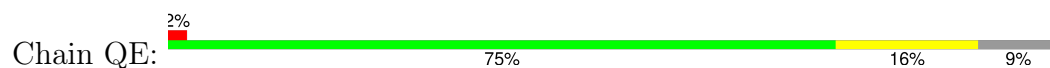
- Molecule 4: 30S ribosomal protein S4



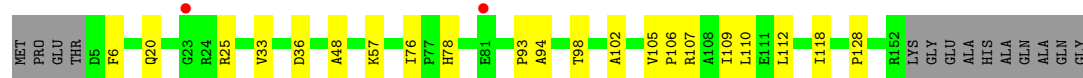
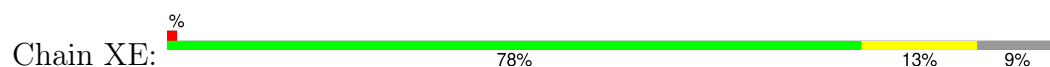
- Molecule 4: 30S ribosomal protein S4



- Molecule 5: 30S ribosomal protein S5



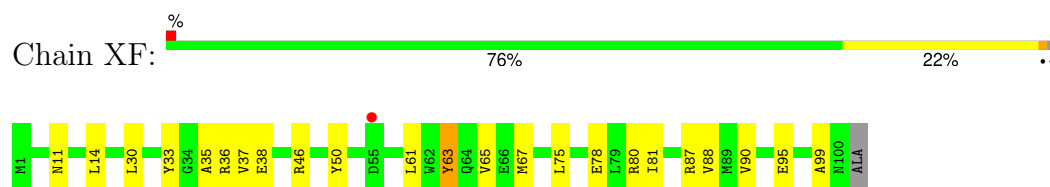
- Molecule 5: 30S ribosomal protein S5



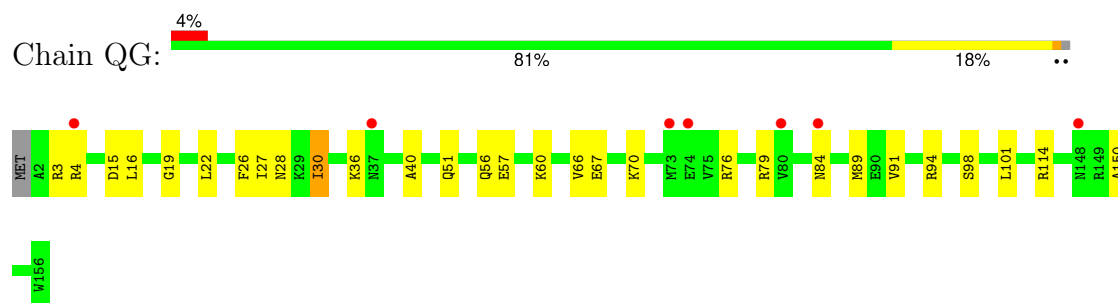
- Molecule 6: 30S ribosomal protein S6



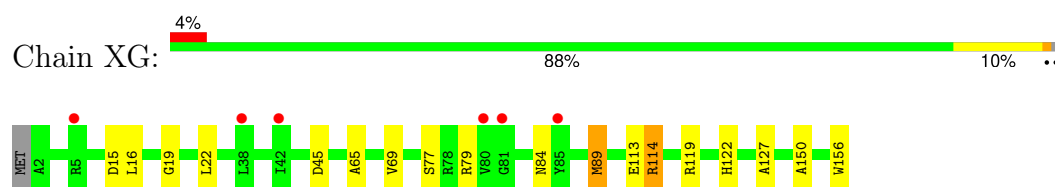
- Molecule 6: 30S ribosomal protein S6



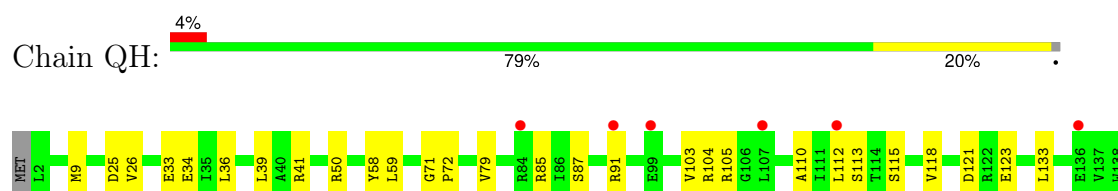
- Molecule 7: 30S ribosomal protein S7



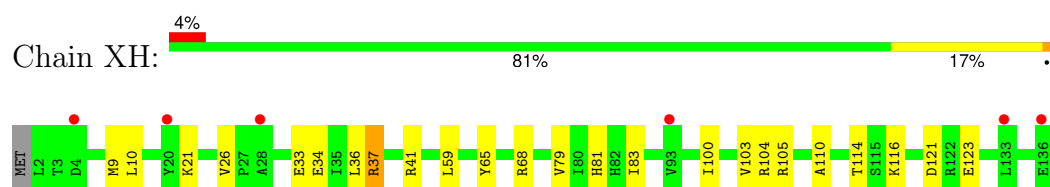
- Molecule 7: 30S ribosomal protein S7



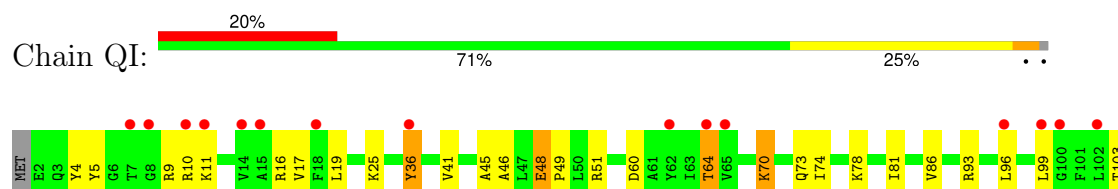
- Molecule 8: 30S ribosomal protein S8

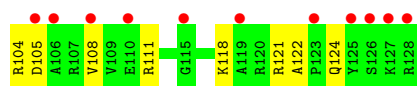


- Molecule 8: 30S ribosomal protein S8



- Molecule 9: 30S ribosomal protein S9

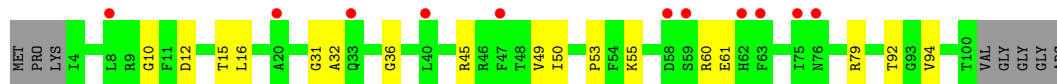
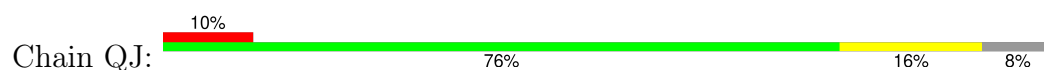




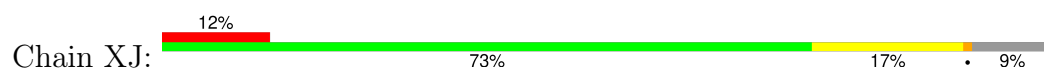
- Molecule 9: 30S ribosomal protein S9



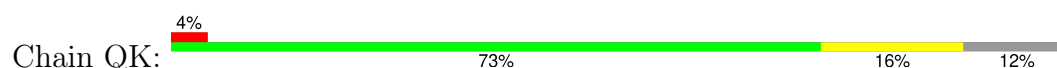
- Molecule 10: 30S ribosomal protein S10



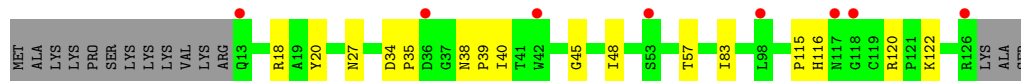
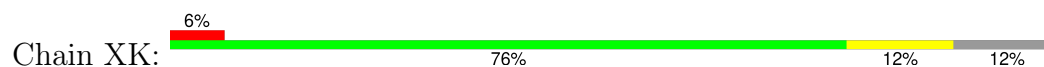
- Molecule 10: 30S ribosomal protein S10



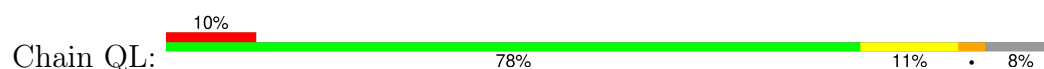
- Molecule 11: 30S ribosomal protein S11

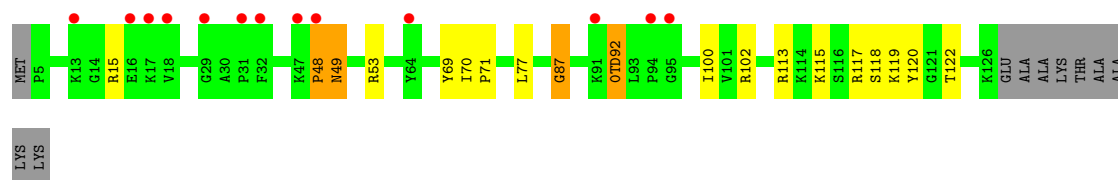


- Molecule 11: 30S ribosomal protein S11

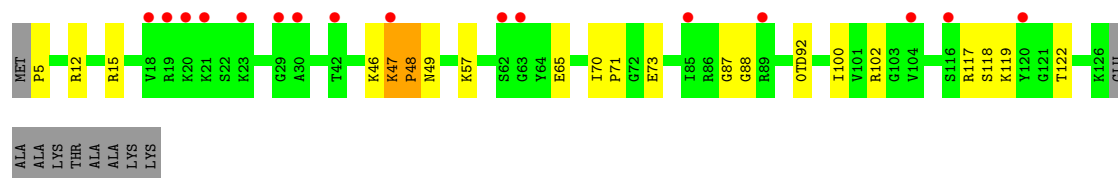
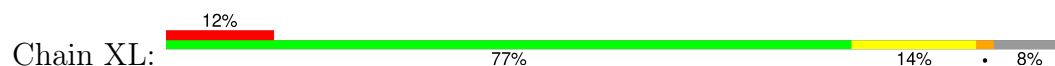


- Molecule 12: 30S ribosomal protein S12

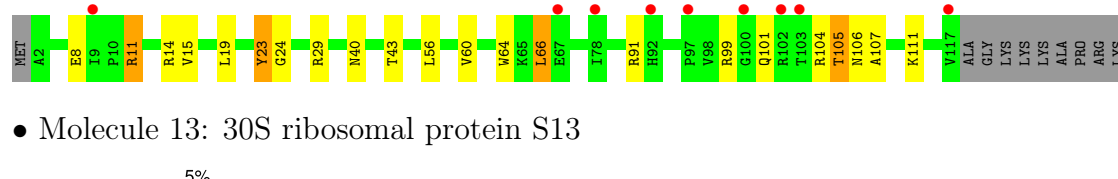
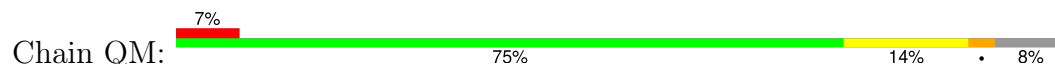




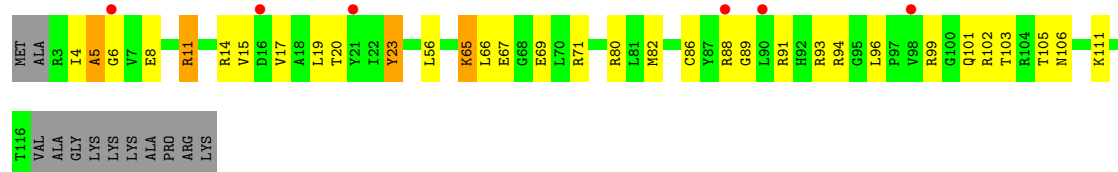
- Molecule 12: 30S ribosomal protein S12



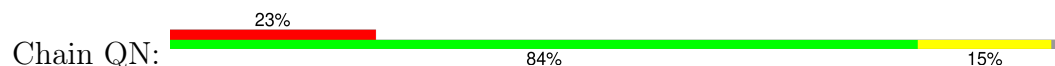
- Molecule 13: 30S ribosomal protein S13



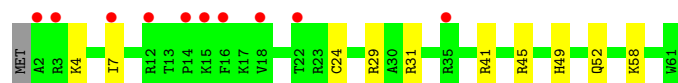
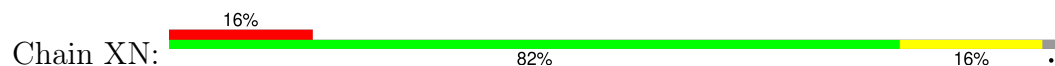
- Molecule 13: 30S ribosomal protein S13



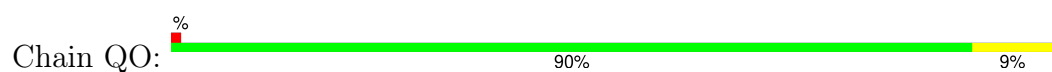
- Molecule 14: 30S ribosomal protein S14 type Z



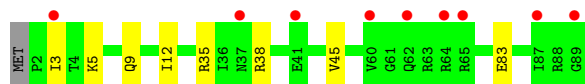
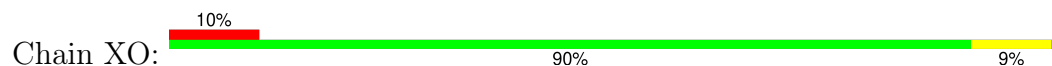
- Molecule 14: 30S ribosomal protein S14 type Z



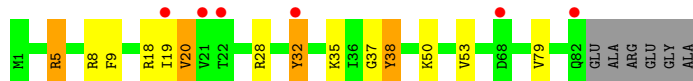
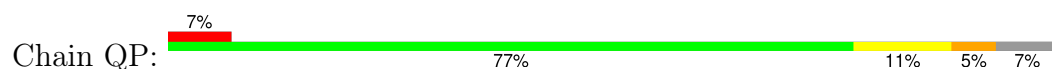
- Molecule 15: 30S ribosomal protein S15



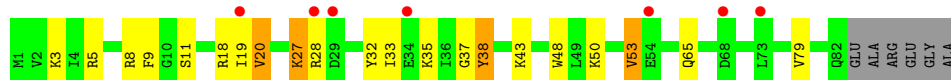
- Molecule 15: 30S ribosomal protein S15



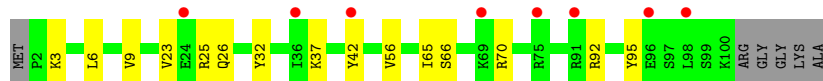
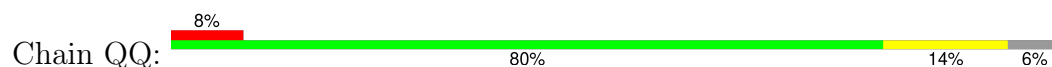
- Molecule 16: 30S ribosomal protein S16



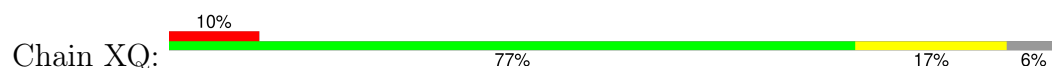
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



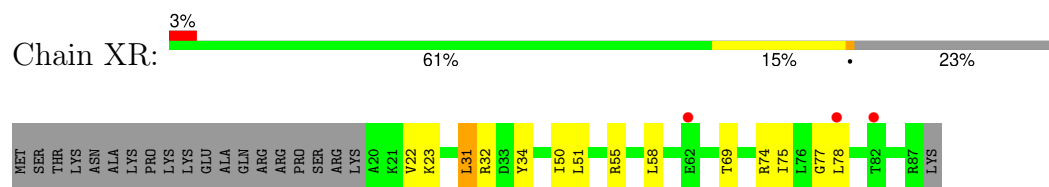
- Molecule 17: 30S ribosomal protein S17



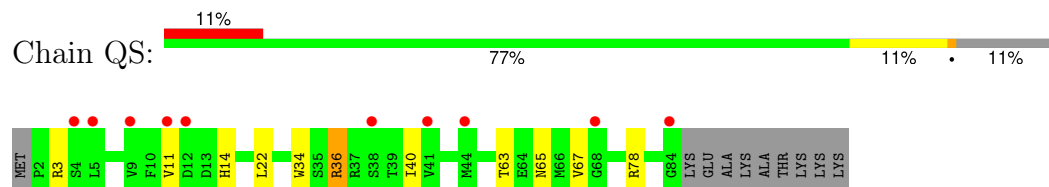
- Molecule 18: 30S ribosomal protein S18



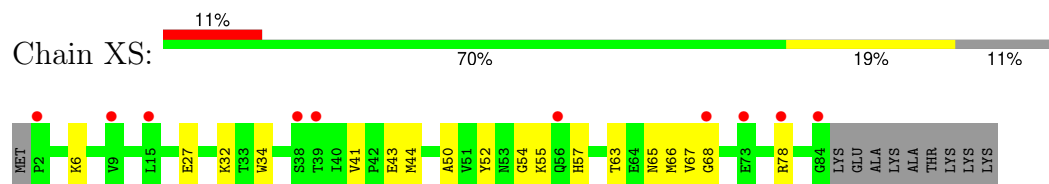
- Molecule 18: 30S ribosomal protein S18



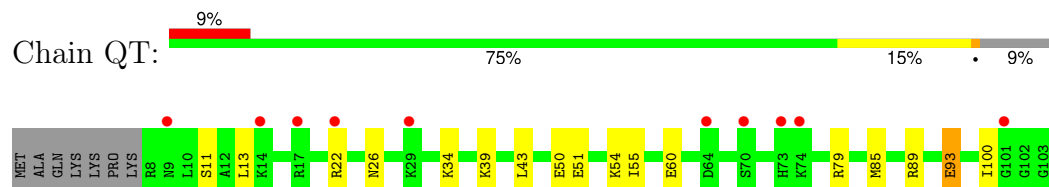
- Molecule 19: 30S ribosomal protein S19



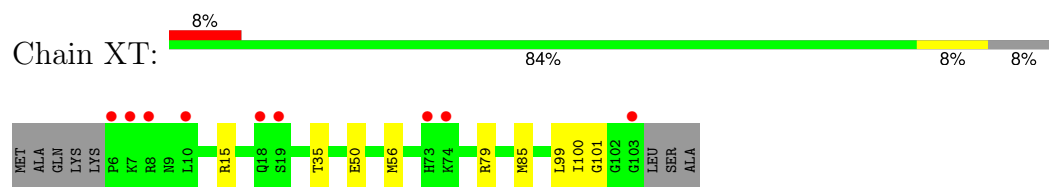
- Molecule 19: 30S ribosomal protein S19



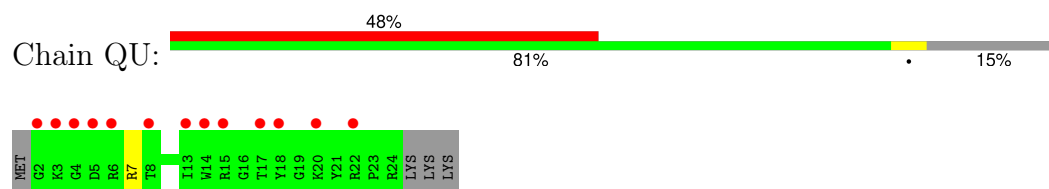
- Molecule 20: 30S ribosomal protein S20



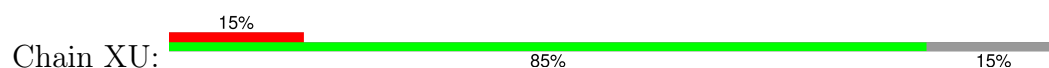
- Molecule 20: 30S ribosomal protein S20

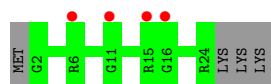


- Molecule 21: 30S ribosomal protein Thx

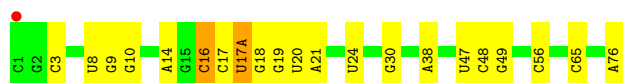
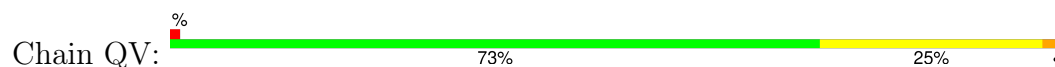


- Molecule 21: 30S ribosomal protein Thx

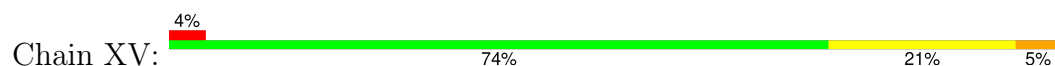




- Molecule 22: P-site tRNAfMet



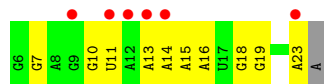
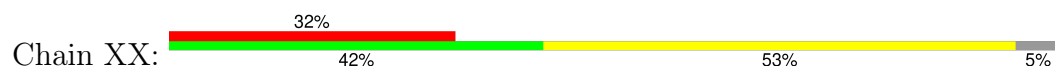
- Molecule 22: P-site tRNAfMet



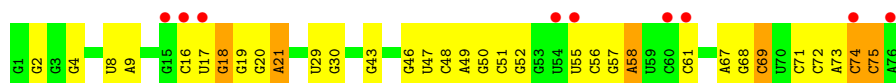
- Molecule 23: mRNA



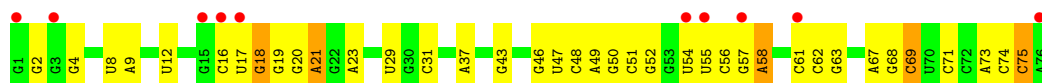
- Molecule 23: mRNA



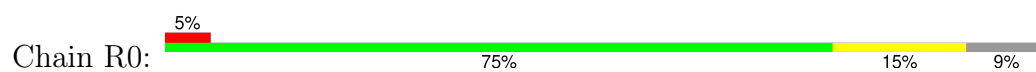
- Molecule 24: A-site tRNAAla(GGC) U32-A38



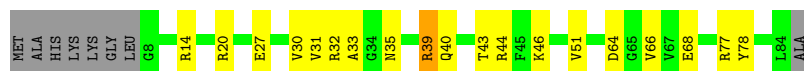
- Molecule 24: A-site tRNAAla(GGC) U32-A38



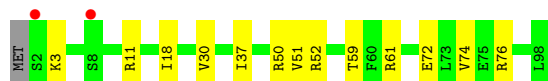
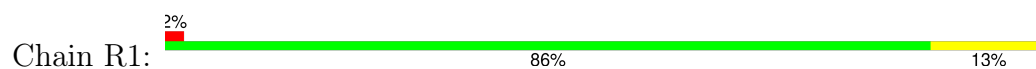
- Molecule 25: 50S ribosomal protein L27



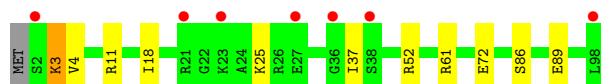
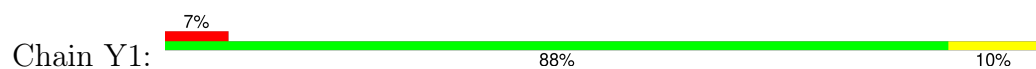
- Molecule 25: 50S ribosomal protein L27



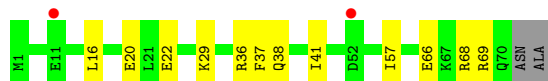
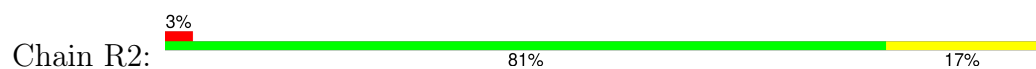
- Molecule 26: 50S ribosomal protein L28



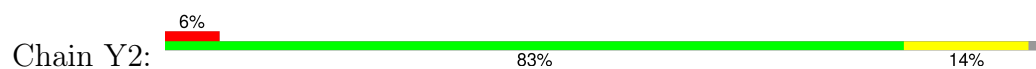
- Molecule 26: 50S ribosomal protein L28



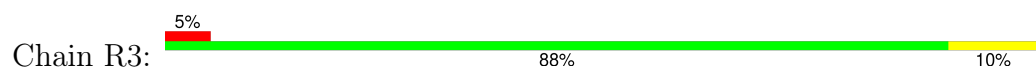
- Molecule 27: 50S ribosomal protein L29



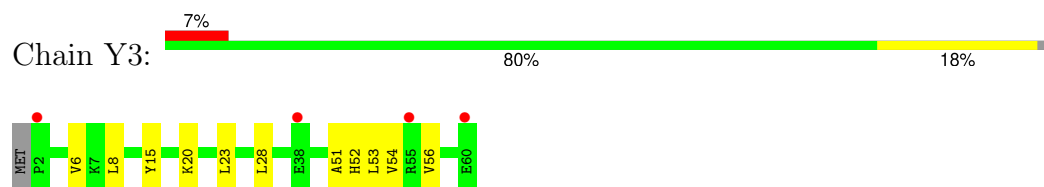
- Molecule 27: 50S ribosomal protein L29



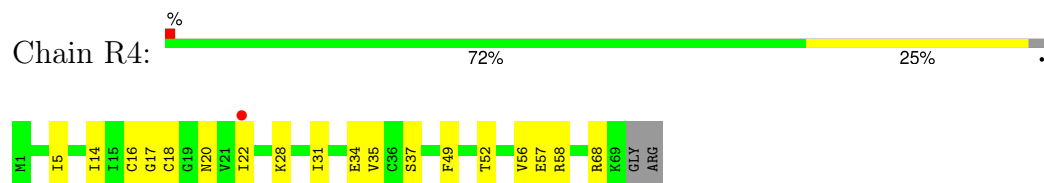
- Molecule 28: 50S ribosomal protein L30



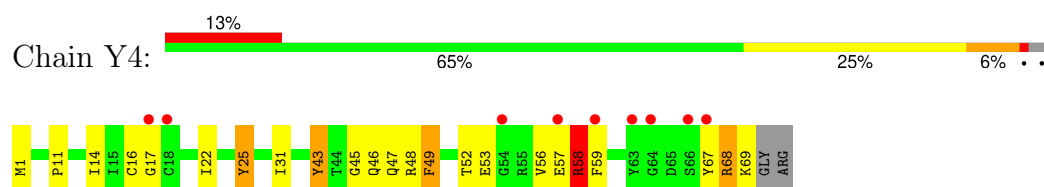
- Molecule 28: 50S ribosomal protein L30



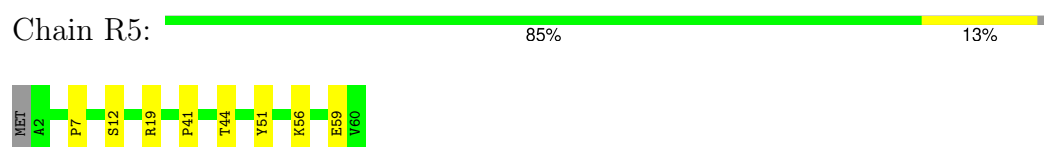
- Molecule 29: 50S ribosomal protein L31



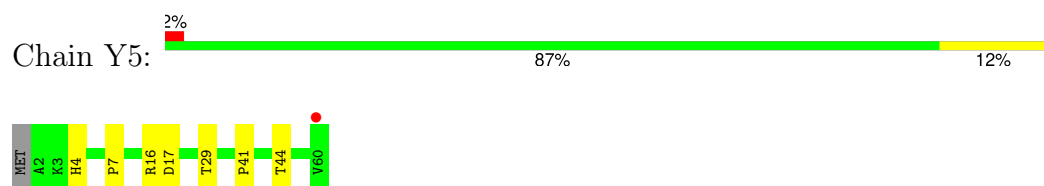
- Molecule 29: 50S ribosomal protein L31



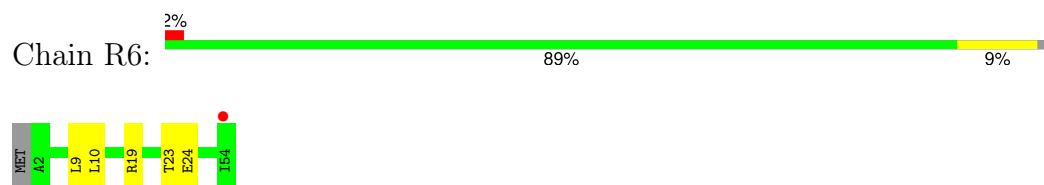
- Molecule 30: 50S ribosomal protein L32



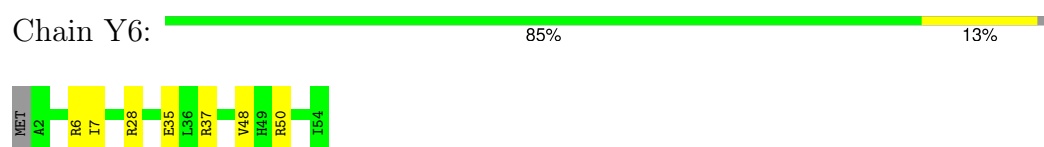
- Molecule 30: 50S ribosomal protein L32



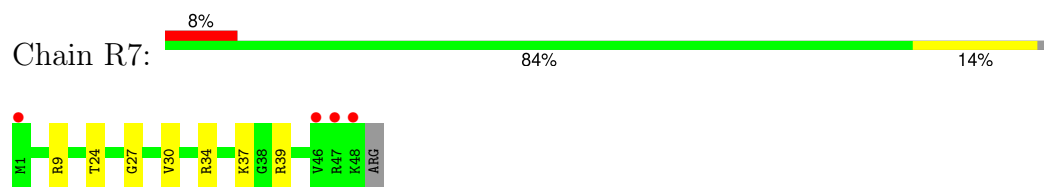
- Molecule 31: 50S ribosomal protein L33



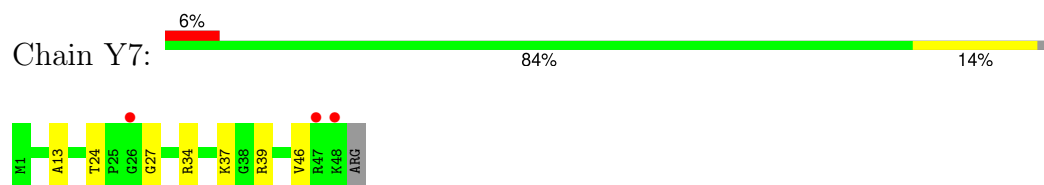
- Molecule 31: 50S ribosomal protein L33



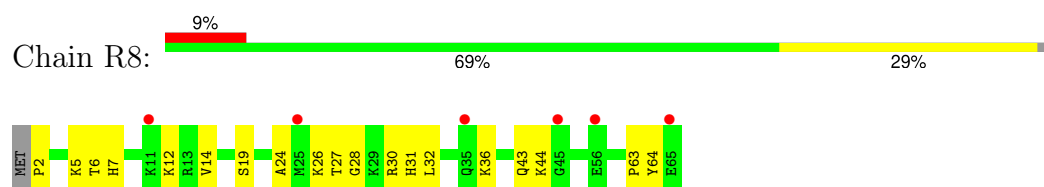
- Molecule 32: 50S ribosomal protein L34



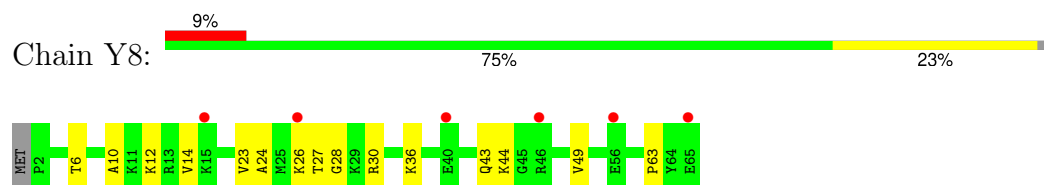
- Molecule 32: 50S ribosomal protein L34



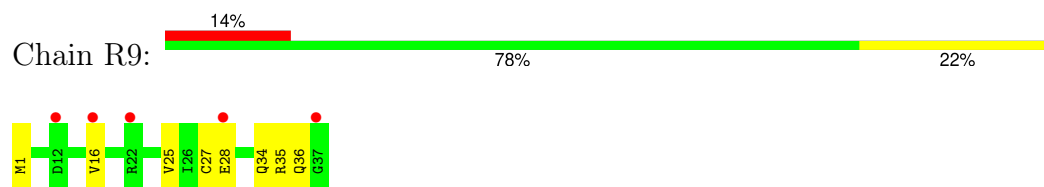
- Molecule 33: 50S ribosomal protein L35



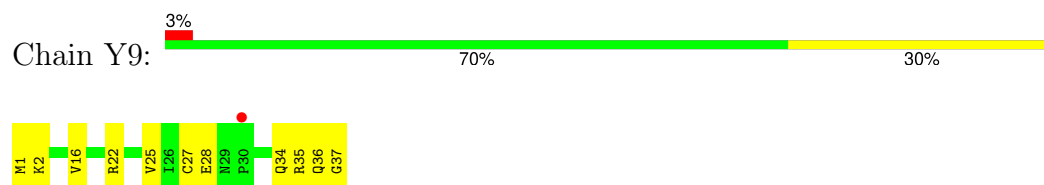
- Molecule 33: 50S ribosomal protein L35



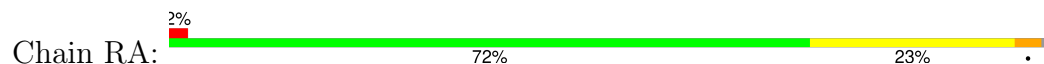
- Molecule 34: 50S ribosomal protein L36



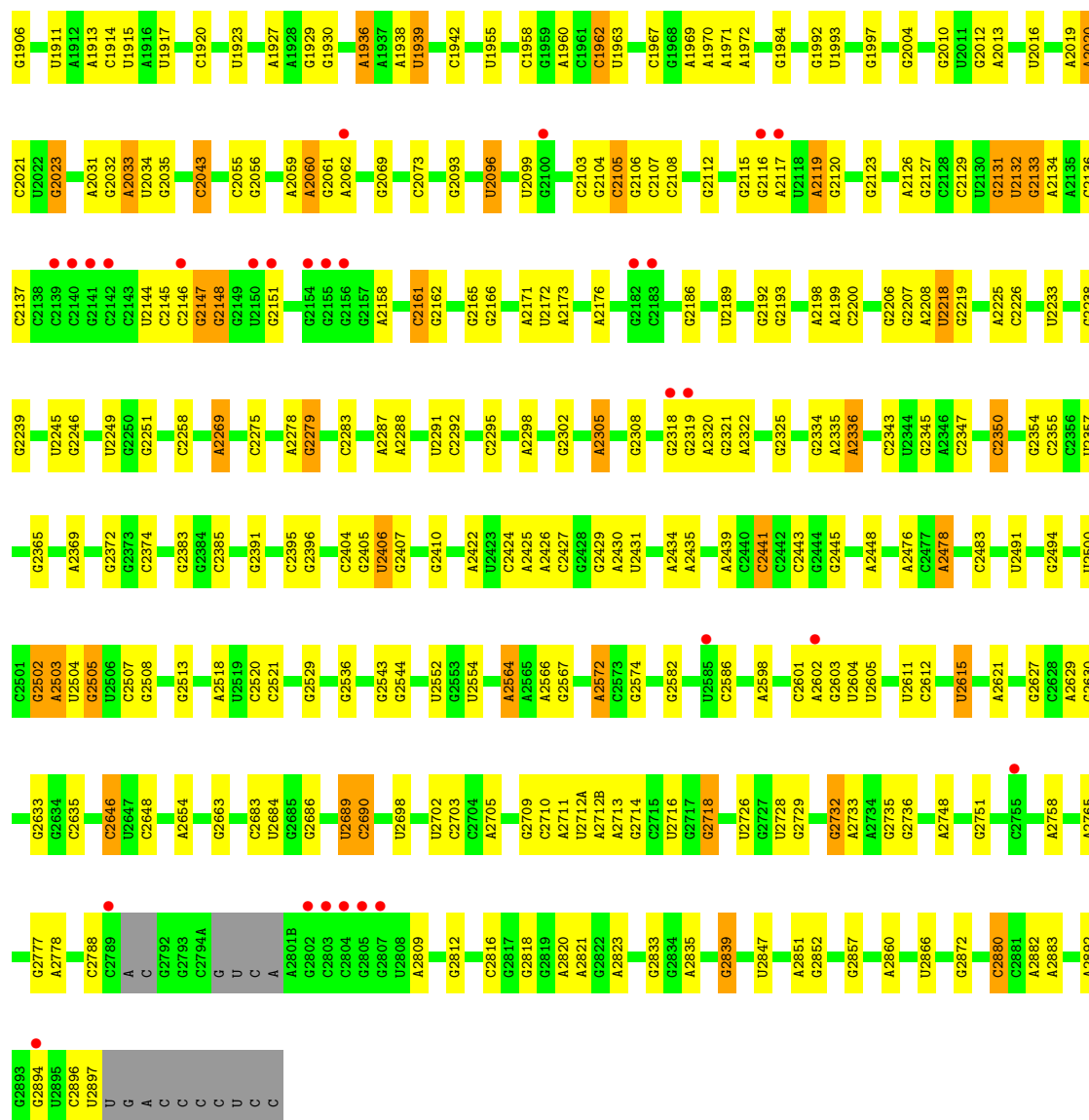
- Molecule 34: 50S ribosomal protein L36



- Molecule 35: 23S rRNA

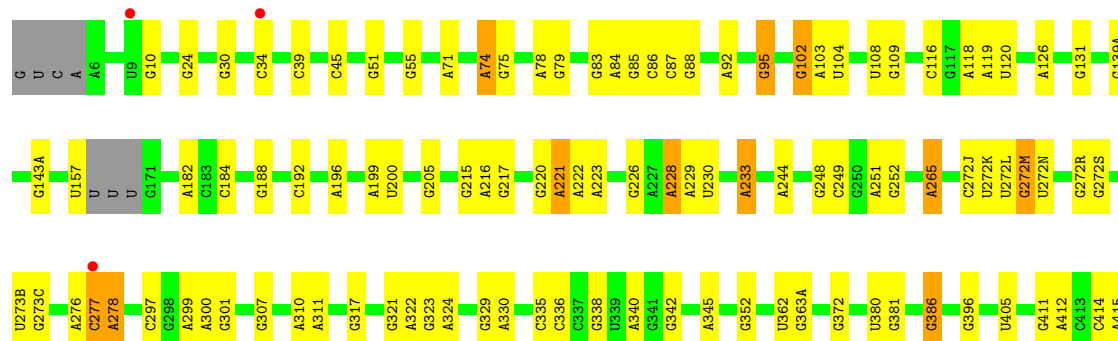


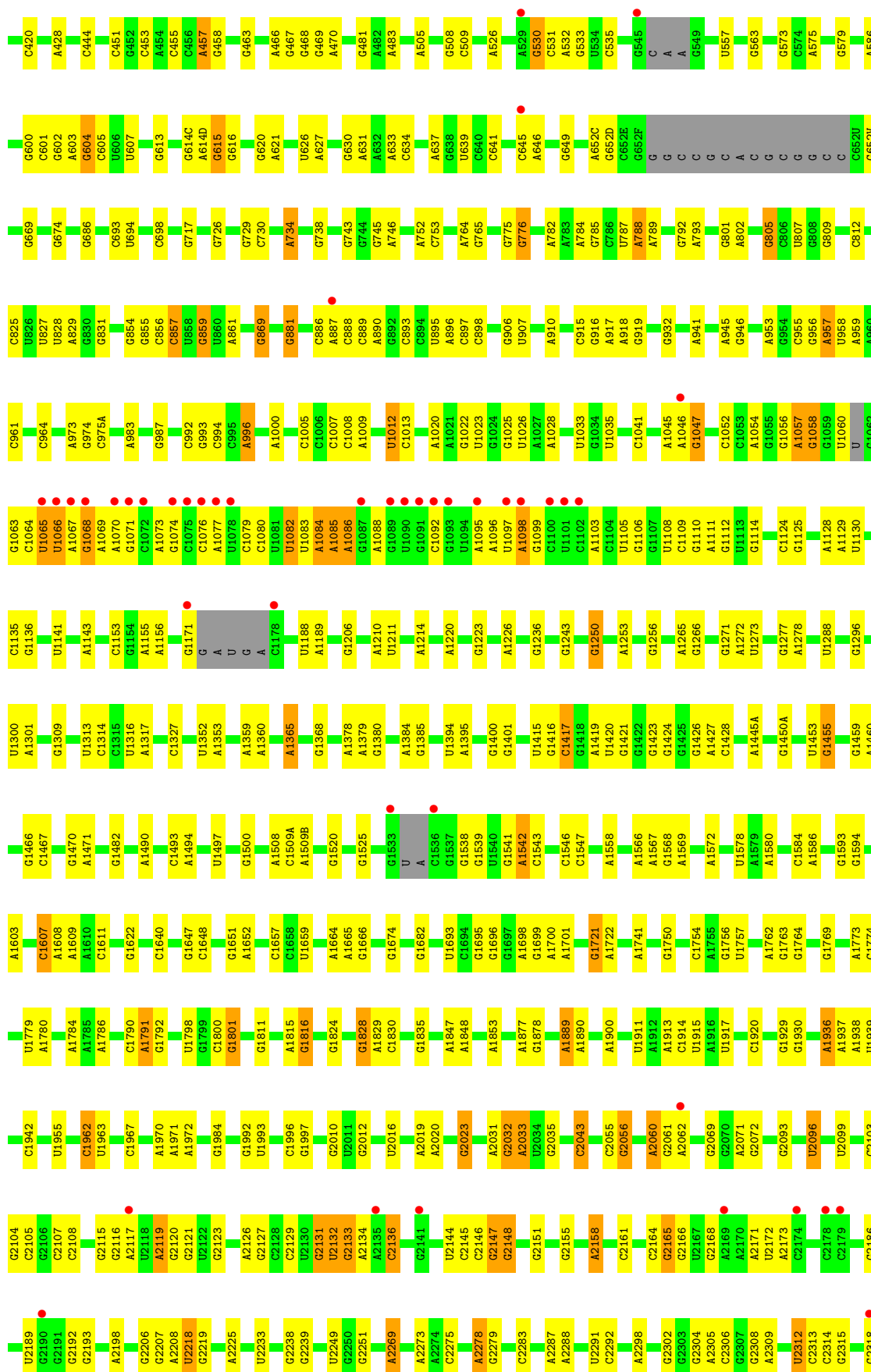


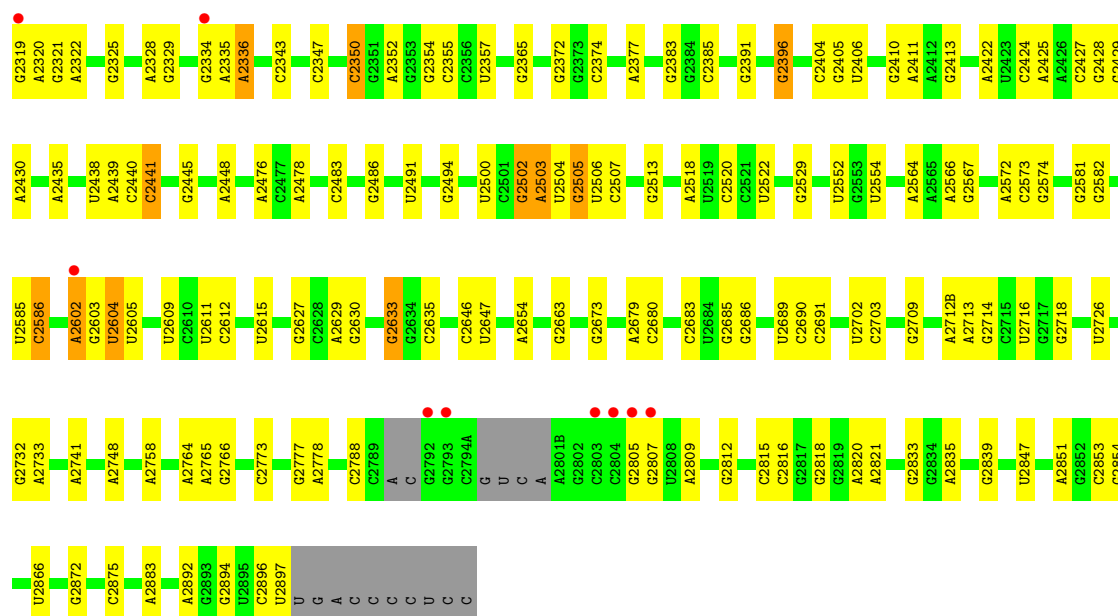


• Molecule 35: 23S rRNA

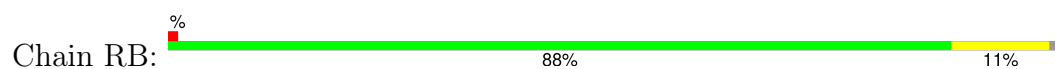
Chain YA: 2% 72% 23% . .



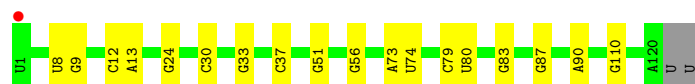
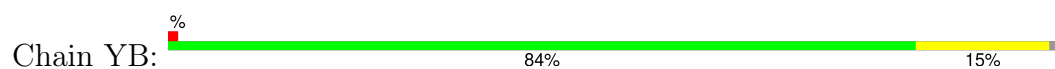




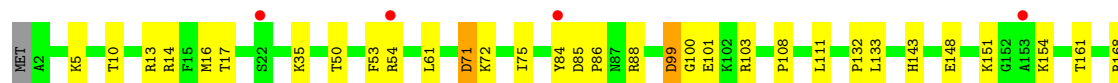
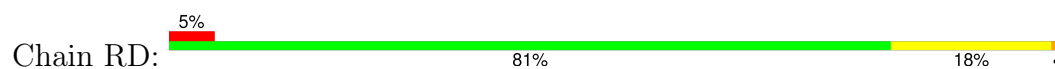
- Molecule 36: 5S rRNA



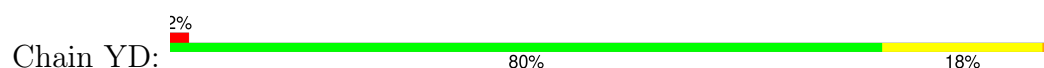
- Molecule 36: 5S rRNA

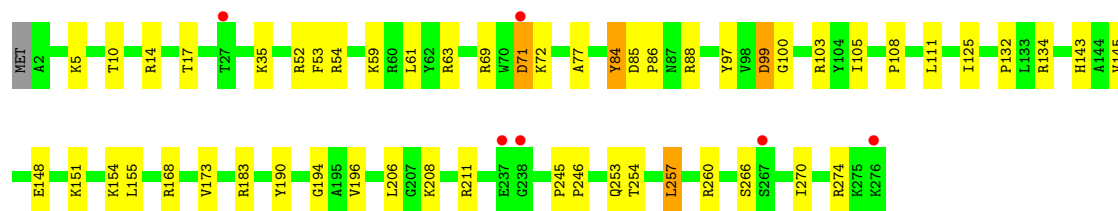


- Molecule 37: 50S ribosomal protein L2

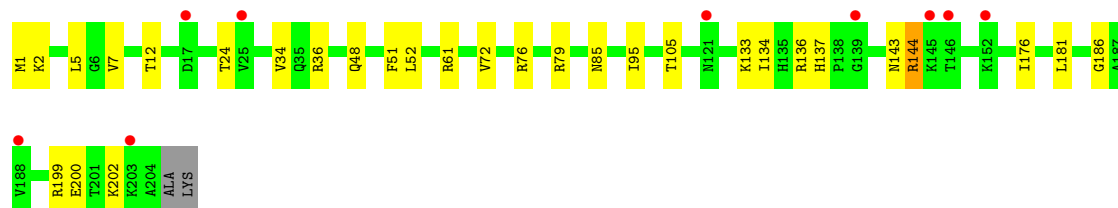
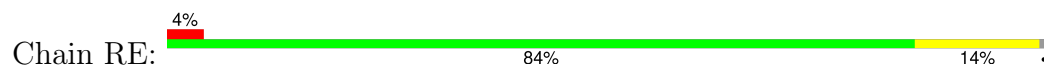


- Molecule 37: 50S ribosomal protein L2

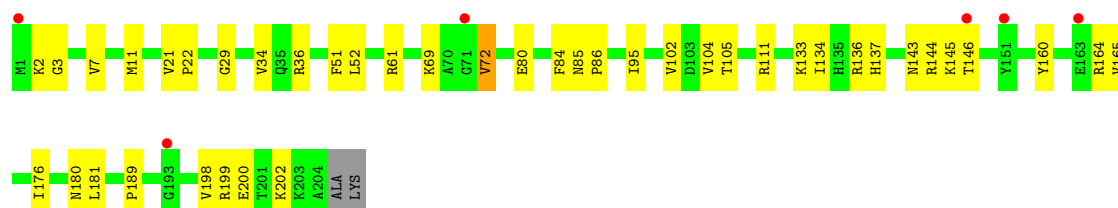
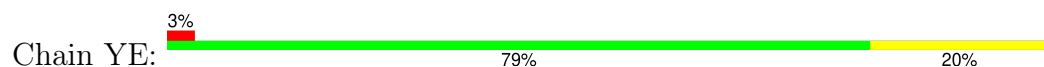




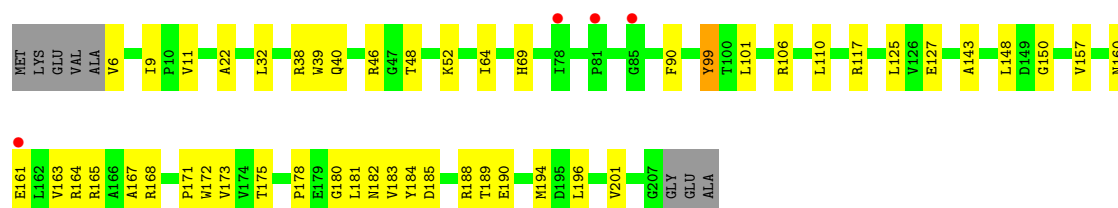
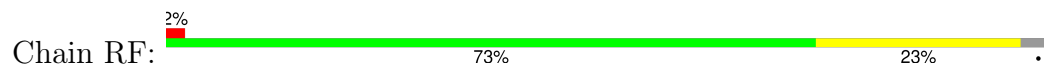
• Molecule 38: 50S ribosomal protein L3



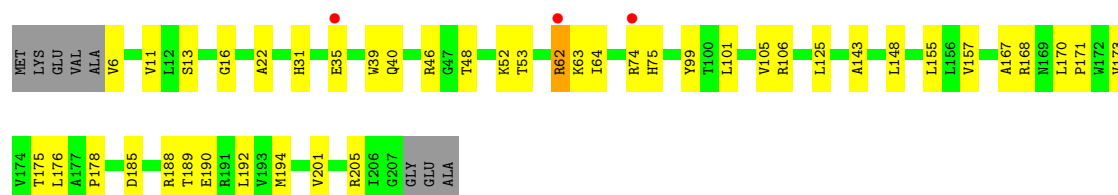
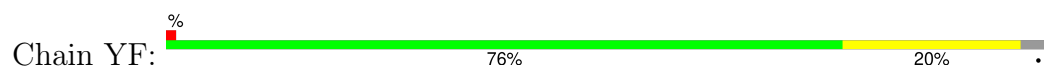
• Molecule 38: 50S ribosomal protein L3



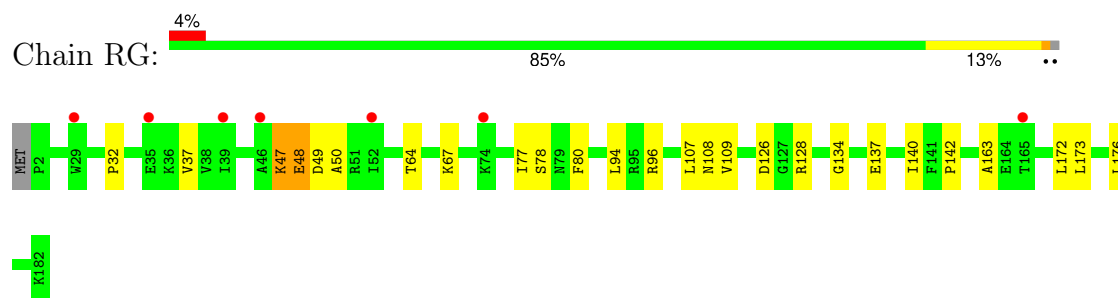
• Molecule 39: 50S ribosomal protein L4



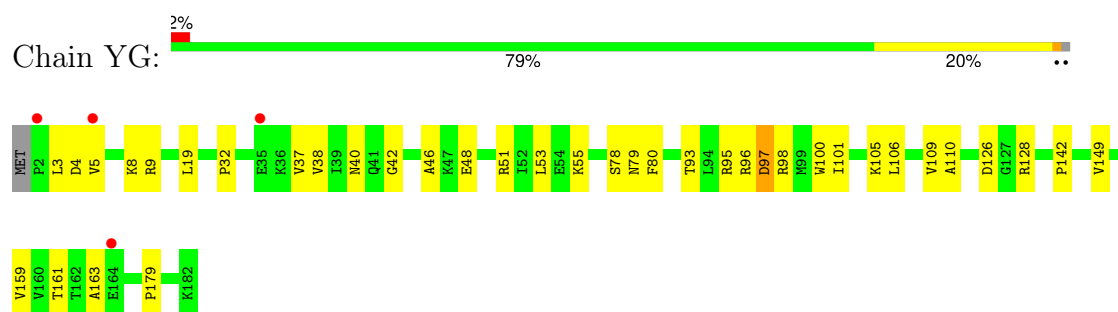
• Molecule 39: 50S ribosomal protein L4



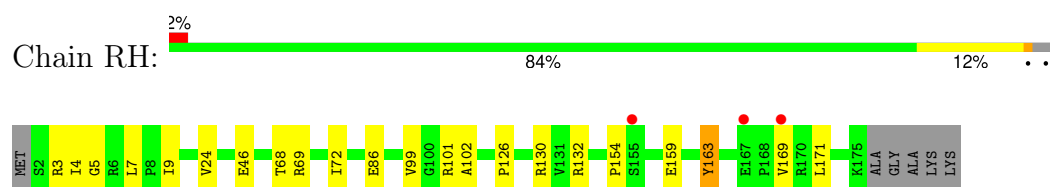
- Molecule 40: 50S ribosomal protein L5



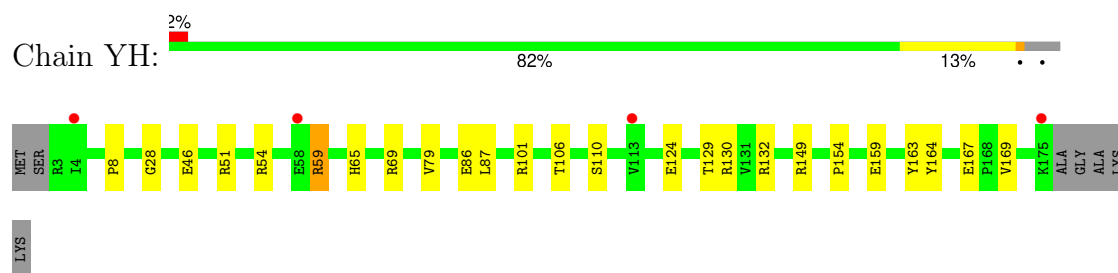
- Molecule 40: 50S ribosomal protein L5



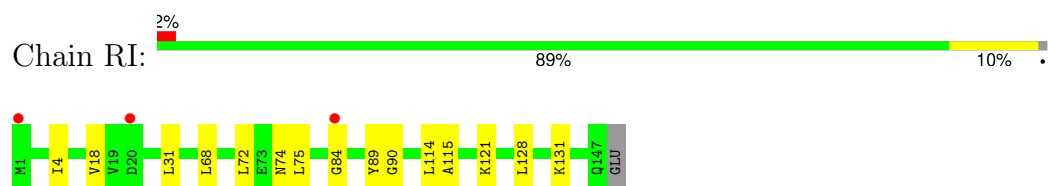
- Molecule 41: 50S ribosomal protein L6



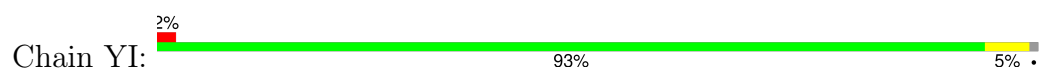
- Molecule 41: 50S ribosomal protein L6



- Molecule 42: 50S ribosomal protein L9

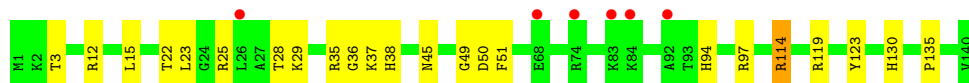
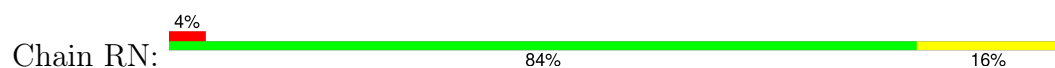


- Molecule 42: 50S ribosomal protein L9

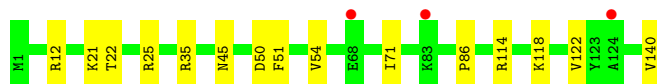
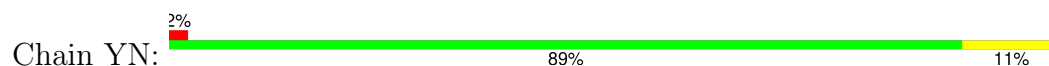




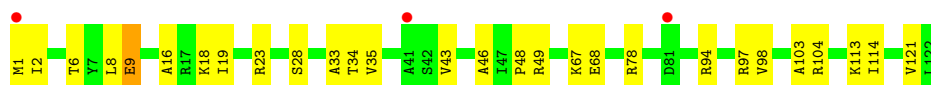
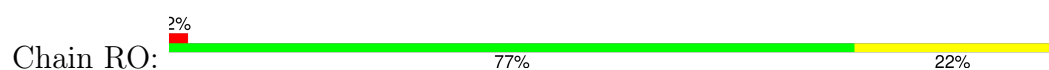
- Molecule 43: 50S ribosomal protein L13



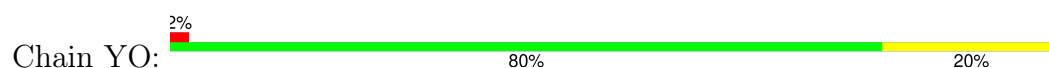
- Molecule 43: 50S ribosomal protein L13



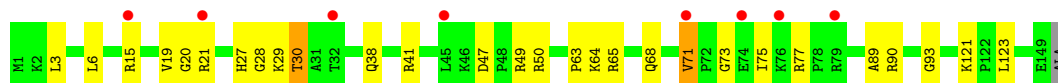
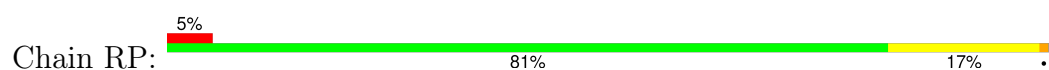
- Molecule 44: 50S ribosomal protein L14



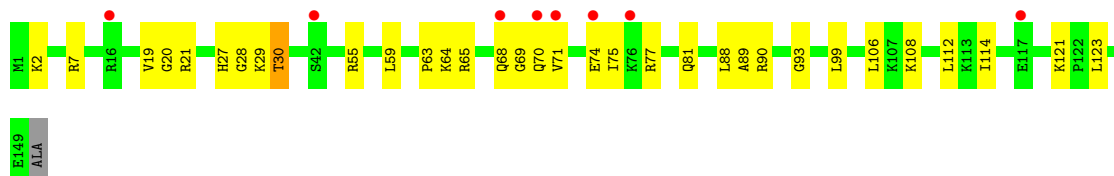
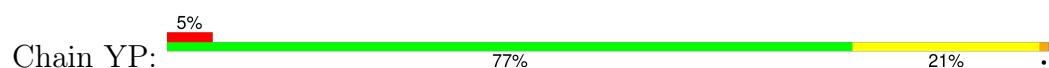
- Molecule 44: 50S ribosomal protein L14



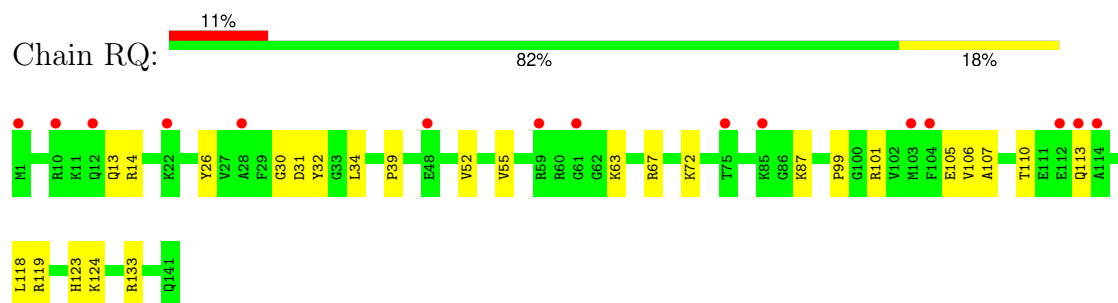
- Molecule 45: 50S ribosomal protein L15



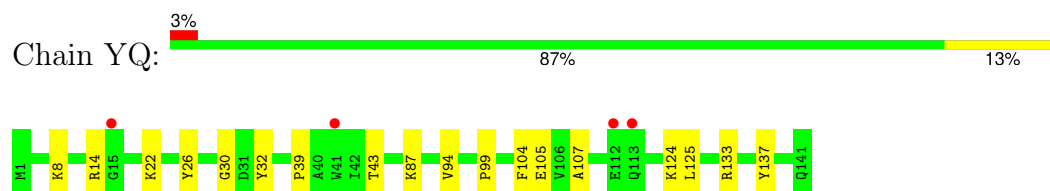
- Molecule 45: 50S ribosomal protein L15



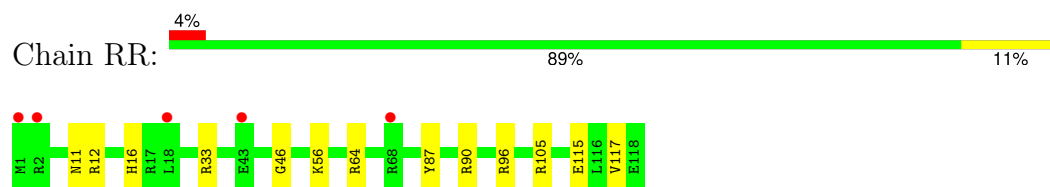
- Molecule 46: 50S ribosomal protein L16



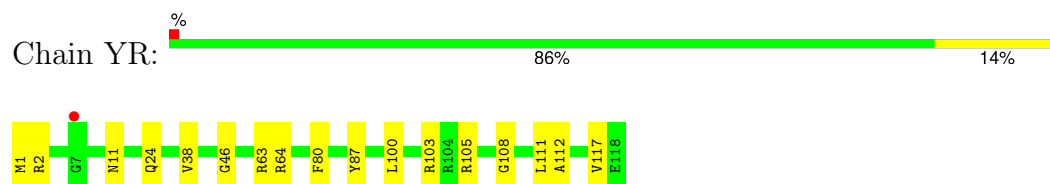
- Molecule 46: 50S ribosomal protein L16



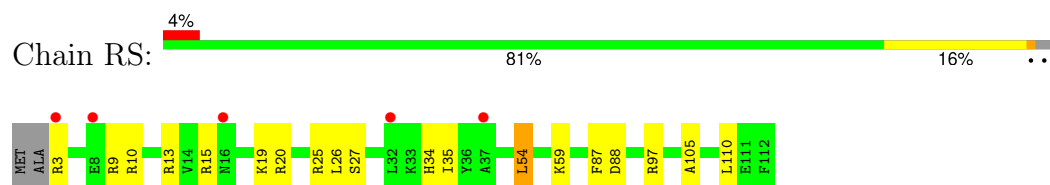
- Molecule 47: 50S ribosomal protein L17



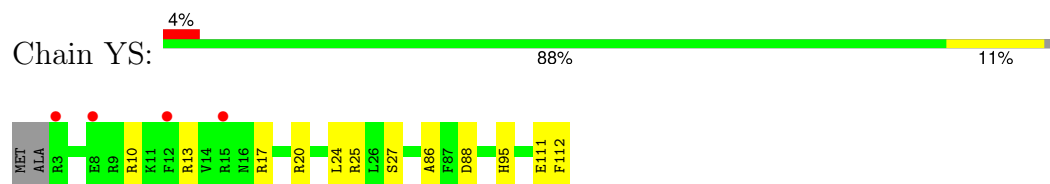
- Molecule 47: 50S ribosomal protein L17



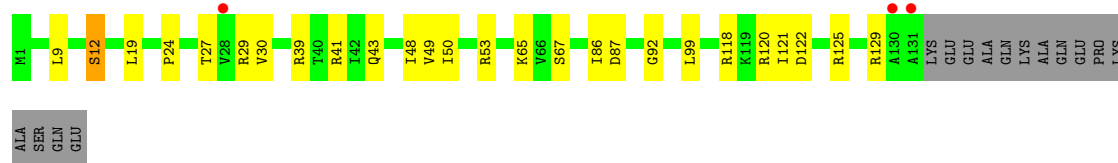
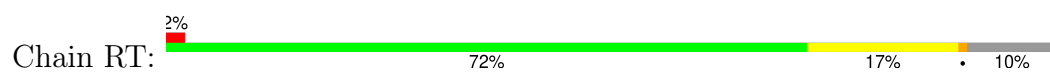
- Molecule 48: 50S ribosomal protein L18



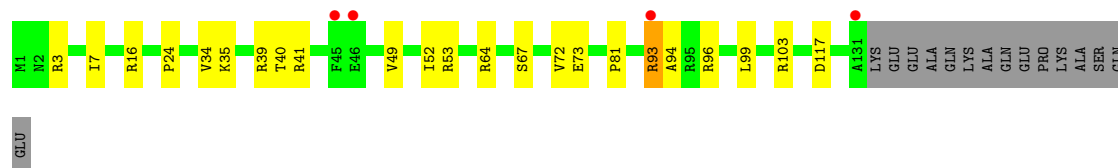
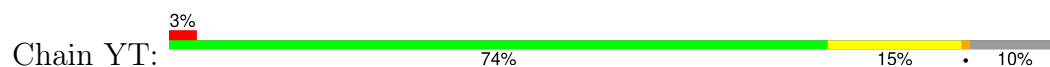
- Molecule 48: 50S ribosomal protein L18



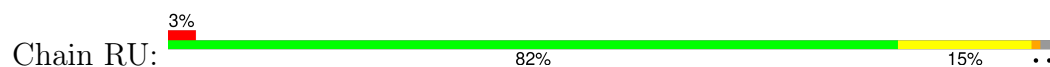
- Molecule 49: 50S ribosomal protein L19



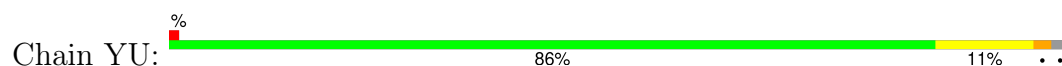
- Molecule 49: 50S ribosomal protein L19



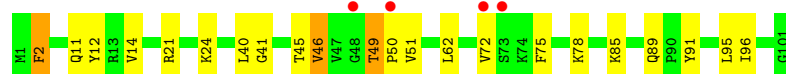
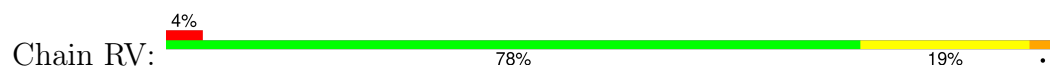
- Molecule 50: 50S ribosomal protein L20



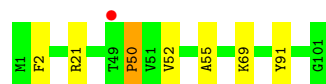
- Molecule 50: 50S ribosomal protein L20



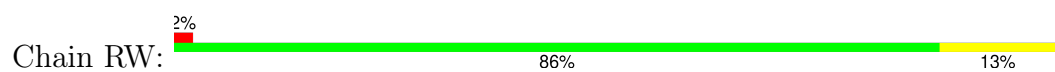
- Molecule 51: 50S ribosomal protein L21



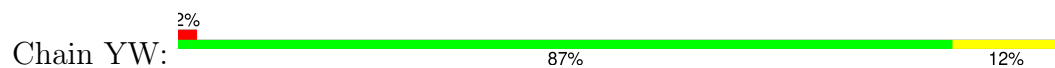
- Molecule 51: 50S ribosomal protein L21



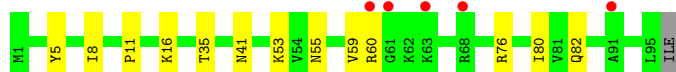
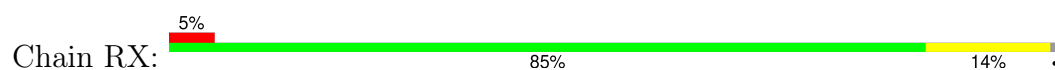
- Molecule 52: 50S ribosomal protein L22



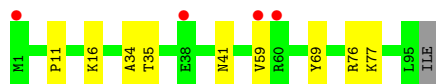
- Molecule 52: 50S ribosomal protein L22



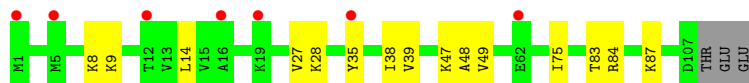
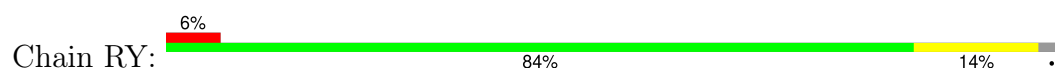
- Molecule 53: 50S ribosomal protein L23



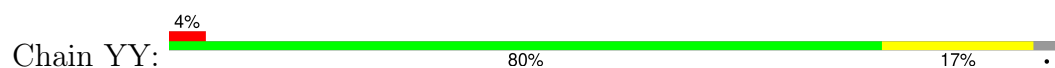
- Molecule 53: 50S ribosomal protein L23



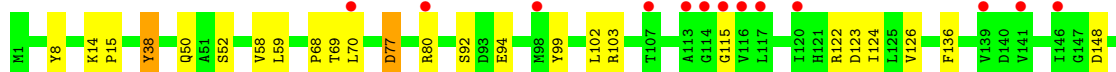
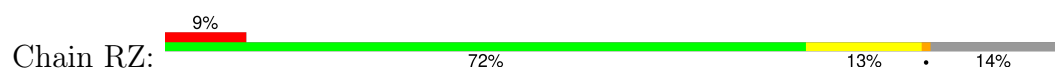
- Molecule 54: 50S ribosomal protein L24

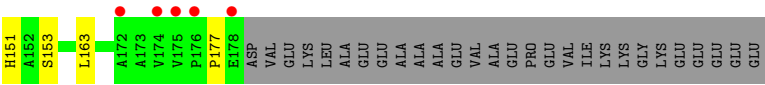


- Molecule 54: 50S ribosomal protein L24

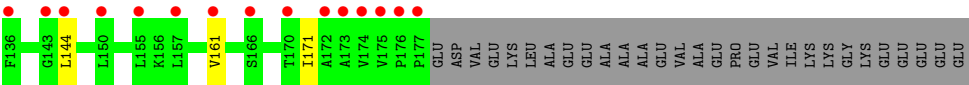
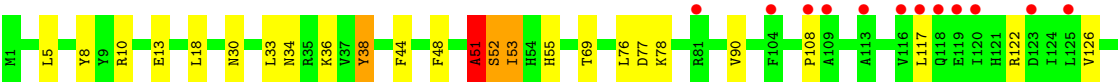
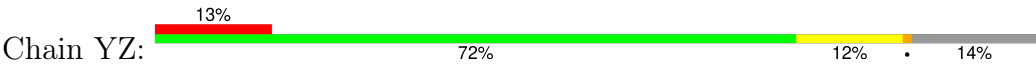


- Molecule 55: 50S ribosomal protein L25





● Molecule 55: 50S ribosomal protein L25



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.38Å 445.83Å 616.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.2 (50.00-3.10) 95.2 (50.00-3.10)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.231 , 0.268 0.231 , 0.267	Depositor DCC
R_{free} test set	48817 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	293819	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, 5MU, MA6, 5MC, SF4, ZN, OMG, PAR, UR3, 2MG, 4OC, M2G, MG, OMC, OMU, PSU, 0TD, 2MA

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	QA	0.37	0/35795	0.38	7/55864 (0.0%)
1	XA	0.39	0/35890	0.39	5/56012 (0.0%)
2	QB	0.41	0/1876	1.14	20/2533 (0.8%)
2	XB	0.40	0/1860	1.03	11/2518 (0.4%)
3	QC	0.35	0/1582	0.81	4/2137 (0.2%)
3	XC	0.42	0/1566	0.89	7/2119 (0.3%)
4	QD	0.48	0/1695	1.01	13/2274 (0.6%)
4	XD	0.43	0/1698	0.89	4/2277 (0.2%)
5	QE	0.36	0/1149	0.76	2/1548 (0.1%)
5	XE	0.38	0/1149	0.77	0/1548
6	QF	0.45	0/827	0.80	2/1120 (0.2%)
6	XF	0.45	0/829	0.80	1/1123 (0.1%)
7	QG	0.37	0/1254	0.86	3/1683 (0.2%)
7	XG	0.42	0/1248	0.87	6/1676 (0.4%)
8	QH	0.40	0/1118	0.85	2/1506 (0.1%)
8	XH	0.40	0/1108	0.84	4/1494 (0.3%)
9	QI	0.36	0/1005	0.97	7/1351 (0.5%)
9	XI	0.36	0/985	0.93	4/1329 (0.3%)
10	QJ	0.40	0/732	0.96	3/993 (0.3%)
10	XJ	0.43	0/723	0.85	2/984 (0.2%)
11	QK	0.38	0/849	0.79	2/1150 (0.2%)
11	XK	0.38	0/848	0.80	3/1149 (0.3%)
12	QL	0.49	0/937	1.03	4/1260 (0.3%)
12	XL	0.52	0/937	1.02	3/1260 (0.2%)
13	QM	0.38	0/924	1.03	9/1242 (0.7%)
13	XM	0.42	0/905	1.05	7/1217 (0.6%)
14	QN	0.37	0/501	0.80	0/664
14	XN	0.39	0/501	0.79	0/664
15	QO	0.41	0/739	0.91	4/985 (0.4%)
15	XO	0.40	0/739	0.90	3/985 (0.3%)
16	QP	0.41	0/697	0.99	5/939 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	XP	0.43	0/693	0.97	6/935 (0.6%)
17	QQ	0.42	0/836	0.82	1/1117 (0.1%)
17	XQ	0.40	0/836	0.85	2/1117 (0.2%)
18	QR	0.38	0/560	0.78	2/746 (0.3%)
18	XR	0.42	0/560	0.79	2/746 (0.3%)
19	QS	0.40	0/663	0.97	4/895 (0.4%)
19	XS	0.38	0/660	0.97	4/893 (0.4%)
20	QT	0.36	0/734	0.84	4/969 (0.4%)
20	XT	0.36	0/736	0.75	0/976
21	QU	0.32	0/203	0.67	0/266
21	XU	0.36	0/203	0.73	0/266
22	QV	0.33	0/1832	0.35	0/2855
22	XV	0.38	0/1832	0.38	0/2855
23	QX	0.31	0/443	0.51	0/690
23	XX	0.31	0/443	0.53	0/690
24	QY	0.28	0/1816	0.39	0/2830
24	XY	0.33	0/1816	0.42	0/2830
25	R0	0.44	0/616	0.93	2/821 (0.2%)
25	Y0	0.48	0/616	0.97	3/821 (0.4%)
26	R1	0.44	0/761	0.76	0/1013
26	Y1	0.47	0/766	0.78	2/1018 (0.2%)
27	R2	0.43	0/590	0.81	0/781
27	Y2	0.48	0/594	0.95	2/785 (0.3%)
28	R3	0.43	0/474	0.91	2/635 (0.3%)
28	Y3	0.48	0/469	0.90	1/630 (0.2%)
29	R4	0.46	0/559	1.22	6/754 (0.8%)
29	Y4	0.48	0/549	1.28	13/741 (1.8%)
30	R5	0.48	0/473	0.86	1/639 (0.2%)
30	Y5	0.48	0/469	0.78	0/635
31	R6	0.48	0/460	0.91	1/613 (0.2%)
31	Y6	0.50	0/456	0.89	2/608 (0.3%)
32	R7	0.49	0/426	0.92	1/561 (0.2%)
32	Y7	0.49	0/426	0.90	0/561
33	R8	0.46	0/525	0.76	0/691
33	Y8	0.50	0/525	0.75	0/691
34	R9	0.45	0/310	0.79	0/407
34	Y9	0.52	0/310	0.79	0/407
35	RA	0.42	0/68903	0.40	3/107552 (0.0%)
35	YA	0.47	0/68903	0.41	3/107552 (0.0%)
36	RB	0.37	0/2876	0.36	0/4486
36	YB	0.43	0/2878	0.38	0/4490
37	RD	0.49	0/2181	0.87	6/2940 (0.2%)
37	YD	0.52	0/2186	0.85	6/2944 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	RE	0.44	0/1592	0.89	3/2149 (0.1%)
38	YE	0.51	0/1592	0.91	5/2149 (0.2%)
39	RF	0.50	0/1618	0.94	8/2191 (0.4%)
39	YF	0.49	0/1614	0.91	3/2186 (0.1%)
40	RG	0.41	0/1451	0.92	8/1961 (0.4%)
40	YG	0.44	0/1449	0.87	5/1957 (0.3%)
41	RH	0.40	0/1356	0.86	4/1834 (0.2%)
41	YH	0.45	0/1350	0.78	4/1826 (0.2%)
42	RI	0.39	0/1109	0.90	6/1512 (0.4%)
42	YI	0.42	0/1091	0.80	1/1490 (0.1%)
43	RN	0.44	0/1148	0.78	3/1547 (0.2%)
43	YN	0.48	0/1144	0.80	1/1543 (0.1%)
44	RO	0.47	0/943	0.84	3/1269 (0.2%)
44	YO	0.51	0/943	0.82	0/1269
45	RP	0.45	0/1152	0.88	3/1533 (0.2%)
45	YP	0.51	0/1152	0.88	4/1533 (0.3%)
46	RQ	0.39	0/1143	0.77	0/1527
46	YQ	0.45	0/1143	0.80	0/1527
47	RR	0.45	0/982	0.84	0/1312
47	YR	0.48	0/982	0.85	1/1312 (0.1%)
48	RS	0.40	0/887	0.91	4/1180 (0.3%)
48	YS	0.44	0/880	0.84	1/1172 (0.1%)
49	RT	0.42	0/1105	0.81	2/1477 (0.1%)
49	YT	0.43	0/1097	0.83	2/1468 (0.1%)
50	RU	0.44	0/977	0.88	5/1301 (0.4%)
50	YU	0.49	0/977	0.92	7/1301 (0.5%)
51	RV	0.50	0/786	1.02	4/1053 (0.4%)
51	YV	0.49	0/782	0.88	3/1049 (0.3%)
52	RW	0.43	0/897	0.77	1/1205 (0.1%)
52	YW	0.47	0/897	0.75	1/1205 (0.1%)
53	RX	0.43	0/764	0.81	0/1025
53	YX	0.45	0/764	0.81	1/1025 (0.1%)
54	RY	0.41	0/823	0.85	0/1099
54	YY	0.48	0/823	0.89	0/1100
55	RZ	0.39	0/1438	0.95	6/1955 (0.3%)
55	YZ	0.43	0/1413	1.00	8/1924 (0.4%)
All	All	0.43	0/316097	0.57	333/473222 (0.1%)

There are no bond length outliers.

All (333) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	RV	49	THR	N-CA-C	-13.80	90.09	110.24
55	RZ	38	TYR	CA-CB-CG	11.45	134.50	113.90
2	QB	232	PRO	CA-C-N	11.02	152.25	120.97
2	QB	232	PRO	C-N-CA	11.02	152.25	120.97
13	XM	80	ARG	N-CA-C	-10.71	98.52	111.69
41	RH	101	ARG	N-CA-C	-10.62	100.45	113.41
2	QB	23	ARG	N-CA-C	-10.60	98.47	114.16
12	QL	119	LYS	N-CA-C	-10.42	93.73	110.20
13	QM	23	TYR	CA-CB-CG	10.26	132.37	113.90
50	YU	52	ARG	CG-CD-NE	10.05	134.11	112.00
29	Y4	68	ARG	N-CA-C	9.99	122.17	111.28
29	R4	52	THR	N-CA-C	-9.88	97.17	111.30
16	QP	38	TYR	CA-CB-CG	9.78	131.50	113.90
12	XL	119	LYS	N-CA-C	-9.70	93.66	109.96
37	YD	84	TYR	CA-CB-CG	9.65	131.27	113.90
8	XH	79	VAL	N-CA-C	-9.60	101.41	111.58
55	YZ	38	TYR	CA-CB-CG	9.58	131.15	113.90
50	RU	52	ARG	CG-CD-NE	9.39	132.66	112.00
50	YU	9	VAL	N-CA-C	9.26	119.86	110.23
2	QB	10	LEU	N-CA-C	-9.16	102.49	114.31
55	RZ	122	ARG	N-CA-C	-8.97	102.05	113.72
37	RD	84	TYR	CA-CB-CG	8.92	129.96	113.90
39	YF	64	ILE	N-CA-C	8.78	120.62	110.62
3	XC	39	ILE	N-CA-C	-8.69	101.94	110.72
13	XM	23	TYR	CA-CB-CG	8.59	129.36	113.90
16	XP	38	TYR	CA-CB-CG	8.32	128.87	113.90
25	R0	44	ARG	N-CA-C	-8.28	101.80	112.23
39	RF	99	TYR	CA-CB-CG	8.23	128.71	113.90
17	XQ	65	ILE	N-CA-C	-8.18	105.28	111.90
3	XC	125	GLU	N-CA-C	-7.99	103.67	113.50
50	RU	9	VAL	N-CA-C	7.98	118.53	110.23
8	QH	79	VAL	N-CA-C	-7.97	101.12	112.35
38	YE	69	LYS	N-CA-C	-7.83	102.82	111.36
13	XM	66	LEU	N-CA-C	7.70	122.81	111.34
40	RG	48	GLU	CA-C-N	7.64	136.13	121.54
40	RG	48	GLU	C-N-CA	7.64	136.13	121.54
2	XB	19	HIS	N-CA-C	7.49	120.30	107.93
4	QD	8	VAL	N-CA-C	7.49	121.59	113.43
39	RF	64	ILE	N-CA-C	7.35	119.00	110.62
2	QB	126	GLU	CA-C-N	7.32	135.15	121.97
2	QB	126	GLU	C-N-CA	7.32	135.15	121.97
9	QI	36	TYR	CA-CB-CG	7.29	127.03	113.90
12	QL	48	PRO	CA-C-N	7.29	135.46	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	QL	48	PRO	C-N-CA	7.29	135.46	121.54
45	RP	73	GLY	N-CA-C	7.27	118.90	111.56
39	YF	62	ARG	N-CA-C	-7.25	98.75	110.20
2	QB	190	THR	N-CA-C	7.21	120.01	111.71
45	RP	30	THR	N-CA-C	-7.21	105.67	114.75
19	QS	14	HIS	N-CA-C	-7.19	103.48	112.90
11	XK	116	HIS	CA-C-N	7.16	135.21	121.54
11	XK	116	HIS	C-N-CA	7.16	135.21	121.54
4	QD	196	LEU	N-CA-C	-7.15	100.78	110.36
45	YP	99	LEU	N-CA-C	-7.14	102.90	111.69
2	XB	23	ARG	N-CA-C	-7.13	101.82	111.87
9	QI	99	LEU	N-CA-C	-7.11	104.64	113.38
13	QM	11	ARG	N-CA-C	-7.10	101.37	110.53
9	XI	96	LEU	N-CA-C	-7.09	105.25	114.04
3	XC	21	ARG	N-CA-C	7.05	120.40	107.99
2	QB	8	LYS	CA-C-N	7.01	134.93	121.54
2	QB	8	LYS	C-N-CA	7.01	134.93	121.54
12	QL	87	GLY	N-CA-C	7.00	129.76	113.18
12	XL	48	PRO	N-CA-C	6.99	126.87	112.47
19	QS	34	TRP	N-CA-C	-6.92	103.23	113.61
42	RI	74	ASN	N-CA-C	-6.91	101.41	111.30
13	QM	15	VAL	N-CA-C	6.91	117.67	110.62
1	QA	266	G	P-O3'-C3'	6.89	130.54	120.20
9	QI	96	LEU	N-CA-C	-6.85	104.07	113.18
39	RF	32	LEU	N-CA-C	-6.84	103.91	111.36
29	Y4	58	ARG	N-CA-CB	6.83	122.03	110.49
41	RH	9	ILE	N-CA-C	6.81	113.75	107.56
3	XC	29	TYR	CA-CB-CG	6.80	126.14	113.90
51	RV	12	TYR	CA-CB-CG	6.78	126.10	113.90
4	XD	8	VAL	N-CA-C	6.77	117.38	111.90
45	YP	71	VAL	N-CA-C	6.74	122.38	112.61
3	QC	19	GLU	N-CA-C	-6.72	105.09	113.28
55	YZ	51	ALA	CA-C-N	6.71	134.36	121.54
55	YZ	51	ALA	C-N-CA	6.71	134.36	121.54
17	QQ	65	ILE	N-CA-C	-6.70	106.26	112.96
15	XO	12	ILE	N-CA-C	-6.68	103.97	110.72
29	Y4	57	GLU	CA-C-N	6.64	134.23	121.54
29	Y4	57	GLU	C-N-CA	6.64	134.23	121.54
26	Y1	3	LYS	N-CA-C	6.64	118.74	109.31
55	YZ	171	ILE	N-CA-C	6.64	119.60	112.96
11	XK	40	ILE	N-CA-C	-6.59	106.41	111.62
1	XA	266	G	P-O3'-C3'	6.58	130.08	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	RN	114	ARG	N-CA-C	-6.58	105.07	113.23
38	RE	144	ARG	N-CA-CB	6.58	116.22	109.51
2	XB	19	HIS	CA-C-N	6.57	134.09	121.54
2	XB	19	HIS	C-N-CA	6.57	134.09	121.54
1	QA	266	G	C2'-C3'-O3'	6.49	119.24	109.50
41	RH	46	GLU	N-CA-C	-6.49	100.27	108.45
40	RG	47	LYS	CA-C-N	6.49	133.93	121.54
40	RG	47	LYS	C-N-CA	6.49	133.93	121.54
30	R5	59	GLU	N-CA-C	-6.48	98.71	109.46
19	XS	27	GLU	N-CA-C	6.46	119.27	108.73
29	R4	57	GLU	CA-C-N	6.46	133.87	121.54
29	R4	57	GLU	C-N-CA	6.46	133.87	121.54
12	XL	87	GLY	N-CA-C	6.43	128.42	113.18
16	XP	5	ARG	N-CA-C	6.41	116.74	108.34
55	YZ	122	ARG	N-CA-C	-6.39	105.30	113.23
50	YU	52	ARG	CD-NE-CZ	6.39	133.34	124.40
15	QO	12	ILE	N-CA-C	-6.38	104.28	110.72
3	QC	29	TYR	CA-CB-CG	6.37	125.37	113.90
15	QO	65	ARG	N-CA-C	-6.37	104.41	111.36
1	XA	266	G	C2'-C3'-O3'	6.37	119.05	109.50
45	YP	69	GLY	N-CA-C	6.34	117.97	111.95
19	XS	67	VAL	N-CA-C	6.33	116.96	110.82
9	QI	41	VAL	N-CA-C	-6.32	103.74	113.16
4	QD	185	PHE	CA-CB-CG	6.30	120.10	113.80
35	YA	272(M)	G	P-O3'-C3'	6.30	127.26	119.70
2	QB	23	ARG	CA-C-N	6.29	132.15	120.95
2	QB	23	ARG	C-N-CA	6.29	132.15	120.95
13	XM	11	ARG	N-CA-C	6.29	118.94	111.71
7	XG	69	VAL	N-CA-C	-6.29	107.12	113.47
1	QA	1442(A)	G	P-O3'-C3'	6.28	127.24	119.70
45	RP	71	VAL	N-CA-C	6.25	119.85	112.35
48	RS	20	ARG	N-CA-C	6.25	118.09	111.28
37	YD	71	ASP	N-CA-C	-6.24	104.02	111.69
3	XC	36	ASP	N-CA-C	-6.23	104.57	111.36
41	YH	101	ARG	N-CA-C	-6.23	106.00	113.97
10	QJ	31	GLY	CA-C-N	6.22	133.42	121.54
10	QJ	31	GLY	C-N-CA	6.22	133.42	121.54
35	RA	272(M)	G	P-O3'-C3'	6.20	127.14	119.70
25	Y0	44	ARG	N-CA-C	-6.20	104.42	112.23
40	YG	80	PHE	N-CA-C	-6.19	99.19	109.46
7	XG	77	SER	N-CA-C	6.18	118.76	110.35
6	QF	63	TYR	CA-CB-CG	6.18	125.03	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	YF	105	VAL	N-CA-C	-6.17	104.28	111.00
45	YP	30	THR	N-CA-C	-6.17	106.98	114.75
27	Y2	20	GLU	N-CA-C	-6.17	104.82	112.90
42	RI	84	GLY	CA-C-N	6.16	133.31	121.54
42	RI	84	GLY	C-N-CA	6.16	133.31	121.54
3	XC	201	TYR	CA-CB-CG	6.16	124.99	113.90
4	QD	5	ILE	N-CA-C	6.16	122.14	109.34
4	XD	204	ILE	N-CA-C	-6.14	104.52	110.72
2	QB	15	VAL	CA-C-N	6.13	133.26	121.54
2	QB	15	VAL	C-N-CA	6.13	133.26	121.54
35	RA	272(M)	G	OP1-P-O3'	6.13	118.68	105.20
37	RD	71	ASP	N-CA-C	-6.12	104.16	111.69
20	QT	11	SER	N-CA-C	-6.12	105.58	113.16
49	YT	93	ARG	N-CA-C	6.08	118.63	108.73
1	XA	1442(A)	G	P-O3'-C3'	6.07	126.99	119.70
7	XG	114	ARG	N-CA-C	6.04	118.77	111.40
19	QS	36	ARG	N-CA-C	-6.03	105.92	113.28
2	XB	185	ILE	N-CA-C	-6.03	99.73	108.71
37	RD	53	PHE	N-CA-C	6.02	119.94	111.52
35	YA	272(M)	G	OP1-P-O3'	6.02	118.44	105.20
18	QR	70	ILE	N-CA-C	-5.99	104.67	110.72
2	QB	16	HIS	N-CA-C	5.97	123.53	110.80
51	RV	2	PHE	N-CA-CB	5.97	119.67	110.60
16	QP	20	VAL	N-CA-C	5.96	116.95	108.42
4	QD	138	TYR	CA-CB-CG	5.95	124.61	113.90
29	Y4	45	GLY	CA-C-N	5.95	132.90	121.54
29	Y4	45	GLY	C-N-CA	5.95	132.90	121.54
55	YZ	48	PHE	N-CA-C	5.92	117.74	111.28
7	XG	22	LEU	N-CA-C	-5.92	104.78	112.23
9	XI	87	GLN	N-CA-C	-5.90	104.79	112.23
48	RS	59	LYS	N-CA-C	5.90	120.27	112.72
7	XG	45	ASP	N-CA-C	-5.86	104.84	112.23
40	YG	128	ARG	N-CA-C	-5.86	105.78	113.17
50	RU	52	ARG	CD-NE-CZ	5.85	132.59	124.40
50	YU	52	ARG	CB-CG-CD	5.85	124.75	111.30
40	YG	95	ARG	CA-C-N	5.84	132.70	121.54
40	YG	95	ARG	C-N-CA	5.84	132.70	121.54
8	QH	103	VAL	N-CA-C	5.83	116.54	108.84
13	QM	105	THR	CA-C-N	5.83	132.68	121.54
13	QM	105	THR	C-N-CA	5.83	132.68	121.54
29	Y4	43	TYR	CA-CB-CG	5.82	124.38	113.90
4	QD	186	LEU	N-CA-C	5.82	117.49	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	QO	6	GLU	N-CA-C	5.81	117.29	111.07
4	QD	63	LYS	N-CA-C	-5.80	104.59	111.03
29	Y4	52	THR	N-CA-C	-5.79	106.22	113.28
7	QG	91	VAL	N-CA-C	5.79	117.04	109.58
44	RO	94	ARG	N-CA-C	-5.78	106.23	113.28
6	XF	63	TYR	CA-CB-CG	5.77	124.28	113.90
50	YU	50	ARG	N-CA-C	-5.77	104.96	112.23
19	XS	6	LYS	N-CA-C	-5.76	105.08	111.36
7	QG	30	ILE	N-CA-C	-5.75	103.73	111.44
3	QC	201	TYR	CA-CB-CG	5.75	124.25	113.90
29	R4	58	ARG	N-CA-C	5.73	123.01	110.80
2	XB	17	PHE	N-CA-C	5.72	119.08	111.75
39	RF	9	ILE	N-CA-C	5.72	114.12	107.89
39	RF	196	LEU	N-CA-C	-5.71	105.03	112.23
13	XM	15	VAL	N-CA-C	5.69	118.17	111.05
43	YN	51	PHE	N-CA-C	-5.68	99.97	109.24
40	RG	128	ARG	N-CA-C	-5.66	106.42	113.38
50	RU	51	LYS	N-CA-C	-5.66	104.58	112.45
27	Y2	9	GLN	N-CA-C	-5.65	105.20	111.36
52	RW	99	ARG	N-CA-C	5.65	117.99	110.53
31	Y6	7	ILE	N-CA-C	5.64	116.20	110.05
48	YS	111	GLU	N-CA-C	5.64	117.97	107.99
40	YG	95	ARG	N-CA-C	-5.64	100.22	109.80
35	YA	1065	U	P-O3'-C3'	5.63	128.65	120.20
41	YH	59	ARG	N-CA-C	5.63	117.42	111.28
15	XO	45	VAL	N-CA-C	-5.63	106.21	111.45
20	QT	13	LEU	N-CA-C	-5.63	105.23	111.36
40	RG	96	ARG	N-CA-C	5.63	122.79	110.80
49	RT	121	ILE	N-CA-C	-5.63	104.86	111.00
15	XO	83	GLU	N-CA-C	-5.62	104.77	111.69
38	YE	72	VAL	N-CA-C	5.62	117.77	108.99
37	YD	10	THR	N-CA-C	-5.62	99.78	108.55
43	RN	51	PHE	N-CA-C	-5.61	101.33	110.20
4	QD	178	VAL	CA-C-N	5.59	132.22	121.54
4	QD	178	VAL	C-N-CA	5.59	132.22	121.54
4	QD	156	GLU	N-CA-C	5.58	117.37	111.28
38	RE	76	ARG	N-CA-C	5.57	118.19	111.40
16	XP	33	ILE	N-CA-C	5.54	115.63	110.42
16	QP	5	ARG	N-CA-C	5.54	115.59	108.34
49	YT	7	ILE	N-CA-C	-5.53	105.46	110.82
4	QD	163	GLU	N-CA-C	-5.52	105.28	112.23
18	QR	31	LEU	N-CA-C	-5.52	105.28	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	YD	257	LEU	N-CA-C	5.51	117.08	109.15
16	XP	20	VAL	N-CA-C	5.50	116.28	108.42
16	XP	27	LYS	N-CA-C	-5.47	103.16	110.55
41	YH	129	THR	N-CA-C	-5.47	107.15	113.88
26	Y1	72	GLU	N-CA-C	-5.47	105.40	111.36
35	RA	1065	U	P-O3'-C3'	5.47	128.40	120.20
39	RF	183	VAL	N-CA-C	5.47	116.19	110.62
29	R4	49	PHE	CB-CA-C	-5.46	101.77	110.84
51	YV	50	PRO	CA-C-N	5.45	129.26	121.96
51	YV	50	PRO	C-N-CA	5.45	129.26	121.96
37	RD	50	THR	N-CA-C	-5.44	106.32	113.12
10	QJ	92	THR	N-CA-C	5.44	117.02	111.14
5	QE	26	PHE	N-CA-C	5.42	117.87	110.55
25	Y0	40	GLN	N-CA-C	5.42	116.51	108.60
29	Y4	67	TYR	CA-CB-CG	5.42	123.65	113.90
43	RN	23	LEU	N-CA-C	5.42	116.87	110.97
2	QB	78	GLN	N-CA-C	5.41	117.18	111.28
8	XH	37	ARG	N-CA-C	-5.41	105.42	112.23
42	RI	31	LEU	N-CA-C	5.41	120.84	113.16
50	RU	40	PHE	N-CA-C	-5.40	105.47	111.36
37	YD	99	ASP	N-CA-C	-5.40	106.19	112.89
2	QB	187	LEU	N-CA-C	-5.39	100.38	108.96
28	R3	31	LEU	N-CA-C	-5.37	102.53	110.48
29	Y4	46	GLN	CA-C-N	5.37	131.80	121.54
29	Y4	46	GLN	C-N-CA	5.37	131.80	121.54
37	YD	53	PHE	N-CA-C	5.36	118.64	111.24
7	QG	114	ARG	N-CA-C	5.36	117.20	111.36
55	RZ	50	GLN	N-CA-C	-5.36	107.40	114.31
1	QA	1067	A	P-O3'-C3'	5.36	128.23	120.20
3	XC	17	ASP	N-CA-C	-5.36	102.53	110.46
9	XI	70	LYS	N-CA-C	5.36	120.15	111.37
37	RD	99	ASP	N-CA-C	-5.35	106.25	112.89
47	YR	2	ARG	N-CA-C	-5.35	105.03	112.03
52	YW	99	ARG	N-CA-C	5.34	117.43	110.43
17	XQ	42	TYR	CA-CB-CG	5.34	123.51	113.90
11	QK	40	ILE	N-CA-C	-5.33	106.98	111.56
13	QM	66	LEU	N-CA-C	5.33	116.88	109.31
44	RO	9	GLU	N-CA-C	-5.33	103.36	110.55
55	RZ	148	ASP	N-CA-C	-5.32	102.87	110.59
1	XA	1067	A	P-O3'-C3'	5.32	128.19	120.20
41	RH	163	TYR	CA-CB-CG	5.32	123.48	113.90
3	QC	161	GLU	N-CA-C	-5.31	105.66	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	YU	40	PHE	N-CA-C	-5.31	105.58	111.36
4	QD	140	VAL	N-CA-C	-5.31	101.99	109.21
9	QI	48	GLU	N-CA-C	5.30	120.89	113.57
39	RF	190	GLU	N-CA-C	-5.30	106.65	113.23
32	R7	30	VAL	N-CA-C	-5.30	105.55	110.53
9	QI	64	THR	N-CA-C	-5.29	101.54	109.95
16	QP	32	TYR	CA-CB-CG	5.27	123.39	113.90
2	QB	22	LYS	CA-C-N	5.27	129.29	120.70
2	QB	22	LYS	C-N-CA	5.27	129.29	120.70
50	YU	29	SER	N-CA-C	-5.27	107.51	114.31
37	RD	10	THR	N-CA-C	-5.26	100.34	108.55
20	QT	55	ILE	N-CA-C	-5.25	105.41	110.72
51	RV	46	VAL	N-CA-C	5.25	115.42	107.80
41	YH	110	SER	N-CA-C	-5.25	106.46	112.92
4	XD	116	GLN	N-CA-C	-5.25	105.23	111.69
18	XR	31	LEU	N-CA-C	-5.24	106.73	113.23
40	RG	109	VAL	N-CA-C	5.23	116.06	111.56
53	YX	69	TYR	N-CA-C	5.23	116.78	108.67
5	QE	111	GLU	N-CA-C	-5.22	105.27	111.69
2	QB	20	GLU	N-CA-C	5.22	121.91	110.80
29	R4	68	ARG	N-CA-C	5.21	118.31	109.76
42	RI	89	TYR	N-CA-C	-5.21	105.51	111.14
28	Y3	56	VAL	N-CA-C	5.21	115.46	108.17
55	YZ	77	ASP	N-CA-C	-5.20	101.66	109.15
2	XB	129	GLU	CA-C-N	5.20	138.47	122.71
2	XB	129	GLU	C-N-CA	5.20	138.47	122.71
19	XS	34	TRP	N-CA-C	-5.20	105.61	112.94
42	RI	68	LEU	N-CA-C	-5.20	105.69	112.23
51	YV	2	PHE	N-CA-C	-5.19	101.53	109.41
10	XJ	34	VAL	N-CA-C	5.18	115.56	107.99
15	QO	45	VAL	N-CA-C	-5.18	106.03	110.74
39	RF	127	GLU	N-CA-C	-5.17	105.26	112.45
55	RZ	59	LEU	N-CA-C	5.17	117.18	108.96
19	QS	11	VAL	N-CA-C	-5.17	100.80	108.45
25	R0	40	GLN	N-CA-C	5.17	116.66	108.96
48	RS	34	HIS	N-CA-C	5.15	117.10	109.69
29	Y4	25	TYR	CA-CB-CG	5.14	123.16	113.90
2	QB	12	GLU	N-CA-C	-5.14	106.25	112.88
13	XM	65	LYS	N-CA-C	-5.14	102.08	110.20
38	RE	12	THR	N-CA-C	-5.14	101.97	108.45
13	XM	5	ALA	N-CA-C	5.14	121.74	110.80
11	QK	102	GLY	N-CA-C	-5.13	107.59	116.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Y6	28	ARG	N-CA-C	-5.13	105.38	111.69
44	RO	113	LYS	N-CA-C	-5.12	105.77	111.36
1	QA	1065	U	P-O3'-C3'	5.11	127.87	120.20
9	QI	70	LYS	N-CA-C	5.11	117.24	111.11
1	QA	991	U	P-O3'-C3'	5.11	127.86	120.20
9	XI	51	ARG	N-CA-C	-5.10	106.90	113.23
25	Y0	39	ARG	N-CA-C	-5.10	100.42	108.73
55	YZ	53	ILE	N-CA-C	-5.10	106.61	112.98
1	XA	1065	U	P-O3'-C3'	5.10	127.85	120.20
18	XR	22	VAL	N-CA-C	-5.09	105.57	113.16
4	QD	204	ILE	N-CA-C	-5.09	105.58	110.72
42	YI	126	TYR	CA-CB-CG	5.09	123.06	113.90
29	Y4	49	PHE	N-CA-C	5.09	121.64	110.80
16	XP	53	VAL	N-CA-C	5.08	117.44	111.09
31	R6	9	LEU	N-CA-C	5.08	115.75	108.74
1	QA	687	A	P-O3'-C3'	5.07	127.81	120.20
38	YE	61	ARG	N-CA-C	5.07	120.50	113.45
28	R3	54	VAL	N-CA-C	5.06	115.20	108.11
13	QM	66	LEU	CA-C-N	5.06	129.24	121.19
13	QM	66	LEU	C-N-CA	5.06	129.24	121.19
49	RT	12	SER	N-CA-C	5.05	117.52	111.71
4	XD	38	TYR	CA-CB-CG	5.05	122.99	113.90
55	RZ	77	ASP	N-CA-C	-5.05	100.85	108.67
6	QF	65	VAL	N-CA-C	5.04	116.12	108.96
20	QT	93	GLU	N-CA-C	-5.04	105.97	111.82
8	XH	100	ILE	N-CA-C	-5.04	104.01	108.95
13	QM	23	TYR	CB-CA-C	5.04	117.42	110.16
2	XB	127	ILE	CA-C-N	5.04	131.16	121.54
2	XB	127	ILE	C-N-CA	5.04	131.16	121.54
38	YE	202	LYS	N-CA-C	-5.03	106.56	113.30
8	XH	103	VAL	N-CA-C	5.03	115.48	108.84
38	YE	102	VAL	N-CA-C	5.02	117.23	108.95
2	XB	87	ARG	N-CA-C	-5.02	106.00	111.82
10	XJ	50	ILE	N-CA-C	-5.02	103.02	109.30
16	QP	9	PHE	N-CA-C	-5.02	102.13	109.81
40	RG	107	LEU	N-CA-C	5.01	117.48	111.71
48	RS	54	LEU	N-CA-C	-5.01	105.53	111.69
7	XG	89	MET	N-CA-C	5.01	117.57	109.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32246	0	16295	176	0
1	XA	32331	0	16337	186	0
2	QB	1842	0	1861	27	0
2	XB	1825	0	1828	23	0
3	QC	1558	0	1557	29	0
3	XC	1542	0	1517	16	0
4	QD	1665	0	1691	35	0
4	XD	1668	0	1707	26	0
5	QE	1133	0	1191	16	0
5	XE	1133	0	1191	14	0
6	QF	814	0	808	8	0
6	XF	816	0	808	20	0
7	QG	1235	0	1249	17	0
7	XG	1229	0	1238	11	0
8	QH	1098	0	1143	18	0
8	XH	1088	0	1126	14	0
9	QI	986	0	990	25	0
9	XI	966	0	953	25	0
10	QJ	719	0	672	10	0
10	XJ	710	0	661	15	0
11	QK	834	0	838	12	0
11	XK	833	0	836	12	0
12	QL	932	0	981	17	0
12	XL	932	0	981	11	0
13	QM	914	0	954	14	0
13	XM	895	0	920	23	0
14	QN	492	0	529	11	0
14	XN	492	0	529	11	0
15	QO	728	0	760	2	0
15	XO	728	0	760	3	0
16	QP	681	0	697	20	0
16	XP	677	0	686	22	0
17	QQ	823	0	891	10	0
17	XQ	823	0	891	10	0
18	QR	555	0	618	5	0
18	XR	555	0	618	12	0
19	QS	648	0	658	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XS	645	0	635	17	0
20	QT	732	0	809	9	0
20	XT	733	0	795	9	0
21	QU	199	0	208	1	0
21	XU	199	0	208	0	0
22	QV	1640	0	837	6	0
22	XV	1640	0	837	7	0
23	QX	394	0	197	1	0
23	XX	394	0	197	1	0
24	QY	1625	0	822	5	0
24	XY	1625	0	822	7	0
25	R0	608	0	622	8	0
25	Y0	608	0	622	12	0
26	R1	754	0	823	10	0
26	Y1	759	0	837	7	0
27	R2	588	0	643	8	0
27	Y2	592	0	654	6	0
28	R3	469	0	518	2	0
28	Y3	464	0	514	8	0
29	R4	546	0	522	9	0
29	Y4	536	0	514	12	0
30	R5	459	0	476	8	0
30	Y5	455	0	465	6	0
31	R6	453	0	473	2	0
31	Y6	449	0	469	3	0
32	R7	418	0	466	5	0
32	Y7	418	0	466	4	0
33	R8	517	0	582	16	0
33	Y8	517	0	582	12	0
34	R9	307	0	335	5	0
34	Y9	307	0	335	8	0
35	RA	61758	0	31137	286	0
35	YA	61758	0	31138	275	0
36	RB	2572	0	1304	3	0
36	YB	2573	0	1306	7	0
37	RD	2131	0	2205	41	0
37	YD	2136	0	2217	44	0
38	RE	1559	0	1618	21	0
38	YE	1559	0	1618	35	0
39	RF	1583	0	1624	43	0
39	YF	1579	0	1618	29	0
40	RG	1426	0	1445	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	YG	1424	0	1441	22	0
41	RH	1330	0	1407	16	0
41	YH	1324	0	1402	14	0
42	RI	1094	0	1127	5	0
42	YI	1076	0	1094	4	0
43	RN	1121	0	1195	16	0
43	YN	1117	0	1184	9	0
44	RO	933	0	996	19	0
44	YO	933	0	996	18	0
45	RP	1135	0	1212	22	0
45	YP	1135	0	1212	24	0
46	RQ	1122	0	1179	18	0
46	YQ	1122	0	1179	14	0
47	RR	968	0	1033	10	0
47	YR	968	0	1033	12	0
48	RS	877	0	938	10	0
48	YS	870	0	923	8	0
49	RT	1091	0	1151	17	0
49	YT	1083	0	1136	15	0
50	RU	959	0	1019	15	0
50	YU	959	0	1019	11	0
51	RV	775	0	841	15	0
51	YV	771	0	830	8	0
52	RW	886	0	940	9	0
52	YW	886	0	940	9	0
53	RX	750	0	814	11	0
53	YX	750	0	814	6	0
54	RY	810	0	892	10	0
54	YY	810	0	887	14	0
55	RZ	1406	0	1418	17	0
55	YZ	1381	0	1386	15	0
56	QA	221	0	0	0	0
56	QB	1	0	0	0	0
56	QD	4	0	0	0	0
56	QE	4	0	0	0	0
56	QF	2	0	0	0	0
56	QG	2	0	0	0	0
56	QH	2	0	0	0	0
56	QI	1	0	0	0	0
56	QK	1	0	0	0	0
56	QL	3	0	0	0	0
56	QN	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	QO	2	0	0	0	0
56	QP	1	0	0	0	0
56	QT	1	0	0	0	0
56	QV	5	0	0	0	0
56	R0	3	0	0	0	0
56	R1	1	0	0	0	0
56	R3	3	0	0	0	0
56	R5	2	0	0	0	0
56	R6	1	0	0	0	0
56	R7	3	0	0	0	0
56	R9	1	0	0	0	0
56	RA	709	0	0	0	0
56	RB	17	0	0	0	0
56	RD	8	0	0	0	0
56	RE	4	0	0	0	0
56	RF	4	0	0	0	0
56	RG	4	0	0	0	0
56	RH	2	0	0	0	0
56	RN	2	0	0	0	0
56	RO	1	0	0	0	0
56	RP	3	0	0	0	0
56	RQ	4	0	0	0	0
56	RR	2	0	0	0	0
56	RT	4	0	0	0	0
56	RU	2	0	0	0	0
56	RV	3	0	0	0	0
56	RW	1	0	0	0	0
56	RZ	1	0	0	0	0
56	XA	193	0	0	0	0
56	XE	2	0	0	0	0
56	XF	2	0	0	0	0
56	XJ	1	0	0	0	0
56	XL	2	0	0	0	0
56	XR	1	0	0	0	0
56	XT	1	0	0	0	0
56	XV	3	0	0	0	0
56	XY	1	0	0	0	0
56	Y0	1	0	0	0	0
56	Y1	2	0	0	0	0
56	Y3	1	0	0	0	0
56	Y5	1	0	0	0	0
56	Y6	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	Y7	2	0	0	0	0
56	Y8	1	0	0	0	0
56	YA	707	0	0	0	0
56	YB	20	0	0	0	0
56	YD	7	0	0	0	0
56	YE	5	0	0	0	0
56	YF	3	0	0	0	0
56	YG	3	0	0	0	0
56	YI	1	0	0	0	0
56	YN	1	0	0	0	0
56	YO	1	0	0	0	0
56	YP	2	0	0	0	0
56	YQ	2	0	0	0	0
56	YR	2	0	0	0	0
56	YT	3	0	0	0	0
56	YV	1	0	0	0	0
56	YW	2	0	0	0	0
57	QA	42	0	45	1	0
57	XA	42	0	45	2	0
58	QD	8	0	0	0	0
58	XD	8	0	0	1	0
59	QN	1	0	0	0	0
59	R4	1	0	0	0	0
59	R5	1	0	0	0	0
59	R6	1	0	0	0	0
59	R9	1	0	0	0	0
59	RY	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y4	1	0	0	0	0
59	Y5	1	0	0	0	0
59	Y6	1	0	0	0	0
59	Y9	1	0	0	0	0
59	YY	1	0	0	0	0
All	All	293819	0	196213	1818	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (1818) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:RZ:8:TYR:HB2	55:RZ:38:TYR:CE1	1.78	1.17
16:QP:20:VAL:HG21	16:QP:32:TYR:HD2	1.09	1.13
55:RZ:8:TYR:HB2	55:RZ:38:TYR:CD1	1.90	1.07
35:RA:660:G:H5'	39:RF:99:TYR:CE2	1.94	1.03
16:QP:20:VAL:HG21	16:QP:32:TYR:CD2	1.94	1.02
4:QD:38:TYR:HE2	4:QD:45:GLN:HG2	1.26	1.00
16:XP:20:VAL:HG21	16:XP:32:TYR:CD2	1.96	0.99
3:QC:159:GLY:N	3:QC:193:TYR:HE2	1.60	0.99
35:RA:660:G:C5'	39:RF:99:TYR:CE2	2.47	0.97
35:RA:660:G:C5'	39:RF:99:TYR:HE2	1.78	0.95
35:YA:2604:U:H5''	35:YA:2604:U:H6	1.31	0.94
16:XP:20:VAL:HG21	16:XP:32:TYR:HD2	1.30	0.94
16:QP:38:TYR:CD1	16:QP:50:LYS:HB3	2.04	0.91
55:RZ:8:TYR:CB	55:RZ:38:TYR:CE1	2.56	0.87
35:YA:1567:A:C5	37:YD:84:TYR:HE2	1.92	0.87
35:RA:528:A:H2	43:RN:114:ARG:NH2	1.72	0.86
16:QP:38:TYR:CE1	16:QP:50:LYS:HB3	2.12	0.85
3:QC:159:GLY:HA2	3:QC:193:TYR:CE2	2.11	0.85
38:YE:84:PHE:CD2	38:YE:86:PRO:HD3	2.11	0.84
19:XS:41:VAL:CG2	19:XS:43:GLU:OE1	2.25	0.84
35:RA:528:A:H2	43:RN:114:ARG:HH21	1.21	0.83
35:YA:1567:A:C5	37:YD:84:TYR:CE2	2.68	0.82
19:XS:41:VAL:HB	19:XS:43:GLU:OE1	1.80	0.82
3:QC:159:GLY:CA	3:QC:193:TYR:HE2	1.92	0.81
35:RA:660:G:H4'	39:RF:99:TYR:HE2	1.45	0.80
35:RA:660:G:H5'	39:RF:99:TYR:CD2	2.17	0.79
19:XS:41:VAL:HG23	19:XS:43:GLU:OE1	1.80	0.79
3:QC:159:GLY:HA2	3:QC:193:TYR:CD2	2.18	0.79
35:YA:1567:A:N7	37:YD:84:TYR:HE2	1.80	0.79
1:QA:1422:G:H5''	44:RO:48:PRO:HB3	1.65	0.79
4:QD:98:GLU:OE1	4:QD:189:PRO:CG	2.30	0.78
39:RF:39:TRP:HA	39:RF:99:TYR:HE1	1.48	0.78
1:XA:1330:U:H4'	13:XM:23:TYR:CD1	2.17	0.78
4:QD:38:TYR:CE2	4:QD:45:GLN:HG2	2.15	0.78
1:QA:1330:U:H4'	13:QM:23:TYR:CD1	2.18	0.77
50:RU:49:HIS:HA	50:RU:52:ARG:HB3	1.66	0.77
4:QD:98:GLU:OE2	4:QD:194:LEU:HD23	1.83	0.77
55:RZ:8:TYR:CB	55:RZ:38:TYR:HE1	1.97	0.77
1:QA:626:U:H4'	16:QP:38:TYR:CE2	2.20	0.76
16:QP:38:TYR:CE1	16:QP:50:LYS:CB	2.69	0.76
29:Y4:11:PRO:HG3	29:Y4:25:TYR:CE2	2.21	0.76
35:YA:2604:U:H5''	35:YA:2604:U:C6	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:QC:159:GLY:H	3:QC:193:TYR:HE2	1.33	0.75
1:QA:626:U:H4'	16:QP:38:TYR:HE2	1.51	0.74
19:XS:43:GLU:OE1	19:XS:43:GLU:N	2.20	0.74
3:QC:159:GLY:CA	3:QC:193:TYR:CE2	2.69	0.74
19:XS:41:VAL:CB	19:XS:43:GLU:OE1	2.35	0.74
35:RA:660:G:C4'	39:RF:99:TYR:HE2	2.00	0.74
50:YU:49:HIS:HA	50:YU:52:ARG:HB3	1.70	0.74
1:XA:1043:C:OP1	1:XA:1043:C:H4'	1.87	0.74
1:QA:1086:U:H3	1:QA:1099:G:H22	1.36	0.73
3:QC:184:TYR:HE1	3:QC:201:TYR:HE1	1.36	0.73
1:XA:626:U:H4'	16:XP:38:TYR:CE2	2.24	0.73
1:XA:501:C:OP1	12:XL:117:ARG:NH2	2.22	0.72
4:QD:98:GLU:OE1	4:QD:189:PRO:HG3	1.90	0.72
38:YE:84:PHE:CE2	38:YE:86:PRO:HD3	2.24	0.72
41:RH:154:PRO:HB3	41:RH:163:TYR:CE1	2.24	0.72
1:XA:1422:G:H5''	44:YO:48:PRO:HB3	1.71	0.71
1:XA:1393:U:HO2'	1:XA:1501:C:HO2'	1.39	0.71
4:QD:68:TYR:HE2	4:QD:103:ASN:ND2	1.88	0.71
48:YS:25:ARG:NH1	48:YS:88:ASP:OD2	2.22	0.71
3:QC:184:TYR:CE1	3:QC:201:TYR:CE1	2.79	0.71
1:XA:1249:C:O2'	9:XI:73:GLN:NE2	2.24	0.70
6:XF:50:TYR:HE1	18:XR:77:GLY:HA2	1.55	0.70
35:YA:1041:C:H42	35:YA:1114:G:H1	1.39	0.70
3:QC:159:GLY:N	3:QC:193:TYR:CE2	2.53	0.70
10:QJ:10:GLY:HA3	10:QJ:16:LEU:HD21	1.72	0.70
16:QP:38:TYR:HE1	16:QP:50:LYS:HB2	1.55	0.70
24:QY:4:G:H1	24:QY:69:C:H42	1.37	0.70
35:RA:2131:G:H5''	35:RA:2132:U:H5'	1.74	0.70
1:XA:664:G:H22	1:XA:741:G:H1	1.38	0.69
1:QA:236:G:H5''	17:QQ:42:TYR:OH	1.92	0.69
40:RG:47:LYS:NZ	40:RG:80:PHE:O	2.25	0.69
1:QA:559:A:H4'	1:QA:560:U:H3'	1.72	0.69
2:QB:185:ILE:HG22	2:QB:199:TYR:HB2	1.74	0.69
16:QP:5:ARG:HH12	16:QP:28:ARG:HA	1.56	0.69
35:RA:528:A:C2	43:RN:114:ARG:NH2	2.60	0.69
35:RA:660:G:C5'	39:RF:99:TYR:CD2	2.76	0.69
1:QA:544:G:OP1	4:QD:59:ARG:NH2	2.25	0.69
1:XA:544:G:OP1	4:XD:59:ARG:NH2	2.26	0.69
35:RA:881:G:H1	35:RA:895:U:H3	1.39	0.69
33:Y8:30:ARG:HH21	45:YP:63:PRO:HB2	1.57	0.69
35:YA:1056:G:H21	35:YA:1103:A:H62	1.39	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:XB:122:PHE:HE2	2:XB:139:LYS:HD3	1.58	0.68
1:QA:429:U:OP1	4:QD:13:ARG:NH1	2.27	0.68
16:QP:38:TYR:HE1	16:QP:50:LYS:CB	2.07	0.68
1:XA:1130:A:O2'	9:XI:3:GLN:NE2	2.26	0.68
27:R2:66:GLU:HA	27:R2:69:ARG:HD3	1.76	0.67
44:RO:35:VAL:HG11	44:RO:103:ALA:HB3	1.76	0.67
35:RA:83:G:H1	35:RA:102:G:HO2'	1.41	0.67
35:RA:1153:C:OP1	50:RU:92:ARG:NH2	2.25	0.67
51:YV:21:ARG:NE	51:YV:91:TYR:HE2	1.93	0.67
1:QA:1295:G:O2'	13:QM:14:ARG:NH1	2.27	0.67
2:QB:8:LYS:O	2:QB:217:ARG:NH2	2.28	0.67
4:QD:98:GLU:OE1	4:QD:189:PRO:HG2	1.94	0.67
1:XA:559:A:H4'	1:XA:560:U:H3'	1.77	0.67
34:R9:27:CYS:SG	34:R9:28:GLU:N	2.68	0.66
5:XE:102:ALA:HB1	5:XE:106:PRO:HG2	1.77	0.66
25:Y0:39:ARG:HH21	35:YA:2355:C:H1'	1.61	0.66
3:QC:184:TYR:HE1	3:QC:201:TYR:CE1	2.13	0.66
52:RW:14:PRO:HG2	52:RW:78:GLU:HG2	1.76	0.66
35:RA:958:U:OP2	46:RQ:14:ARG:NH1	2.29	0.66
16:QP:38:TYR:HD1	16:QP:50:LYS:HB3	1.60	0.66
35:YA:881:G:H1	35:YA:895:U:H3	1.43	0.66
35:RA:1041:C:H42	35:RA:1114:G:H1	1.44	0.66
20:XT:100:ILE:HG22	20:XT:101:GLY:H	1.59	0.66
9:QI:86:VAL:HG21	9:QI:93:ARG:HE	1.59	0.66
29:R4:16:CYS:SG	29:R4:17:GLY:N	2.69	0.66
55:YZ:51:ALA:HB1	55:YZ:55:HIS:HB2	1.78	0.66
8:XH:114:THR:HG23	8:XH:116:LYS:H	1.61	0.66
10:XJ:57:LYS:HE2	10:XJ:60:ARG:HH22	1.60	0.66
55:YZ:10:ARG:HE	55:YZ:36:LYS:HB3	1.61	0.65
1:XA:8:A:N6	4:XD:205:GLU:O	2.29	0.65
35:YA:2131:G:H5''	35:YA:2132:U:H5'	1.77	0.65
39:RF:157:VAL:HB	39:RF:194:MET:HG2	1.78	0.65
35:YA:2506:U:C2	35:YA:2585:U:O4	2.49	0.65
35:YA:2298:A:H62	35:YA:2318:G:H8	1.44	0.65
1:QA:501:C:OP1	12:QL:117:ARG:NH2	2.29	0.65
1:QA:545:C:OP1	4:QD:61:LYS:NZ	2.29	0.65
4:XD:98:GLU:HA	4:XD:103:ASN:HD22	1.62	0.65
12:XL:47:LYS:O	12:XL:49:ASN:N	2.30	0.65
35:YA:483:A:H5''	54:YY:50:ARG:HE	1.61	0.65
38:YE:84:PHE:HE2	38:YE:86:PRO:HG3	1.62	0.65
2:QB:187:LEU:HA	2:QB:201:ILE:HB	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1123:A:H4'	10:XJ:36:GLY:HA3	1.78	0.65
6:XF:81:ILE:HD11	37:YD:125:ILE:HB	1.79	0.65
51:RV:21:ARG:HH11	51:RV:91:TYR:HE2	1.45	0.65
29:Y4:14:ILE:HB	29:Y4:22:ILE:HB	1.79	0.65
35:YA:2010:G:H5''	52:YW:42:ARG:HB2	1.79	0.65
39:RF:143:ALA:HB1	39:RF:148:LEU:HB2	1.78	0.64
13:XM:6:GLY:HA3	13:XM:67:GLU:HG3	1.78	0.64
35:YA:1153:C:OP1	50:YU:92:ARG:NH2	2.29	0.64
4:QD:4:TYR:O	4:QD:6:GLY:N	2.31	0.64
37:RD:85:ASP:OD2	37:RD:88:ARG:NH1	2.29	0.64
38:RE:2:LYS:HB2	38:RE:95:ILE:HD12	1.78	0.64
17:QQ:26:GLN:HG2	17:QQ:37:LYS:HG2	1.78	0.64
35:RA:2010:G:H5''	52:RW:42:ARG:HB2	1.79	0.64
6:XF:87:ARG:NH1	18:XR:75:ILE:O	2.31	0.64
1:XA:1101:A:N7	2:XB:175:ARG:NH2	2.46	0.64
55:RZ:115:GLY:HA2	55:RZ:177:PRO:HD3	1.79	0.64
38:YE:84:PHE:HE2	38:YE:86:PRO:CG	2.10	0.64
1:QA:664:G:H22	1:QA:741:G:H1	1.45	0.63
33:R8:6:THR:HG22	33:R8:63:PRO:HD2	1.81	0.63
35:YA:39:C:O2	39:YF:46:ARG:NH2	2.28	0.63
9:QI:121:ARG:NH1	9:QI:122:ALA:O	2.30	0.63
4:QD:18:LYS:NZ	4:QD:31:CYS:SG	2.72	0.63
1:XA:626:U:H4'	16:XP:38:TYR:HE2	1.61	0.63
34:Y9:27:CYS:SG	34:Y9:28:GLU:N	2.71	0.63
5:QE:102:ALA:HB1	5:QE:106:PRO:HG2	1.79	0.63
35:RA:1791:A:H5'	37:RD:206:LEU:HD12	1.81	0.63
3:QC:108:ASN:ND2	3:QC:144:SER:OG	2.32	0.63
22:QV:9:G:O2'	22:QV:10:G:N7	2.32	0.63
29:Y4:16:CYS:SG	29:Y4:17:GLY:N	2.72	0.63
35:YA:1824:G:N3	37:YD:254:THR:OG1	2.32	0.63
35:YA:2604:U:H6	35:YA:2604:U:C5'	2.10	0.63
35:RA:2851:A:O2'	47:RR:64:ARG:NH2	2.32	0.62
35:YA:1470:G:N2	35:YA:1520:G:OP2	2.31	0.62
35:YA:2032:G:N2	38:YE:146:THR:OG1	2.32	0.62
33:R8:30:ARG:HH21	45:RP:63:PRO:HB2	1.63	0.62
4:QD:68:TYR:CE2	4:QD:103:ASN:ND2	2.67	0.62
12:QL:71:PRO:O	12:QL:102:ARG:NH1	2.33	0.62
35:RA:1607:C:N4	35:RA:1622:G:OP2	2.30	0.62
49:RT:125:ARG:O	49:RT:129:ARG:NH1	2.32	0.62
35:RA:993:G:N3	51:RV:89:GLN:NE2	2.46	0.62
48:YS:25:ARG:HD3	48:YS:27:SER:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R8:28:GLY:O	33:R8:36:LYS:NZ	2.31	0.62
43:RN:12:ARG:NH1	43:RN:50:ASP:OD2	2.32	0.62
35:YA:1721:G:H8	35:YA:1741:A:H62	1.46	0.62
17:QQ:66:SER:O	17:QQ:70:ARG:NH1	2.33	0.62
26:R1:51:VAL:HG11	26:R1:74:VAL:HG21	1.81	0.62
29:R4:34:GLU:OE1	29:R4:35:VAL:HG23	2.00	0.62
38:RE:36:ARG:NH1	38:RE:85:ASN:OD1	2.33	0.62
3:XC:56:ASP:HB2	3:XC:67:THR:HB	1.82	0.62
37:YD:108:PRO:HD2	37:YD:111:LEU:HD22	1.80	0.62
54:YY:9:LYS:NZ	54:YY:28:LYS:O	2.30	0.62
1:QA:539:A:OP2	12:QL:115:LYS:NZ	2.33	0.62
2:QB:54:THR:HG22	2:QB:199:TYR:HB3	1.81	0.62
35:RA:1195:G:OP2	45:RP:15:ARG:NH1	2.32	0.62
35:YA:993:G:OP1	50:YU:50:ARG:NH2	2.31	0.62
39:YF:157:VAL:HB	39:YF:194:MET:HG2	1.81	0.62
35:RA:1695:G:N7	37:RD:14:ARG:NH2	2.48	0.62
41:YH:86:GLU:OE2	41:YH:130:ARG:NH1	2.33	0.62
17:XQ:26:GLN:HG2	17:XQ:37:LYS:HG2	1.82	0.61
37:RD:108:PRO:HD2	37:RD:111:LEU:HD22	1.82	0.61
40:YG:48:GLU:O	40:YG:51:ARG:NH1	2.33	0.61
1:QA:352:C:O2	1:QA:355:C:N4	2.32	0.61
1:QA:626:U:H5''	16:QP:38:TYR:HD2	1.64	0.61
3:XC:184:TYR:HE1	3:XC:201:TYR:HE1	1.48	0.61
1:QA:1497:G:H1'	1:QA:1518:MA6:H2	1.82	0.61
1:QA:1328:C:O2'	13:QM:29:ARG:NH2	2.34	0.61
3:QC:56:ASP:HB2	3:QC:67:THR:HB	1.83	0.61
1:QA:1137:C:O2	1:QA:1138:G:N2	2.34	0.61
51:RV:40:LEU:HB2	51:RV:46:VAL:HG22	1.82	0.61
35:YA:83:G:H1	35:YA:102:G:HO2'	1.45	0.61
35:RA:807:U:O2'	35:RA:2060:A:N1	2.33	0.61
17:XQ:66:SER:O	17:XQ:70:ARG:NH1	2.34	0.61
24:XY:18:G:N2	24:XY:58:A:OP1	2.33	0.61
35:YA:2413:G:H21	45:YP:70:GLN:HE22	1.48	0.61
45:YP:93:GLY:H	45:YP:123:LEU:HD22	1.66	0.61
38:YE:84:PHE:CE2	38:YE:86:PRO:CD	2.84	0.61
43:YN:22:THR:HB	43:YN:25:ARG:HB2	1.83	0.61
35:RA:660:G:H5''	39:RF:99:TYR:CE2	2.35	0.60
44:RO:23:ARG:NH2	44:RO:28:SER:O	2.34	0.60
35:YA:958:U:OP2	46:YQ:14:ARG:NH1	2.34	0.60
35:YA:1567:A:N7	37:YD:84:TYR:CE2	2.67	0.60
44:YO:35:VAL:HG11	44:YO:103:ALA:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:737:A:H1'	6:QF:73:ASN:HD21	1.66	0.60
25:Y0:20:ARG:HH12	35:YA:2357:U:H5'	1.66	0.60
1:QA:8:A:N6	4:QD:205:GLU:O	2.32	0.60
9:QI:17:VAL:HG21	9:QI:81:ILE:HG22	1.84	0.60
26:Y1:52:ARG:NH1	35:YA:2218:U:O2	2.35	0.60
7:QG:150:ALA:HB1	11:QK:57:THR:HG21	1.83	0.60
1:XA:974:A:OP2	14:XN:41:ARG:NH1	2.34	0.60
8:QH:110:ALA:HB3	8:QH:121:ASP:HB3	1.82	0.60
35:RA:613:G:N2	35:RA:614(D):A:O2'	2.35	0.60
35:YA:2292:C:OP1	48:YS:17:ARG:NH2	2.34	0.60
2:QB:69:LEU:HB3	2:QB:162:ILE:HG22	1.82	0.60
24:QY:74:C:H42	35:RA:2508:G:H5'	1.65	0.60
55:RZ:99:TYR:HB3	55:RZ:123:ASP:HB2	1.82	0.60
38:YE:105:THR:OG1	38:YE:199:ARG:NH2	2.34	0.60
35:RA:1824:G:N3	37:RD:254:THR:OG1	2.35	0.60
3:QC:58:GLU:HB2	3:QC:65:ALA:HB3	1.84	0.60
40:RG:64:THR:HB	40:RG:94:LEU:HD21	1.83	0.60
49:RT:92:GLY:O	49:RT:120:ARG:NH2	2.34	0.60
16:XP:38:TYR:HE1	16:XP:50:LYS:CB	2.13	0.60
1:XA:954:G:H21	1:XA:1227:A:H62	1.48	0.60
30:Y5:29:THR:HG21	35:YA:2815:C:H5'	1.83	0.60
35:YA:674:G:H1'	39:YF:74:ARG:HD3	1.83	0.60
37:YD:85:ASP:OD2	37:YD:88:ARG:NH1	2.32	0.60
35:YA:301:G:OP2	54:YY:84:ARG:NH2	2.34	0.60
35:YA:336:C:O2'	54:YY:35:TYR:OH	2.20	0.60
35:RA:987:G:O2'	35:RA:1000:A:N3	2.34	0.59
3:XC:110:ASN:OD1	3:XC:140:ARG:NH1	2.35	0.59
50:YU:97:ASP:OD1	50:YU:101:ARG:NH1	2.34	0.59
37:YD:143:HIS:ND1	37:YD:194:GLY:O	2.33	0.59
38:YE:29:GLY:HA2	38:YE:180:ASN:HB3	1.83	0.59
1:XA:978:A:H61	1:XA:1316:G:H1'	1.66	0.59
1:XA:427:U:OP1	4:XD:13:ARG:NH1	2.35	0.59
1:XA:1406:U:O2	1:XA:1517:G:N2	2.35	0.59
1:QA:425:G:O3'	4:QD:45:GLN:NE2	2.35	0.59
4:QD:20:TYR:CD2	4:QD:26:CYS:HB3	2.37	0.59
35:YA:2602:A:H2'	35:YA:2602:A:N3	2.18	0.59
1:QA:974:A:OP2	14:QN:41:ARG:NH1	2.35	0.59
3:QC:21:ARG:NH2	3:QC:58:GLU:OE2	2.36	0.59
35:RA:2096:U:H3	35:RA:2193:G:H1	1.50	0.59
16:XP:8:ARG:HB3	16:XP:28:ARG:HH12	1.66	0.59
1:QA:111:G:HO2'	1:QA:389:A:HO2'	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1330:U:H4'	13:QM:23:TYR:CE1	2.37	0.59
35:RA:1815:A:OP2	37:RD:54:ARG:NH2	2.36	0.59
2:XB:68:ILE:HG12	2:XB:161:ALA:HB3	1.84	0.59
8:XH:10:LEU:HD22	8:XH:83:ILE:HD11	1.84	0.59
55:YZ:8:TYR:HB2	55:YZ:38:TYR:CE1	2.38	0.59
35:RA:181:A:H1'	35:RA:435:C:H5'	1.85	0.59
1:XA:508:C:OP1	4:XD:209:ARG:NH2	2.35	0.59
1:XA:1500:A:H5''	1:XA:1508:G:H5''	1.84	0.59
10:XJ:17:ASP:OD1	10:XJ:70:ARG:NH1	2.35	0.59
1:QA:1013:G:N2	1:QA:1016:A:OP2	2.36	0.59
33:R8:14:VAL:HG12	33:R8:24:ALA:HB2	1.85	0.59
20:XT:56:MET:HE3	20:XT:85:MET:HG2	1.85	0.59
37:YD:260:ARG:NH2	37:YD:266:SER:OG	2.36	0.59
40:YG:19:LEU:HD23	40:YG:32:PRO:HD2	1.85	0.59
54:YY:15:VAL:HG21	54:YY:42:VAL:HG11	1.84	0.59
1:QA:933:G:O6	7:QG:3:ARG:NH2	2.36	0.58
46:RQ:13:GLN:O	46:RQ:72:LYS:NZ	2.33	0.58
48:RS:105:ALA:HB1	48:RS:110:LEU:HD12	1.85	0.58
5:XE:33:VAL:HG21	5:XE:109:ILE:HA	1.85	0.58
35:YA:693:C:O2'	35:YA:1353:A:N3	2.34	0.58
35:RA:1791:A:H4'	37:RD:206:LEU:HB2	1.85	0.58
35:YA:987:G:O2'	35:YA:1000:A:N3	2.35	0.58
55:YZ:8:TYR:HB2	55:YZ:38:TYR:CD1	2.38	0.58
28:R3:15:TYR:O	28:R3:20:LYS:NZ	2.37	0.58
39:RF:101:LEU:O	39:RF:106:ARG:NH1	2.35	0.58
41:RH:159:GLU:HG3	41:RH:171:LEU:HD11	1.85	0.58
24:XY:4:G:H1	24:XY:69:C:H42	1.50	0.58
35:YA:1058:G:N2	35:YA:1080:C:O2	2.35	0.58
35:YA:2096:U:H3	35:YA:2193:G:H1	1.50	0.58
45:YP:29:LYS:HD3	45:YP:30:THR:HG23	1.85	0.58
20:QT:51:GLU:HA	20:QT:54:LYS:HE2	1.84	0.58
25:R0:14:ARG:NH1	35:RA:2279:G:O6	2.36	0.58
33:R8:30:ARG:NH2	45:RP:64:LYS:O	2.36	0.58
35:YA:2604:U:C6	35:YA:2604:U:C5'	2.85	0.58
16:XP:18:ARG:NH1	16:XP:32:TYR:OH	2.36	0.58
35:RA:2298:A:H62	35:RA:2318:G:H8	1.51	0.58
33:Y8:43:GLN:NE2	35:YA:2365:G:O6	2.30	0.58
35:YA:526:A:O2'	35:YA:2043:C:O2	2.21	0.58
40:YG:55:LYS:HZ1	40:YG:149:VAL:HA	1.69	0.58
24:XY:75:C:O2'	35:YA:2573:C:N4	2.37	0.58
35:YA:631:A:OP1	45:YP:65:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1155:A:OP1	50:YU:55:ARG:HG2	2.04	0.58
34:R9:36:GLN:NE2	35:RA:1124:C:O2	2.36	0.58
35:RA:956:G:H2'	35:RA:957:A:H2'	1.86	0.58
17:QQ:9:VAL:HG22	17:QQ:56:VAL:HG22	1.85	0.58
1:XA:1286:A:H2'	1:XA:1287:A:H4'	1.85	0.58
24:XY:20:G:N2	24:XY:21:A:O2'	2.37	0.58
35:YA:2574:G:N3	38:YE:143:ASN:ND2	2.52	0.58
1:QA:779:C:O2'	11:QK:120:ARG:NH1	2.37	0.58
1:QA:528:C:N4	12:QL:49:ASN:OD1	2.34	0.57
35:RA:39:C:O2	39:RF:46:ARG:NH2	2.33	0.57
35:RA:340:A:O2'	39:RF:168:ARG:NH2	2.37	0.57
35:RA:1800:C:OP2	37:RD:183:ARG:NH2	2.37	0.57
27:Y2:16:LEU:O	27:Y2:67:LYS:NZ	2.36	0.57
35:YA:1791:A:H5'	37:YD:206:LEU:HD12	1.86	0.57
35:YA:2483:C:N3	46:YQ:124:LYS:NZ	2.42	0.57
1:XA:1086:U:H3	1:XA:1099:G:H22	1.52	0.57
35:RA:1791:A:N6	35:RA:1828:G:O2'	2.34	0.57
35:RA:2627:G:N2	35:RA:2777:G:OP2	2.36	0.57
3:XC:40:ARG:HH12	14:XN:52:GLN:HG2	1.69	0.57
35:RA:994:C:OP1	50:RU:53:ARG:NH2	2.37	0.57
12:XL:70:ILE:HG13	12:XL:100:ILE:HD12	1.86	0.57
39:YF:190:GLU:HA	45:YP:2:LYS:HE3	1.86	0.57
1:QA:977:A:N6	1:QA:1224:G:OP1	2.29	0.57
28:R3:8:LEU:HB2	28:R3:28:LEU:HD13	1.86	0.57
35:RA:500:G:N1	35:RA:503:A:OP2	2.37	0.57
35:RA:631:A:OP1	45:RP:65:ARG:NH1	2.37	0.57
35:RA:1162:G:H4'	51:RV:24:LYS:HB3	1.87	0.57
4:XD:18:LYS:HD2	58:XD:301:SF4:S2	2.44	0.57
25:R0:20:ARG:HH12	35:RA:2357:U:H5'	1.69	0.57
35:RA:143(A):G:H4'	53:RX:35:THR:HG21	1.87	0.57
37:RD:143:HIS:ND1	37:RD:194:GLY:O	2.34	0.57
44:RO:104:ARG:NH2	44:RO:121:VAL:O	2.38	0.57
35:YA:859:G:O2'	35:YA:916:G:O6	2.22	0.57
13:QM:99:ARG:HB2	13:QM:101:GLN:HE22	1.69	0.57
35:RA:615:G:OP1	39:RF:40:GLN:NE2	2.38	0.57
41:RH:154:PRO:HG3	41:RH:163:TYR:CD1	2.40	0.57
28:Y3:15:TYR:O	28:Y3:20:LYS:NZ	2.37	0.57
31:Y6:35:GLU:OE2	31:Y6:50:ARG:NH1	2.38	0.57
1:XA:1295:G:O2'	13:XM:14:ARG:NH1	2.38	0.57
35:RA:1009:A:OP2	43:RN:37:LYS:NZ	2.35	0.57
35:YA:1791:A:N6	35:YA:1828:G:O2'	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:RF:11:VAL:HG22	39:RF:125:LEU:HB2	1.86	0.56
45:RP:93:GLY:H	45:RP:123:LEU:HD22	1.70	0.56
13:XM:8:GLU:OE2	13:XM:11:ARG:NH2	2.38	0.56
10:QJ:49:VAL:HG23	14:QN:41:ARG:HB2	1.86	0.56
26:R1:52:ARG:NH1	35:RA:2218:U:O2	2.38	0.56
35:RA:2839:G:H5'	47:RR:46:GLY:HA2	1.87	0.56
33:Y8:28:GLY:O	33:Y8:36:LYS:NZ	2.36	0.56
35:YA:1651:G:N7	47:YR:11:ASN:ND2	2.52	0.56
47:YR:103:ARG:NH1	47:YR:108:GLY:O	2.38	0.56
1:QA:1318:A:OP1	19:QS:3:ARG:NH2	2.37	0.56
54:RY:47:LYS:NZ	54:RY:48:ALA:O	2.39	0.56
1:XA:545:C:OP1	4:XD:61:LYS:NZ	2.38	0.56
1:XA:626:U:H5''	16:XP:38:TYR:HD2	1.69	0.56
19:XS:63:THR:HG23	19:XS:65:ASN:H	1.70	0.56
35:YA:458:G:O2'	35:YA:469:G:O6	2.24	0.56
35:YA:1695:G:N7	37:YD:14:ARG:NH2	2.54	0.56
26:R1:3:LYS:NZ	35:RA:1366:A:OP1	2.38	0.56
49:RT:122:ASP:OD1	49:RT:125:ARG:NH2	2.35	0.56
1:XA:1003:G:H1	1:XA:1035:A:H61	1.52	0.56
29:Y4:43:TYR:OH	40:YG:179:PRO:HG3	2.05	0.56
40:RG:137:GLU:HG3	40:RG:140:ILE:HG12	1.88	0.56
5:QE:7:GLU:OE1	5:QE:37:ARG:NE	2.35	0.56
25:Y0:51:VAL:O	48:YS:20:ARG:NH2	2.39	0.56
34:Y9:22:ARG:HH12	35:YA:2741:A:H5''	1.71	0.56
35:YA:1466:G:HO2'	35:YA:1546:C:HO2'	1.50	0.56
1:QA:1226:C:O2'	13:QM:111:LYS:NZ	2.34	0.56
35:RA:297:C:OP1	54:RY:87:LYS:NZ	2.38	0.56
50:RU:97:ASP:OD1	50:RU:101:ARG:NH1	2.38	0.56
55:RZ:126:VAL:HG12	55:RZ:163:LEU:HA	1.86	0.56
8:XH:9:MET:HG3	8:XH:26:VAL:HG11	1.87	0.56
1:QA:619:U:N3	4:QD:134:ASP:OD1	2.38	0.56
1:XA:1321:C:O2'	19:XS:78:ARG:NH1	2.39	0.56
19:XS:50:ALA:HB1	19:XS:57:HIS:HB3	1.88	0.56
38:YE:84:PHE:CE2	38:YE:86:PRO:CG	2.88	0.56
1:QA:7:G:O2'	5:QE:120:THR:O	2.23	0.56
1:QA:345:C:OP2	49:RT:39:ARG:NH2	2.39	0.56
12:QL:117:ARG:HB2	12:QL:122:THR:HB	1.86	0.56
38:RE:105:THR:OG1	38:RE:199:ARG:NH2	2.38	0.56
1:XA:1226:C:O2'	13:XM:111:LYS:NZ	2.37	0.56
4:QD:157:LEU:O	4:QD:161:ASN:ND2	2.38	0.56
1:XA:562:C:H1'	12:XL:15:ARG:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:XB:74:LYS:NZ	2:XB:206:ASP:OD1	2.37	0.56
2:XB:187:LEU:HA	2:XB:201:ILE:HB	1.87	0.56
29:Y4:53:GLU:HG3	29:Y4:56:VAL:HB	1.87	0.56
35:YA:615:G:OP1	39:YF:40:GLN:NE2	2.39	0.56
35:YA:2144:U:O2	35:YA:2148:G:N1	2.34	0.56
30:R5:19:ARG:NH2	35:RA:1264:G:OP1	2.38	0.55
1:XA:352:C:O2	1:XA:355:C:N4	2.39	0.55
2:XB:195:ASP:O	8:XH:68:ARG:NH2	2.39	0.55
20:XT:50:GLU:HB2	20:XT:99:LEU:HD22	1.88	0.55
50:YU:83:LEU:HD13	50:YU:88:ILE:HB	1.89	0.55
35:RA:1250:G:OP2	45:RP:21:ARG:NH1	2.39	0.55
35:RA:1266:G:O5'	52:RW:15:ARG:NH2	2.39	0.55
1:XA:662:G:O2'	1:XA:836:G:OP1	2.25	0.55
3:XC:184:TYR:CE1	3:XC:201:TYR:CE1	2.94	0.55
12:XL:71:PRO:O	12:XL:102:ARG:NH1	2.39	0.55
13:XM:19:LEU:HD11	13:XM:56:LEU:HD21	1.87	0.55
37:YD:72:LYS:NZ	37:YD:99:ASP:OD2	2.40	0.55
1:QA:1316:G:O2'	1:QA:1318:A:N7	2.39	0.55
35:RA:1638:C:O2	35:RA:2698:U:O2'	2.24	0.55
35:RA:2635:C:O2'	38:RE:48:GLN:NE2	2.38	0.55
51:RV:21:ARG:HD3	51:RV:91:TYR:HE2	1.72	0.55
1:XA:1152:A:OP1	10:XJ:70:ARG:NH2	2.39	0.55
41:YH:124:GLU:HB2	41:YH:132:ARG:HB3	1.89	0.55
1:QA:297:G:N2	1:QA:300:A:OP2	2.40	0.55
1:QA:1249:C:O2'	9:QI:73:GLN:NE2	2.39	0.55
8:QH:9:MET:HG3	8:QH:26:VAL:HG11	1.87	0.55
35:RA:1066:U:O2'	35:RA:1068:G:OP2	2.21	0.55
35:RA:1721:G:H8	35:RA:1741:A:H62	1.53	0.55
38:RE:7:VAL:HG13	38:RE:51:PHE:HE2	1.72	0.55
49:RT:29:ARG:HB3	49:RT:87:ASP:HB2	1.88	0.55
39:YF:143:ALA:HB1	39:YF:148:LEU:HB2	1.87	0.55
44:YO:104:ARG:NH2	44:YO:121:VAL:O	2.38	0.55
24:QY:20:G:N2	24:QY:21:A:O2'	2.38	0.55
27:R2:16:LEU:HB3	27:R2:20:GLU:HG3	1.89	0.55
35:RA:526:A:O2'	35:RA:2043:C:O2	2.23	0.55
41:RH:86:GLU:OE2	41:RH:132:ARG:NH2	2.37	0.55
49:RT:65:LYS:HE3	49:RT:67:SER:HB2	1.89	0.55
3:XC:70:VAL:HG12	3:XC:72:LYS:H	1.72	0.55
11:XK:34:ASP:OD1	11:XK:38:ASN:N	2.40	0.55
32:Y7:24:THR:HG23	32:Y7:27:GLY:H	1.71	0.55
1:QA:922:G:H4'	5:QE:20:GLN:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1320:C:O2	19:QS:36:ARG:NH2	2.35	0.55
35:RA:1246:A:OP1	39:RF:38:ARG:NH2	2.37	0.55
1:QA:978:A:O2'	1:QA:1322:C:N3	2.39	0.55
1:QA:1178:G:OP1	9:QI:93:ARG:NH1	2.40	0.55
9:QI:11:LYS:HA	9:QI:108:VAL:HG12	1.88	0.55
33:R8:43:GLN:NE2	35:RA:2365:G:O6	2.38	0.55
35:RA:919:G:N2	35:RA:2269:A:OP2	2.40	0.55
43:RN:123:TYR:OH	43:RN:130:HIS:NE2	2.37	0.55
35:RA:604:G:OP2	45:RP:90:ARG:NH1	2.40	0.55
35:YA:451:C:OP1	39:YF:52:LYS:NZ	2.39	0.55
35:RA:993:G:OP1	50:RU:50:ARG:NH2	2.39	0.55
1:XA:1414:U:H3	1:XA:1486:G:H1	1.54	0.55
3:XC:184:TYR:HE1	3:XC:201:TYR:CE1	2.25	0.55
35:YA:918:A:N3	36:YB:80:U:O2'	2.40	0.55
37:YD:168:ARG:HG2	37:YD:173:VAL:HG12	1.89	0.55
1:QA:573:A:N3	1:QA:883:C:O2'	2.36	0.55
6:QF:41:GLU:OE1	18:QR:35:ARG:NH1	2.37	0.55
35:RA:458:G:O2'	35:RA:469:G:O6	2.24	0.55
35:RA:2683:C:OP1	49:RT:53:ARG:NH2	2.34	0.55
39:RF:40:GLN:HE22	39:RF:182:ASN:HB2	1.72	0.55
55:RZ:8:TYR:HB3	55:RZ:38:TYR:HE1	1.71	0.55
1:XA:79:G:H1	1:XA:90:U:H3	1.55	0.55
8:QH:41:ARG:NH2	8:QH:123:GLU:OE1	2.40	0.54
35:YA:604:G:OP2	45:YP:90:ARG:NH1	2.39	0.54
35:YA:2291:U:O2'	35:YA:2374:C:O2	2.24	0.54
38:YE:84:PHE:CE2	38:YE:86:PRO:HB3	2.42	0.54
9:QI:10:ARG:HG3	9:QI:11:LYS:H	1.72	0.54
35:RA:237:C:O2	35:RA:609:A:O2'	2.25	0.54
25:Y0:30:VAL:HG22	25:Y0:66:VAL:HG22	1.89	0.54
4:QD:20:TYR:HD2	4:QD:26:CYS:HB3	1.72	0.54
9:QI:49:PRO:HD2	9:QI:81:ILE:HD11	1.89	0.54
35:RA:861:A:N3	36:RB:79:C:O2'	2.40	0.54
35:YA:613:G:N2	35:YA:614(D):A:O2'	2.40	0.54
35:YA:807:U:O2'	35:YA:2060:A:N1	2.41	0.54
35:YA:2788:C:O2'	35:YA:2809:A:N3	2.35	0.54
44:YO:23:ARG:NH2	44:YO:28:SER:O	2.40	0.54
1:QA:261:U:OP2	20:QT:79:ARG:NH2	2.40	0.54
1:QA:1147:C:HO2'	9:QI:5:TYR:HH	1.52	0.54
35:RA:600:G:N2	35:RA:605:C:O3'	2.40	0.54
35:RA:907:U:O2'	46:RQ:101:ARG:NH2	2.38	0.54
35:RA:2073:C:HO2'	35:RA:2598:A:HO2'	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:XF:36:ARG:NH2	6:XF:38:GLU:OE2	2.41	0.54
1:QA:1003:G:H1	1:QA:1035:A:H61	1.56	0.54
1:QA:1484:C:HO2'	35:RA:1960:A:HO2'	1.48	0.54
35:RA:660:G:H4'	39:RF:99:TYR:CE2	2.34	0.54
46:RQ:32:TYR:CE1	46:RQ:133:ARG:HG3	2.42	0.54
1:XA:676:A:H1'	11:XK:115:PRO:HB3	1.89	0.54
32:Y7:34:ARG:HG3	32:Y7:39:ARG:HG3	1.90	0.54
38:YE:36:ARG:NH1	38:YE:85:ASN:OD1	2.41	0.54
1:QA:692:U:OP2	11:QK:26:ASN:ND2	2.37	0.54
7:QG:94:ARG:NH1	7:QG:98:SER:OG	2.41	0.54
35:RA:2115:G:N1	35:RA:2119:A:OP2	2.36	0.54
45:RP:29:LYS:HD3	45:RP:30:THR:HG23	1.89	0.54
1:XA:1060:C:OP1	14:XN:45:ARG:NH2	2.41	0.54
1:XA:1101:A:N6	2:XB:176:GLU:OE2	2.40	0.54
36:RB:117:G:H4'	48:RS:54:LEU:HD22	1.89	0.54
35:YA:1652:A:N6	47:YR:11:ASN:OD1	2.34	0.54
54:YY:47:LYS:NZ	54:YY:48:ALA:O	2.41	0.54
35:YA:2683:C:OP1	49:YT:53:ARG:NH2	2.36	0.54
46:YQ:137:TYR:HB3	55:YZ:76:LEU:HD11	1.90	0.54
37:RD:5:LYS:HG2	37:RD:17:THR:HG22	1.90	0.54
55:RZ:92:SER:OG	55:RZ:94:GLU:OE1	2.25	0.54
35:YA:307:G:N1	35:YA:310:A:OP2	2.39	0.54
1:XA:626:U:C5'	16:XP:38:TYR:HD2	2.21	0.54
40:YG:46:ALA:HB2	40:YG:53:LEU:HD12	1.90	0.54
2:QB:28:PHE:HD1	2:QB:194:PRO:HG3	1.73	0.53
35:RA:2012:G:OP1	52:RW:11:ARG:NH2	2.41	0.53
29:Y4:31:ILE:HG21	40:YG:142:PRO:HB2	1.89	0.53
35:YA:184:C:O2'	35:YA:217:G:N3	2.42	0.53
46:YQ:32:TYR:CE1	46:YQ:133:ARG:HG3	2.43	0.53
5:QE:33:VAL:HG21	5:QE:109:ILE:HA	1.89	0.53
7:QG:15:ASP:OD1	7:QG:19:GLY:N	2.42	0.53
35:RA:2033:A:O2'	35:RA:2035:G:OP2	2.25	0.53
38:RE:176:ILE:HB	38:RE:181:LEU:HB2	1.90	0.53
44:RO:9:GLU:OE2	44:RO:18:LYS:NZ	2.39	0.53
2:XB:47:THR:OG1	2:XB:48:MET:N	2.39	0.53
34:Y9:16:VAL:HG22	34:Y9:25:VAL:HG22	1.90	0.53
35:YA:1754:C:N3	35:YA:2716:U:O2'	2.33	0.53
46:YQ:30:GLY:N	46:YQ:105:GLU:OE2	2.41	0.53
1:QA:1368:G:OP1	9:QI:111:ARG:NH2	2.41	0.53
35:RA:2245:U:H5''	35:RA:2246:G:H5'	1.91	0.53
1:XA:977:A:N6	1:XA:1224:G:OP1	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:XC:152:ILE:HD11	3:XC:199:LYS:HD2	1.89	0.53
4:XD:59:ARG:HH21	4:XD:62:GLN:HG3	1.71	0.53
20:XT:50:GLU:HG3	20:XT:100:ILE:HD11	1.90	0.53
25:Y0:77:ARG:NH2	35:YA:857:C:OP2	2.40	0.53
35:YA:1607:C:N4	35:YA:1622:G:OP2	2.34	0.53
39:YF:62:ARG:HD2	39:YF:63:LYS:C	2.33	0.53
45:YP:89:ALA:O	45:YP:121:LYS:NZ	2.38	0.53
35:YA:1066:U:O2'	35:YA:1068:G:OP2	2.21	0.53
35:RA:1398:C:OP1	53:RX:53:LYS:NZ	2.40	0.53
35:RA:2258:C:O2'	35:RA:2427:C:OP2	2.26	0.53
35:RA:2502:G:H5''	35:RA:2503:2MA:H5''	1.91	0.53
35:YA:2115:G:N1	35:YA:2119:A:OP2	2.41	0.53
39:YF:185:ASP:OD1	39:YF:188:ARG:NH1	2.41	0.53
4:QD:168:ARG:HH22	37:YD:134:ARG:HH21	1.57	0.53
35:RA:1788:C:OP1	37:RD:222:ARG:NH2	2.41	0.53
1:XA:578:C:O2'	1:XA:728:A:N3	2.38	0.53
1:XA:811:C:O2'	1:XA:901:A:N1	2.42	0.53
35:YA:300:A:OP1	54:YY:86:ARG:NH2	2.42	0.53
38:YE:2:LYS:HB2	38:YE:95:ILE:HD12	1.91	0.53
35:RA:1801:G:OP2	37:RD:154:LYS:NZ	2.42	0.53
39:RF:46:ARG:HG3	39:RF:48:THR:HG23	1.91	0.53
6:XF:99:ALA:HB2	18:XR:31:LEU:HD11	1.91	0.53
34:Y9:36:GLN:NE2	35:YA:1124:C:O2	2.42	0.53
52:YW:22:ASP:OD1	52:YW:25:ARG:NH1	2.38	0.53
1:QA:437:U:O2'	4:QD:123:HIS:ND1	2.39	0.53
16:QP:53:VAL:HG13	16:QP:79:VAL:HG12	1.90	0.53
35:RA:2572:A:OP1	35:RA:2574:G:O2'	2.25	0.53
1:XA:765:G:N1	1:XA:812:C:O2'	2.37	0.53
1:XA:976:G:OP2	1:XA:1358:U:O2'	2.27	0.53
13:XM:99:ARG:HB2	13:XM:101:GLN:HE22	1.73	0.53
35:YA:2033:A:O2'	35:YA:2035:G:OP2	2.24	0.53
1:QA:662:G:O2'	1:QA:836:G:OP1	2.27	0.53
3:QC:191:THR:OG1	3:QC:194:GLY:O	2.27	0.53
18:QR:32:ARG:HA	18:QR:69:THR:HG21	1.91	0.53
39:RF:117:ARG:NH2	39:RF:189:THR:O	2.42	0.53
4:XD:109:GLY:HA3	4:XD:165:MET:HG3	1.90	0.53
9:XI:7:THR:OG1	9:XI:83:ARG:NH1	2.39	0.53
35:YA:2851:A:O2'	47:YR:64:ARG:NH2	2.41	0.53
42:YI:23:PRO:HB3	42:YI:27:ARG:HE	1.73	0.53
24:QY:18:G:N2	24:QY:58:A:OP1	2.41	0.53
40:RG:32:PRO:HB2	40:RG:172:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:RU:89:GLU:O	51:RV:11:GLN:NE2	2.35	0.53
6:XF:33:TYR:HB2	6:XF:75:LEU:HD12	1.91	0.53
35:YA:600:G:N2	35:YA:605:C:O3'	2.42	0.53
1:QA:1218:C:OP2	14:QN:9:LYS:NZ	2.41	0.52
8:QH:36:LEU:HD23	8:QH:39:LEU:HD12	1.91	0.52
16:XP:20:VAL:HG23	16:XP:35:LYS:HA	1.91	0.52
35:YA:2404:C:O3'	45:YP:77:ARG:NH2	2.40	0.52
1:QA:792:A:O2'	1:QA:794:A:N7	2.42	0.52
4:QD:98:GLU:HA	4:QD:103:ASN:HD22	1.75	0.52
7:QG:76:ARG:HD3	7:QG:89:MET:HG3	1.92	0.52
35:RA:574:C:N4	35:RA:2034:U:OP1	2.41	0.52
35:RA:1817:G:OP1	37:RD:88:ARG:NH2	2.41	0.52
55:RZ:69:THR:OG1	55:RZ:70:LEU:N	2.42	0.52
1:XA:824:C:H2'	1:XA:825:G:H8	1.73	0.52
3:XC:39:ILE:HG23	3:XC:91:LEU:HD11	1.89	0.52
40:YG:161:THR:HG22	40:YG:163:ALA:H	1.74	0.52
35:RA:1693:U:O2'	37:RD:14:ARG:NH2	2.42	0.52
1:XA:67:C:O2'	1:XA:171:A:N3	2.35	0.52
26:Y1:11:ARG:NH2	35:YA:1365:A:O2'	2.42	0.52
42:YI:92:VAL:HG23	42:YI:120:ILE:HB	1.91	0.52
1:QA:677:U:H3	1:QA:713:G:H22	1.58	0.52
46:RQ:31:ASP:N	46:RQ:106:VAL:O	2.42	0.52
30:Y5:16:ARG:NH1	30:Y5:17:ASP:OD1	2.43	0.52
1:QA:738:C:OP1	6:QF:4:TYR:OH	2.24	0.52
9:QI:48:GLU:HG3	9:QI:51:ARG:HH11	1.75	0.52
32:R7:39:ARG:NH2	35:RA:468:G:N7	2.51	0.52
47:RR:56:LYS:NZ	47:RR:90:ARG:O	2.43	0.52
54:RY:14:LEU:HB2	54:RY:75:ILE:HD11	1.92	0.52
1:XA:486:U:H2'	1:XA:487:A:H8	1.74	0.52
1:XA:1030(D):G:H2'	1:XA:1030(E):A:H8	1.73	0.52
44:YO:98:VAL:HG21	44:YO:114:ILE:HG23	1.92	0.52
2:QB:88:ALA:HB2	2:QB:219:VAL:HG13	1.92	0.52
5:QE:105:VAL:HG21	5:QE:128:PRO:HB3	1.90	0.52
35:RA:859:G:O2'	35:RA:916:G:O6	2.25	0.52
44:RO:98:VAL:HG21	44:RO:114:ILE:HG23	1.91	0.52
1:XA:413:G:N7	4:XD:35:ARG:NH1	2.57	0.52
9:XI:121:ARG:NH1	9:XI:122:ALA:O	2.43	0.52
19:XS:32:LYS:HA	19:XS:50:ALA:HB3	1.92	0.52
35:YA:805:G:N2	35:YA:829:A:OP1	2.40	0.52
1:QA:157:G:H1	1:QA:164:U:H3	1.57	0.52
1:QA:1003:G:N2	1:QA:1025:U:O4	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1286:A:H2'	1:QA:1287:A:H4'	1.91	0.52
1:QA:1438:G:OP2	20:QT:34:LYS:NZ	2.37	0.52
3:QC:20:SER:OG	3:QC:22:TRP:NE1	2.43	0.52
35:RA:99:U:O4	54:RY:8:LYS:NZ	2.37	0.52
1:XA:950:U:H3	1:XA:1231:G:H1	1.58	0.52
35:YA:86:C:H4'	35:YA:104:U:H1'	1.92	0.52
38:YE:2:LYS:HG2	38:YE:200:GLU:HB2	1.92	0.52
43:YN:114:ARG:O	43:YN:118:LYS:NZ	2.37	0.52
44:YO:87:ILE:HD12	44:YO:91:LEU:HA	1.91	0.52
1:QA:954:G:H21	1:QA:1227:A:H62	1.57	0.52
2:QB:93:VAL:HG11	2:QB:101:MET:HE1	1.90	0.52
31:R6:23:THR:OG1	31:R6:24:GLU:N	2.41	0.52
52:YW:69:LEU:HB3	52:YW:107:LEU:HD23	1.90	0.52
35:RA:200:U:O2	35:RA:386:G:N2	2.43	0.52
35:RA:2646:C:OP2	35:RA:2732:G:O2'	2.22	0.52
35:RA:2684:U:O2'	44:RO:68:GLU:OE2	2.24	0.52
55:RZ:103:ARG:HE	55:RZ:136:PHE:HD2	1.58	0.52
2:XB:88:ALA:HB2	2:XB:219:VAL:HG13	1.92	0.52
33:Y8:6:THR:HG22	33:Y8:63:PRO:HD2	1.92	0.52
35:YA:641:C:O2'	35:YA:2350:C:OP1	2.23	0.52
35:YA:906:G:OP1	46:YQ:26:TYR:OH	2.22	0.52
35:YA:2313:C:O4'	40:YG:40:ASN:ND2	2.43	0.52
32:Y7:37:LYS:NZ	35:YA:468:G:OP2	2.42	0.52
35:YA:24:G:O2'	52:YW:78:GLU:O	2.26	0.52
35:YA:2602:A:N3	35:YA:2602:A:C2'	2.73	0.52
1:QA:235:C:H2'	1:QA:236:G:H8	1.74	0.51
1:QA:742:G:OP2	15:QO:35:ARG:NH2	2.42	0.51
8:QH:36:LEU:HD12	8:QH:59:LEU:HD23	1.92	0.51
35:RA:1819:A:H5''	37:RD:161:THR:HG21	1.92	0.51
1:XA:35:G:N3	12:XL:118:SER:OG	2.42	0.51
35:YA:221:A:N1	35:YA:265:A:O2'	2.41	0.51
35:YA:2627:G:N2	35:YA:2777:G:OP2	2.42	0.51
35:YA:2718:G:O2'	35:YA:2847:U:OP1	2.26	0.51
53:YX:34:ALA:O	53:YX:77:LYS:NZ	2.42	0.51
1:QA:475:G:H2'	1:QA:476:G:H8	1.75	0.51
7:QG:26:PHE:HD1	7:QG:101:LEU:HD22	1.75	0.51
1:XA:410:G:H21	1:XA:432:A:H62	1.59	0.51
1:XA:922:G:H4'	5:XE:20:GLN:HA	1.92	0.51
1:XA:1147:C:O2	9:XI:16:ARG:NH1	2.43	0.51
1:XA:1386:G:H2'	1:XA:1387:G:H8	1.75	0.51
6:XF:37:VAL:HA	6:XF:65:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y5:29:THR:O	30:Y5:29:THR:OG1	2.26	0.51
39:YF:101:LEU:O	39:YF:106:ARG:NH1	2.42	0.51
1:QA:950:U:H3	1:QA:1231:G:H1	1.56	0.51
26:R1:76:ARG:O	35:RA:272(Q):G:O2'	2.28	0.51
35:RA:577:G:O2'	35:RA:1254:A:OP1	2.27	0.51
35:RA:2133:G:O2'	35:RA:2158:A:N1	2.43	0.51
43:RN:49:GLY:O	43:RN:119:ARG:NH1	2.43	0.51
35:YA:2306:C:N4	40:YG:42:GLY:O	2.43	0.51
47:YR:38:VAL:HG22	47:YR:112:ALA:HB2	1.91	0.51
51:YV:21:ARG:CD	51:YV:91:TYR:HE2	2.24	0.51
54:RY:83:THR:OG1	54:RY:84:ARG:N	2.44	0.51
1:XA:390:C:O3'	16:XP:28:ARG:NH2	2.42	0.51
1:XA:1077:G:N2	1:XA:1080:A:OP2	2.35	0.51
35:YA:299:A:N1	35:YA:322:A:O2'	2.41	0.51
1:QA:339:C:OP2	44:RO:97:ARG:NH2	2.44	0.51
35:RA:116:C:O2'	35:RA:126:A:N3	2.41	0.51
35:RA:2705:A:O2'	35:RA:2852:G:OP1	2.27	0.51
1:XA:73:G:H1	1:XA:96:U:H3	1.57	0.51
3:XC:153:VAL:HG22	3:XC:198:VAL:HG22	1.90	0.51
29:Y4:68:ARG:NH2	29:Y4:69:LYS:O	2.44	0.51
37:YD:148:GLU:HB3	37:YD:151:LYS:HD2	1.93	0.51
40:YG:4:ASP:OD2	40:YG:9:ARG:NH2	2.43	0.51
35:RA:1666:G:HO2'	44:RO:6:THR:HG1	1.55	0.51
1:XA:1316:G:O2'	1:XA:1318:A:N7	2.43	0.51
8:XH:81:HIS:N	8:XH:138:TRP:O	2.44	0.51
27:Y2:48:HIS:ND1	35:YA:95:G:O2'	2.37	0.51
33:Y8:26:LYS:HD3	33:Y8:44:LYS:HA	1.93	0.51
34:Y9:25:VAL:HB	34:Y9:34:GLN:HB2	1.93	0.51
35:YA:1791:A:H4'	37:YD:206:LEU:HB2	1.92	0.51
43:YN:54:VAL:HB	43:YN:122:VAL:HG22	1.91	0.51
35:RA:2115:G:O2'	35:RA:2166:G:N2	2.43	0.51
49:RT:19:LEU:HD13	49:RT:86:ILE:HD12	1.92	0.51
9:XI:28:VAL:HG12	9:XI:63:ILE:HB	1.93	0.51
35:YA:1266:G:O2'	35:YA:2012:G:O6	2.27	0.51
39:YF:63:LYS:NZ	39:YF:75:HIS:O	2.38	0.51
1:XA:401:C:OP2	4:XD:73:ARG:NH2	2.43	0.51
1:XA:403:C:OP2	4:XD:74:GLN:NE2	2.44	0.51
1:XA:993:G:O2'	1:XA:994:A:N7	2.43	0.51
1:XA:1525:G:OP1	11:XK:120:ARG:NH2	2.44	0.51
7:XG:89:MET:HE1	7:XG:156:TRP:H	1.75	0.51
13:XM:65:LYS:HB2	13:XM:69:GLU:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:QE:102:ALA:HB3	5:QE:107:ARG:HB2	1.93	0.51
16:QP:19:ILE:HB	16:QP:37:GLY:HA3	1.92	0.51
35:RA:453:C:O2	35:RA:457:A:O2'	2.28	0.51
35:RA:2144:U:HO2'	35:RA:2147:G:H1	1.57	0.51
7:XG:113:GLU:HB2	7:XG:119:ARG:HG2	1.92	0.51
16:XP:8:ARG:NH2	16:XP:11:SER:O	2.44	0.51
35:YA:1266:G:O5'	52:YW:15:ARG:NH2	2.44	0.51
40:YG:37:VAL:HG22	40:YG:159:VAL:HG12	1.93	0.51
46:YQ:22:LYS:O	55:YZ:78:LYS:NZ	2.44	0.51
47:RR:33:ARG:NH2	47:RR:115:GLU:OE1	2.42	0.51
55:RZ:77:ASP:OD2	55:RZ:80:ARG:NH1	2.40	0.51
1:XA:376:G:H1	1:XA:387:U:H3	1.59	0.51
9:XI:53:VAL:HG23	9:XI:55:ALA:H	1.76	0.51
1:QA:1123:A:H4'	10:QJ:36:GLY:HA3	1.93	0.50
29:R4:5:ILE:HD12	40:RG:67:LYS:HE2	1.92	0.50
39:RF:185:ASP:OD1	39:RF:188:ARG:NH1	2.42	0.50
8:XH:21:LYS:O	8:XH:65:TYR:OH	2.29	0.50
25:Y0:27:GLU:HG3	25:Y0:68:GLU:HA	1.94	0.50
39:YF:62:ARG:HD2	39:YF:63:LYS:O	2.10	0.50
46:YQ:30:GLY:HA2	46:YQ:107:ALA:HB2	1.94	0.50
1:QA:765:G:N1	1:QA:812:C:O2'	2.38	0.50
1:QA:1101:A:N6	2:QB:176:GLU:OE2	2.44	0.50
35:RA:1056:G:H21	35:RA:1103:A:H62	1.59	0.50
5:XE:48:ALA:HB2	5:XE:57:LYS:HD3	1.93	0.50
35:YA:2302:G:N2	40:YG:126:ASP:OD1	2.40	0.50
3:QC:175:LEU:HD21	3:QC:201:TYR:HE2	1.76	0.50
5:QE:33:VAL:HG13	5:QE:112:LEU:HD22	1.92	0.50
6:QF:11:ASN:HB3	6:QF:14:LEU:HG	1.93	0.50
37:RD:148:GLU:HB3	37:RD:151:LYS:HD2	1.93	0.50
41:RH:7:LEU:O	41:RH:69:ARG:NE	2.43	0.50
43:RN:22:THR:HB	43:RN:25:ARG:HB2	1.93	0.50
52:RW:86:LEU:HD22	52:RW:96:ILE:HD11	1.93	0.50
22:XV:33:U:N3	22:XV:36:U:OP2	2.31	0.50
33:Y8:14:VAL:HG12	33:Y8:24:ALA:HB2	1.93	0.50
35:YA:1426:G:O2'	35:YA:1572:A:N6	2.45	0.50
48:YS:10:ARG:HG3	48:YS:13:ARG:HH21	1.76	0.50
35:RA:1043:C:HO2'	35:RA:1048:A:HO2'	1.59	0.50
35:RA:2291:U:O2'	35:RA:2374:C:O2	2.28	0.50
46:RQ:30:GLY:HA2	46:RQ:107:ALA:HB2	1.92	0.50
26:Y1:4:VAL:HG12	26:Y1:11:ARG:HG2	1.94	0.50
35:RA:1779:U:OP2	35:RA:1784:A:N6	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2199:A:N1	35:RA:2226:C:N4	2.57	0.50
30:Y5:41:PRO:O	30:Y5:44:THR:OG1	2.30	0.50
39:YF:46:ARG:HB3	39:YF:48:THR:HG23	1.94	0.50
1:QA:626:U:H5''	16:QP:38:TYR:CD2	2.45	0.50
10:QJ:53:PRO:O	14:QN:41:ARG:NH2	2.44	0.50
26:R1:50:ARG:HG2	26:R1:59:THR:HG22	1.93	0.50
35:RA:2816:C:O2	35:RA:2883:A:O2'	2.29	0.50
1:XA:978:A:OP2	1:XA:1363(A):C:N4	2.43	0.50
1:XA:1289:A:N1	1:XA:1371:G:O2'	2.42	0.50
39:YF:168:ARG:HG2	39:YF:175:THR:HG21	1.93	0.50
2:QB:88:ALA:O	2:QB:226:ARG:NH2	2.45	0.50
11:QK:32:ILE:HG13	11:QK:72:ALA:HB2	1.94	0.50
33:R8:12:LYS:NZ	35:RA:249:C:O2	2.40	0.50
2:XB:84:GLU:HB3	2:XB:219:VAL:HG21	1.92	0.50
2:XB:121:LEU:HD23	2:XB:127:ILE:HD12	1.94	0.50
35:YA:1223:G:O6	51:YV:69:LYS:NZ	2.44	0.50
39:YF:155:LEU:HD23	39:YF:192:LEU:HD13	1.93	0.50
1:QA:1149:C:OP2	9:QI:9:ARG:NH2	2.45	0.50
35:RA:221:A:N1	35:RA:265:A:O2'	2.44	0.50
43:RN:15:LEU:HB2	43:RN:135:PRO:HB2	1.93	0.50
1:XA:618:C:H5'	1:XA:619:U:H5''	1.94	0.50
1:XA:1330:U:H4'	13:XM:23:TYR:CE1	2.46	0.50
26:Y1:3:LYS:HB2	26:Y1:61:ARG:HH11	1.77	0.50
29:Y4:1:MET:SD	40:YG:98:ARG:NH1	2.85	0.50
35:RA:693:C:O2'	35:RA:1353:A:N3	2.41	0.50
1:XA:1005:A:O3'	1:XA:1037:C:O2'	2.30	0.50
35:YA:1801:G:OP2	37:YD:154:LYS:NZ	2.44	0.50
1:QA:975:A:H4'	1:QA:976:G:H5''	1.93	0.49
18:QR:23:LYS:HD2	18:QR:58:LEU:HD23	1.94	0.49
35:RA:299:A:N3	35:RA:319:C:O2'	2.45	0.49
6:XF:11:ASN:HB3	6:XF:14:LEU:HG	1.94	0.49
35:YA:601:C:O2'	35:YA:605:C:OP1	2.28	0.49
35:YA:1296:G:OP1	35:YA:2709:G:O2'	2.26	0.49
1:QA:278:G:OP2	17:QQ:92:ARG:NH2	2.40	0.49
1:QA:993:G:O2'	1:QA:994:A:N7	2.44	0.49
35:RA:2882:A:H5'	47:RR:96:ARG:HG3	1.93	0.49
1:XA:757:U:O2'	1:XA:879:C:O2	2.30	0.49
8:XH:41:ARG:NH2	8:XH:123:GLU:OE2	2.45	0.49
35:YA:116:C:O2'	35:YA:126:A:N3	2.37	0.49
54:YY:20:TYR:HB3	54:YY:23:ARG:HG3	1.94	0.49
1:QA:769:G:H4'	1:QA:1513:A:H4'	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:953:G:N7	13:QM:104:ARG:NH2	2.53	0.49
35:RA:1853:A:N3	35:RA:2233:U:O2'	2.41	0.49
44:RO:19:ILE:HG22	44:RO:43:VAL:HA	1.93	0.49
35:YA:1098:A:H3'	35:YA:1099:G:H8	1.77	0.49
35:YA:2875:C:OP1	49:YT:3:ARG:NH1	2.45	0.49
38:YE:7:VAL:HG23	38:YE:51:PHE:HE2	1.77	0.49
52:YW:86:LEU:HD22	52:YW:96:ILE:HD11	1.95	0.49
54:YY:14:LEU:HB2	54:YY:75:ILE:HD11	1.92	0.49
1:QA:410:G:H21	1:QA:432:A:H62	1.59	0.49
13:QM:24:GLY:O	13:QM:29:ARG:NH1	2.46	0.49
35:RA:392:C:H5''	35:RA:409:C:H5''	1.93	0.49
35:YA:2680:C:H5'	38:YE:189:PRO:HA	1.95	0.49
39:YF:11:VAL:HG22	39:YF:125:LEU:HB2	1.93	0.49
35:RA:336:C:HO2'	54:RY:35:TYR:HH	1.60	0.49
35:RA:831:G:O2'	45:RP:38:GLN:OE1	2.27	0.49
1:XA:28:G:O2'	1:XA:296:U:OP1	2.28	0.49
1:XA:1129:C:OP1	9:XI:16:ARG:NH1	2.46	0.49
10:XJ:11:PHE:HE1	10:XJ:67:THR:HG22	1.77	0.49
10:XJ:67:THR:O	10:XJ:67:THR:OG1	2.30	0.49
26:Y1:25:LYS:NZ	35:YA:2396:G:OP1	2.45	0.49
35:YA:1047:G:H21	35:YA:1111:A:H62	1.59	0.49
1:QA:1255:G:OP2	10:QJ:45:ARG:NH2	2.45	0.49
18:XR:32:ARG:HA	18:XR:69:THR:HG21	1.94	0.49
35:YA:1277:G:O2'	47:YR:24:GLN:OE1	2.23	0.49
39:YF:6:VAL:N	39:YF:22:ALA:O	2.45	0.49
53:YX:59:VAL:HB	53:YX:76:ARG:HG3	1.95	0.49
1:QA:28:G:O2'	1:QA:296:U:OP1	2.29	0.49
1:QA:407:G:H5''	4:QD:115:ARG:HG2	1.94	0.49
4:QD:88:VAL:HA	5:QE:97:GLY:HA3	1.94	0.49
35:RA:1490:A:O2'	37:RD:99:ASP:OD1	2.30	0.49
1:XA:501:C:O2	1:XA:549:C:O2'	2.29	0.49
1:XA:1098:C:OP2	2:XB:144:ARG:NH1	2.46	0.49
35:YA:994:C:OP1	50:YU:53:ARG:NH2	2.45	0.49
35:RA:299:A:N1	35:RA:322:A:O2'	2.42	0.49
2:XB:69:LEU:HB3	2:XB:162:ILE:HG22	1.95	0.49
2:XB:122:PHE:CE2	2:XB:139:LYS:HD3	2.43	0.49
1:QA:1219:U:OP1	14:QN:19:ARG:NH2	2.46	0.49
8:QH:91:ARG:NE	17:QQ:32:TYR:O	2.45	0.49
9:QI:118:LYS:HB2	9:QI:121:ARG:HB3	1.93	0.49
29:R4:31:ILE:HG21	40:RG:142:PRO:HB2	1.95	0.49
33:Y8:26:LYS:HD3	33:Y8:44:LYS:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:955:C:OP1	46:YQ:87:LYS:NZ	2.40	0.49
57:QA:1821:PAR:N64	57:QA:1821:PAR:O44	2.44	0.49
25:R0:32:ARG:H	25:R0:35:ASN:ND2	2.09	0.49
35:RA:1022:G:N2	35:RA:1023:U:O4	2.41	0.49
39:RF:165:ARG:HG3	39:RF:168:ARG:HH12	1.78	0.49
51:RV:72:VAL:HG13	51:RV:85:LYS:HB3	1.94	0.49
1:XA:792:A:O2'	1:XA:794:A:N7	2.40	0.49
2:XB:16:HIS:HB2	2:XB:204:ASN:HB3	1.94	0.49
13:XM:23:TYR:HE2	13:XM:71:ARG:HG2	1.78	0.49
13:XM:102:ARG:NH2	13:XM:105:THR:OG1	2.43	0.49
41:YH:159:GLU:HG2	41:YH:169:VAL:HG11	1.94	0.49
1:QA:380:G:N2	1:QA:383:A:OP2	2.39	0.48
1:QA:401:C:O2'	1:QA:621:A:N3	2.42	0.48
35:RA:643:A:N1	35:RA:2369:A:O2'	2.43	0.48
39:RF:167:ALA:HB1	39:RF:173:VAL:HG11	1.95	0.48
45:RP:89:ALA:O	45:RP:121:LYS:NZ	2.36	0.48
6:XF:50:TYR:CE1	18:XR:77:GLY:HA2	2.43	0.48
8:XH:34:GLU:OE1	8:XH:37:ARG:NH2	2.46	0.48
35:YA:996:A:OP2	50:YU:93:LYS:NZ	2.39	0.48
44:YO:16:ALA:HA	44:YO:46:ALA:HA	1.94	0.48
1:QA:186:C:O2'	20:QT:85:MET:SD	2.69	0.48
1:QA:811:C:O2'	1:QA:901:A:N1	2.46	0.48
33:R8:27:THR:HG22	45:RP:63:PRO:HD3	1.94	0.48
34:R9:25:VAL:HB	34:R9:34:GLN:HB2	1.94	0.48
1:QA:663:A:H61	1:QA:742:G:H1	1.59	0.48
1:QA:978:A:H61	1:QA:1316:G:H1'	1.78	0.48
13:QM:8:GLU:OE2	13:QM:11:ARG:NH1	2.46	0.48
35:RA:271:A:N3	35:RA:365:C:O2'	2.43	0.48
45:RP:19:VAL:HG12	45:RP:27:HIS:HB3	1.95	0.48
2:XB:126:GLU:O	2:XB:130:ARG:NH1	2.46	0.48
3:XC:9:GLY:HA3	14:YN:49:HIS:HA	1.95	0.48
14:YN:24:CYS:HB3	14:YN:29:ARG:H	1.78	0.48
39:YF:167:ALA:HA	39:YF:170:LEU:HD23	1.95	0.48
2:QB:27:LYS:O	2:QB:30:ARG:NH1	2.46	0.48
6:QF:37:VAL:HA	6:QF:65:VAL:HG12	1.95	0.48
3:XC:152:ILE:HG12	3:XC:199:LYS:HB2	1.94	0.48
35:YA:1022:G:N2	35:YA:1023:U:O4	2.40	0.48
35:YA:1657:C:OP1	38:YE:136:ARG:N	2.46	0.48
37:RD:168:ARG:HG2	37:RD:173:VAL:HG12	1.95	0.48
52:RW:18:ARG:NH1	52:RW:76:VAL:O	2.46	0.48
1:QA:978:A:OP2	1:QA:1363(A):C:N4	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:R4:18:CYS:SG	29:R4:20:ASN:ND2	2.87	0.48
35:RA:1082:U:O4	35:RA:1086:A:N6	2.47	0.48
42:RI:4:ILE:HG12	42:RI:18:VAL:HG22	1.95	0.48
51:RV:21:ARG:HD3	51:RV:91:TYR:CE2	2.48	0.48
28:Y3:8:LEU:HD13	28:Y3:23:LEU:HD11	1.95	0.48
41:YH:106:THR:O	41:YH:106:THR:OG1	2.31	0.48
7:QG:57:GLU:HG3	7:QG:60:LYS:H	1.79	0.48
39:RF:164:ARG:HG3	39:RF:175:THR:HB	1.96	0.48
41:RH:3:ARG:HE	41:RH:4:ILE:H	1.62	0.48
1:XA:1309:G:N7	13:XM:99:ARG:NH2	2.61	0.48
10:XJ:9:ARG:HG2	10:XJ:69:ASN:HD22	1.79	0.48
35:YA:139(A):G:H21	53:YX:41:ASN:HD21	1.61	0.48
35:YA:919:G:N2	35:YA:2269:A:OP2	2.46	0.48
1:QA:1414:U:H3	1:QA:1486:G:H1	1.61	0.48
35:RA:220:G:O2'	35:RA:233:A:N3	2.40	0.48
44:RO:16:ALA:HA	44:RO:46:ALA:HA	1.95	0.48
51:RV:41:GLY:HA2	51:RV:45:THR:HA	1.95	0.48
35:YA:223:A:O2'	35:YA:420:C:O2	2.29	0.48
35:YA:1682:G:OP1	35:YA:1699:G:N1	2.46	0.48
44:YO:1:MET:HG3	44:YO:67:LYS:HG2	1.95	0.48
54:YY:39:VAL:HB	54:YY:42:VAL:HB	1.96	0.48
33:R8:26:LYS:HD3	33:R8:44:LYS:HG2	1.95	0.48
35:RA:307:G:N1	35:RA:310:A:OP2	2.47	0.48
37:RD:71:ASP:HB2	37:RD:103:ARG:HH12	1.79	0.48
1:XA:280:C:OP1	17:XQ:91:ARG:NH1	2.43	0.48
1:XA:461:A:O2'	1:XA:471:G:N7	2.44	0.48
1:XA:1085:U:H5''	1:XA:1086:U:H5	1.79	0.48
6:XF:80:ARG:NH1	6:XF:88:VAL:O	2.47	0.48
35:YA:861:A:N3	36:YB:79:C:O2'	2.45	0.48
35:YA:1568:G:H5''	37:YD:61:LEU:HG	1.95	0.48
39:YF:167:ALA:HB1	39:YF:173:VAL:HG11	1.96	0.48
35:RA:117:G:OP2	35:RA:119:A:O2'	2.26	0.48
35:RA:579:G:O2'	35:RA:2019:A:OP1	2.30	0.48
35:RA:2751:G:H4'	41:RH:4:ILE:HD11	1.96	0.48
38:RE:134:ILE:HA	38:RE:137:HIS:HD2	1.77	0.48
1:XA:380:G:N2	1:XA:383:A:OP2	2.35	0.48
17:XQ:28:PRO:HA	17:XQ:35:VAL:HA	1.96	0.48
41:YH:154:PRO:HB3	41:YH:163:TYR:CZ	2.48	0.48
49:YT:34:VAL:O	49:YT:41:ARG:N	2.43	0.48
55:YZ:69:THR:HG22	55:YZ:90:VAL:HA	1.95	0.48
16:QP:20:VAL:HG23	16:QP:35:LYS:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R5:41:PRO:O	30:R5:44:THR:OG1	2.32	0.47
33:R8:19:SER:OG	35:RA:651:G:OP1	2.31	0.47
35:RA:1155:A:P	50:RU:55:ARG:HG2	2.54	0.47
42:RI:90:GLY:O	42:RI:121:LYS:NZ	2.37	0.47
1:XA:718:G:O6	18:XR:74:ARG:NH1	2.47	0.47
3:XC:8:ILE:HG23	3:XC:16:ARG:HE	1.78	0.47
27:Y2:22:GLU:OE2	27:Y2:68:ARG:NH2	2.47	0.47
35:YA:2572:A:OP1	35:YA:2574:G:O2'	2.30	0.47
1:QA:1261:A:H62	1:QA:1274:G:H21	1.62	0.47
9:QI:46:ALA:HB2	9:QI:74:ILE:HG23	1.95	0.47
27:R2:22:GLU:OE2	27:R2:68:ARG:NH2	2.46	0.47
35:RA:918:A:N3	36:RB:80:U:O2'	2.46	0.47
35:RA:1657:C:OP1	38:RE:136:ARG:N	2.47	0.47
35:RA:2574:G:N3	38:RE:143:ASN:ND2	2.61	0.47
45:RP:47:ASP:OD2	45:RP:49:ARG:NH2	2.43	0.47
35:YA:535:C:O3'	50:YU:53:ARG:NH1	2.47	0.47
37:YD:5:LYS:HG2	37:YD:17:THR:HG22	1.96	0.47
44:YO:80:ASP:OD2	49:YT:64:ARG:NH2	2.47	0.47
49:YT:73:GLU:OE2	49:YT:103:ARG:NH2	2.46	0.47
1:QA:376:G:H1	1:QA:387:U:H3	1.62	0.47
1:QA:1172:C:H2'	1:QA:1173:G:H8	1.79	0.47
1:QA:1422:G:O3'	44:RO:49:ARG:NH1	2.46	0.47
35:RA:1833:U:O2'	35:RA:1969:A:N1	2.46	0.47
35:RA:1859:A:N6	35:RA:1883:G:O2'	2.46	0.47
19:XS:43:GLU:N	19:XS:43:GLU:CD	2.71	0.47
25:Y0:33:ALA:N	25:Y0:64:ASP:OD1	2.45	0.47
35:YA:1250:G:OP2	45:YP:21:ARG:NH1	2.47	0.47
35:YA:1490:A:O2'	37:YD:99:ASP:OD1	2.29	0.47
35:YA:1798:U:OP2	37:YD:274:ARG:NH2	2.42	0.47
1:QA:642:A:N3	8:QH:113:SER:OG	2.44	0.47
32:R7:37:LYS:NZ	35:RA:468:G:OP2	2.47	0.47
35:RA:1155:A:OP1	50:RU:55:ARG:HG2	2.14	0.47
35:RA:1394:U:O2	53:RX:16:LYS:NZ	2.45	0.47
37:RD:183:ARG:HG3	37:RD:270:ILE:HG12	1.96	0.47
44:RO:1:MET:HG3	44:RO:67:LYS:HG2	1.95	0.47
5:XE:94:ALA:HB1	5:XE:98:THR:HG21	1.97	0.47
19:XS:41:VAL:HG22	19:XS:44:MET:HE3	1.96	0.47
25:Y0:32:ARG:H	25:Y0:35:ASN:ND2	2.12	0.47
38:YE:144:ARG:HB3	38:YE:145:LYS:H	1.51	0.47
29:R4:37:SER:HB2	40:RG:108:ASN:HA	1.95	0.47
35:RA:223:A:O2'	35:RA:420:C:O2	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:660:G:H5''	39:RF:99:TYR:CD2	2.47	0.47
48:RS:27:SER:HA	48:RS:88:ASP:HB3	1.96	0.47
4:XD:68:TYR:OH	4:XD:98:GLU:OE2	2.21	0.47
10:XJ:50:ILE:HB	14:XN:41:ARG:HE	1.79	0.47
19:XS:63:THR:HG22	19:XS:66:MET:HE3	1.97	0.47
35:YA:2853:C:H2'	35:YA:2854:G:H8	1.79	0.47
38:YE:104:VAL:HG22	38:YE:198:VAL:HG22	1.97	0.47
40:YG:106:LEU:HA	40:YG:110:ALA:HB3	1.96	0.47
1:QA:1442(B):G:C8	49:RT:118:ARG:HG2	2.50	0.47
22:QV:16:C:H4'	22:QV:17(A):U:H5''	1.95	0.47
35:RA:2144:U:O2	35:RA:2148:G:N1	2.43	0.47
46:RQ:39:PRO:HB3	46:RQ:99:PRO:HD3	1.96	0.47
53:RX:59:VAL:HB	53:RX:76:ARG:HG3	1.96	0.47
9:XI:19:LEU:HB3	9:XI:59:PHE:HD2	1.79	0.47
1:QA:123:C:OP1	1:QA:311:C:O2'	2.27	0.47
1:QA:562:C:H1'	12:QL:15:ARG:HB3	1.96	0.47
1:QA:593:G:H1	1:QA:646:U:H3	1.63	0.47
6:QF:50:TYR:OH	18:QR:74:ARG:O	2.32	0.47
7:QG:28:ASN:OD1	7:QG:36:LYS:NZ	2.48	0.47
7:QG:51:GLN:NE2	7:QG:56:GLN:O	2.47	0.47
8:QH:85:ARG:NE	8:QH:87:SER:O	2.30	0.47
20:QT:50:GLU:HG3	20:QT:100:ILE:HD11	1.95	0.47
25:R0:27:GLU:HG3	25:R0:68:GLU:HA	1.96	0.47
34:R9:16:VAL:HG22	34:R9:25:VAL:HG22	1.96	0.47
1:XA:235:C:H2'	1:XA:236:G:H8	1.79	0.47
1:XA:261:U:OP2	20:XT:79:ARG:NH2	2.48	0.47
2:XB:71:VAL:HA	2:XB:93:VAL:HG22	1.97	0.47
3:XC:58:GLU:HB3	10:XJ:92:THR:HG21	1.95	0.47
26:Y1:18:ILE:HG12	26:Y1:37:ILE:HG12	1.97	0.47
35:YA:463:G:N2	35:YA:466:A:OP2	2.39	0.47
44:YO:19:ILE:HG22	44:YO:43:VAL:HA	1.97	0.47
49:YT:24:PRO:HA	49:YT:49:VAL:HG13	1.97	0.47
1:QA:1005:A:O2'	1:QA:1036:G:N2	2.47	0.47
1:QA:1358:U:H5''	14:QN:34:TYR:HA	1.95	0.47
35:RA:1074:G:C2	35:RA:1075:C:H1'	2.50	0.47
46:RQ:26:TYR:O	46:RQ:67:ARG:NH1	2.43	0.47
16:XP:38:TYR:CE1	16:XP:50:LYS:CB	2.97	0.47
27:Y2:55:ARG:HH12	35:YA:74:A:H5'	1.80	0.47
22:QV:56:C:O2	40:RG:78:SER:OG	2.32	0.47
25:R0:43:THR:HG22	35:RA:2336:A:H61	1.79	0.47
33:R8:26:LYS:HD3	33:R8:44:LYS:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R9:1:MET:SD	34:R9:35:ARG:HB2	2.55	0.47
1:XA:949:A:N7	13:XM:106:ASN:ND2	2.63	0.47
13:XM:94:ARG:HB3	13:XM:96:LEU:HD13	1.96	0.47
16:XP:8:ARG:NH1	16:XP:9:PHE:O	2.48	0.47
35:YA:530:G:N1	35:YA:2023:G:OP1	2.37	0.47
38:YE:134:ILE:HA	38:YE:137:HIS:HD2	1.80	0.47
1:QA:73:G:H1	1:QA:96:U:H3	1.63	0.47
35:RA:321:G:O2'	35:RA:340:A:N3	2.46	0.47
35:RA:854:G:H2'	35:RA:855:G:H8	1.80	0.47
1:XA:1220:G:N2	19:XS:54:GLY:O	2.46	0.47
18:XR:23:LYS:HD2	18:XR:58:LEU:HD23	1.97	0.47
35:YA:745:G:O6	35:YA:746:A:N6	2.48	0.47
51:YV:21:ARG:NE	51:YV:91:TYR:CE2	2.79	0.47
52:YW:35:ILE:O	52:YW:39:THR:OG1	2.29	0.47
1:QA:689:C:OP1	11:QK:27:ASN:ND2	2.44	0.46
4:QD:166:LYS:HD2	4:QD:178:VAL:HG11	1.97	0.46
19:QS:40:ILE:HG22	19:QS:67:VAL:HG13	1.97	0.46
24:QY:75:C:O2	35:RA:2507:C:O2'	2.29	0.46
35:RA:2483:C:N3	46:RQ:124:LYS:NZ	2.55	0.46
35:RA:2718:G:O2'	35:RA:2847:U:OP1	2.33	0.46
1:XA:975:A:H4'	1:XA:976:G:H5''	1.96	0.46
2:XB:212:GLN:O	2:XB:216:SER:OG	2.27	0.46
35:YA:2405:G:O2'	35:YA:2411:A:N6	2.45	0.46
35:YA:2680:C:O2'	38:YE:11:MET:SD	2.72	0.46
37:YD:71:ASP:HB2	37:YD:103:ARG:HH12	1.80	0.46
45:YP:88:LEU:HD11	45:YP:114:ILE:HD12	1.98	0.46
1:QA:932:C:H5''	7:QG:4:ARG:HE	1.80	0.46
3:QC:184:TYR:HD1	3:QC:201:TYR:CD1	2.34	0.46
20:QT:43:LEU:HD13	20:QT:51:GLU:HB3	1.97	0.46
30:R5:12:SER:HB3	35:RA:2020:A:H5'	1.98	0.46
1:XA:634:C:H2'	1:XA:635:G:H8	1.80	0.46
1:XA:1330:U:H5'	13:XM:23:TYR:HD1	1.80	0.46
6:XF:46:ARG:HH21	18:XR:78:LEU:HD22	1.80	0.46
10:XJ:6:ILE:HB	10:XJ:72:VAL:HG13	1.97	0.46
12:XL:57:LYS:HE3	12:XL:65:GLU:HG2	1.96	0.46
16:QP:32:TYR:CE2	16:QP:35:LYS:HB2	2.51	0.46
35:RA:1769:G:O2'	35:RA:1958:C:OP1	2.28	0.46
45:RP:20:GLY:HA2	45:RP:28:GLY:HA2	1.98	0.46
49:RT:27:THR:HG22	49:RT:48:ILE:HG12	1.96	0.46
1:XA:345:C:OP2	49:YT:39:ARG:NH2	2.47	0.46
12:XL:5:PRO:HD2	12:XL:15:ARG:HH22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:586:A:N1	35:YA:809:G:O2'	2.45	0.46
35:YA:793:A:OP2	35:YA:2071:A:O2'	2.33	0.46
35:YA:1453:U:O2'	35:YA:1455:G:N7	2.46	0.46
35:YA:2816:C:O2	35:YA:2883:A:O2'	2.29	0.46
39:YF:157:VAL:HG22	39:YF:176:LEU:HB2	1.98	0.46
3:QC:71:ALA:HA	3:QC:106:VAL:HG22	1.96	0.46
35:RA:1266:G:O2'	35:RA:2012:G:O6	2.28	0.46
35:RA:1288:U:O2'	35:RA:1647:G:N2	2.47	0.46
1:XA:619:U:N3	4:XD:134:ASP:OD1	2.38	0.46
1:XA:1414:U:H2'	1:XA:1415:G:H8	1.80	0.46
35:YA:2503:2MA:O2'	35:YA:2505:G:OP2	2.25	0.46
38:YE:84:PHE:CZ	38:YE:86:PRO:HB3	2.51	0.46
1:QA:35:G:N3	12:QL:118:SER:OG	2.48	0.46
35:RA:2105:C:H2'	35:RA:2106:G:C8	2.51	0.46
35:RA:2689:U:H4'	35:RA:2690:C:H5'	1.97	0.46
51:RV:49:THR:O	51:RV:51:VAL:N	2.49	0.46
1:XA:867:G:O2'	1:XA:873:A:N1	2.43	0.46
1:XA:1251:A:N3	1:XA:1369:C:O2'	2.41	0.46
4:XD:63:LYS:HD2	4:XD:198:VAL:HG12	1.97	0.46
5:XE:76:ILE:HG13	5:XE:93:PRO:HG3	1.96	0.46
8:XH:110:ALA:HB3	8:XH:121:ASP:HB3	1.97	0.46
16:XP:43:LYS:HG2	16:XP:48:TRP:CD2	2.51	0.46
35:YA:694:U:OP1	37:YD:59:LYS:NZ	2.44	0.46
35:YA:2304:G:H22	35:YA:2312:U:H3	1.61	0.46
35:YA:2685:G:H5'	44:YO:68:GLU:OE2	2.15	0.46
55:YZ:108:PRO:HG2	55:YZ:117:LEU:HD21	1.96	0.46
1:QA:1329:A:N7	21:QU:7:ARG:NH2	2.63	0.46
33:R8:64:TYR:OH	35:RA:592:G:O2'	2.28	0.46
35:RA:521:G:H2'	35:RA:522:G:H8	1.81	0.46
35:RA:2478:A:O2'	35:RA:2536:G:N2	2.49	0.46
1:XA:486:U:H2'	1:XA:487:A:C8	2.50	0.46
1:XA:689:C:OP1	11:XK:27:ASN:ND2	2.48	0.46
1:XA:769:G:OP2	1:XA:803:G:O2'	2.32	0.46
8:XH:33:GLU:HG2	8:XH:59:LEU:HD21	1.96	0.46
11:XK:18:ARG:NH2	11:XK:35:PRO:O	2.48	0.46
14:XN:29:ARG:HG2	14:XN:31:ARG:H	1.80	0.46
35:YA:958:U:O2	36:YB:90:A:O2'	2.27	0.46
35:YA:1815:A:OP2	37:YD:54:ARG:NH2	2.42	0.46
38:YE:111:ARG:HG3	47:YR:1:MET:HE1	1.97	0.46
43:YN:12:ARG:NH1	43:YN:50:ASP:OD2	2.48	0.46
52:YW:14:PRO:HG2	52:YW:78:GLU:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:QB:68:ILE:HD12	2:QB:161:ALA:HB3	1.96	0.46
9:QI:10:ARG:NH1	9:QI:105:ASP:OD2	2.48	0.46
10:QJ:12:ASP:HB3	10:QJ:15:THR:HG22	1.98	0.46
30:R5:7:PRO:O	35:RA:2016:U:O2'	2.31	0.46
33:R8:7:HIS:CD2	45:RP:50:ARG:HD3	2.51	0.46
35:RA:530:G:N1	35:RA:2023:G:OP1	2.36	0.46
35:RA:743:G:O2'	35:RA:1659:U:OP1	2.32	0.46
35:RA:1084:A:H8	35:RA:1085:A:H4'	1.80	0.46
35:RA:1666:G:O2'	44:RO:6:THR:OG1	2.27	0.46
35:RA:2711:A:H5''	35:RA:2712(A):U:H5''	1.98	0.46
35:RA:2788:C:OP1	38:RE:61:ARG:NH2	2.49	0.46
54:RY:9:LYS:NZ	54:RY:28:LYS:O	2.43	0.46
1:XA:1498:UR3:OP2	23:XX:16:A:O2'	2.32	0.46
13:XM:82:MET:HE3	13:XM:93:ARG:HG2	1.98	0.46
35:YA:1394:U:O2	53:YX:16:LYS:NZ	2.45	0.46
44:YO:8:LEU:HB2	44:YO:19:ILE:HG13	1.97	0.46
46:YQ:43:THR:HG22	46:YQ:94:VAL:HG12	1.98	0.46
1:QA:824:C:H2'	1:QA:825:G:H8	1.81	0.46
35:RA:2059:A:HO2'	39:RF:69:HIS:HD1	1.63	0.46
39:RF:6:VAL:N	39:RF:22:ALA:O	2.48	0.46
41:RH:3:ARG:HE	41:RH:5:GLY:H	1.64	0.46
41:RH:7:LEU:HD22	41:RH:69:ARG:HH21	1.80	0.46
1:XA:1518:MA6:O5'	1:XA:1518:MA6:H8	2.15	0.46
28:Y3:51:ALA:HA	28:Y3:54:VAL:HG12	1.98	0.46
35:YA:630:G:N2	35:YA:633:A:OP2	2.41	0.46
37:YD:108:PRO:HA	37:YD:196:VAL:HA	1.97	0.46
1:QA:1222:G:H5''	19:QS:78:ARG:HD2	1.97	0.46
7:QG:79:ARG:HA	7:QG:84:ASN:HA	1.98	0.46
9:QI:9:ARG:HB2	9:QI:104:ARG:HE	1.81	0.46
35:RA:660:G:OP1	39:RF:99:TYR:HD2	1.99	0.46
35:RA:675:A:N3	35:RA:2443:C:O2'	2.48	0.46
35:RA:1007:C:H5''	43:RN:35:ARG:NH1	2.31	0.46
35:RA:2295:C:OP1	48:RS:10:ARG:NH1	2.49	0.46
35:RA:2521:C:O2'	35:RA:2564:A:N3	2.45	0.46
43:RN:94:HIS:HB3	43:RN:97:ARG:HD3	1.98	0.46
1:XA:1000:U:H2'	1:XA:1001(A):A:H8	1.78	0.46
19:XS:68:GLY:H	29:Y4:58:ARG:HH12	1.63	0.46
35:YA:1423:G:H2'	35:YA:1424:G:H8	1.81	0.46
26:R1:3:LYS:HB3	26:R1:61:ARG:HH22	1.81	0.46
35:RA:776:G:N7	35:RA:793:A:O2'	2.49	0.46
35:RA:1223:G:N2	35:RA:1226:A:OP2	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:RF:110:LEU:HD11	39:RF:181:LEU:HG	1.97	0.46
1:XA:742:G:OP2	15:XO:35:ARG:NH2	2.49	0.46
7:XG:15:ASP:OD1	7:XG:19:GLY:N	2.48	0.46
35:YA:1936:A:OP2	35:YA:1962:5MC:N4	2.46	0.46
1:QA:976:G:OP2	1:QA:1358:U:O2'	2.34	0.45
1:QA:1122:U:O4	1:QA:1123:A:N6	2.49	0.45
35:RA:1231:G:H2'	35:RA:1232:G:C8	2.51	0.45
35:RA:2788:C:O2'	35:RA:2809:A:N3	2.42	0.45
1:XA:148:G:H2'	1:XA:149:A:C8	2.51	0.45
1:XA:278:G:OP2	17:XQ:92:ARG:NH2	2.44	0.45
16:XP:53:VAL:HG12	16:XP:79:VAL:HG22	1.97	0.45
35:YA:1394:U:H4'	35:YA:1603:A:H4'	1.98	0.45
35:YA:1824:G:H5''	37:YD:52:ARG:HH21	1.80	0.45
37:YD:145:VAL:HB	37:YD:155:LEU:HB2	1.98	0.45
2:QB:178:ARG:HG2	8:QH:72:PRO:HA	1.98	0.45
26:R1:72:GLU:OE2	26:R1:76:ARG:HD2	2.16	0.45
35:RA:1012:U:O4	43:RN:28:THR:OG1	2.29	0.45
1:XA:427:U:O2'	1:XA:541:G:OP1	2.30	0.45
1:XA:475:G:H2'	1:XA:476:G:H8	1.82	0.45
4:XD:133:VAL:HG11	4:XD:138:TYR:HD2	1.80	0.45
35:YA:2314:C:H2'	35:YA:2315:G:C8	2.52	0.45
40:YG:97:ASP:HA	40:YG:100:TRP:HD1	1.80	0.45
43:YN:71:ILE:HA	43:YN:86:PRO:HA	1.98	0.45
35:RA:276:A:H5''	35:RA:277:C:H5'	1.98	0.45
35:RA:1568:G:H5''	37:RD:61:LEU:HG	1.98	0.45
35:RA:2735:G:H2'	35:RA:2736:G:H8	1.81	0.45
1:XA:1129:C:H2'	1:XA:1139:G:N7	2.31	0.45
1:XA:1458:G:OP1	20:XT:35:THR:OG1	2.31	0.45
4:XD:148:VAL:HG11	4:XD:158:ILE:HG21	1.99	0.45
35:YA:956:G:OP2	46:YQ:14:ARG:NH2	2.49	0.45
35:YA:1541:G:OP2	35:YA:1542:A:O2'	2.31	0.45
35:YA:1567:A:H3'	37:YD:86:PRO:HG3	1.99	0.45
35:YA:1816:G:O6	37:YD:35:LYS:NZ	2.42	0.45
36:YB:74:U:H1'	55:YZ:34:ASN:HD21	1.82	0.45
1:QA:279:A:OP2	17:QQ:95:TYR:OH	2.34	0.45
2:QB:164:VAL:HG21	2:QB:174:VAL:HG12	1.99	0.45
5:QE:145:LYS:NZ	5:QE:149:GLU:OE2	2.49	0.45
7:QG:22:LEU:HD21	7:QG:66:VAL:HG11	1.98	0.45
12:QL:70:ILE:HG12	12:QL:77:LEU:HD12	1.98	0.45
27:R2:29:LYS:HG2	27:R2:57:ILE:HD13	1.98	0.45
32:R7:34:ARG:HG3	32:R7:39:ARG:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:805:G:N2	35:RA:829:A:OP1	2.50	0.45
35:RA:1798:U:OP2	37:RD:273:ARG:NH2	2.49	0.45
35:YA:220:G:O2'	35:YA:233:A:N3	2.41	0.45
35:YA:621:A:OP2	45:YP:108:LYS:NZ	2.50	0.45
35:YA:1020:A:N1	35:YA:1141:U:O2'	2.45	0.45
5:QE:48:ALA:HB2	5:QE:57:LYS:HD3	1.98	0.45
15:QO:5:LYS:O	15:QO:9:GLN:HG2	2.17	0.45
22:QV:24:U:O2'	35:RA:1923:U:OP1	2.34	0.45
35:RA:641:C:O2'	35:RA:2350:C:OP1	2.26	0.45
35:RA:995:C:O2	43:RN:3:THR:OG1	2.32	0.45
35:RA:2431:U:N3	35:RA:2434:A:OP2	2.36	0.45
37:RD:72:LYS:HE3	37:RD:101:GLU:HB3	1.97	0.45
39:RF:150:GLY:HA2	39:RF:172:TRP:CD2	2.52	0.45
39:RF:160:ASN:HB3	39:RF:163:VAL:HG12	1.98	0.45
17:XQ:9:VAL:HG22	17:XQ:56:VAL:HG22	1.99	0.45
3:QC:24:ALA:HB3	3:QC:29:TYR:HB2	1.98	0.45
13:QM:60:VAL:HG12	13:QM:64:TRP:HZ3	1.80	0.45
41:RH:159:GLU:HG2	41:RH:169:VAL:HG11	1.98	0.45
48:RS:35:ILE:HB	48:RS:97:ARG:HH21	1.81	0.45
50:RU:66:ASN:HD21	50:RU:70:ARG:HH21	1.65	0.45
55:RZ:8:TYR:C	55:RZ:38:TYR:HD1	2.24	0.45
1:XA:520:A:O2'	12:XL:73:GLU:OE1	2.34	0.45
1:XA:736:C:O2'	6:XF:90:VAL:O	2.32	0.45
1:XA:744:C:O2'	1:XA:851:G:N2	2.48	0.45
6:XF:35:ALA:HA	6:XF:67:MET:HB3	1.99	0.45
22:XV:58:A:O2'	22:XV:60:U:OP2	2.26	0.45
35:YA:698:C:O2'	35:YA:734:A:N6	2.50	0.45
35:YA:1035:U:OP1	41:YH:59:ARG:NH2	2.49	0.45
35:YA:1288:U:O2'	35:YA:1647:G:N2	2.48	0.45
35:YA:2133:G:O2'	35:YA:2158:A:N1	2.49	0.45
1:QA:1255:G:O2'	1:QA:1258:G:N3	2.45	0.45
1:QA:1393:U:HO2'	1:QA:1501:C:HO2'	1.62	0.45
1:QA:1485:U:H2'	1:QA:1486:G:C8	2.52	0.45
3:QC:184:TYR:CD1	3:QC:201:TYR:CE1	3.05	0.45
35:RA:1754:C:N3	35:RA:2716:U:O2'	2.38	0.45
39:RF:178:PRO:HB2	39:RF:201:VAL:HG11	1.98	0.45
1:XA:181:G:O2'	1:XA:183:G:N7	2.49	0.45
1:XA:1199:U:O2'	1:XA:1202:G:OP1	2.33	0.45
35:YA:1098:A:H3'	35:YA:1099:G:C8	2.52	0.45
35:YA:1853:A:N3	35:YA:2233:U:O2'	2.39	0.45
55:YZ:126:VAL:HG11	55:YZ:161:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1069:C:O2'	1:QA:1192:C:O2	2.27	0.45
8:QH:33:GLU:OE2	8:QH:50:ARG:NE	2.47	0.45
14:QN:24:CYS:HB3	14:QN:29:ARG:H	1.81	0.45
35:RA:1312:U:O4	53:RX:60:ARG:HD3	2.17	0.45
37:RD:132:PRO:HG3	37:RD:190:TYR:CE1	2.52	0.45
54:RY:28:LYS:N	54:RY:38:ILE:O	2.44	0.45
1:XA:1192:C:O2	5:XE:25:ARG:NH2	2.50	0.45
31:Y6:37:ARG:HA	31:Y6:48:VAL:HA	1.99	0.45
35:YA:1415:U:O2'	35:YA:1417:C:OP1	2.30	0.45
35:YA:2581:G:OP2	35:YA:2581:G:N2	2.41	0.45
1:QA:1456:G:O3'	20:QT:39:LYS:NZ	2.50	0.45
7:QG:27:ILE:HD12	7:QG:40:ALA:HA	1.98	0.45
32:R7:24:THR:HG23	32:R7:27:GLY:H	1.82	0.45
35:RA:265:A:N1	35:RA:427:U:O2'	2.46	0.45
46:RQ:30:GLY:N	46:RQ:105:GLU:OE2	2.48	0.45
22:XV:49:G:H1	22:XV:65:C:H42	1.63	0.45
26:Y1:86:SER:OG	26:Y1:89:GLU:OE1	2.29	0.45
35:YA:30:G:O2'	35:YA:1214:A:N3	2.42	0.45
35:YA:272(L):U:P	42:YI:50:ARG:HH22	2.40	0.45
35:YA:2352:A:N6	35:YA:2365:G:O2'	2.50	0.45
51:YV:21:ARG:CD	51:YV:91:TYR:CE2	3.00	0.45
51:YV:21:ARG:CZ	51:YV:91:TYR:HE2	2.29	0.45
4:QD:105:VAL:HG13	4:QD:110:PHE:HB2	1.99	0.45
13:QM:19:LEU:HD11	13:QM:56:LEU:HD21	1.99	0.45
20:QT:89:ARG:O	20:QT:93:GLU:HG2	2.17	0.45
35:RA:557:U:O2'	43:RN:45:ASN:O	2.35	0.45
35:RA:1417:C:O2'	35:RA:1587:A:N3	2.45	0.45
39:RF:101:LEU:HD23	39:RF:106:ARG:HG2	2.00	0.45
1:XA:1073:U:O2	2:XB:104:ASN:ND2	2.50	0.45
5:XE:6:PHE:HD1	5:XE:36:ASP:HB3	1.82	0.45
5:XE:33:VAL:HG13	5:XE:112:LEU:HD22	1.98	0.45
6:XF:30:LEU:HB3	6:XF:35:ALA:HB3	1.99	0.45
9:XI:9:ARG:HG2	9:XI:14:VAL:HG12	1.99	0.45
13:XM:86:CYS:SG	13:XM:89:GLY:N	2.87	0.45
35:YA:964:C:O2'	35:YA:2273:A:N3	2.46	0.45
35:YA:2012:G:OP1	52:YW:11:ARG:NH2	2.49	0.45
37:YD:132:PRO:HG3	37:YD:190:TYR:CE1	2.52	0.45
38:YE:84:PHE:CE2	38:YE:86:PRO:CB	3.00	0.45
35:RA:984:A:H5''	35:RA:985:C:H5	1.81	0.44
43:RN:25:ARG:O	43:RN:29:LYS:NZ	2.45	0.44
1:XA:1309:G:P	13:XM:88:ARG:HH21	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1105:U:H2'	35:YA:1106:G:H8	1.80	0.44
38:YE:176:ILE:HB	38:YE:181:LEU:HB2	1.99	0.44
51:YV:21:ARG:HD3	51:YV:91:TYR:CE2	2.52	0.44
1:QA:447:G:O6	1:QA:485:G:O2'	2.34	0.44
1:QA:806:C:H2'	1:QA:807:A:H8	1.82	0.44
10:QJ:61:GLU:OE1	14:QN:45:ARG:NE	2.47	0.44
35:RA:588:U:H1'	39:RF:90:PHE:HB3	1.99	0.44
35:RA:1651:G:N7	47:RR:11:ASN:ND2	2.64	0.44
35:RA:1939:5MU:OP1	35:RA:2604:U:O2'	2.34	0.44
38:RE:24:THR:OG1	38:RE:186:GLY:O	2.30	0.44
1:XA:543:C:OP2	4:XD:10:ARG:NH2	2.48	0.44
18:XR:51:LEU:HD13	18:XR:55:ARG:HG2	2.00	0.44
35:YA:2119:A:H61	35:YA:2168:G:H21	1.64	0.44
37:YD:77:ALA:HA	37:YD:97:TYR:HA	2.00	0.44
37:YD:183:ARG:HG3	37:YD:270:ILE:HG12	1.99	0.44
1:QA:426:G:OP1	4:QD:38:TYR:OH	2.36	0.44
9:QI:36:TYR:HE1	9:QI:70:LYS:HE2	1.83	0.44
35:RA:728:G:H4'	37:RD:13:ARG:HE	1.82	0.44
35:RA:1327:C:HO2'	47:RR:105:ARG:HH12	1.59	0.44
35:RA:1514:U:H2'	35:RA:1515:G:H8	1.82	0.44
35:RA:2441:C:OP2	35:RA:2586:C:O2'	2.28	0.44
37:RD:75:ILE:HG21	37:RD:99:ASP:HB2	2.00	0.44
1:XA:790:A:OP1	22:XV:38:A:O2'	2.24	0.44
5:XE:105:VAL:HG21	5:XE:128:PRO:HB3	1.99	0.44
7:XG:79:ARG:HA	7:XG:84:ASN:HA	1.99	0.44
11:XK:45:GLY:HA2	11:XK:48:ILE:HD12	2.00	0.44
36:YB:87:G:N2	36:YB:90:A:OP2	2.40	0.44
43:YN:21:LYS:NZ	43:YN:140:VAL:OXT	2.39	0.44
1:QA:718:G:H5'	11:QK:117:ASN:OD1	2.18	0.44
2:QB:9:GLU:HG2	2:QB:11:LEU:H	1.82	0.44
5:QE:78:HIS:HA	8:QH:105:ARG:HG3	1.99	0.44
20:QT:22:ARG:O	20:QT:26:ASN:ND2	2.51	0.44
35:RA:586:A:N1	35:RA:809:G:O2'	2.46	0.44
35:RA:1188:U:H2'	35:RA:1189:A:H8	1.81	0.44
35:RA:1792:G:O2'	35:RA:1830:C:OP1	2.33	0.44
35:RA:2200:C:O2	35:RA:2226:C:N4	2.49	0.44
1:XA:624:C:H2'	1:XA:625:G:H8	1.82	0.44
1:XA:978:A:O2'	1:XA:1322:C:N3	2.47	0.44
5:XE:110:LEU:HD13	5:XE:118:ILE:HG21	1.97	0.44
32:Y7:13:ALA:HB2	32:Y7:46:VAL:HG11	1.99	0.44
35:YA:1792:G:O2'	35:YA:1830:C:OP1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:YG:38:VAL:HG22	40:YG:93:THR:HG23	1.99	0.44
1:QA:184:G:H2'	1:QA:185:A:H8	1.81	0.44
1:QA:790:A:OP1	22:QV:38:A:O2'	2.30	0.44
9:QI:16:ARG:HB2	9:QI:64:THR:HG22	1.99	0.44
10:QJ:16:LEU:HD22	10:QJ:94:VAL:HG12	2.00	0.44
35:RA:463:G:N2	35:RA:466:A:OP2	2.39	0.44
38:RE:1:MET:HE1	38:RE:202:LYS:HG2	1.99	0.44
1:XA:328:C:H4'	1:XA:329:A:H5'	1.99	0.44
9:XI:5:TYR:N	9:XI:87:GLN:OE1	2.50	0.44
41:YH:154:PRO:HB3	41:YH:163:TYR:CE1	2.53	0.44
47:YR:63:ARG:HG2	47:YR:80:PHE:CE2	2.53	0.44
1:QA:396:G:O2'	1:QA:398:C:OP1	2.26	0.44
43:RN:36:GLY:HA2	43:RN:38:HIS:CE1	2.53	0.44
1:XA:1368:G:OP1	9:XI:111:ARG:NH2	2.50	0.44
6:XF:95:GLU:O	18:XR:32:ARG:NH1	2.50	0.44
13:XM:17:VAL:O	13:XM:20:THR:OG1	2.27	0.44
35:YA:2522:U:O2'	35:YA:2647:U:OP1	2.31	0.44
37:YD:108:PRO:HB3	37:YD:143:HIS:CE1	2.53	0.44
54:YY:83:THR:OG1	54:YY:84:ARG:N	2.51	0.44
1:QA:128:G:O2'	17:QQ:3:LYS:NZ	2.38	0.44
35:RA:184:C:O2'	35:RA:217:G:N3	2.50	0.44
35:RA:807:U:OP2	45:RP:41:ARG:NH2	2.51	0.44
35:RA:1936:A:OP2	35:RA:1962:5MC:N4	2.48	0.44
35:RA:2404:C:O3'	45:RP:77:ARG:NH2	2.51	0.44
41:RH:126:PRO:HG2	41:RH:130:ARG:HH21	1.82	0.44
45:RP:3:LEU:HD23	45:RP:6:LEU:HD12	2.00	0.44
1:XA:111:G:H5''	16:XP:27:LYS:HG2	1.99	0.44
1:XA:297:G:N2	1:XA:300:A:OP2	2.48	0.44
2:XB:71:VAL:HG13	2:XB:164:VAL:HA	1.99	0.44
2:XB:207:ALA:O	2:XB:210:SER:OG	2.32	0.44
6:XF:33:TYR:HE2	6:XF:78:GLU:HG3	1.82	0.44
9:XI:50:LEU:HD23	9:XI:85:LEU:HD11	1.98	0.44
35:YA:2377:A:O2'	48:YS:112:PHE:O	2.30	0.44
35:YA:2500:U:O2'	35:YA:2504:U:OP1	2.32	0.44
1:QA:1073:U:O2	2:QB:104:ASN:ND2	2.51	0.44
35:RA:139(A):G:H21	53:RX:41:ASN:HD21	1.66	0.44
35:RA:729:G:C5	37:RD:208:LYS:HB2	2.52	0.44
35:RA:873:G:O3'	46:RQ:63:LYS:NZ	2.50	0.44
9:XI:16:ARG:HH21	9:XI:18:PHE:HZ	1.66	0.44
35:YA:956:G:H2'	35:YA:957:A:H2'	1.99	0.44
47:YR:100:LEU:HD12	47:YR:111:LEU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1377:A:OP2	7:QG:94:ARG:NE	2.51	0.44
26:R1:11:ARG:NH2	35:RA:1365:A:O2'	2.51	0.44
35:RA:475:U:H4'	35:RA:510:C:H5'	2.00	0.44
51:RV:14:VAL:HB	51:RV:96:ILE:HG13	2.00	0.44
1:XA:1074:G:H1	1:XA:1083:U:H3	1.66	0.44
1:XA:1240:U:OP1	7:XG:119:ARG:NH2	2.46	0.44
1:XA:1316:G:N1	1:XA:1319:A:OP2	2.51	0.44
16:XP:19:ILE:HB	16:XP:37:GLY:HA3	1.99	0.44
19:XS:68:GLY:H	29:Y4:58:ARG:NH1	2.16	0.44
35:YA:639:U:H3	35:YA:649:G:H1	1.66	0.44
35:YA:992:C:OP1	50:YU:47:TYR:OH	2.32	0.44
1:QA:189(C):C:H42	1:QA:189(J):G:H1	1.66	0.43
11:QK:20:TYR:CE1	11:QK:83:ILE:HD13	2.53	0.43
35:RA:814:C:O2'	35:RA:1224:C:N3	2.51	0.43
49:RT:9:LEU:O	49:RT:12:SER:OG	2.27	0.43
55:RZ:102:LEU:HD11	55:RZ:124:ILE:HG12	2.00	0.43
1:XA:96:U:H2'	1:XA:97:G:H8	1.82	0.43
1:XA:123:C:OP1	1:XA:311:C:O2'	2.31	0.43
6:XF:61:LEU:HD12	6:XF:63:TYR:HE1	1.83	0.43
29:Y4:11:PRO:HG3	29:Y4:25:TYR:CD2	2.53	0.43
33:Y8:12:LYS:NZ	35:YA:249:C:O2	2.35	0.43
45:YP:19:VAL:HG12	45:YP:27:HIS:HB3	2.00	0.43
11:QK:34:ASP:OD1	11:QK:38:ASN:N	2.51	0.43
18:QR:34:TYR:HD1	18:QR:34:TYR:H	1.64	0.43
32:R7:9:ARG:NH2	35:RA:1311:G:N7	2.65	0.43
41:RH:68:THR:O	41:RH:72:ILE:HG12	2.18	0.43
41:RH:126:PRO:HG2	41:RH:130:ARG:HE	1.83	0.43
42:RI:114:LEU:HD11	42:RI:128:LEU:HB3	2.00	0.43
4:XD:20:TYR:HD1	4:XD:26:CYS:HB3	1.83	0.43
4:XD:59:ARG:HA	4:XD:59:ARG:HE	1.83	0.43
7:XG:16:LEU:HD11	9:XI:45:ALA:HB2	2.00	0.43
17:XQ:52:LYS:HE3	17:XQ:52:LYS:HB3	1.83	0.43
35:YA:1664:A:H61	35:YA:1996:C:H42	1.66	0.43
35:YA:2773:C:H5''	38:YE:164:ARG:HG2	2.00	0.43
55:YZ:52:SER:OG	55:YZ:53:ILE:N	2.51	0.43
1:QA:142:G:H2'	1:QA:143:A:H8	1.82	0.43
4:QD:10:ARG:HB2	4:QD:40:PRO:HG3	2.00	0.43
4:QD:140:VAL:HG11	4:QD:146:ILE:HD11	2.00	0.43
49:RT:50:ILE:HB	49:RT:99:LEU:HB2	1.99	0.43
15:XO:5:LYS:O	15:XO:9:GLN:HG2	2.19	0.43
29:Y4:43:TYR:CZ	40:YG:179:PRO:HG3	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:2115:G:O2'	35:YA:2166:G:N2	2.51	0.43
35:YA:2635:C:O2'	38:YE:80:GLU:OE1	2.32	0.43
39:YF:155:LEU:HD11	39:YF:176:LEU:HD12	1.99	0.43
40:YG:109:VAL:HG11	40:YG:142:PRO:HB3	2.00	0.43
1:QA:1516:G:N2	1:QA:1519:MA6:OP2	2.49	0.43
2:QB:179:LYS:HD3	8:QH:72:PRO:HG3	1.99	0.43
35:RA:955:C:OP1	46:RQ:87:LYS:NZ	2.43	0.43
35:RA:956:G:OP2	46:RQ:14:ARG:NH2	2.52	0.43
49:RT:24:PRO:HA	49:RT:49:VAL:HG13	2.00	0.43
1:XA:107:G:N7	20:XT:15:ARG:NH2	2.67	0.43
1:XA:824:C:H2'	1:XA:825:G:C8	2.53	0.43
1:XA:986:A:H1'	19:XS:55:LYS:HA	1.99	0.43
13:XM:23:TYR:CE2	13:XM:71:ARG:HG2	2.52	0.43
34:Y9:2:LYS:NZ	35:YA:2478:A:OP2	2.48	0.43
49:YT:35:LYS:HA	49:YT:40:THR:HA	1.99	0.43
49:YT:93:ARG:HB3	49:YT:117:ASP:HB2	2.00	0.43
1:QA:1129:C:H2'	1:QA:1139:G:N7	2.33	0.43
5:QE:6:PHE:HD1	5:QE:36:ASP:HB3	1.83	0.43
8:QH:112:LEU:HB3	8:QH:133:LEU:HA	2.00	0.43
27:R2:36:ARG:NH2	53:RX:5:TYR:O	2.40	0.43
30:R5:12:SER:OG	35:RA:2021:C:OP1	2.32	0.43
35:RA:647:G:N3	35:RA:2350:C:O2'	2.51	0.43
35:RA:1151:G:O2'	50:RU:77:SER:O	2.37	0.43
35:RA:2572:A:H2'	38:RE:144:ARG:HD3	2.01	0.43
52:RW:35:ILE:O	52:RW:39:THR:OG1	2.31	0.43
1:XA:601:C:H2'	1:XA:602:A:H8	1.83	0.43
1:XA:626:U:H4'	16:XP:38:TYR:CD2	2.53	0.43
4:XD:98:GLU:HG3	4:XD:194:LEU:HD11	2.01	0.43
5:XE:78:HIS:ND1	8:XH:104:ARG:HD2	2.33	0.43
33:Y8:23:VAL:HG22	33:Y8:49:VAL:HG22	2.01	0.43
33:Y8:30:ARG:NH2	45:YP:64:LYS:O	2.52	0.43
35:YA:1009:A:N3	35:YA:1153:C:O2'	2.42	0.43
35:YA:2164:C:H3'	35:YA:2165:G:H8	1.83	0.43
1:QA:444:C:H2'	1:QA:445:G:H8	1.84	0.43
1:QA:1005:A:O3'	1:QA:1037:C:O2'	2.37	0.43
44:RO:8:LEU:HB2	44:RO:19:ILE:HG13	2.00	0.43
48:RS:3:ARG:HH21	48:RS:9:ARG:HH12	1.67	0.43
1:XA:1133:G:H2'	1:XA:1134:G:H8	1.82	0.43
1:XA:1133:G:H2'	1:XA:1134:G:C8	2.54	0.43
35:YA:743:G:O2'	35:YA:1659:U:OP1	2.31	0.43
41:YH:87:LEU:HD23	41:YH:164:TYR:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:YS:24:LEU:O	48:YS:86:ALA:N	2.48	0.43
1:QA:1031:G:H2'	1:QA:1032:G:C8	2.53	0.43
12:QL:71:PRO:HB2	12:QL:120:TYR:HE1	1.84	0.43
35:RA:1466:G:O2'	35:RA:1546:C:O2'	2.28	0.43
35:RA:1566:A:OP1	37:RD:211:ARG:NH1	2.51	0.43
35:RA:1816:G:O6	37:RD:35:LYS:NZ	2.50	0.43
35:RA:2013:A:H2	52:RW:88:ARG:HH22	1.66	0.43
48:RS:26:LEU:HD23	48:RS:87:PHE:HD1	1.84	0.43
49:RT:50:ILE:HA	49:RT:99:LEU:HD12	2.00	0.43
1:XA:943:U:H1'	9:XI:124:GLN:HE22	1.84	0.43
35:YA:297:C:OP1	54:YY:87:LYS:NZ	2.43	0.43
35:YA:380:U:H2'	35:YA:381:G:H8	1.83	0.43
35:YA:1779:U:OP2	35:YA:1784:A:N6	2.34	0.43
35:YA:2438:U:O2'	35:YA:2440:C:OP1	2.36	0.43
41:YH:28:GLY:HA3	41:YH:79:VAL:HB	2.01	0.43
1:QA:730:G:C5	1:QA:731:G:H1'	2.54	0.43
12:QL:70:ILE:HG13	12:QL:100:ILE:HD12	1.99	0.43
35:RA:906:G:O2'	46:RQ:67:ARG:NH2	2.46	0.43
22:XV:76:A:H2'	35:YA:2602:A:N6	2.33	0.43
24:XY:37:A:O2'	35:YA:1913:A:N1	2.50	0.43
35:YA:453:C:O2	35:YA:457:A:O2'	2.35	0.43
35:YA:1156:A:OP1	50:YU:55:ARG:HD2	2.19	0.43
35:YA:1327:C:HO2'	47:YR:105:ARG:HH12	1.60	0.43
1:QA:522:C:H41	12:QL:53:ARG:HH22	1.67	0.43
1:QA:640:A:N3	8:QH:115:SER:OG	2.40	0.43
1:QA:806:C:H2'	1:QA:807:A:C8	2.54	0.43
1:QA:985:C:H2'	1:QA:986:A:C8	2.54	0.43
29:R4:14:ILE:HB	29:R4:22:ILE:HB	2.00	0.43
29:R4:34:GLU:OE1	29:R4:35:VAL:CG2	2.66	0.43
35:RA:2728:U:H2'	35:RA:2729:G:C8	2.54	0.43
40:RG:77:ILE:HG23	40:RG:80:PHE:HB2	2.01	0.43
1:XA:626:U:H5''	16:XP:38:TYR:CD2	2.52	0.43
1:XA:1030(D):G:H2'	1:XA:1030(E):A:C8	2.54	0.43
44:YO:122:LEU:HD13	49:YT:72:VAL:HG11	2.00	0.43
2:QB:54:THR:O	2:QB:58:ILE:HG12	2.19	0.43
4:QD:168:ARG:HH22	37:YD:134:ARG:NH2	2.17	0.43
35:RA:2880:C:O3'	47:RR:90:ARG:NH1	2.52	0.43
37:RD:275:LYS:HD3	37:RD:275:LYS:HA	1.80	0.43
44:RO:2:ILE:HB	44:RO:33:ALA:HB3	2.01	0.43
50:RU:83:LEU:HD13	50:RU:88:ILE:HB	2.01	0.43
1:XA:410:G:H3'	4:XD:25:ARG:HH22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:919:A:O2'	1:XA:1080:A:N1	2.41	0.43
2:XB:80:ILE:HG21	2:XB:211:ILE:HD12	2.01	0.43
7:XG:150:ALA:HB1	11:XK:57:THR:HG21	2.01	0.43
8:XH:36:LEU:HD12	8:XH:59:LEU:HD23	2.01	0.43
31:Y6:6:ARG:HA	31:Y6:6:ARG:HD2	1.88	0.43
35:YA:244:A:H4'	45:YP:74:GLU:HB2	2.01	0.43
35:YA:869:G:H1'	46:YQ:8:LYS:HD2	2.01	0.43
35:YA:2839:G:H5'	47:YR:46:GLY:HA2	2.01	0.43
40:YG:5:VAL:HG23	40:YG:8:LYS:H	1.84	0.43
1:QA:522:C:OP2	12:QL:69:TYR:OH	2.28	0.42
3:QC:159:GLY:HA2	3:QC:193:TYR:HD2	1.75	0.42
8:QH:25:ASP:HB3	8:QH:58:TYR:HD2	1.83	0.42
26:R1:30:VAL:O	35:RA:2395:C:O2'	2.35	0.42
27:R2:36:ARG:NH2	53:RX:8:ILE:O	2.51	0.42
35:RA:1231:G:H2'	35:RA:1232:G:H8	1.84	0.42
1:XA:148:G:H2'	1:XA:149:A:H8	1.83	0.42
1:XA:237:C:O3'	17:XQ:25:ARG:NH2	2.51	0.42
1:XA:403:C:H4'	4:XD:122:ARG:HH11	1.84	0.42
1:XA:1131:G:OP1	9:XI:20:ARG:NH2	2.52	0.42
35:YA:2502:G:H5''	35:YA:2503:2MA:H5''	2.00	0.42
35:YA:2679:A:H5'	38:YE:165:VAL:HG21	2.01	0.42
39:YF:155:LEU:HB2	39:YF:189:THR:HG21	2.01	0.42
44:YO:68:GLU:HB3	44:YO:78:ARG:HB2	2.00	0.42
45:YP:20:GLY:HA2	45:YP:28:GLY:HA2	2.01	0.42
49:YT:94:ALA:HB1	49:YT:99:LEU:HD21	2.01	0.42
3:QC:37:GLN:NE2	14:QN:52:GLN:OE1	2.36	0.42
35:RA:576:U:H2'	35:RA:577:G:C8	2.54	0.42
35:RA:685:A:OP1	35:RA:686:G:N2	2.52	0.42
35:RA:1567:A:H3'	37:RD:86:PRO:HG3	2.01	0.42
38:RE:134:ILE:HA	38:RE:137:HIS:CD2	2.54	0.42
50:RU:102:GLU:HG3	51:RV:2:PHE:CZ	2.54	0.42
55:RZ:58:VAL:HA	55:RZ:68:PRO:HA	2.01	0.42
1:XA:184:G:H2'	1:XA:185:A:H8	1.84	0.42
1:XA:624:C:H2'	1:XA:625:G:C8	2.54	0.42
15:XO:3:ILE:HG22	15:XO:38:ARG:HH21	1.84	0.42
35:YA:83:G:O2'	35:YA:102:G:N2	2.51	0.42
35:YA:226:G:H21	35:YA:228:A:H62	1.67	0.42
35:YA:335:C:O2	54:YY:70:SER:OG	2.38	0.42
35:YA:1277:G:H2'	35:YA:1278:A:C8	2.54	0.42
55:YZ:30:ASN:OD1	55:YZ:33:LEU:N	2.41	0.42
35:RA:602:G:N2	35:RA:655:A:OP2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:RD:245:PRO:HA	37:RD:246:PRO:HD3	1.94	0.42
37:RD:247:ALA:HA	37:RD:253:GLN:HA	2.00	0.42
1:XA:946:A:O2'	1:XA:1333:A:N3	2.45	0.42
1:XA:1286:A:N6	1:XA:1354:C:O3'	2.52	0.42
12:XL:117:ARG:HB2	12:XL:122:THR:HB	2.02	0.42
13:XM:4:ILE:HG13	13:XM:5:ALA:H	1.84	0.42
41:YH:46:GLU:OE2	41:YH:51:ARG:NH2	2.50	0.42
41:YH:149:ARG:NH2	41:YH:167:GLU:OE2	2.47	0.42
51:YV:52:VAL:HG21	51:YV:55:ALA:HB3	2.01	0.42
55:YZ:13:GLU:HG3	55:YZ:18:LEU:HD21	2.01	0.42
1:QA:328:C:H4'	1:QA:329:A:H5'	2.00	0.42
1:QA:977:A:O2'	1:QA:979:C:OP2	2.34	0.42
4:QD:61:LYS:HE2	4:QD:206:PHE:CE2	2.54	0.42
27:R2:38:GLN:HA	27:R2:41:ILE:HG12	2.01	0.42
30:R5:51:TYR:HE1	30:R5:56:LYS:HD3	1.84	0.42
35:RA:1682:G:OP2	35:RA:1699:G:N2	2.52	0.42
35:RA:2564:A:OP1	35:RA:2648:C:O2'	2.37	0.42
39:RF:161:GLU:O	39:RF:165:ARG:HB2	2.20	0.42
44:RO:68:GLU:HB3	44:RO:78:ARG:HB2	2.02	0.42
46:RQ:52:VAL:HA	46:RQ:55:VAL:HG22	2.01	0.42
50:RU:66:ASN:OD1	50:RU:70:ARG:NE	2.51	0.42
11:XK:20:TYR:CE1	11:XK:83:ILE:HD12	2.54	0.42
16:XP:3:LYS:HG2	16:XP:65:GLN:HB2	2.01	0.42
27:Y2:37:PHE:CD1	53:YX:11:PRO:HD3	2.55	0.42
35:YA:272(R):G:H2'	35:YA:272(S):G:H8	1.84	0.42
35:YA:414:C:H2'	35:YA:415:A:C8	2.54	0.42
35:YA:616:G:O2'	39:YF:205:ARG:NH1	2.53	0.42
35:YA:626:U:O4	45:YP:81:GLN:NE2	2.53	0.42
35:YA:2328:A:H2'	35:YA:2329:G:C8	2.54	0.42
40:YG:78:SER:OG	40:YG:79:ASN:N	2.52	0.42
41:YH:54:ARG:HD2	41:YH:65:HIS:ND1	2.35	0.42
41:YH:86:GLU:OE2	41:YH:132:ARG:NH2	2.52	0.42
1:QA:346:G:OP1	49:RT:41:ARG:NH1	2.52	0.42
1:QA:522:C:H41	12:QL:53:ARG:NH2	2.17	0.42
1:QA:552:U:H4'	12:QL:87:GLY:HA3	2.02	0.42
1:QA:626:U:C5'	16:QP:38:TYR:HD2	2.30	0.42
1:QA:652:U:O4	1:QA:752:G:O2'	2.32	0.42
3:QC:153:VAL:HG22	3:QC:198:VAL:HG22	2.00	0.42
4:QD:18:LYS:HE3	4:QD:20:TYR:CE2	2.54	0.42
35:RA:698:C:O2'	35:RA:734:A:N6	2.52	0.42
35:RA:1423:G:H2'	35:RA:1424:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2543:G:H2'	35:RA:2544:G:C8	2.54	0.42
45:RP:65:ARG:O	45:RP:68:GLN:NE2	2.53	0.42
53:RX:53:LYS:HB3	53:RX:82:GLN:HB3	2.01	0.42
1:XA:96:U:H2'	1:XA:97:G:C8	2.55	0.42
6:XF:30:LEU:HD23	6:XF:75:LEU:HD11	2.02	0.42
35:YA:1028:A:N3	35:YA:2486:G:O2'	2.49	0.42
35:YA:1665:A:H1'	44:YO:1:MET:HB2	2.01	0.42
35:YA:1666:G:HO2'	44:YO:6:THR:HG1	1.59	0.42
46:YQ:104:PHE:HE2	46:YQ:125:LEU:HD11	1.85	0.42
1:QA:1106:G:H5''	3:QC:172:ARG:HG2	2.01	0.42
1:QA:1412:C:H2'	1:QA:1413:A:C8	2.55	0.42
2:QB:84:GLU:HB3	2:QB:219:VAL:HG21	2.02	0.42
3:QC:19:GLU:HG2	3:QC:55:VAL:O	2.18	0.42
9:QI:4:TYR:HB2	9:QI:19:LEU:HB2	2.00	0.42
25:R0:77:ARG:NH2	35:RA:857:C:OP2	2.52	0.42
35:RA:442:G:N3	39:RF:48:THR:OG1	2.42	0.42
35:RA:2633:G:H5''	35:RA:2812:G:H5'	2.02	0.42
39:RF:165:ARG:HG3	39:RF:168:ARG:NH1	2.35	0.42
39:RF:184:TYR:CE2	39:RF:188:ARG:HD2	2.55	0.42
1:XA:142:G:H2'	1:XA:143:A:H8	1.84	0.42
1:XA:673:G:H4'	6:XF:87:ARG:HH12	1.84	0.42
14:YN:4:LYS:HA	14:YN:7:ILE:HG12	2.02	0.42
30:Y5:7:PRO:O	35:YA:2016:U:O2'	2.37	0.42
35:YA:78:A:H2'	35:YA:79:G:H8	1.83	0.42
35:YA:200:U:O2	35:YA:386:G:N2	2.52	0.42
13:QM:66:LEU:HD13	13:QM:66:LEU:HA	1.88	0.42
33:R8:2:PRO:O	35:RA:666:G:N2	2.52	0.42
35:RA:1638:C:OP1	35:RA:2710:C:O2'	2.36	0.42
40:RG:37:VAL:HG13	40:RG:94:LEU:HB2	2.02	0.42
40:RG:173:LEU:HD13	40:RG:176:LEU:HD12	2.01	0.42
1:XA:769:G:H4'	1:XA:1513:A:H4'	2.02	0.42
17:XQ:62:SER:OG	17:XQ:72:ARG:NE	2.43	0.42
28:Y3:52:HIS:CD2	28:Y3:53:LEU:HG	2.55	0.42
35:YA:1223:G:N2	35:YA:1226:A:OP2	2.43	0.42
35:YA:1500:G:H21	37:YD:100:GLY:HA3	1.85	0.42
35:YA:2441:C:OP2	35:YA:2586:C:O2'	2.35	0.42
35:YA:2602:A:H4'	35:YA:2603:G:C5'	2.50	0.42
39:YF:178:PRO:HB2	39:YF:201:VAL:HG21	2.01	0.42
1:QA:523:A:H61	12:QL:92:0TD:CG	2.31	0.42
1:QA:981:U:O4	1:QA:1223:C:N4	2.53	0.42
2:QB:163:PHE:HA	2:QB:185:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:QE:6:PHE:CD1	5:QE:36:ASP:HB3	2.54	0.42
35:RA:572:A:OP2	51:RV:78:LYS:NZ	2.41	0.42
41:RH:3:ARG:NE	41:RH:5:GLY:H	2.18	0.42
7:XG:113:GLU:OE2	7:XG:122:HIS:ND1	2.38	0.42
8:XH:104:ARG:HA	8:XH:104:ARG:HD3	1.85	0.42
10:XJ:40:LEU:HB2	10:XJ:69:ASN:HB2	2.02	0.42
28:Y3:52:HIS:CG	36:YB:83:G:H4'	2.54	0.42
35:YA:1069:A:C6	35:YA:1095:A:H4'	2.55	0.42
35:YA:2679:A:OP2	38:YE:160:TYR:OH	2.27	0.42
1:QA:165:C:H2'	1:QA:166:G:H8	1.85	0.42
35:RA:411:G:OP2	35:RA:2406:U:O2'	2.37	0.42
35:RA:1296:G:OP1	35:RA:2709:G:O2'	2.26	0.42
1:XA:192:U:H5'	20:XT:101:GLY:HA3	2.01	0.42
4:XD:50:ARG:HA	4:XD:51:PRO:HD3	1.92	0.42
9:XI:42:ARG:NH2	9:XI:71:SER:OG	2.53	0.42
9:XI:73:GLN:O	9:XI:77:ILE:HG12	2.20	0.42
35:YA:2633:G:H5''	35:YA:2812:G:H5'	2.00	0.42
39:YF:31:HIS:NE2	39:YF:35:GLU:OE2	2.53	0.42
16:QP:18:ARG:NH1	16:QP:32:TYR:OH	2.53	0.42
19:QS:22:LEU:HA	19:QS:22:LEU:HD13	1.82	0.42
35:RA:1478:G:O2'	35:RA:1558:A:N7	2.50	0.42
38:RE:5:LEU:HD11	38:RE:79:ARG:HB2	2.02	0.42
41:RH:99:VAL:N	41:RH:102:ALA:O	2.51	0.42
42:RI:115:ALA:HB2	42:RI:131:LYS:HE2	2.02	0.42
46:RQ:34:LEU:HB2	46:RQ:118:LEU:HD22	2.01	0.42
50:RU:44:ASN:HD21	51:RV:75:PHE:HB3	1.84	0.42
1:XA:356:A:N3	1:XA:368:U:O2'	2.37	0.42
1:XA:476:G:H2'	1:XA:477:A:H8	1.84	0.42
1:XA:779:C:H5''	11:XK:122:LYS:HG2	2.02	0.42
1:XA:1356:G:H2'	1:XA:1357:A:C8	2.55	0.42
1:XA:1408:A:N1	57:XA:1794:PAR:O61	2.51	0.42
9:XI:9:ARG:H	9:XI:79:LEU:HD23	1.85	0.42
17:XQ:6:LEU:HD23	17:XQ:23:VAL:HG11	2.02	0.42
35:YA:602:G:O2'	35:YA:604:G:O2'	2.33	0.42
35:YA:1188:U:H2'	35:YA:1189:A:H8	1.84	0.42
35:YA:1309:G:O2'	35:YA:1611:C:O2'	2.33	0.42
35:YA:1567:A:C6	37:YD:84:TYR:CD2	3.08	0.42
35:YA:1790:C:H2'	35:YA:1791:A:C5	2.55	0.42
37:YD:253:GLN:HB2	37:YD:257:LEU:HD12	2.01	0.42
38:YE:34:VAL:HG12	38:YE:72:VAL:HG21	2.01	0.42
40:YG:101:ILE:HG22	40:YG:105:LYS:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:142:G:H2'	1:QA:143:A:C8	2.54	0.41
1:QA:673:G:H5''	6:QF:87:ARG:NH1	2.35	0.41
1:QA:1366:C:O2'	10:QJ:60:ARG:NH2	2.47	0.41
31:R6:10:LEU:HD13	31:R6:19:ARG:HG2	2.02	0.41
35:RA:1466:G:HO2'	35:RA:1546:C:HO2'	1.59	0.41
35:RA:2503:2MA:O2'	35:RA:2505:G:OP2	2.25	0.41
41:RH:24:VAL:HG21	41:RH:72:ILE:HD12	2.02	0.41
48:RS:10:ARG:HG3	48:RS:13:ARG:HH21	1.84	0.41
1:XA:407:G:H2'	1:XA:408:A:C8	2.54	0.41
1:XA:407:G:OP1	4:XD:115:ARG:NH1	2.53	0.41
1:XA:684:A:O2'	11:XK:39:PRO:O	2.35	0.41
1:XA:1060:C:H5''	10:XJ:51:ARG:HG2	2.02	0.41
1:XA:1491:G:N7	57:XA:1794:PAR:O53	2.47	0.41
25:Y0:31:VAL:HB	25:Y0:35:ASN:HD22	1.85	0.41
35:YA:557:U:O2'	43:YN:45:ASN:O	2.34	0.41
35:YA:1057:A:H62	35:YA:1086:A:H3'	1.84	0.41
2:QB:181:PHE:CE1	8:QH:71:GLY:HA2	2.55	0.41
35:RA:1688:U:O2	35:RA:1700:A:H5'	2.20	0.41
35:RA:2857:G:N2	35:RA:2860:A:OP2	2.34	0.41
1:XA:1031:G:H2'	1:XA:1032:G:C8	2.55	0.41
1:XA:1179:A:O3'	9:XI:103:THR:OG1	2.37	0.41
24:XY:75:C:O2	35:YA:2507:C:O2'	2.28	0.41
28:Y3:6:VAL:HG12	28:Y3:28:LEU:HD11	2.01	0.41
35:YA:2405:G:H5'	45:YP:75:ILE:HD13	2.03	0.41
40:YG:3:LEU:HD11	40:YG:101:ILE:HD11	2.01	0.41
41:YH:8:PRO:O	41:YH:69:ARG:NH2	2.46	0.41
1:QA:749:C:H2'	1:QA:750:G:H8	1.85	0.41
14:QN:29:ARG:HG2	14:QN:31:ARG:H	1.84	0.41
35:RA:1657:C:H4'	38:RE:133:LYS:HB3	2.03	0.41
35:RA:1889:A:H2'	35:RA:1890:A:C8	2.55	0.41
1:XA:966:M2G:HM13	1:XA:967:5MC:H1'	2.02	0.41
1:XA:1149:C:P	9:XI:9:ARG:HH21	2.43	0.41
3:XC:150:LYS:HG3	3:XC:169:ALA:HB2	2.02	0.41
4:XD:194:LEU:HB3	4:XD:196:LEU:HD12	2.01	0.41
10:XJ:61:GLU:OE1	14:XN:45:ARG:NE	2.48	0.41
10:XJ:61:GLU:OE2	14:XN:49:HIS:NE2	2.40	0.41
28:Y3:8:LEU:HA	28:Y3:54:VAL:HG23	2.01	0.41
35:YA:87:C:H5''	35:YA:88:G:H5'	2.03	0.41
39:YF:39:TRP:NE1	39:YF:99:TYR:O	2.52	0.41
47:YR:87:TYR:OH	47:YR:117:VAL:O	2.37	0.41
2:QB:155:LEU:HD21	2:QB:159:PRO:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:QE:76:ILE:HG13	5:QE:93:PRO:HG3	2.02	0.41
11:QK:65:ALA:HB1	11:QK:98:LEU:HD12	2.03	0.41
35:RA:272(Q):G:H2'	35:RA:272(R):G:C8	2.55	0.41
35:RA:581:C:H2'	35:RA:582:G:C8	2.55	0.41
35:RA:1082:U:H6	35:RA:1082:U:H2'	1.71	0.41
35:RA:1516:C:H2'	35:RA:1517:G:H8	1.85	0.41
35:RA:2302:G:O2'	40:RG:126:ASP:O	2.33	0.41
37:RD:72:LYS:NZ	37:RD:99:ASP:OD2	2.53	0.41
37:RD:260:ARG:NH2	37:RD:266:SER:OG	2.53	0.41
46:RQ:110:THR:HG23	46:RQ:113:GLN:H	1.85	0.41
1:XA:652:U:O4	1:XA:752:G:O2'	2.30	0.41
1:XA:1005:A:O2'	1:XA:1036:G:N2	2.53	0.41
25:Y0:43:THR:HG22	35:YA:2336:A:H61	1.86	0.41
30:Y5:4:HIS:O	35:YA:2056:G:N2	2.53	0.41
35:YA:184:C:H1'	35:YA:217:G:H1'	2.01	0.41
35:YA:579:G:O2'	35:YA:2019:A:OP1	2.38	0.41
35:YA:2136:C:N4	35:YA:2155:G:O6	2.52	0.41
45:YP:65:ARG:O	45:YP:68:GLN:NE2	2.52	0.41
1:QA:521:G:N7	12:QL:53:ARG:NH1	2.67	0.41
1:QA:1230:C:H5'	22:QV:30:G:H5''	2.03	0.41
1:QA:1403:C:N4	23:QX:18:G:OP1	2.52	0.41
4:QD:79:PHE:HE1	4:QD:204:ILE:HD13	1.85	0.41
8:QH:34:GLU:HB3	8:QH:118:VAL:HG21	2.01	0.41
19:QS:63:THR:OG1	19:QS:65:ASN:OD1	2.35	0.41
35:RA:1593:G:H2'	35:RA:1594:G:C8	2.56	0.41
35:RA:1638:C:O3'	35:RA:2709:G:N2	2.53	0.41
1:XA:476:G:H2'	1:XA:477:A:C8	2.55	0.41
1:XA:673:G:H2'	1:XA:674:G:C8	2.55	0.41
33:Y8:10:ALA:HA	45:YP:59:LEU:HD11	2.01	0.41
35:YA:483:A:O2'	54:YY:49:VAL:O	2.25	0.41
35:YA:801:G:O6	39:YF:53:THR:OG1	2.38	0.41
35:YA:1538:G:H2'	35:YA:1539:G:H8	1.86	0.41
35:YA:1567:A:C6	37:YD:84:TYR:CE2	3.06	0.41
36:YB:37:C:O2	48:YS:95:HIS:NE2	2.48	0.41
1:QA:1179:A:O3'	9:QI:103:THR:OG1	2.34	0.41
1:QA:1343:G:H4'	9:QI:122:ALA:HB3	2.02	0.41
2:QB:101:MET:HA	2:QB:108:ILE:HG21	2.02	0.41
4:QD:103:ASN:CG	4:QD:114:ARG:HE	2.28	0.41
30:R5:7:PRO:HA	35:RA:2615:U:C2	2.56	0.41
35:RA:323:G:C8	39:RF:171:PRO:HG3	2.55	0.41
35:RA:1057:A:N6	35:RA:1087:G:OP2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:RD:13:ARG:NH1	37:RD:16:MET:SD	2.94	0.41
39:RF:182:ASN:OD1	39:RF:182:ASN:N	2.44	0.41
53:RX:55:ASN:HB2	53:RX:80:ILE:HB	2.03	0.41
1:XA:1524:C:H5''	11:XK:120:ARG:HH12	1.85	0.41
9:XI:50:LEU:HB3	9:XI:56:LEU:HA	2.02	0.41
35:YA:1243:G:O2'	45:YP:7:ARG:NH2	2.52	0.41
42:YI:114:LEU:HD23	42:YI:130:TYR:HA	2.02	0.41
1:QA:237:C:O3'	17:QQ:25:ARG:NH2	2.54	0.41
2:QB:82:ARG:HG3	2:QB:92:TYR:CZ	2.55	0.41
3:QC:130:VAL:HG21	3:QC:157:ILE:HG23	2.02	0.41
3:QC:184:TYR:CD1	3:QC:201:TYR:CD1	3.08	0.41
9:QI:78:LYS:HB2	9:QI:78:LYS:HE2	1.84	0.41
26:R1:18:ILE:HG12	26:R1:37:ILE:HG12	2.03	0.41
35:RA:451:C:OP1	39:RF:52:LYS:NZ	2.46	0.41
35:RA:2305:A:H5''	40:RG:134:GLY:HA3	2.02	0.41
35:RA:2513:G:N2	38:RE:143:ASN:HD21	2.19	0.41
38:RE:34:VAL:HG12	38:RE:72:VAL:HG21	2.03	0.41
47:RR:12:ARG:HB3	47:RR:16:HIS:HB3	2.02	0.41
47:RR:87:TYR:OH	47:RR:117:VAL:O	2.27	0.41
52:RW:69:LEU:HB3	52:RW:107:LEU:HD23	2.03	0.41
1:XA:84:U:O2'	1:XA:89:C:N4	2.54	0.41
1:XA:677:U:O2	1:XA:777:A:O2'	2.35	0.41
1:XA:719:C:O2'	18:XR:50:ILE:O	2.33	0.41
5:XE:102:ALA:H	5:XE:107:ARG:HH21	1.67	0.41
7:XG:150:ALA:O	11:XK:57:THR:OG1	2.29	0.41
13:XM:91:ARG:HH22	13:XM:103:THR:HG21	1.84	0.41
35:YA:108:U:H2'	35:YA:109:G:H8	1.86	0.41
35:YA:1889:A:H2'	35:YA:1890:A:C8	2.56	0.41
44:YO:120:GLU:OE1	49:YT:67:SER:OG	2.37	0.41
1:QA:6:G:H4'	1:QA:298:A:H4'	2.03	0.41
1:QA:444:C:H2'	1:QA:445:G:C8	2.55	0.41
1:QA:943:U:H1'	9:QI:124:GLN:HE22	1.85	0.41
2:QB:84:GLU:HG3	2:QB:215:LEU:HB3	2.02	0.41
33:R8:31:HIS:ND1	33:R8:32:LEU:HG	2.36	0.41
35:RA:252:G:OP1	45:RP:50:ARG:NH1	2.53	0.41
35:RA:635:C:O2'	35:RA:639:U:OP1	2.36	0.41
44:RO:34:THR:OG1	44:RO:35:VAL:N	2.54	0.41
1:XA:108:G:N1	20:XT:15:ARG:HG2	2.36	0.41
1:XA:673:G:H4'	6:XF:87:ARG:NH1	2.36	0.41
33:Y8:27:THR:HG22	45:YP:63:PRO:HD3	2.03	0.41
35:YA:1657:C:H4'	38:YE:133:LYS:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:YZ:5:LEU:HD11	55:YZ:44:PHE:HA	2.02	0.41
1:QA:9:G:H2'	1:QA:10:A:H8	1.86	0.41
1:QA:744:C:O2'	1:QA:851:G:N2	2.51	0.41
2:QB:158:LEU:HA	2:QB:159:PRO:HD3	1.98	0.41
6:QF:24:GLU:O	6:QF:28:ARG:N	2.52	0.41
9:QI:25:LYS:N	9:QI:60:ASP:OD1	2.50	0.41
10:QJ:50:ILE:HB	14:QN:41:ARG:HE	1.85	0.41
11:QK:43:SER:HB3	11:QK:68:ALA:HB2	2.03	0.41
17:QQ:6:LEU:HD23	17:QQ:23:VAL:HG11	2.03	0.41
27:R2:37:PHE:CD1	53:RX:11:PRO:HD3	2.55	0.41
35:RA:679:C:H2'	35:RA:680:G:C8	2.56	0.41
35:RA:2500:U:O2'	35:RA:2504:U:OP1	2.30	0.41
38:RE:1:MET:HG3	38:RE:200:GLU:HB3	2.03	0.41
48:RS:25:ARG:NE	48:RS:88:ASP:OD2	2.50	0.41
1:XA:881:G:P	12:XL:12:ARG:HH22	2.44	0.41
1:XA:1510:U:H2'	1:XA:1511:G:C8	2.55	0.41
7:XG:65:ALA:HB1	7:XG:127:ALA:HB3	2.03	0.41
18:XR:34:TYR:H	18:XR:34:TYR:HD1	1.69	0.41
19:XS:52:TYR:HB2	19:XS:57:HIS:CE1	2.56	0.41
22:XV:15:G:N2	22:XV:21:A:N3	2.69	0.41
25:Y0:14:ARG:O	35:YA:2278:A:N6	2.54	0.41
34:Y9:37:GLY:HA2	35:YA:1125:G:H5'	2.03	0.41
35:YA:143(A):G:H4'	53:YX:35:THR:HG21	2.02	0.41
35:YA:251:A:C5	35:YA:252:G:H1'	2.56	0.41
35:YA:277:C:H4'	35:YA:278:A:H8	1.86	0.41
35:YA:321:G:O2'	35:YA:340:A:N3	2.53	0.41
35:YA:776:G:N7	35:YA:793:A:O2'	2.54	0.41
35:YA:825:C:O2	45:YP:55:ARG:NH1	2.54	0.41
35:YA:1082:U:H6	35:YA:1082:U:H2'	1.73	0.41
35:YA:1538:G:H2'	35:YA:1539:G:C8	2.56	0.41
35:YA:2071:A:H2'	35:YA:2072:G:H8	1.85	0.41
35:YA:2513:G:N2	38:YE:143:ASN:HD21	2.19	0.41
1:QA:41:G:H2'	1:QA:42:G:H8	1.85	0.41
1:QA:1287:A:H2	1:QA:1353:G:H1'	1.86	0.41
7:QG:67:GLU:HA	7:QG:70:LYS:HD3	2.01	0.41
37:RD:260:ARG:HH22	37:RD:270:ILE:HD12	1.85	0.41
55:RZ:14:LYS:HA	55:RZ:15:PRO:HD3	1.97	0.41
34:Y9:1:MET:SD	34:Y9:35:ARG:HB2	2.61	0.41
35:YA:276:A:H5''	35:YA:277:C:H5'	2.03	0.41
35:YA:729:G:O5'	37:YD:208:LYS:NZ	2.54	0.41
35:YA:854:G:H2'	35:YA:855:G:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1568:G:OP1	37:YD:63:ARG:NH1	2.42	0.41
35:YA:2144:U:HO2'	35:YA:2147:G:H1	1.66	0.41
49:YT:16:ARG:HH21	49:YT:81:PRO:HA	1.86	0.41
1:QA:624:C:H2'	1:QA:625:G:C8	2.56	0.40
1:QA:924:C:H2'	1:QA:925:G:C8	2.56	0.40
1:QA:1226:C:P	13:QM:91:ARG:HH12	2.44	0.40
7:QG:26:PHE:O	7:QG:30:ILE:HG12	2.21	0.40
8:QH:104:ARG:HD3	8:QH:104:ARG:HA	1.91	0.40
35:RA:483:A:O2'	54:RY:49:VAL:O	2.35	0.40
35:RA:855:G:H1	35:RA:922:U:H3	1.68	0.40
35:RA:2161:C:H2'	35:RA:2162:G:H8	1.86	0.40
35:RA:2405:G:H5'	45:RP:75:ILE:HD13	2.02	0.40
38:RE:2:LYS:HG2	38:RE:200:GLU:HB2	2.03	0.40
49:RT:30:VAL:HG22	49:RT:86:ILE:HG12	2.02	0.40
1:XA:157:G:H1	1:XA:164:U:H3	1.68	0.40
1:XA:1000:U:H2'	1:XA:1001(A):A:C8	2.56	0.40
2:XB:54:THR:HG22	2:XB:199:TYR:HB3	2.02	0.40
8:XH:105:ARG:HD3	8:XH:105:ARG:HA	1.94	0.40
9:XI:48:GLU:OE2	9:XI:51:ARG:NE	2.44	0.40
35:YA:2805:G:H2'	35:YA:2807:G:C8	2.56	0.40
38:YE:21:VAL:HA	38:YE:22:PRO:HD3	1.94	0.40
44:YO:8:LEU:HD13	44:YO:82:ASN:HB3	2.03	0.40
1:QA:1294:G:H2'	1:QA:1295:G:H8	1.86	0.40
1:QA:1484:C:O2'	35:RA:1960:A:O2'	2.24	0.40
2:QB:177:ALA:HB1	2:QB:182:ILE:HB	2.03	0.40
3:QC:3:ASN:OD1	3:QC:3:ASN:N	2.54	0.40
7:QG:16:LEU:HD21	9:QI:45:ALA:HB2	2.02	0.40
25:R0:23:VAL:HG22	25:R0:38:VAL:HG22	2.03	0.40
30:R5:19:ARG:HH11	30:R5:19:ARG:HD3	1.78	0.40
35:RA:459:U:H2'	35:RA:460:A:H8	1.86	0.40
35:RA:535:C:O3'	50:RU:53:ARG:NH1	2.54	0.40
37:RD:133:LEU:HB3	37:RD:173:VAL:HG21	2.03	0.40
37:RD:231:HIS:CD2	37:RD:249:PRO:HG3	2.55	0.40
42:RI:72:LEU:HA	42:RI:75:LEU:HD22	2.03	0.40
44:RO:104:ARG:HH22	49:RT:43:GLN:CD	2.29	0.40
46:RQ:119:ARG:O	46:RQ:123:HIS:ND1	2.50	0.40
48:RS:15:ARG:O	48:RS:19:LYS:HG2	2.21	0.40
55:RZ:151:HIS:CE1	55:RZ:153:SER:HB2	2.57	0.40
13:XM:99:ARG:HB2	13:XM:101:GLN:NE2	2.36	0.40
16:XP:20:VAL:HG21	16:XP:32:TYR:CE2	2.50	0.40
24:XY:62:C:H2'	24:XY:63:G:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y2:55:ARG:HB3	27:Y2:59:ARG:HH12	1.87	0.40
35:YA:85:G:O2'	35:YA:103:A:N1	2.42	0.40
35:YA:323:G:C8	39:YF:171:PRO:HG3	2.56	0.40
38:YE:3:GLY:HA2	38:YE:199:ARG:HA	2.03	0.40
49:YT:24:PRO:HD3	49:YT:52:ILE:HD12	2.03	0.40
1:QA:537:G:H5''	12:QL:113:ARG:HH12	1.86	0.40
1:QA:718:G:C8	11:QK:116:HIS:HB3	2.56	0.40
5:QE:50:GLU:HB2	5:QE:53:LEU:HD13	2.02	0.40
13:QM:40:ASN:HB3	13:QM:43:THR:HG23	2.02	0.40
25:R0:39:ARG:HH21	35:RA:2355:C:H1'	1.85	0.40
35:RA:1500:G:H21	37:RD:100:GLY:HA3	1.86	0.40
35:RA:2572:A:O2'	38:RE:144:ARG:NH1	2.54	0.40
37:RD:16:MET:SD	37:RD:211:ARG:NH2	2.88	0.40
51:RV:62:LEU:HD11	51:RV:95:LEU:HB2	2.03	0.40
1:XA:1229:A:O2'	22:XV:30:G:OP1	2.38	0.40
1:XA:1239:A:O2'	7:XG:114:ARG:O	2.36	0.40
3:XC:108:ASN:HD21	3:XC:144:SER:HB3	1.87	0.40
28:Y3:8:LEU:HB2	28:Y3:28:LEU:HD13	2.02	0.40
35:YA:192:C:O2'	35:YA:802:A:N3	2.47	0.40
35:YA:1007:C:H5''	43:YN:35:ARG:NH1	2.36	0.40
35:YA:1084:A:H8	35:YA:1085:A:H4'	1.86	0.40
35:YA:1316:U:H2'	35:YA:1317:A:H8	1.86	0.40
35:YA:1754:C:OP1	49:YT:96:ARG:NH1	2.55	0.40
37:YD:69:ARG:HH11	37:YD:105:ILE:HG21	1.87	0.40
1:QA:392:G:OP1	16:QP:8:ARG:NH2	2.51	0.40
1:QA:1184:G:H2'	1:QA:1185:G:H8	1.86	0.40
4:QD:53:ASP:HB3	4:QD:57:ARG:NH1	2.36	0.40
11:QK:99:GLN:HG2	11:QK:105:VAL:HG21	2.04	0.40
33:R8:5:LYS:HG2	35:RA:242:G:C8	2.56	0.40
35:RA:521:G:H2'	35:RA:522:G:C8	2.57	0.40
54:RY:27:VAL:HG12	54:RY:39:VAL:HG22	2.04	0.40
5:XE:6:PHE:CD1	5:XE:36:ASP:HB3	2.57	0.40
25:Y0:46:LYS:HB2	25:Y0:78:TYR:CD1	2.56	0.40
35:YA:1593:G:H2'	35:YA:1594:G:C8	2.57	0.40
1:QA:56:U:H2'	1:QA:57:G:C8	2.56	0.40
29:R4:28:LYS:HD2	29:R4:31:ILE:HD11	2.03	0.40
35:RA:390:A:C6	45:RP:71:VAL:HG21	2.56	0.40
35:RA:614(D):A:C4	39:RF:180:GLY:HA3	2.57	0.40
40:RG:32:PRO:HB3	40:RG:163:ALA:HB2	2.03	0.40
1:XA:107:G:OP1	1:XA:325:A:N6	2.55	0.40
1:XA:1053:G:N7	1:XA:1200:C:H5''	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1095:U:P	1:XA:1108:G:H1	2.44	0.40
9:XI:24:GLY:N	9:XI:60:ASP:OD1	2.37	0.40
10:XJ:61:GLU:OE2	14:YN:58:LYS:NZ	2.51	0.40
35:YA:787:U:H5''	35:YA:788:A:H5'	2.03	0.40
35:YA:1012:U:C4	43:YN:25:ARG:HD3	2.56	0.40
35:YA:1400:G:H2'	35:YA:1401:G:C8	2.57	0.40
37:YD:206:LEU:HA	37:YD:211:ARG:HD2	2.03	0.40
37:YD:245:PRO:HA	37:YD:246:PRO:HD3	1.94	0.40
38:YE:134:ILE:HA	38:YE:137:HIS:CD2	2.57	0.40
39:YF:13:SER:OG	39:YF:16:GLY:O	2.29	0.40
45:YP:106:LEU:HD11	45:YP:112:LEU:HB2	2.04	0.40
46:YQ:39:PRO:HB3	46:YQ:99:PRO:HD3	2.03	0.40
55:YZ:108:PRO:HB3	55:YZ:144:LEU:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
2	QB	229/256 (90%)	202 (88%)	19 (8%)	8 (4%)	3	16
2	XB	229/256 (90%)	204 (89%)	22 (10%)	3 (1%)	9	35
3	QC	204/239 (85%)	197 (97%)	7 (3%)	0	100	100
3	XC	204/239 (85%)	195 (96%)	9 (4%)	0	100	100
4	QD	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	24	57
4	XD	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
5	QE	146/162 (90%)	140 (96%)	6 (4%)	0	100	100
5	XE	146/162 (90%)	141 (97%)	5 (3%)	0	100	100
6	QF	98/101 (97%)	98 (100%)	0	0	100	100
6	XF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	QG	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
7	XG	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
8	QH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
8	XH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
9	QI	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
9	XI	124/128 (97%)	111 (90%)	13 (10%)	0	100	100
10	QJ	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	3	18
10	XJ	94/105 (90%)	84 (89%)	8 (8%)	2 (2%)	5	25
11	QK	112/129 (87%)	107 (96%)	5 (4%)	0	100	100
11	XK	112/129 (87%)	108 (96%)	4 (4%)	0	100	100
12	QL	119/132 (90%)	105 (88%)	12 (10%)	2 (2%)	7	30
12	XL	119/132 (90%)	109 (92%)	6 (5%)	4 (3%)	3	16
13	QM	114/126 (90%)	107 (94%)	4 (4%)	3 (3%)	4	21
13	XM	112/126 (89%)	106 (95%)	6 (5%)	0	100	100
14	QN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
14	XN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
15	QO	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	10	37
15	XO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	QP	80/88 (91%)	79 (99%)	1 (1%)	0	100	100
16	XP	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
17	QQ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	XQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
18	QR	66/88 (75%)	66 (100%)	0	0	100	100
18	XR	66/88 (75%)	66 (100%)	0	0	100	100
19	QS	81/93 (87%)	78 (96%)	3 (4%)	0	100	100
19	XS	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
20	QT	94/106 (89%)	91 (97%)	3 (3%)	0	100	100
20	XT	96/106 (91%)	92 (96%)	4 (4%)	0	100	100
21	QU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
21	XU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
25	R0	75/85 (88%)	74 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Y0	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
26	R1	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
26	Y1	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
27	R2	68/72 (94%)	68 (100%)	0	0	100	100
27	Y2	68/72 (94%)	68 (100%)	0	0	100	100
28	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	Y3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
29	R4	67/71 (94%)	59 (88%)	7 (10%)	1 (2%)	8	32
29	Y4	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1	4
30	R5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
30	Y5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
31	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
31	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
32	R7	46/49 (94%)	46 (100%)	0	0	100	100
32	Y7	46/49 (94%)	46 (100%)	0	0	100	100
33	R8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
33	Y8	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
34	R9	35/37 (95%)	35 (100%)	0	0	100	100
34	Y9	35/37 (95%)	35 (100%)	0	0	100	100
37	RD	273/276 (99%)	263 (96%)	10 (4%)	0	100	100
37	YD	273/276 (99%)	264 (97%)	9 (3%)	0	100	100
38	RE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	24	57
38	YE	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	24	57
39	RF	200/210 (95%)	196 (98%)	4 (2%)	0	100	100
39	YF	200/210 (95%)	198 (99%)	2 (1%)	0	100	100
40	RG	179/182 (98%)	163 (91%)	13 (7%)	3 (2%)	7	30
40	YG	179/182 (98%)	161 (90%)	16 (9%)	2 (1%)	11	39
41	RH	172/180 (96%)	166 (96%)	6 (4%)	0	100	100
41	YH	171/180 (95%)	165 (96%)	6 (4%)	0	100	100
42	RI	145/148 (98%)	134 (92%)	11 (8%)	0	100	100
42	YI	144/148 (97%)	140 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	RN	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
43	YN	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
44	RO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
44	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
45	RP	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
45	YP	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
46	RQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
46	YQ	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
47	RR	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
47	YR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
48	RS	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
48	YS	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
49	RT	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
49	YT	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
50	RU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
50	YU	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
51	RV	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	41
51	YV	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	12	41
52	RW	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
52	YW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
53	RX	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
53	YX	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
54	RY	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
54	YY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
55	RZ	176/206 (85%)	164 (93%)	11 (6%)	1 (1%)	21	52
55	YZ	175/206 (85%)	165 (94%)	8 (5%)	2 (1%)	11	39
All	All	11389/12128 (94%)	10866 (95%)	478 (4%)	45 (0%)	30	61

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	17	PHE
2	QB	127	ILE

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Mol	Chain	Res	Type
4	QD	5	ILE
10	QJ	32	ALA
10	QJ	79	ARG
12	QL	48	PRO
13	QM	106	ASN
40	RG	48	GLU
40	RG	49	ASP
51	RV	50	PRO
10	XJ	79	ARG
12	XL	47	LYS
29	Y4	47	GLN
29	Y4	49	PHE
29	Y4	59	PHE
40	YG	96	ARG
55	YZ	52	SER
2	QB	9	GLU
2	QB	21	ARG
2	QB	126	GLU
10	QJ	55	LYS
12	QL	49	ASN
29	R4	56	VAL
40	RG	50	ALA
10	XJ	55	LYS
12	XL	48	PRO
29	Y4	58	ARG
2	QB	22	LYS
13	QM	107	ALA
15	QO	88	ARG
2	XB	9	GLU
2	XB	126	GLU
55	YZ	51	ALA
2	QB	8	LYS
13	QM	105	THR
55	RZ	52	SER
12	XL	46	LYS
29	Y4	48	ARG
40	YG	97	ASP
51	YV	50	PRO
38	RE	52	LEU
38	YE	52	LEU
12	XL	88	GLY
2	XB	125	PRO

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Mol	Chain	Res	Type
2	QB	125	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	191/220 (87%)	191 (100%)	0	100	100
2	XB	187/220 (85%)	187 (100%)	0	100	100
3	QC	144/188 (77%)	144 (100%)	0	100	100
3	XC	140/188 (74%)	140 (100%)	0	100	100
4	QD	171/181 (94%)	171 (100%)	0	100	100
4	XD	172/181 (95%)	172 (100%)	0	100	100
5	QE	114/123 (93%)	114 (100%)	0	100	100
5	XE	114/123 (93%)	114 (100%)	0	100	100
6	QF	85/90 (94%)	85 (100%)	0	100	100
6	XF	85/90 (94%)	85 (100%)	0	100	100
7	QG	120/127 (94%)	120 (100%)	0	100	100
7	XG	119/127 (94%)	119 (100%)	0	100	100
8	QH	116/119 (98%)	116 (100%)	0	100	100
8	XH	114/119 (96%)	114 (100%)	0	100	100
9	QI	91/99 (92%)	91 (100%)	0	100	100
9	XI	88/99 (89%)	88 (100%)	0	100	100
10	QJ	68/92 (74%)	68 (100%)	0	100	100
10	XJ	68/92 (74%)	68 (100%)	0	100	100
11	QK	83/99 (84%)	83 (100%)	0	100	100
11	XK	83/99 (84%)	83 (100%)	0	100	100
12	QL	96/108 (89%)	96 (100%)	0	100	100
12	XL	96/108 (89%)	96 (100%)	0	100	100
13	QM	90/101 (89%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	XM	87/101 (86%)	87 (100%)	0	100	100
14	QN	49/50 (98%)	49 (100%)	0	100	100
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	78/80 (98%)	78 (100%)	0	100	100
15	XO	78/80 (98%)	78 (100%)	0	100	100
16	QP	69/74 (93%)	69 (100%)	0	100	100
16	XP	68/74 (92%)	68 (100%)	0	100	100
17	QQ	94/97 (97%)	94 (100%)	0	100	100
17	XQ	94/97 (97%)	94 (100%)	0	100	100
18	QR	59/77 (77%)	59 (100%)	0	100	100
18	XR	59/77 (77%)	59 (100%)	0	100	100
19	QS	68/80 (85%)	68 (100%)	0	100	100
19	XS	67/80 (84%)	67 (100%)	0	100	100
20	QT	71/82 (87%)	70 (99%)	1 (1%)	59	76
20	XT	70/82 (85%)	70 (100%)	0	100	100
21	QU	18/22 (82%)	18 (100%)	0	100	100
21	XU	18/22 (82%)	18 (100%)	0	100	100
25	R0	61/67 (91%)	61 (100%)	0	100	100
25	Y0	61/67 (91%)	61 (100%)	0	100	100
26	R1	79/83 (95%)	79 (100%)	0	100	100
26	Y1	81/83 (98%)	81 (100%)	0	100	100
27	R2	65/67 (97%)	65 (100%)	0	100	100
27	Y2	66/67 (98%)	66 (100%)	0	100	100
28	R3	51/52 (98%)	51 (100%)	0	100	100
28	Y3	50/52 (96%)	50 (100%)	0	100	100
29	R4	58/63 (92%)	58 (100%)	0	100	100
29	Y4	54/63 (86%)	54 (100%)	0	100	100
30	R5	51/52 (98%)	51 (100%)	0	100	100
30	Y5	50/52 (96%)	50 (100%)	0	100	100
31	R6	51/52 (98%)	51 (100%)	0	100	100
31	Y6	50/52 (96%)	50 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	R7	41/42 (98%)	41 (100%)	0	100	100
32	Y7	41/42 (98%)	41 (100%)	0	100	100
33	R8	54/55 (98%)	54 (100%)	0	100	100
33	Y8	54/55 (98%)	54 (100%)	0	100	100
34	R9	34/34 (100%)	34 (100%)	0	100	100
34	Y9	34/34 (100%)	34 (100%)	0	100	100
37	RD	214/218 (98%)	214 (100%)	0	100	100
37	YD	215/218 (99%)	215 (100%)	0	100	100
38	RE	164/166 (99%)	164 (100%)	0	100	100
38	YE	164/166 (99%)	164 (100%)	0	100	100
39	RF	160/166 (96%)	160 (100%)	0	100	100
39	YF	159/166 (96%)	159 (100%)	0	100	100
40	RG	144/156 (92%)	144 (100%)	0	100	100
40	YG	142/156 (91%)	142 (100%)	0	100	100
41	RH	144/148 (97%)	144 (100%)	0	100	100
41	YH	143/148 (97%)	143 (100%)	0	100	100
42	RI	111/124 (90%)	111 (100%)	0	100	100
42	YI	108/124 (87%)	108 (100%)	0	100	100
43	RN	119/119 (100%)	119 (100%)	0	100	100
43	YN	118/119 (99%)	118 (100%)	0	100	100
44	RO	100/100 (100%)	100 (100%)	0	100	100
44	YO	100/100 (100%)	100 (100%)	0	100	100
45	RP	115/116 (99%)	115 (100%)	0	100	100
45	YP	115/116 (99%)	115 (100%)	0	100	100
46	RQ	111/111 (100%)	111 (100%)	0	100	100
46	YQ	111/111 (100%)	111 (100%)	0	100	100
47	RR	101/101 (100%)	101 (100%)	0	100	100
47	YR	101/101 (100%)	101 (100%)	0	100	100
48	RS	87/88 (99%)	87 (100%)	0	100	100
48	YS	85/88 (97%)	85 (100%)	0	100	100
49	RT	115/127 (91%)	115 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	YT	113/127 (89%)	113 (100%)	0	100	100
50	RU	93/94 (99%)	93 (100%)	0	100	100
50	YU	93/94 (99%)	93 (100%)	0	100	100
51	RV	81/82 (99%)	81 (100%)	0	100	100
51	YV	80/82 (98%)	80 (100%)	0	100	100
52	RW	90/92 (98%)	90 (100%)	0	100	100
52	YW	90/92 (98%)	90 (100%)	0	100	100
53	RX	77/78 (99%)	77 (100%)	0	100	100
53	YX	77/78 (99%)	77 (100%)	0	100	100
54	RY	86/91 (94%)	86 (100%)	0	100	100
54	YY	86/91 (94%)	86 (100%)	0	100	100
55	RZ	152/179 (85%)	152 (100%)	0	100	100
55	YZ	148/179 (83%)	148 (100%)	0	100	100
All	All	9329/10064 (93%)	9328 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	QT	60	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
3	QC	108	ASN
4	QD	45	GLN
4	QD	129	ASN
4	QD	201	GLN
5	QE	127	ASN
6	QF	73	ASN
7	QG	148	ASN
9	QI	73	GLN
9	QI	124	GLN
10	QJ	69	ASN
12	QL	80	HIS
13	QM	101	GLN
14	QN	49	HIS

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Mol	Chain	Res	Type
15	QO	37	ASN
16	QP	13	HIS
19	QS	23	ASN
19	QS	57	HIS
20	QT	16	HIS
31	R6	26	ASN
33	R8	35	GLN
34	R9	34	GLN
37	RD	166	GLN
38	RE	48	GLN
38	RE	137	HIS
39	RF	8	GLN
39	RF	40	GLN
40	RG	26	GLN
40	RG	108	ASN
41	RH	74	ASN
42	RI	133	HIS
42	RI	139	GLN
43	RN	94	HIS
44	RO	89	ASN
45	RP	70	GLN
46	RQ	57	HIS
47	RR	13	HIS
47	RR	71	GLN
49	RT	90	GLN
52	RW	61	ASN
53	RX	41	ASN
55	RZ	73	GLN
55	RZ	75	ASN
2	XB	113	HIS
3	XC	108	ASN
3	XC	139	GLN
5	XE	20	GLN
5	XE	127	ASN
6	XF	73	ASN
6	XF	100	ASN
7	XG	64	GLN
9	XI	73	GLN
9	XI	124	GLN
10	XJ	69	ASN
12	XL	80	HIS
13	XM	106	ASN

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Mol	Chain	Res	Type
15	XO	9	GLN
15	XO	37	ASN
15	XO	62	GLN
19	XS	65	ASN
20	XT	16	HIS
34	Y9	34	GLN
37	YD	87	ASN
39	YF	29	ASN
39	YF	40	GLN
43	YN	94	HIS
45	YP	70	GLN
47	YR	13	HIS
47	YR	71	GLN
49	YT	58	ASN
52	YW	61	ASN
53	YX	41	ASN
55	YZ	55	HIS
55	YZ	121	HIS
55	YZ	151	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1497/1522 (98%)	239 (15%)	15 (1%)
1	XA	1501/1522 (98%)	230 (15%)	15 (0%)
22	QV	76/77 (98%)	15 (19%)	0
22	XV	76/77 (98%)	13 (17%)	0
23	QX	17/19 (89%)	6 (35%)	1 (5%)
23	XX	17/19 (89%)	8 (47%)	1 (5%)
24	QY	75/76 (98%)	31 (41%)	0
24	XY	75/76 (98%)	33 (44%)	0
35	RA	2858/2915 (98%)	453 (15%)	16 (0%)
35	YA	2858/2915 (98%)	454 (15%)	15 (0%)
36	RB	119/122 (97%)	10 (8%)	0
36	YB	119/122 (97%)	11 (9%)	0
All	All	9288/9462 (98%)	1503 (16%)	63 (0%)

All (1503) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	5	U

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Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	22	G
1	QA	32	A
1	QA	39	G
1	QA	47	C
1	QA	48	C
1	QA	50	A
1	QA	51	A
1	QA	52	G
1	QA	61	G
1	QA	66	G
1	QA	78	G
1	QA	101	A
1	QA	105	G
1	QA	116	A
1	QA	121	C
1	QA	129(B)	G
1	QA	131	C
1	QA	151	A
1	QA	163	C
1	QA	174	C
1	QA	182	U
1	QA	189(F)	U
1	QA	189(G)	U
1	QA	189(H)	G
1	QA	195	A
1	QA	197	A
1	QA	202	U
1	QA	203	U
1	QA	204	U
1	QA	216	G
1	QA	220	G
1	QA	247	G
1	QA	251	G
1	QA	266	G
1	QA	267	C
1	QA	289	G
1	QA	301	G
1	QA	321	A
1	QA	328	C
1	QA	332	G

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Mol	Chain	Res	Type
1	QA	346	G
1	QA	350	G
1	QA	351	G
1	QA	352	C
1	QA	353	A
1	QA	354	G
1	QA	356	A
1	QA	367	U
1	QA	372	C
1	QA	373	A
1	QA	384	G
1	QA	388	G
1	QA	397	A
1	QA	398	C
1	QA	406	G
1	QA	412	A
1	QA	413	G
1	QA	424	G
1	QA	429	U
1	QA	439	A
1	QA	452	A
1	QA	461	A
1	QA	470	C
1	QA	482	A
1	QA	484	G
1	QA	485	G
1	QA	496	A
1	QA	498	U
1	QA	508	C
1	QA	509	A
1	QA	510	A
1	QA	511	C
1	QA	518	C
1	QA	521	G
1	QA	532	A
1	QA	533	A
1	QA	547	A
1	QA	559	A
1	QA	560	U
1	QA	561	U
1	QA	564	C
1	QA	567	G

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Mol	Chain	Res	Type
1	QA	572	A
1	QA	573	A
1	QA	576	G
1	QA	577	G
1	QA	596	C
1	QA	630	G
1	QA	631	G
1	QA	653	A
1	QA	665	A
1	QA	666	G
1	QA	687	A
1	QA	688	G
1	QA	695	A
1	QA	721	G
1	QA	723	U
1	QA	731	G
1	QA	734	G
1	QA	749	C
1	QA	755	G
1	QA	760	G
1	QA	774	G
1	QA	777	A
1	QA	793	U
1	QA	794	A
1	QA	815	A
1	QA	816	A
1	QA	817	C
1	QA	821	G
1	QA	828	A
1	QA	829	G
1	QA	836	G
1	QA	840	C
1	QA	841	U
1	QA	848	C
1	QA	851	G
1	QA	902	G
1	QA	914	A
1	QA	916	G
1	QA	926	G
1	QA	927	G
1	QA	934	C
1	QA	942	G

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Mol	Chain	Res	Type
1	QA	960	U
1	QA	961	U
1	QA	968	A
1	QA	969	A
1	QA	971	G
1	QA	974	A
1	QA	975	A
1	QA	976	G
1	QA	977	A
1	QA	981	U
1	QA	982	U
1	QA	992	U
1	QA	993	G
1	QA	1002	G
1	QA	1004	A
1	QA	1005	A
1	QA	1006	C
1	QA	1009	G
1	QA	1020	U
1	QA	1022	G
1	QA	1023	G
1	QA	1025	U
1	QA	1026	G
1	QA	1027	C
1	QA	1028	C
1	QA	1029	C
1	QA	1030(B)	G
1	QA	1030(C)	C
1	QA	1031	G
1	QA	1036	G
1	QA	1044	A
1	QA	1053	G
1	QA	1054	C
1	QA	1065	U
1	QA	1066	C
1	QA	1068	G
1	QA	1070	U
1	QA	1081	G
1	QA	1094	G
1	QA	1095	U
1	QA	1101	A
1	QA	1108	G

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Mol	Chain	Res	Type
1	QA	1117	G
1	QA	1125	U
1	QA	1129	C
1	QA	1130	A
1	QA	1136	U
1	QA	1137	C
1	QA	1139	G
1	QA	1146	A
1	QA	1147	C
1	QA	1152	A
1	QA	1157	A
1	QA	1159	U
1	QA	1183	A
1	QA	1187	G
1	QA	1196	U
1	QA	1197	G
1	QA	1201	A
1	QA	1211	U
1	QA	1214	C
1	QA	1224	G
1	QA	1227	A
1	QA	1228	C
1	QA	1236	A
1	QA	1238	A
1	QA	1250	A
1	QA	1256	A
1	QA	1257	U
1	QA	1258	G
1	QA	1260	C
1	QA	1270	C
1	QA	1278	U
1	QA	1279	A
1	QA	1280	A
1	QA	1282	C
1	QA	1287	A
1	QA	1300	G
1	QA	1302	U
1	QA	1303	C
1	QA	1305	G
1	QA	1320	C
1	QA	1340	A
1	QA	1346	A

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Mol	Chain	Res	Type
1	QA	1347	G
1	QA	1353	G
1	QA	1363(A)	C
1	QA	1370	G
1	QA	1397	C
1	QA	1399	C
1	QA	1404	5MC
1	QA	1419	G
1	QA	1442(A)	G
1	QA	1442(B)	G
1	QA	1447	A
1	QA	1452	C
1	QA	1456	G
1	QA	1469	G
1	QA	1487	G
1	QA	1490	C
1	QA	1492	A
1	QA	1497	G
1	QA	1499	A
1	QA	1503	A
1	QA	1504	G
1	QA	1506	U
1	QA	1517	G
1	QA	1519	MA6
1	QA	1520	G
1	QA	1529	G
1	QA	1530	G
1	QA	1531	A
22	QV	3	C
22	QV	8	U
22	QV	14	A
22	QV	16	C
22	QV	17	C
22	QV	17(A)	U
22	QV	18	G
22	QV	19	G
22	QV	20	U
22	QV	21	A
22	QV	47	U
22	QV	48	C
22	QV	49	G
22	QV	65	C

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Mol	Chain	Res	Type
22	QV	76	A
23	QX	7	G
23	QX	10	G
23	QX	11	U
23	QX	13	A
23	QX	15	A
23	QX	19	G
24	QY	2	G
24	QY	8	U
24	QY	9	A
24	QY	16	C
24	QY	17	U
24	QY	18	G
24	QY	19	G
24	QY	21	A
24	QY	29	U
24	QY	30	G
24	QY	43	G
24	QY	46	G
24	QY	47	U
24	QY	48	C
24	QY	49	A
24	QY	50	G
24	QY	51	C
24	QY	52	G
24	QY	55	U
24	QY	56	C
24	QY	57	G
24	QY	58	A
24	QY	61	C
24	QY	67	A
24	QY	68	G
24	QY	69	C
24	QY	71	C
24	QY	72	C
24	QY	73	A
24	QY	74	C
24	QY	75	C
35	RA	10	G
35	RA	15	G
35	RA	34	C
35	RA	45	C

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Mol	Chain	Res	Type
35	RA	51	G
35	RA	71	A
35	RA	74	A
35	RA	75	G
35	RA	84	A
35	RA	102	G
35	RA	118	A
35	RA	119	A
35	RA	120	U
35	RA	131	G
35	RA	157	U
35	RA	182	A
35	RA	188	G
35	RA	196	A
35	RA	199	A
35	RA	205	G
35	RA	214	G
35	RA	216	A
35	RA	221	A
35	RA	222	A
35	RA	229	A
35	RA	230	U
35	RA	248	G
35	RA	265	A
35	RA	272(K)	U
35	RA	272(N)	U
35	RA	273(B)	U
35	RA	273(C)	G
35	RA	278	A
35	RA	311	A
35	RA	317	G
35	RA	324	A
35	RA	329	G
35	RA	330	A
35	RA	331	A
35	RA	338	G
35	RA	342	G
35	RA	345	A
35	RA	352	G
35	RA	362	U
35	RA	363(A)	G
35	RA	372	G

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Mol	Chain	Res	Type
35	RA	386	G
35	RA	396	G
35	RA	405	U
35	RA	411	G
35	RA	412	A
35	RA	428	A
35	RA	444	C
35	RA	455	C
35	RA	457	A
35	RA	467	G
35	RA	470	A
35	RA	481	G
35	RA	491	G
35	RA	505	A
35	RA	508	G
35	RA	509	C
35	RA	530	G
35	RA	531	C
35	RA	532	A
35	RA	533	G
35	RA	563	G
35	RA	573	G
35	RA	575	A
35	RA	583	G
35	RA	586	A
35	RA	603	A
35	RA	604	G
35	RA	607	U
35	RA	614(B)	U
35	RA	614(C)	G
35	RA	615	G
35	RA	620	G
35	RA	627	A
35	RA	634	C
35	RA	637	A
35	RA	645	C
35	RA	646	A
35	RA	652(C)	A
35	RA	652(D)	G
35	RA	652(V)	G
35	RA	669	G
35	RA	686	G

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Mol	Chain	Res	Type
35	RA	717	G
35	RA	726	G
35	RA	730	C
35	RA	734	A
35	RA	753	C
35	RA	764	A
35	RA	765	G
35	RA	775	G
35	RA	776	G
35	RA	782	A
35	RA	784	A
35	RA	785	G
35	RA	788	A
35	RA	789	A
35	RA	792	G
35	RA	805	G
35	RA	812	C
35	RA	827	U
35	RA	828	U
35	RA	831	G
35	RA	857	C
35	RA	859	G
35	RA	881	G
35	RA	886	C
35	RA	887	A
35	RA	888	C
35	RA	889	C
35	RA	890	A
35	RA	893	C
35	RA	896	A
35	RA	897	C
35	RA	898	C
35	RA	899	A
35	RA	907	U
35	RA	910	A
35	RA	915	C
35	RA	917	A
35	RA	932	G
35	RA	941	A
35	RA	945	A
35	RA	946	G
35	RA	953	A

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Mol	Chain	Res	Type
35	RA	957	A
35	RA	959	A
35	RA	961	C
35	RA	974	G
35	RA	975(A)	C
35	RA	983	A
35	RA	996	A
35	RA	1005	C
35	RA	1012	U
35	RA	1013	C
35	RA	1022	G
35	RA	1025	G
35	RA	1026	U
35	RA	1033	U
35	RA	1045	A
35	RA	1046	A
35	RA	1047	G
35	RA	1051	G
35	RA	1052	C
35	RA	1054	A
35	RA	1058	G
35	RA	1060	U
35	RA	1063	G
35	RA	1064	C
35	RA	1065	U
35	RA	1066	U
35	RA	1067	A
35	RA	1068	G
35	RA	1070	A
35	RA	1071	G
35	RA	1073	A
35	RA	1074	G
35	RA	1076	C
35	RA	1077	A
35	RA	1079	C
35	RA	1082	U
35	RA	1083	U
35	RA	1084	A
35	RA	1085	A
35	RA	1086	A
35	RA	1088	A
35	RA	1090	U

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Mol	Chain	Res	Type
35	RA	1092	C
35	RA	1094	U
35	RA	1096	A
35	RA	1097	U
35	RA	1098	A
35	RA	1108	U
35	RA	1109	C
35	RA	1110	G
35	RA	1112	G
35	RA	1128	A
35	RA	1130	U
35	RA	1135	C
35	RA	1136	G
35	RA	1155	A
35	RA	1171	G
35	RA	1188	U
35	RA	1206	G
35	RA	1211	U
35	RA	1220	A
35	RA	1236	G
35	RA	1247	A
35	RA	1250	G
35	RA	1253	A
35	RA	1256	G
35	RA	1265	A
35	RA	1271	G
35	RA	1272	A
35	RA	1273	U
35	RA	1300	U
35	RA	1301	A
35	RA	1314	C
35	RA	1341	U
35	RA	1352	U
35	RA	1359	A
35	RA	1360	A
35	RA	1365	A
35	RA	1368	G
35	RA	1379	A
35	RA	1384	A
35	RA	1385	G
35	RA	1395	A
35	RA	1416	G

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Mol	Chain	Res	Type
35	RA	1417	C
35	RA	1419	A
35	RA	1420	U
35	RA	1421	G
35	RA	1427	A
35	RA	1428	C
35	RA	1429	G
35	RA	1445(A)	A
35	RA	1450(A)	G
35	RA	1455	G
35	RA	1459	G
35	RA	1460	A
35	RA	1461	G
35	RA	1467	C
35	RA	1471	A
35	RA	1482	G
35	RA	1490	A
35	RA	1493	C
35	RA	1494	A
35	RA	1497	U
35	RA	1508	A
35	RA	1509(A)	C
35	RA	1509(B)	A
35	RA	1542	A
35	RA	1543	C
35	RA	1554	A
35	RA	1558	A
35	RA	1566	A
35	RA	1569	A
35	RA	1578	U
35	RA	1580	A
35	RA	1584	C
35	RA	1586	A
35	RA	1608	A
35	RA	1609	A
35	RA	1640	C
35	RA	1648	C
35	RA	1674	G
35	RA	1696	G
35	RA	1700	A
35	RA	1701	A
35	RA	1721	G

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Mol	Chain	Res	Type
35	RA	1722	A
35	RA	1750	G
35	RA	1756	G
35	RA	1762	A
35	RA	1763	G
35	RA	1764	G
35	RA	1773	A
35	RA	1774	C
35	RA	1780	A
35	RA	1786	A
35	RA	1791	A
35	RA	1800	C
35	RA	1801	G
35	RA	1816	G
35	RA	1828	G
35	RA	1829	A
35	RA	1835	G
35	RA	1847	A
35	RA	1848	A
35	RA	1877	A
35	RA	1878	G
35	RA	1900	A
35	RA	1906	G
35	RA	1913	A
35	RA	1914	C
35	RA	1927	A
35	RA	1929	G
35	RA	1930	G
35	RA	1936	A
35	RA	1938	A
35	RA	1955	U
35	RA	1963	U
35	RA	1967	C
35	RA	1970	A
35	RA	1971	A
35	RA	1972	A
35	RA	1984	G
35	RA	1992	G
35	RA	1993	U
35	RA	1997	G
35	RA	2004	G
35	RA	2020	A

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Mol	Chain	Res	Type
35	RA	2023	G
35	RA	2031	A
35	RA	2032	G
35	RA	2033	A
35	RA	2043	C
35	RA	2055	C
35	RA	2056	G
35	RA	2060	A
35	RA	2061	G
35	RA	2062	A
35	RA	2069	G
35	RA	2093	G
35	RA	2096	U
35	RA	2099	U
35	RA	2103	C
35	RA	2104	G
35	RA	2105	C
35	RA	2107	C
35	RA	2108	C
35	RA	2112	G
35	RA	2116	G
35	RA	2117	A
35	RA	2119	A
35	RA	2120	G
35	RA	2123	G
35	RA	2126	A
35	RA	2127	G
35	RA	2129	C
35	RA	2131	G
35	RA	2132	U
35	RA	2133	G
35	RA	2134	A
35	RA	2136	C
35	RA	2137	C
35	RA	2145	C
35	RA	2146	C
35	RA	2147	G
35	RA	2148	G
35	RA	2151	G
35	RA	2161	C
35	RA	2165	G
35	RA	2172	U

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Mol	Chain	Res	Type
35	RA	2173	A
35	RA	2176	A
35	RA	2186	G
35	RA	2189	U
35	RA	2192	G
35	RA	2198	A
35	RA	2206	G
35	RA	2207	G
35	RA	2208	A
35	RA	2218	U
35	RA	2219	G
35	RA	2225	A
35	RA	2238	G
35	RA	2239	G
35	RA	2249	U
35	RA	2269	A
35	RA	2275	C
35	RA	2278	A
35	RA	2279	G
35	RA	2283	C
35	RA	2287	A
35	RA	2288	A
35	RA	2292	C
35	RA	2305	A
35	RA	2308	G
35	RA	2319	G
35	RA	2320	A
35	RA	2321	G
35	RA	2322	A
35	RA	2325	G
35	RA	2334	G
35	RA	2335	A
35	RA	2336	A
35	RA	2343	C
35	RA	2345	G
35	RA	2347	C
35	RA	2350	C
35	RA	2354	G
35	RA	2372	G
35	RA	2383	G
35	RA	2385	C
35	RA	2391	G

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Mol	Chain	Res	Type
35	RA	2396	G
35	RA	2406	U
35	RA	2407	G
35	RA	2410	G
35	RA	2422	A
35	RA	2424	C
35	RA	2425	A
35	RA	2426	A
35	RA	2429	G
35	RA	2430	A
35	RA	2435	A
35	RA	2439	A
35	RA	2441	C
35	RA	2445	G
35	RA	2448	A
35	RA	2476	A
35	RA	2478	A
35	RA	2491	U
35	RA	2494	G
35	RA	2502	G
35	RA	2505	G
35	RA	2518	A
35	RA	2520	C
35	RA	2529	G
35	RA	2554	U
35	RA	2564	A
35	RA	2566	A
35	RA	2567	G
35	RA	2572	A
35	RA	2582	G
35	RA	2602	A
35	RA	2603	G
35	RA	2611	U
35	RA	2612	C
35	RA	2615	U
35	RA	2621	A
35	RA	2629	A
35	RA	2630	G
35	RA	2646	C
35	RA	2654	A
35	RA	2663	G
35	RA	2686	G

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Mol	Chain	Res	Type
35	RA	2689	U
35	RA	2690	C
35	RA	2702	U
35	RA	2703	C
35	RA	2712(B)	A
35	RA	2713	A
35	RA	2714	G
35	RA	2718	G
35	RA	2726	U
35	RA	2732	G
35	RA	2733	A
35	RA	2748	A
35	RA	2758	A
35	RA	2765	A
35	RA	2778	A
35	RA	2818	G
35	RA	2820	A
35	RA	2821	A
35	RA	2823	A
35	RA	2833	G
35	RA	2835	A
35	RA	2839	G
35	RA	2866	U
35	RA	2872	G
35	RA	2880	C
35	RA	2892	A
35	RA	2894	G
35	RA	2896	C
35	RA	2897	U
36	RB	8	U
36	RB	9	G
36	RB	12	C
36	RB	13	A
36	RB	30	C
36	RB	33	G
36	RB	51	G
36	RB	56	G
36	RB	73	A
36	RB	110	G
1	XA	5	U
1	XA	7	G
1	XA	9	G

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Mol	Chain	Res	Type
1	XA	31	G
1	XA	32	A
1	XA	39	G
1	XA	47	C
1	XA	48	C
1	XA	51	A
1	XA	59	A
1	XA	61	G
1	XA	66	G
1	XA	88	A
1	XA	89	C
1	XA	101	A
1	XA	105	G
1	XA	116	A
1	XA	121	C
1	XA	129(B)	G
1	XA	131	C
1	XA	144	G
1	XA	151	A
1	XA	163	C
1	XA	174	C
1	XA	182	U
1	XA	189(G)	U
1	XA	189(I)	G
1	XA	195	A
1	XA	197	A
1	XA	202	U
1	XA	203	U
1	XA	204	U
1	XA	216	G
1	XA	220	G
1	XA	247	G
1	XA	250	A
1	XA	251	G
1	XA	266	G
1	XA	267	C
1	XA	289	G
1	XA	301	G
1	XA	321	A
1	XA	328	C
1	XA	332	G
1	XA	346	G

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Mol	Chain	Res	Type
1	XA	350	G
1	XA	351	G
1	XA	352	C
1	XA	353	A
1	XA	354	G
1	XA	356	A
1	XA	367	U
1	XA	372	C
1	XA	373	A
1	XA	384	G
1	XA	388	G
1	XA	397	A
1	XA	398	C
1	XA	406	G
1	XA	412	A
1	XA	413	G
1	XA	424	G
1	XA	429	U
1	XA	439	A
1	XA	452	A
1	XA	461	A
1	XA	470	C
1	XA	482	A
1	XA	484	G
1	XA	485	G
1	XA	496	A
1	XA	498	U
1	XA	509	A
1	XA	510	A
1	XA	511	C
1	XA	518	C
1	XA	521	G
1	XA	532	A
1	XA	533	A
1	XA	547	A
1	XA	559	A
1	XA	561	U
1	XA	564	C
1	XA	572	A
1	XA	573	A
1	XA	576	G
1	XA	577	G

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Mol	Chain	Res	Type
1	XA	596	C
1	XA	630	G
1	XA	631	G
1	XA	653	A
1	XA	665	A
1	XA	666	G
1	XA	687	A
1	XA	688	G
1	XA	695	A
1	XA	703	G
1	XA	721	G
1	XA	723	U
1	XA	731	G
1	XA	749	C
1	XA	755	G
1	XA	759	A
1	XA	777	A
1	XA	793	U
1	XA	794	A
1	XA	815	A
1	XA	816	A
1	XA	817	C
1	XA	821	G
1	XA	828	A
1	XA	829	G
1	XA	836	G
1	XA	840	C
1	XA	841	U
1	XA	848	C
1	XA	851	G
1	XA	891	U
1	XA	902	G
1	XA	914	A
1	XA	916	G
1	XA	926	G
1	XA	927	G
1	XA	934	C
1	XA	960	U
1	XA	961	U
1	XA	968	A
1	XA	969	A
1	XA	971	G

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Mol	Chain	Res	Type
1	XA	974	A
1	XA	975	A
1	XA	976	G
1	XA	977	A
1	XA	992	U
1	XA	993	G
1	XA	1002	G
1	XA	1003	G
1	XA	1004	A
1	XA	1005	A
1	XA	1006	C
1	XA	1020	U
1	XA	1023	G
1	XA	1025	U
1	XA	1026	G
1	XA	1027	C
1	XA	1028	C
1	XA	1030(B)	G
1	XA	1030(C)	C
1	XA	1031	G
1	XA	1043	C
1	XA	1044	A
1	XA	1053	G
1	XA	1054	C
1	XA	1065	U
1	XA	1066	C
1	XA	1068	G
1	XA	1081	G
1	XA	1094	G
1	XA	1095	U
1	XA	1100	C
1	XA	1101	A
1	XA	1117	G
1	XA	1125	U
1	XA	1129	C
1	XA	1130	A
1	XA	1136	U
1	XA	1137	C
1	XA	1138	G
1	XA	1139	G
1	XA	1146	A
1	XA	1147	C

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Mol	Chain	Res	Type
1	XA	1152	A
1	XA	1157	A
1	XA	1158	C
1	XA	1159	U
1	XA	1183	A
1	XA	1196	U
1	XA	1197	G
1	XA	1201	A
1	XA	1211	U
1	XA	1214	C
1	XA	1224	G
1	XA	1227	A
1	XA	1236	A
1	XA	1238	A
1	XA	1250	A
1	XA	1256	A
1	XA	1257	U
1	XA	1258	G
1	XA	1260	C
1	XA	1270	C
1	XA	1278	U
1	XA	1279	A
1	XA	1280	A
1	XA	1282	C
1	XA	1285	A
1	XA	1286	A
1	XA	1287	A
1	XA	1300	G
1	XA	1302	U
1	XA	1303	C
1	XA	1305	G
1	XA	1317	C
1	XA	1320	C
1	XA	1340	A
1	XA	1347	G
1	XA	1353	G
1	XA	1363(A)	C
1	XA	1363(B)	A
1	XA	1370	G
1	XA	1397	C
1	XA	1399	C
1	XA	1419	G

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Mol	Chain	Res	Type
1	XA	1442(A)	G
1	XA	1442(B)	G
1	XA	1447	A
1	XA	1456	G
1	XA	1469	G
1	XA	1487	G
1	XA	1492	A
1	XA	1497	G
1	XA	1499	A
1	XA	1503	A
1	XA	1504	G
1	XA	1506	U
1	XA	1517	G
1	XA	1520	G
1	XA	1529	G
1	XA	1530	G
1	XA	1531	A
22	XV	3	C
22	XV	8	U
22	XV	16	C
22	XV	17(A)	U
22	XV	18	G
22	XV	19	G
22	XV	20	U
22	XV	21	A
22	XV	47	U
22	XV	48	C
22	XV	49	G
22	XV	65	C
22	XV	76	A
23	XX	7	G
23	XX	10	G
23	XX	11	U
23	XX	13	A
23	XX	14	A
23	XX	15	A
23	XX	19	G
23	XX	23	A
24	XY	2	G
24	XY	8	U
24	XY	9	A
24	XY	12	U

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Mol	Chain	Res	Type
24	XY	16	C
24	XY	17	U
24	XY	18	G
24	XY	19	G
24	XY	21	A
24	XY	23	A
24	XY	29	U
24	XY	31	C
24	XY	43	G
24	XY	46	G
24	XY	47	U
24	XY	48	C
24	XY	49	A
24	XY	50	G
24	XY	51	C
24	XY	52	G
24	XY	54	U
24	XY	55	U
24	XY	56	C
24	XY	57	G
24	XY	58	A
24	XY	61	C
24	XY	67	A
24	XY	68	G
24	XY	69	C
24	XY	71	C
24	XY	73	A
24	XY	74	C
24	XY	75	C
35	YA	10	G
35	YA	34	C
35	YA	45	C
35	YA	51	G
35	YA	55	G
35	YA	71	A
35	YA	74	A
35	YA	75	G
35	YA	84	A
35	YA	92	A
35	YA	95	G
35	YA	102	G
35	YA	118	A

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Mol	Chain	Res	Type
35	YA	119	A
35	YA	120	U
35	YA	131	G
35	YA	157	U
35	YA	182	A
35	YA	188	G
35	YA	196	A
35	YA	199	A
35	YA	205	G
35	YA	215	G
35	YA	216	A
35	YA	221	A
35	YA	222	A
35	YA	228	A
35	YA	229	A
35	YA	230	U
35	YA	233	A
35	YA	248	G
35	YA	265	A
35	YA	272(J)	C
35	YA	272(K)	U
35	YA	272(N)	U
35	YA	273(B)	U
35	YA	273(C)	G
35	YA	277	C
35	YA	278	A
35	YA	311	A
35	YA	317	G
35	YA	324	A
35	YA	329	G
35	YA	330	A
35	YA	338	G
35	YA	342	G
35	YA	345	A
35	YA	352	G
35	YA	362	U
35	YA	363(A)	G
35	YA	372	G
35	YA	386	G
35	YA	396	G
35	YA	405	U
35	YA	411	G

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Mol	Chain	Res	Type
35	YA	412	A
35	YA	428	A
35	YA	444	C
35	YA	455	C
35	YA	457	A
35	YA	467	G
35	YA	470	A
35	YA	481	G
35	YA	505	A
35	YA	508	G
35	YA	509	C
35	YA	530	G
35	YA	531	C
35	YA	532	A
35	YA	533	G
35	YA	563	G
35	YA	573	G
35	YA	575	A
35	YA	603	A
35	YA	604	G
35	YA	607	U
35	YA	614(C)	G
35	YA	615	G
35	YA	620	G
35	YA	627	A
35	YA	634	C
35	YA	637	A
35	YA	645	C
35	YA	646	A
35	YA	652(C)	A
35	YA	652(D)	G
35	YA	652(V)	G
35	YA	669	G
35	YA	686	G
35	YA	717	G
35	YA	726	G
35	YA	730	C
35	YA	734	A
35	YA	738	G
35	YA	753	C
35	YA	764	A
35	YA	765	G

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Mol	Chain	Res	Type
35	YA	775	G
35	YA	776	G
35	YA	782	A
35	YA	784	A
35	YA	785	G
35	YA	788	A
35	YA	789	A
35	YA	792	G
35	YA	805	G
35	YA	812	C
35	YA	827	U
35	YA	828	U
35	YA	831	G
35	YA	857	C
35	YA	859	G
35	YA	869	G
35	YA	881	G
35	YA	886	C
35	YA	887	A
35	YA	888	C
35	YA	889	C
35	YA	890	A
35	YA	893	C
35	YA	896	A
35	YA	897	C
35	YA	898	C
35	YA	907	U
35	YA	910	A
35	YA	915	C
35	YA	917	A
35	YA	932	G
35	YA	941	A
35	YA	945	A
35	YA	946	G
35	YA	953	A
35	YA	957	A
35	YA	959	A
35	YA	961	C
35	YA	973	A
35	YA	974	G
35	YA	975(A)	C
35	YA	983	A

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Mol	Chain	Res	Type
35	YA	996	A
35	YA	1005	C
35	YA	1008	C
35	YA	1012	U
35	YA	1013	C
35	YA	1025	G
35	YA	1026	U
35	YA	1033	U
35	YA	1045	A
35	YA	1046	A
35	YA	1047	G
35	YA	1052	C
35	YA	1054	A
35	YA	1058	G
35	YA	1060	U
35	YA	1063	G
35	YA	1064	C
35	YA	1065	U
35	YA	1066	U
35	YA	1067	A
35	YA	1068	G
35	YA	1070	A
35	YA	1071	G
35	YA	1073	A
35	YA	1074	G
35	YA	1076	C
35	YA	1077	A
35	YA	1079	C
35	YA	1082	U
35	YA	1083	U
35	YA	1084	A
35	YA	1085	A
35	YA	1086	A
35	YA	1088	A
35	YA	1092	C
35	YA	1096	A
35	YA	1097	U
35	YA	1098	A
35	YA	1108	U
35	YA	1109	C
35	YA	1110	G
35	YA	1112	G

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Mol	Chain	Res	Type
35	YA	1128	A
35	YA	1129	A
35	YA	1130	U
35	YA	1135	C
35	YA	1136	G
35	YA	1143	A
35	YA	1171	G
35	YA	1206	G
35	YA	1211	U
35	YA	1220	A
35	YA	1236	G
35	YA	1250	G
35	YA	1253	A
35	YA	1256	G
35	YA	1265	A
35	YA	1271	G
35	YA	1272	A
35	YA	1273	U
35	YA	1300	U
35	YA	1301	A
35	YA	1313	U
35	YA	1314	C
35	YA	1352	U
35	YA	1359	A
35	YA	1360	A
35	YA	1365	A
35	YA	1368	G
35	YA	1378	A
35	YA	1379	A
35	YA	1380	G
35	YA	1384	A
35	YA	1385	G
35	YA	1395	A
35	YA	1416	G
35	YA	1417	C
35	YA	1419	A
35	YA	1420	U
35	YA	1421	G
35	YA	1427	A
35	YA	1428	C
35	YA	1445(A)	A
35	YA	1450(A)	G

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Mol	Chain	Res	Type
35	YA	1455	G
35	YA	1459	G
35	YA	1460	A
35	YA	1467	C
35	YA	1471	A
35	YA	1482	G
35	YA	1493	C
35	YA	1494	A
35	YA	1497	U
35	YA	1508	A
35	YA	1509(A)	C
35	YA	1509(B)	A
35	YA	1525	G
35	YA	1542	A
35	YA	1543	C
35	YA	1547	C
35	YA	1558	A
35	YA	1566	A
35	YA	1569	A
35	YA	1578	U
35	YA	1580	A
35	YA	1584	C
35	YA	1586	A
35	YA	1607	C
35	YA	1608	A
35	YA	1609	A
35	YA	1640	C
35	YA	1648	C
35	YA	1674	G
35	YA	1693	U
35	YA	1696	G
35	YA	1698	A
35	YA	1700	A
35	YA	1701	A
35	YA	1721	G
35	YA	1722	A
35	YA	1750	G
35	YA	1756	G
35	YA	1757	U
35	YA	1762	A
35	YA	1763	G
35	YA	1764	G

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Mol	Chain	Res	Type
35	YA	1769	G
35	YA	1773	A
35	YA	1774	C
35	YA	1780	A
35	YA	1786	A
35	YA	1791	A
35	YA	1800	C
35	YA	1801	G
35	YA	1811	G
35	YA	1816	G
35	YA	1828	G
35	YA	1829	A
35	YA	1835	G
35	YA	1847	A
35	YA	1848	A
35	YA	1877	A
35	YA	1878	G
35	YA	1889	A
35	YA	1900	A
35	YA	1914	C
35	YA	1929	G
35	YA	1930	G
35	YA	1936	A
35	YA	1937	A
35	YA	1938	A
35	YA	1955	U
35	YA	1963	U
35	YA	1967	C
35	YA	1970	A
35	YA	1971	A
35	YA	1972	A
35	YA	1984	G
35	YA	1992	G
35	YA	1993	U
35	YA	1997	G
35	YA	2020	A
35	YA	2023	G
35	YA	2031	A
35	YA	2032	G
35	YA	2033	A
35	YA	2043	C
35	YA	2055	C

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Mol	Chain	Res	Type
35	YA	2056	G
35	YA	2060	A
35	YA	2061	G
35	YA	2062	A
35	YA	2069	G
35	YA	2093	G
35	YA	2096	U
35	YA	2099	U
35	YA	2103	C
35	YA	2104	G
35	YA	2105	C
35	YA	2107	C
35	YA	2108	C
35	YA	2116	G
35	YA	2117	A
35	YA	2119	A
35	YA	2120	G
35	YA	2121	G
35	YA	2123	G
35	YA	2127	G
35	YA	2129	C
35	YA	2131	G
35	YA	2132	U
35	YA	2133	G
35	YA	2134	A
35	YA	2136	C
35	YA	2145	C
35	YA	2146	C
35	YA	2147	G
35	YA	2148	G
35	YA	2151	G
35	YA	2158	A
35	YA	2161	C
35	YA	2165	G
35	YA	2172	U
35	YA	2173	A
35	YA	2186	G
35	YA	2189	U
35	YA	2192	G
35	YA	2198	A
35	YA	2206	G
35	YA	2207	G

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Mol	Chain	Res	Type
35	YA	2208	A
35	YA	2218	U
35	YA	2219	G
35	YA	2225	A
35	YA	2238	G
35	YA	2239	G
35	YA	2249	U
35	YA	2269	A
35	YA	2275	C
35	YA	2278	A
35	YA	2279	G
35	YA	2283	C
35	YA	2287	A
35	YA	2288	A
35	YA	2305	A
35	YA	2308	G
35	YA	2309	A
35	YA	2312	U
35	YA	2319	G
35	YA	2320	A
35	YA	2321	G
35	YA	2322	A
35	YA	2325	G
35	YA	2334	G
35	YA	2335	A
35	YA	2336	A
35	YA	2343	C
35	YA	2347	C
35	YA	2350	C
35	YA	2354	G
35	YA	2372	G
35	YA	2383	G
35	YA	2385	C
35	YA	2391	G
35	YA	2396	G
35	YA	2406	U
35	YA	2410	G
35	YA	2422	A
35	YA	2424	C
35	YA	2425	A
35	YA	2427	C
35	YA	2428	G

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Mol	Chain	Res	Type
35	YA	2429	G
35	YA	2430	A
35	YA	2435	A
35	YA	2439	A
35	YA	2441	C
35	YA	2445	G
35	YA	2448	A
35	YA	2476	A
35	YA	2491	U
35	YA	2494	G
35	YA	2502	G
35	YA	2505	G
35	YA	2518	A
35	YA	2520	C
35	YA	2529	G
35	YA	2554	U
35	YA	2564	A
35	YA	2566	A
35	YA	2567	G
35	YA	2582	G
35	YA	2586	C
35	YA	2602	A
35	YA	2604	U
35	YA	2609	U
35	YA	2611	U
35	YA	2612	C
35	YA	2615	U
35	YA	2629	A
35	YA	2630	G
35	YA	2633	G
35	YA	2646	C
35	YA	2654	A
35	YA	2663	G
35	YA	2673	G
35	YA	2686	G
35	YA	2689	U
35	YA	2690	C
35	YA	2691	C
35	YA	2702	U
35	YA	2703	C
35	YA	2712(B)	A
35	YA	2713	A

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Mol	Chain	Res	Type
35	YA	2714	G
35	YA	2726	U
35	YA	2732	G
35	YA	2733	A
35	YA	2748	A
35	YA	2758	A
35	YA	2764	A
35	YA	2765	A
35	YA	2766	G
35	YA	2778	A
35	YA	2818	G
35	YA	2820	A
35	YA	2821	A
35	YA	2833	G
35	YA	2835	A
35	YA	2866	U
35	YA	2872	G
35	YA	2892	A
35	YA	2894	G
35	YA	2896	C
35	YA	2897	U
36	YB	8	U
36	YB	9	G
36	YB	12	C
36	YB	13	A
36	YB	24	G
36	YB	30	C
36	YB	33	G
36	YB	51	G
36	YB	56	G
36	YB	73	A
36	YB	110	G

All (63) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	QA	60	A
1	QA	65	U
1	QA	115	G
1	QA	266	G
1	QA	509	A
1	QA	560	U

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Mol	Chain	Res	Type
1	QA	687	A
1	QA	748	C
1	QA	840	C
1	QA	913	A
1	QA	991	U
1	QA	992	U
1	QA	1065	U
1	QA	1067	A
1	QA	1442(A)	G
23	QX	18	G
35	RA	272(M)	G
35	RA	277	C
35	RA	752	A
35	RA	827	U
35	RA	856	C
35	RA	1057	A
35	RA	1065	U
35	RA	1073	A
35	RA	1210	A
35	RA	1992	G
35	RA	2126	A
35	RA	2171	A
35	RA	2172	U
35	RA	2406	U
35	RA	2601	C
35	RA	2689	U
1	XA	60	A
1	XA	65	U
1	XA	115	G
1	XA	266	G
1	XA	509	A
1	XA	560	U
1	XA	687	A
1	XA	748	C
1	XA	840	C
1	XA	913	A
1	XA	991	U
1	XA	992	U
1	XA	1065	U
1	XA	1067	A
1	XA	1442(A)	G
23	XX	18	G

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Mol	Chain	Res	Type
35	YA	272(M)	G
35	YA	277	C
35	YA	752	A
35	YA	827	U
35	YA	856	C
35	YA	1057	A
35	YA	1065	U
35	YA	1073	A
35	YA	1210	A
35	YA	1992	G
35	YA	2126	A
35	YA	2171	A
35	YA	2172	U
35	YA	2406	U
35	YA	2689	U

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

48 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$
35	PSU	RA	2605	35	18,21,22	1.47	4 (22%)	21,30,33	2.03	4 (19%)
1	MA6	QA	1519	1	23,26,27	1.51	5 (21%)	33,38,41	2.41	13 (39%)
1	MA6	XA	1518	1	23,26,27	1.60	6 (26%)	33,38,41	2.41	12 (36%)
1	MA6	QA	1518	1	23,26,27	1.60	6 (26%)	33,38,41	2.35	10 (30%)
1	2MG	XA	1207	1	23,26,27	1.27	3 (13%)	33,38,41	2.29	10 (30%)
1	5MC	QA	1407	1	19,22,23	1.33	3 (15%)	26,32,35	1.45	2 (7%)
12	0TD	QL	92	12	8,9,10	3.79	1 (12%)	6,11,13	2.26	3 (50%)
1	4OC	QA	1402	1	20,23,24	0.79	0	25,32,35	1.13	2 (8%)
35	2MA	YA	2503	56,35	22,25,26	1.43	5 (22%)	32,37,40	2.31	8 (25%)
35	PSU	YA	1911	35	18,21,22	1.44	4 (22%)	21,30,33	2.03	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	QA	1400	1	19,22,23	1.41	3 (15%)	26,32,35	1.17	2 (7%)
35	2MA	RA	2503	56,35	22,25,26	1.44	5 (22%)	32,37,40	2.44	8 (25%)
1	UR3	XA	1498	1	19,22,23	0.98	2 (10%)	26,32,35	1.71	3 (11%)
1	2MG	QA	1207	1	23,26,27	1.27	4 (17%)	33,38,41	2.26	10 (30%)
35	OMC	YA	1920	35	19,22,23	0.86	2 (10%)	25,31,34	1.19	3 (12%)
1	5MC	XA	1400	1	19,22,23	1.44	3 (15%)	26,32,35	1.21	2 (7%)
35	5MC	RA	1962	56,35	19,22,23	1.30	3 (15%)	26,32,35	1.23	2 (7%)
1	4OC	XA	1402	1	20,23,24	0.81	1 (5%)	25,32,35	1.03	1 (4%)
35	5MC	YA	1942	35	19,22,23	1.41	2 (10%)	26,32,35	1.31	4 (15%)
35	5MU	RA	1939	35	19,22,23	1.42	4 (21%)	27,32,35	2.30	6 (22%)
1	5MC	XA	967	1	19,22,23	1.24	2 (10%)	26,32,35	1.18	3 (11%)
1	M2G	QA	966	1	24,27,28	1.30	5 (20%)	33,40,43	1.78	5 (15%)
1	G7M	XA	527	56,1	23,26,27	2.27	5 (21%)	34,39,42	3.28	10 (29%)
35	OMG	RA	2251	56,35,22	23,26,27	1.25	3 (13%)	32,38,41	1.98	6 (18%)
35	OMU	YA	2552	56,35	19,22,23	1.35	3 (15%)	25,31,34	1.89	5 (20%)
35	5MC	YA	1962	56,35	19,22,23	1.34	3 (15%)	26,32,35	1.17	2 (7%)
1	MA6	XA	1519	1	23,26,27	1.51	6 (26%)	33,38,41	2.40	13 (39%)
1	M2G	XA	966	1	24,27,28	1.29	5 (20%)	33,40,43	1.82	5 (15%)
35	OMG	YA	2251	56,35,22	23,26,27	1.27	3 (13%)	32,38,41	2.08	6 (18%)
35	5MU	YA	1939	35	19,22,23	1.39	4 (21%)	27,32,35	2.26	6 (22%)
35	PSU	RA	1911	35	18,21,22	1.42	4 (22%)	21,30,33	2.09	4 (19%)
35	5MU	RA	1915	35	19,22,23	1.54	5 (26%)	27,32,35	2.68	9 (33%)
1	PSU	QA	516	1	18,21,22	1.40	5 (27%)	21,30,33	1.88	3 (14%)
35	PSU	YA	1917	56,35	18,21,22	1.45	4 (22%)	21,30,33	2.01	3 (14%)
1	5MC	QA	1404	1	19,22,23	1.35	3 (15%)	26,32,35	1.12	3 (11%)
1	G7M	QA	527	56,1	23,26,27	2.32	5 (21%)	34,39,42	3.15	11 (32%)
1	PSU	XA	516	1	18,21,22	1.44	4 (22%)	21,30,33	2.06	5 (23%)
35	OMC	RA	1920	35	19,22,23	0.83	1 (5%)	25,31,34	1.17	3 (12%)
1	5MC	XA	1407	1	19,22,23	1.15	2 (10%)	26,32,35	1.30	2 (7%)
35	PSU	RA	1917	56,35	18,21,22	1.43	4 (22%)	21,30,33	1.96	4 (19%)
1	5MC	QA	967	1	19,22,23	1.56	3 (15%)	26,32,35	1.18	3 (11%)
35	5MU	YA	1915	35	19,22,23	1.48	5 (26%)	27,32,35	2.66	9 (33%)
35	5MC	RA	1942	35	19,22,23	1.50	3 (15%)	26,32,35	1.22	3 (11%)
1	UR3	QA	1498	1	19,22,23	0.93	1 (5%)	26,32,35	1.70	2 (7%)
1	5MC	XA	1404	1	19,22,23	1.28	2 (10%)	26,32,35	1.18	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	OMU	RA	2552	56,35	19,22,23	1.31	2 (10%)	25,31,34	1.87	5 (20%)
12	0TD	XL	92	12	8,9,10	3.41	3 (37%)	6,11,13	1.49	1 (16%)
35	PSU	YA	2605	35	18,21,22	1.51	4 (22%)	21,30,33	2.11	4 (19%)

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
35	PSU	RA	2605	35	-	0/7/25/26	0/2/2/2
1	MA6	QA	1519	1	-	3/11/29/30	0/3/3/3
1	MA6	XA	1518	1	-	3/11/29/30	0/3/3/3
1	MA6	QA	1518	1	-	3/11/29/30	0/3/3/3
1	2MG	XA	1207	1	-	0/9/27/28	0/3/3/3
1	5MC	QA	1407	1	-	0/7/25/26	0/2/2/2
12	0TD	QL	92	12	-	1/7/12/14	-
1	4OC	QA	1402	1	-	2/9/29/30	0/2/2/2
35	2MA	YA	2503	56,35	-	0/7/25/26	0/3/3/3
35	PSU	YA	1911	35	-	0/7/25/26	0/2/2/2
1	5MC	QA	1400	1	-	2/7/25/26	0/2/2/2
35	2MA	RA	2503	56,35	-	0/7/25/26	0/3/3/3
1	UR3	XA	1498	1	-	0/7/25/26	0/2/2/2
1	2MG	QA	1207	1	-	0/9/27/28	0/3/3/3
35	OMC	YA	1920	35	-	0/9/27/28	0/2/2/2
1	5MC	XA	1400	1	-	2/7/25/26	0/2/2/2
35	5MC	RA	1962	56,35	-	0/7/25/26	0/2/2/2
1	4OC	XA	1402	1	-	2/9/29/30	0/2/2/2
35	5MC	YA	1942	35	-	0/7/25/26	0/2/2/2
35	5MU	RA	1939	35	-	0/7/25/26	0/2/2/2
1	5MC	XA	967	1	-	0/7/25/26	0/2/2/2
1	M2G	QA	966	1	-	0/11/29/30	0/3/3/3
1	G7M	XA	527	56,1	-	3/7/25/26	0/3/3/3
35	OMG	RA	2251	56,35,22	-	0/9/27/28	0/3/3/3
35	OMU	YA	2552	56,35	-	0/9/27/28	0/2/2/2
35	5MC	YA	1962	56,35	-	1/7/25/26	0/2/2/2
1	MA6	XA	1519	1	-	4/11/29/30	0/3/3/3
1	M2G	XA	966	1	-	0/11/29/30	0/3/3/3
35	OMG	YA	2251	56,35,22	-	0/9/27/28	0/3/3/3
35	5MU	YA	1939	35	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	PSU	RA	1911	35	-	0/7/25/26	0/2/2/2
35	5MU	RA	1915	35	-	2/7/25/26	0/2/2/2
1	PSU	QA	516	1	-	0/7/25/26	0/2/2/2
35	PSU	YA	1917	56,35	-	0/7/25/26	0/2/2/2
1	5MC	QA	1404	1	-	2/7/25/26	0/2/2/2
1	G7M	QA	527	56,1	-	2/7/25/26	0/3/3/3
1	PSU	XA	516	1	-	0/7/25/26	0/2/2/2
35	OMC	RA	1920	35	-	0/9/27/28	0/2/2/2
1	5MC	XA	1407	1	-	0/7/25/26	0/2/2/2
35	PSU	RA	1917	56,35	-	0/7/25/26	0/2/2/2
1	5MC	QA	967	1	-	0/7/25/26	0/2/2/2
35	5MU	YA	1915	35	-	2/7/25/26	0/2/2/2
35	5MC	RA	1942	35	-	0/7/25/26	0/2/2/2
1	UR3	QA	1498	1	-	0/7/25/26	0/2/2/2
1	5MC	XA	1404	1	-	0/7/25/26	0/2/2/2
35	OMU	RA	2552	56,35	-	1/9/27/28	0/2/2/2
12	0TD	XL	92	12	-	3/7/12/14	-
35	PSU	YA	2605	35	-	0/7/25/26	0/2/2/2

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	QL	92	0TD	CB-CA	-10.41	1.51	1.54
12	XL	92	0TD	CB-CA	-8.91	1.51	1.54
1	QA	527	G7M	C8-N7	7.07	1.45	1.33
1	XA	527	G7M	C8-N7	6.77	1.44	1.33
1	QA	967	5MC	C5-C4	5.55	1.48	1.44
1	QA	527	G7M	C5-N7	-5.26	1.33	1.39
1	XA	527	G7M	C5-N7	-5.15	1.33	1.39
35	RA	1942	5MC	C5-C4	5.13	1.48	1.44
1	XA	1400	5MC	C5-C4	4.81	1.47	1.44
35	YA	1942	5MC	C5-C4	4.75	1.47	1.44
1	QA	1518	MA6	C5-C4	4.70	1.47	1.39
1	QA	1400	5MC	C5-C4	4.67	1.47	1.44
1	XA	1518	MA6	C5-C4	4.51	1.47	1.39
1	QA	1519	MA6	C5-C4	4.49	1.47	1.39
1	QA	1404	5MC	C5-C4	4.43	1.47	1.44
35	YA	1962	5MC	C5-C4	4.36	1.47	1.44
1	QA	1407	5MC	C5-C4	4.32	1.47	1.44
1	XA	1519	MA6	C5-C4	4.25	1.46	1.39
35	YA	2503	2MA	C5-C4	4.06	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	RA	1962	5MC	C5-C4	4.04	1.47	1.44
1	XA	1404	5MC	C5-C4	3.98	1.47	1.44
1	QA	527	G7M	C8-N9	3.93	1.46	1.35
1	XA	527	G7M	C8-N9	3.91	1.46	1.35
35	RA	2503	2MA	C5-C4	3.85	1.46	1.39
1	XA	967	5MC	C5-C4	3.81	1.47	1.44
1	XA	527	G7M	C5-C4	3.56	1.47	1.38
35	YA	2552	OMU	C4-N3	-3.56	1.32	1.38
35	RA	1915	5MU	C4-N3	-3.49	1.32	1.38
35	YA	1915	5MU	C4-N3	-3.42	1.32	1.38
1	QA	527	G7M	C5-C4	3.34	1.46	1.38
1	QA	1518	MA6	C5-C6	3.32	1.49	1.41
1	XA	1407	5MC	C5-C4	3.31	1.46	1.44
1	XA	1518	MA6	C5-C6	3.24	1.49	1.41
35	RA	2552	OMU	C4-N3	-3.24	1.33	1.38
35	RA	1939	5MU	C4-N3	-3.22	1.32	1.38
35	YA	2605	PSU	C4-N3	-3.16	1.32	1.38
35	RA	2605	PSU	C4-N3	-3.07	1.33	1.38
35	RA	1915	5MU	C2-N1	3.07	1.43	1.38
35	YA	1939	5MU	C4-N3	-3.03	1.33	1.38
1	QA	966	M2G	C5-C4	3.02	1.47	1.38
35	YA	1939	5MU	C6-N1	-3.01	1.32	1.38
35	YA	1917	PSU	C4-N3	-3.01	1.33	1.38
35	RA	1962	5MC	C6-N1	-3.00	1.32	1.38
35	YA	2251	OMG	C5-C4	3.00	1.47	1.38
1	XA	516	PSU	C6-C5	2.99	1.38	1.35
1	XA	516	PSU	C4-N3	-2.96	1.33	1.38
1	XA	967	5MC	C6-N1	-2.94	1.33	1.38
35	RA	2251	OMG	C6-N1	-2.93	1.33	1.38
35	YA	2251	OMG	C6-N1	-2.93	1.33	1.38
35	RA	1911	PSU	C4-N3	-2.91	1.33	1.38
35	YA	1915	5MU	C2-N1	2.91	1.43	1.38
1	QA	1207	2MG	C5-C4	2.91	1.46	1.38
1	XA	966	M2G	C6-N1	-2.89	1.33	1.38
35	RA	2251	OMG	C5-C4	2.89	1.46	1.38
35	YA	1962	5MC	C6-N1	-2.88	1.33	1.38
35	YA	1942	5MC	C6-N1	-2.88	1.33	1.38
1	XA	1404	5MC	C6-N1	-2.88	1.33	1.38
35	YA	1911	PSU	C4-N3	-2.88	1.33	1.38
1	QA	1519	MA6	C5-C6	2.87	1.48	1.41
35	YA	1939	5MU	C2-N3	-2.86	1.33	1.38
35	RA	1939	5MU	C6-N1	-2.86	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	RA	1917	PSU	C4-N3	-2.85	1.33	1.38
35	YA	2605	PSU	C6-C5	2.83	1.38	1.35
1	XA	1207	2MG	C6-N1	-2.82	1.33	1.38
1	XA	1519	MA6	C5-C6	2.77	1.48	1.41
1	XA	1207	2MG	C5-C4	2.77	1.46	1.38
1	QA	527	G7M	C6-N1	-2.76	1.33	1.38
35	RA	1939	5MU	C2-N3	-2.76	1.33	1.38
35	RA	1942	5MC	C6-N1	-2.74	1.33	1.38
1	XA	966	M2G	C5-C4	2.74	1.46	1.38
1	QA	1207	2MG	C6-N1	-2.72	1.33	1.38
35	YA	1911	PSU	C6-C5	2.72	1.38	1.35
1	QA	967	5MC	C6-N1	-2.70	1.33	1.38
1	QA	1400	5MC	C6-N1	-2.69	1.33	1.38
1	XA	527	G7M	C6-N1	-2.69	1.33	1.38
35	RA	2503	2MA	C5-N7	-2.68	1.34	1.39
1	XA	1400	5MC	C6-N1	-2.68	1.33	1.38
35	YA	2251	OMG	C5-N7	-2.68	1.33	1.39
1	QA	516	PSU	C4-N3	-2.68	1.33	1.38
35	RA	2605	PSU	C6-C5	2.66	1.38	1.35
1	QA	966	M2G	C6-N1	-2.66	1.33	1.38
35	RA	1911	PSU	C6-C5	2.66	1.38	1.35
35	YA	2503	2MA	C5-N7	-2.66	1.34	1.39
35	RA	1917	PSU	C6-C5	2.64	1.38	1.35
1	XA	1519	MA6	C4-N9	-2.64	1.32	1.37
1	QA	516	PSU	C6-C5	2.59	1.38	1.35
1	QA	1404	5MC	C6-N1	-2.59	1.33	1.38
35	RA	1915	5MU	C6-C5	2.55	1.38	1.34
1	QA	1519	MA6	C5-N7	-2.55	1.34	1.39
1	XA	1400	5MC	C6-C5	2.54	1.38	1.34
1	XA	1407	5MC	C6-N1	-2.53	1.33	1.38
35	YA	1915	5MU	C6-N1	-2.52	1.33	1.38
1	XA	1518	MA6	C4-N9	-2.51	1.32	1.37
35	RA	1915	5MU	C2-N3	-2.50	1.33	1.38
35	YA	2605	PSU	C2-N1	-2.49	1.33	1.36
1	XA	1519	MA6	C5-N7	-2.47	1.34	1.39
35	YA	1915	5MU	C2-N3	-2.46	1.33	1.38
35	YA	2552	OMU	C2-N3	-2.46	1.33	1.38
35	RA	2251	OMG	C5-N7	-2.45	1.34	1.39
1	XA	966	M2G	C5-N7	-2.44	1.34	1.39
35	YA	1920	OMC	C5-C4	-2.43	1.37	1.42
35	RA	2503	2MA	C5-C6	2.43	1.47	1.41
1	XA	1207	2MG	C5-N7	-2.39	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	RA	2605	PSU	C2-N1	-2.39	1.33	1.36
1	QA	1407	5MC	C6-N1	-2.39	1.33	1.38
35	YA	1917	PSU	C2-N3	-2.38	1.33	1.37
35	RA	1915	5MU	C6-N1	-2.38	1.34	1.38
1	QA	1400	5MC	C6-C5	2.37	1.38	1.34
1	QA	966	M2G	C5-N7	-2.37	1.34	1.39
35	YA	1911	PSU	C2-N3	-2.36	1.33	1.37
35	YA	1911	PSU	C2-N1	-2.36	1.33	1.36
35	YA	2605	PSU	C2-N3	-2.36	1.33	1.37
35	YA	1917	PSU	C2-N1	-2.36	1.33	1.36
35	RA	2552	OMU	C2-N3	-2.36	1.33	1.38
1	XA	1518	MA6	C8-N9	-2.36	1.33	1.37
35	RA	1939	5MU	C6-C5	2.35	1.38	1.34
35	RA	1942	5MC	C6-C5	2.35	1.38	1.34
35	YA	1917	PSU	C6-C5	2.33	1.37	1.35
35	RA	2605	PSU	C2-N3	-2.32	1.33	1.37
1	XA	516	PSU	C2-N3	-2.30	1.33	1.37
35	RA	1911	PSU	C2-N3	-2.30	1.33	1.37
35	RA	1917	PSU	C2-N1	-2.29	1.33	1.36
35	YA	2503	2MA	C5-C6	2.28	1.47	1.41
35	RA	1917	PSU	C2-N3	-2.28	1.33	1.37
1	QA	1207	2MG	C5-N7	-2.27	1.34	1.39
35	YA	2503	2MA	C4-N9	-2.27	1.33	1.37
12	XL	92	0TD	OD2-CG	-2.27	1.23	1.30
1	QA	1518	MA6	C5-N7	-2.27	1.34	1.39
35	RA	1920	OMC	C5-C4	-2.26	1.37	1.42
1	QA	1404	5MC	C6-C5	2.26	1.38	1.34
1	QA	966	M2G	C2-N2	2.26	1.39	1.35
1	QA	1407	5MC	C6-C5	2.23	1.38	1.34
1	XA	1498	UR3	C5-C4	-2.23	1.38	1.43
1	QA	1518	MA6	C4-N9	-2.22	1.33	1.37
12	XL	92	0TD	CB-SB	2.21	1.84	1.82
1	QA	967	5MC	C6-C5	2.20	1.38	1.34
1	QA	516	PSU	C2-N1	-2.19	1.33	1.36
1	XA	966	M2G	C2-N2	2.19	1.39	1.35
35	YA	1920	OMC	C6-N1	-2.17	1.32	1.38
35	RA	1911	PSU	C2-N1	-2.15	1.33	1.36
1	XA	1498	UR3	C6-N1	-2.15	1.33	1.38
1	XA	1518	MA6	C5-N7	-2.14	1.35	1.39
1	QA	1519	MA6	C4-N9	-2.14	1.33	1.37
1	XA	516	PSU	C2-N1	-2.13	1.33	1.36
1	QA	1519	MA6	C8-N9	-2.11	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	YA	1939	5MU	C6-C5	2.10	1.38	1.34
1	XA	1519	MA6	C8-N9	-2.10	1.34	1.37
1	QA	1498	UR3	C5-C4	-2.10	1.38	1.43
35	YA	1915	5MU	C6-C5	2.09	1.38	1.34
1	QA	1518	MA6	C8-N9	-2.09	1.34	1.37
35	RA	2503	2MA	C8-N9	-2.09	1.34	1.37
1	XA	1518	MA6	C6-N6	2.07	1.42	1.36
35	RA	1962	5MC	C6-C5	2.06	1.38	1.34
1	XA	966	M2G	C4-N9	-2.05	1.32	1.38
1	QA	516	PSU	C2-N3	-2.05	1.34	1.37
35	RA	2503	2MA	C4-N9	-2.05	1.33	1.37
1	QA	516	PSU	O4'-C1'	-2.05	1.41	1.43
1	QA	966	M2G	C4-N9	-2.03	1.32	1.38
1	XA	1402	4OC	C6-N1	-2.03	1.33	1.38
1	XA	1519	MA6	C8-N7	2.03	1.35	1.31
1	QA	1207	2MG	C4-N9	-2.02	1.32	1.38
35	YA	1962	5MC	C6-C5	2.02	1.37	1.34
35	YA	2503	2MA	C8-N7	2.01	1.35	1.31
35	YA	2552	OMU	C6-N1	-2.00	1.33	1.38
1	QA	1518	MA6	C6-N6	2.00	1.42	1.36

All (247) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	527	G7M	CN7-N7-C8	-10.02	109.61	124.79
35	RA	2503	2MA	C5-C4-N3	-9.19	117.50	127.18
1	QA	527	G7M	CN7-N7-C8	-8.85	111.39	124.79
35	YA	2503	2MA	C5-C4-N3	-8.42	118.31	127.18
1	XA	1207	2MG	C2-N3-C4	7.36	121.20	112.00
35	RA	2503	2MA	N3-C4-N9	7.06	135.95	126.99
1	XA	527	G7M	C8-N7-C5	6.97	116.49	107.78
35	YA	2251	OMG	C5-C4-N3	-6.96	117.31	128.39
1	QA	1207	2MG	C2-N3-C4	6.93	120.67	112.00
1	QA	527	G7M	N9-C8-N7	-6.79	95.99	112.48
1	QA	527	G7M	C8-N7-C5	6.76	116.24	107.78
1	XA	527	G7M	N9-C8-N7	-6.73	96.14	112.48
1	QA	1498	UR3	C4-N3-C2	-6.62	119.26	124.58
1	XA	1498	UR3	C4-N3-C2	-6.58	119.28	124.58
35	RA	1911	PSU	N1-C2-N3	6.50	122.02	115.17
1	XA	1207	2MG	C5-C4-N3	-6.44	118.13	128.39
35	YA	2503	2MA	N3-C4-N9	6.43	135.15	126.99
35	RA	2251	OMG	C5-C4-N3	-6.39	118.22	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1915	5MU	C1'-N1-C2	6.35	129.00	117.59
1	QA	527	G7M	N9-C4-N3	6.35	138.65	125.95
35	YA	2605	PSU	N1-C2-N3	6.33	121.84	115.17
1	XA	516	PSU	N1-C2-N3	6.30	121.81	115.17
35	YA	1915	5MU	C1'-N1-C2	6.27	128.84	117.59
35	YA	1917	PSU	N1-C2-N3	6.20	121.71	115.17
35	YA	1911	PSU	N1-C2-N3	6.13	121.64	115.17
1	QA	1207	2MG	C5-C4-N3	-6.11	118.66	128.39
1	XA	527	G7M	N9-C4-N3	6.11	138.16	125.95
35	RA	1917	PSU	N1-C2-N3	6.04	121.54	115.17
1	QA	966	M2G	C5-C4-N3	-5.95	118.92	128.39
1	XA	966	M2G	C5-C4-N3	-5.88	119.03	128.39
35	RA	2605	PSU	N1-C2-N3	5.87	121.36	115.17
35	RA	1915	5MU	N3-C2-N1	5.87	122.53	114.89
35	YA	2552	OMU	N3-C2-N1	5.80	122.44	114.89
1	QA	516	PSU	N1-C2-N3	5.79	121.28	115.17
1	QA	1519	MA6	C5-C4-N3	-5.78	118.75	126.72
35	RA	1939	5MU	C4-N3-C2	-5.73	119.82	127.34
1	XA	527	G7M	CN7-N7-C5	5.69	133.90	126.80
1	QA	527	G7M	C5-C4-N3	-5.61	117.55	128.15
35	RA	1939	5MU	N3-C2-N1	5.56	122.13	114.89
35	YA	1939	5MU	C4-N3-C2	-5.53	120.09	127.34
1	XA	527	G7M	C5-C4-N3	-5.46	117.84	128.15
1	QA	1518	MA6	C5-C4-N3	-5.36	119.34	126.72
1	QA	1518	MA6	C4-C5-N7	-5.35	104.47	110.58
1	XA	1519	MA6	C5-C4-N3	-5.32	119.39	126.72
1	XA	1518	MA6	C4-C5-N7	-5.32	104.50	110.58
35	RA	2552	OMU	N3-C2-N1	5.31	121.81	114.89
35	YA	1915	5MU	N3-C2-N1	5.31	121.80	114.89
35	YA	1915	5MU	C1'-N1-C6	-5.29	112.44	121.15
35	YA	1939	5MU	N3-C2-N1	5.15	121.59	114.89
35	YA	2251	OMG	N9-C4-N3	5.13	136.20	125.95
1	XA	1518	MA6	C5-C4-N3	-5.12	119.66	126.72
35	YA	2251	OMG	C2-N3-C4	5.10	121.09	112.30
35	RA	2251	OMG	C2-N3-C4	5.00	120.91	112.30
35	RA	1915	5MU	C1'-N1-C6	-4.83	113.20	121.15
35	YA	1915	5MU	C4-N3-C2	-4.82	121.02	127.34
35	RA	2251	OMG	N9-C4-N3	4.80	135.56	125.95
35	RA	1939	5MU	C5-C4-N3	4.77	119.47	115.32
1	QA	527	G7M	C2-N3-C4	4.74	120.46	112.30
35	RA	1915	5MU	C4-N3-C2	-4.69	121.19	127.34
1	XA	1518	MA6	C2-N1-C6	4.69	123.29	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1939	5MU	C5-C4-N3	4.61	119.33	115.32
1	QA	1518	MA6	C2-N1-C6	4.60	123.06	111.83
35	RA	1915	5MU	O2-C2-N3	-4.59	113.03	121.49
35	YA	2552	OMU	C4-N3-C2	-4.59	120.92	126.61
1	XA	1207	2MG	N9-C4-N3	4.55	135.05	125.95
1	QA	1519	MA6	C2-N1-C6	4.53	122.89	111.83
1	XA	1519	MA6	C2-N1-C6	4.50	122.83	111.83
1	QA	966	M2G	N9-C4-N3	4.50	134.94	125.95
1	QA	527	G7M	CN7-N7-C5	4.47	132.37	126.80
1	XA	527	G7M	C2-N3-C4	4.47	119.99	112.30
1	XA	1518	MA6	C9-N6-C6	-4.44	109.22	120.52
35	YA	1939	5MU	O4-C4-C5	-4.44	119.84	124.92
1	XA	966	M2G	N9-C4-N3	4.43	134.81	125.95
1	QA	1519	MA6	C4-C5-N7	-4.40	105.55	110.58
35	RA	2552	OMU	C4-N3-C2	-4.38	121.17	126.61
1	QA	1518	MA6	C9-N6-C6	-4.33	109.51	120.52
35	YA	1915	5MU	C5-C4-N3	4.32	119.08	115.32
35	RA	1911	PSU	C4-N3-C2	-4.28	120.47	126.37
1	XA	966	M2G	C2-N3-C4	4.28	120.43	112.51
35	RA	1939	5MU	C5-C6-N1	-4.26	118.69	123.31
35	YA	1939	5MU	C5-C6-N1	-4.24	118.71	123.31
1	QA	1207	2MG	N9-C4-N3	4.20	134.35	125.95
35	YA	2605	PSU	C4-N3-C2	-4.16	120.64	126.37
1	QA	527	G7M	C8-N9-C4	4.15	117.37	107.09
1	QA	1519	MA6	N3-C4-N9	4.14	134.21	127.17
1	XA	1519	MA6	C4-C5-N7	-4.13	105.86	110.58
1	XA	527	G7M	C8-N9-C4	4.11	117.26	107.09
35	RA	1939	5MU	O4-C4-C5	-4.11	120.22	124.92
1	QA	1407	5MC	O2-C2-N3	-4.10	115.86	122.33
35	RA	2605	PSU	C4-N3-C2	-4.10	120.72	126.37
1	XA	1519	MA6	C10-N6-C6	-4.09	110.11	120.52
35	YA	1911	PSU	C4-N3-C2	-4.07	120.77	126.37
1	QA	1519	MA6	C10-N6-C6	-4.06	110.19	120.52
1	QA	966	M2G	C2-N3-C4	4.06	120.01	112.51
35	YA	1917	PSU	C4-N3-C2	-4.05	120.79	126.37
1	XA	1519	MA6	C9-N6-C6	-4.03	110.26	120.52
1	XA	516	PSU	C4-N3-C2	-4.01	120.85	126.37
35	RA	1962	5MC	C5-C6-N1	-3.98	118.98	123.31
35	YA	1962	5MC	C5-C6-N1	-3.91	119.06	123.31
1	XA	1400	5MC	C5-C6-N1	-3.88	119.10	123.31
35	YA	2605	PSU	O2-C2-N1	-3.87	118.80	122.79
35	RA	1917	PSU	C4-N3-C2	-3.87	121.05	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1911	PSU	O2-C2-N1	-3.84	118.83	122.79
35	YA	1915	5MU	O4-C4-C5	-3.83	120.53	124.92
35	RA	1915	5MU	C5-C4-N3	3.82	118.65	115.32
35	YA	1915	5MU	O2-C2-N3	-3.81	114.45	121.49
35	YA	1917	PSU	O2-C2-N1	-3.80	118.87	122.79
1	XA	516	PSU	O2-C2-N1	-3.78	118.89	122.79
1	QA	1400	5MC	C5-C6-N1	-3.76	119.23	123.31
1	XA	1518	MA6	C2-N3-C4	3.75	120.98	111.83
35	YA	1911	PSU	O2-C2-N1	-3.75	118.92	122.79
1	QA	516	PSU	O2-C2-N1	-3.72	118.95	122.79
35	RA	2605	PSU	O2-C2-N1	-3.71	118.96	122.79
1	QA	1519	MA6	C2-N3-C4	3.69	120.83	111.83
1	XA	1519	MA6	C2-N3-C4	3.68	120.82	111.83
1	XA	1519	MA6	N3-C4-N9	3.68	133.43	127.17
35	RA	2503	2MA	C4-C5-N7	-3.66	106.40	110.58
1	XA	1518	MA6	C10-N6-C9	-3.63	104.53	116.18
1	XA	527	G7M	C1'-N9-C8	-3.60	114.59	126.74
1	QA	1518	MA6	C2-N3-C4	3.59	120.60	111.83
1	XA	1519	MA6	C10-N6-C9	-3.59	104.66	116.18
1	XA	1518	MA6	N1-C2-N3	-3.56	123.19	128.58
35	RA	1942	5MC	C5-C6-N1	-3.56	119.44	123.31
1	XA	1519	MA6	N1-C2-N3	-3.56	123.19	128.58
1	QA	516	PSU	C4-N3-C2	-3.56	121.47	126.37
1	QA	527	G7M	C1'-N9-C8	-3.54	114.79	126.74
35	RA	1915	5MU	C6-N1-C2	-3.52	117.79	121.30
1	QA	1407	5MC	C5-C4-N3	-3.48	118.19	121.75
35	YA	1939	5MU	O2-C2-N1	-3.47	118.28	122.80
1	QA	1519	MA6	C10-N6-C9	-3.44	105.13	116.18
35	RA	1939	5MU	O2-C2-N1	-3.44	118.33	122.80
1	QA	1498	UR3	C5-C4-N3	3.41	119.53	115.04
35	RA	1917	PSU	O2-C2-N1	-3.41	119.27	122.79
1	QA	1518	MA6	C10-N6-C9	-3.38	105.33	116.18
35	YA	2503	2MA	C4-C5-N7	-3.38	106.72	110.58
1	QA	1519	MA6	N1-C2-N3	-3.36	123.50	128.58
1	QA	967	5MC	C5-C6-N1	-3.36	119.67	123.31
1	QA	1207	2MG	C6-C5-N7	3.35	136.38	130.29
1	XA	1518	MA6	C6-C5-N7	3.34	138.77	133.43
35	RA	1915	5MU	O4-C4-C5	-3.30	121.14	124.92
1	QA	1518	MA6	C5-N7-C8	3.29	108.62	103.45
1	XA	1498	UR3	C5-C4-N3	3.28	119.36	115.04
1	XA	1404	5MC	C5-C6-N1	-3.28	119.75	123.31
1	XA	1207	2MG	C6-C5-N7	3.25	136.21	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	1518	MA6	C5-N7-C8	3.25	108.56	103.45
1	QA	1518	MA6	N3-C4-N9	3.24	132.67	127.17
12	QL	92	0TD	OD1-CG-CB	-3.23	115.68	122.44
35	YA	2552	OMU	O2-C2-N1	-3.23	118.60	122.80
1	XA	1518	MA6	N3-C4-N9	3.22	132.64	127.17
1	XA	1407	5MC	O2-C2-N3	-3.22	117.26	122.33
35	RA	2552	OMU	O2-C2-N1	-3.19	118.65	122.80
1	QA	1518	MA6	C6-C5-N7	3.19	138.52	133.43
1	QA	1518	MA6	N1-C2-N3	-3.13	123.84	128.58
1	XA	967	5MC	C5-C6-N1	-3.13	119.92	123.31
1	QA	1404	5MC	C5-C6-N1	-3.12	119.93	123.31
1	XA	966	M2G	C6-C5-N7	3.11	135.96	130.29
1	QA	1519	MA6	C9-N6-C6	-3.11	112.61	120.52
1	XA	1407	5MC	C5-C4-N3	-3.10	118.58	121.75
12	QL	92	0TD	OD2-CG-CB	3.09	119.83	113.15
35	YA	1942	5MC	C5-C6-N1	-2.99	120.07	123.31
35	YA	2503	2MA	N6-C6-N1	2.98	121.05	117.03
12	XL	92	0TD	O-C-CA	-2.98	117.11	124.77
1	QA	1519	MA6	C5-N7-C8	2.94	108.08	103.45
1	XA	1519	MA6	N1-C6-N6	2.94	120.44	116.86
35	YA	1942	5MC	C5-C4-N3	-2.93	118.75	121.75
12	QL	92	0TD	O-C-CA	-2.92	117.26	124.77
1	QA	966	M2G	C6-C5-N7	2.88	135.53	130.29
35	RA	2251	OMG	C6-C5-N7	2.87	135.52	130.29
1	QA	1402	4OC	O2-C2-N3	-2.87	117.81	122.33
1	QA	1207	2MG	C4-C5-N7	-2.87	106.13	110.67
1	QA	1207	2MG	N2-C2-N3	-2.85	116.88	120.51
1	XA	1404	5MC	C5-C4-N3	-2.84	118.85	121.75
1	XA	1207	2MG	C4-C5-N7	-2.81	106.21	110.67
35	RA	2552	OMU	C5-C4-N3	2.79	118.71	114.80
1	QA	1207	2MG	N1-C2-N2	2.78	119.40	116.56
35	RA	2552	OMU	O4-C4-C5	-2.74	120.44	125.16
35	RA	2503	2MA	C5-N7-C8	2.72	107.72	103.45
35	YA	1920	OMC	O2-C2-N3	-2.71	118.06	122.33
1	XA	1400	5MC	C5-C4-N3	-2.70	118.99	121.75
35	RA	1920	OMC	O2-C2-N3	-2.67	118.13	122.33
1	QA	967	5MC	C5-C4-N3	-2.63	119.06	121.75
35	YA	1942	5MC	O2-C2-N3	-2.62	118.20	122.33
35	YA	1915	5MU	C6-N1-C2	-2.60	118.71	121.30
35	YA	2552	OMU	C5-C4-N3	2.56	118.39	114.80
35	YA	2251	OMG	C6-C5-N7	2.54	134.92	130.29
1	XA	1519	MA6	C5-N7-C8	2.54	107.45	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	2552	OMU	O4-C4-C5	-2.53	120.79	125.16
35	RA	2503	2MA	C4-N9-C8	2.53	108.39	105.74
35	YA	2251	OMG	C4-C5-N7	-2.51	106.69	110.67
1	XA	1402	4OC	O2-C2-N3	-2.50	118.38	122.33
1	QA	966	M2G	C4-C5-N7	-2.47	106.75	110.67
1	QA	1207	2MG	C2-N1-C6	-2.47	121.56	124.55
1	QA	1404	5MC	C5-C4-N3	-2.46	119.23	121.75
1	QA	1519	MA6	N1-C6-N6	2.46	119.86	116.86
1	XA	967	5MC	C5-C4-N3	-2.46	119.24	121.75
1	XA	966	M2G	C4-C5-N7	-2.45	106.79	110.67
1	QA	527	G7M	O6-C6-C5	-2.44	122.56	128.01
35	RA	1942	5MC	C5-C4-N3	-2.44	119.25	121.75
1	XA	1519	MA6	C6-C5-N7	2.43	137.31	133.43
35	RA	2605	PSU	C6-C5-C4	-2.43	116.53	118.17
35	YA	2503	2MA	C4-N9-C8	2.42	108.27	105.74
35	YA	1920	OMC	C1'-N1-C2	2.41	123.77	118.44
35	YA	1942	5MC	CM5-C5-C6	-2.40	119.60	122.85
35	RA	1920	OMC	C1'-N1-C2	2.40	123.75	118.44
35	YA	2503	2MA	C2-N1-C6	2.40	121.79	118.10
1	QA	1207	2MG	CM2-N2-C2	-2.39	118.51	123.65
35	YA	2503	2MA	C5-N7-C8	2.39	107.20	103.45
1	XA	1518	MA6	C4-N9-C8	2.38	108.24	105.74
1	XA	1519	MA6	C4-N9-C8	2.36	108.21	105.74
35	RA	2251	OMG	C4-C5-N7	-2.34	106.95	110.67
1	XA	527	G7M	O6-C6-C5	-2.34	122.80	128.01
1	XA	1207	2MG	C2-N1-C6	-2.33	121.73	124.55
35	YA	1920	OMC	N4-C4-N3	2.33	122.08	117.91
1	QA	1404	5MC	O2-C2-N3	-2.33	118.65	122.33
1	QA	527	G7M	C5-C6-N1	2.33	116.65	111.84
1	XA	1207	2MG	N1-C2-N2	2.33	118.94	116.56
35	YA	1911	PSU	C6-C5-C4	-2.28	116.63	118.17
35	RA	1920	OMC	N4-C4-N3	2.28	121.99	117.91
1	QA	1400	5MC	C5-C4-N3	-2.28	119.42	121.75
35	RA	1942	5MC	O2-C2-N3	-2.27	118.75	122.33
35	YA	1915	5MU	C5-C6-N1	-2.25	120.86	123.31
1	XA	1207	2MG	CM2-N2-C2	-2.23	118.86	123.65
1	QA	1519	MA6	C4-N9-C8	2.21	108.06	105.74
35	RA	2251	OMG	O6-C6-C5	-2.21	120.71	126.53
35	RA	1917	PSU	C6-C5-C4	-2.20	116.69	118.17
35	YA	1962	5MC	C5-C4-N3	-2.20	119.50	121.75
1	XA	1498	UR3	C1'-N1-C2	2.19	120.63	117.04
1	QA	1519	MA6	C6-C5-N7	2.19	136.93	133.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	967	5MC	C1'-N1-C6	-2.18	117.55	121.15
35	YA	2605	PSU	C6-C5-C4	-2.18	116.70	118.17
1	QA	1207	2MG	O6-C6-C5	-2.18	120.78	126.53
35	YA	2251	OMG	O6-C6-C5	-2.13	120.91	126.53
35	RA	2503	2MA	N6-C6-N1	2.11	119.88	117.03
35	RA	2503	2MA	N9-C8-N7	-2.11	110.94	113.94
1	QA	1402	4OC	C6-C5-C4	2.10	119.53	117.00
1	XA	1207	2MG	N2-C2-N3	-2.10	117.84	120.51
1	XA	516	PSU	O4'-C1'-C2'	2.09	108.04	105.15
1	XA	1518	MA6	N9-C8-N7	-2.09	110.98	113.94
35	RA	1962	5MC	C5-C4-N3	-2.08	119.62	121.75
35	RA	2503	2MA	C2-N1-C6	2.06	121.27	118.10
1	QA	967	5MC	CM5-C5-C6	-2.05	120.08	122.85
35	YA	2503	2MA	C6-C5-N7	2.03	136.00	132.09
35	RA	1915	5MU	C5-C6-N1	-2.02	121.12	123.31
1	XA	1404	5MC	CM5-C5-C6	-2.02	120.12	122.85
1	XA	1207	2MG	O6-C6-C5	-2.02	121.21	126.53
35	RA	1911	PSU	C5-C6-N1	-2.01	119.35	122.14
1	XA	516	PSU	C6-C5-C4	-2.01	116.82	118.17

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	QA	1518	MA6	C5-C6-N6-C9
1	XA	1518	MA6	C5-C6-N6-C9
1	QA	1519	MA6	O4'-C4'-C5'-O5'
1	XA	1519	MA6	O4'-C4'-C5'-O5'
35	RA	1915	5MU	O4'-C1'-N1-C2
35	RA	1915	5MU	O4'-C1'-N1-C6
35	YA	1915	5MU	O4'-C1'-N1-C2
35	YA	1915	5MU	O4'-C1'-N1-C6
1	QA	1402	4OC	O4'-C4'-C5'-O5'
1	XA	1400	5MC	O4'-C4'-C5'-O5'
1	XA	1402	4OC	O4'-C4'-C5'-O5'
1	QA	1518	MA6	N1-C6-N6-C9
1	XA	1518	MA6	N1-C6-N6-C9
1	QA	1519	MA6	C3'-C4'-C5'-O5'
1	XA	1519	MA6	C3'-C4'-C5'-O5'
1	XA	527	G7M	C3'-C4'-C5'-O5'
1	XA	1519	MA6	C5-C6-N6-C9
1	QA	1400	5MC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	XA	527	G7M	O4'-C4'-C5'-O5'
1	XA	1400	5MC	C3'-C4'-C5'-O5'
1	QA	1402	4OC	C3'-C4'-C5'-O5'
1	QA	1519	MA6	C5-C6-N6-C9
1	QA	1404	5MC	C3'-C4'-C5'-O5'
12	QL	92	0TD	CG-CB-SB-CSB
12	XL	92	0TD	CG-CB-SB-CSB
12	XL	92	0TD	SB-CB-CG-OD1
35	RA	2552	OMU	O4'-C4'-C5'-O5'
1	QA	1518	MA6	C5-C6-N6-C10
1	XA	1518	MA6	C5-C6-N6-C10
1	QA	1400	5MC	C3'-C4'-C5'-O5'
1	QA	1404	5MC	O4'-C4'-C5'-O5'
1	XA	1519	MA6	N1-C6-N6-C9
1	XA	1402	4OC	C3'-C4'-C5'-O5'
1	QA	527	G7M	C4'-C5'-O5'-P
1	XA	527	G7M	C4'-C5'-O5'-P
12	XL	92	0TD	SB-CB-CG-OD2
1	QA	527	G7M	C3'-C4'-C5'-O5'
35	YA	1962	5MC	O4'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	QA	1519	MA6	1	0
1	XA	1518	MA6	1	0
1	QA	1518	MA6	1	0
12	QL	92	0TD	1	0
35	YA	2503	2MA	2	0
35	RA	2503	2MA	2	0
1	XA	1498	UR3	1	0
35	RA	1962	5MC	1	0
35	RA	1939	5MU	1	0
1	XA	967	5MC	1	0
35	YA	1962	5MC	1	0
1	XA	966	M2G	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2027 ligands modelled in this entry, 2023 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	SF4	XD	301	-	0,12,12	-	-	-		
58	SF4	QD	302	-	0,12,12	-	-	-		
57	PAR	XA	1794	-	44,45,45	0.65	0	63,67,67	1.22	7 (11%)
57	PAR	QA	1821	-	44,45,45	0.68	0	63,67,67	1.47	10 (15%)

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	XD	301	-	-	-	0/6/5/5
58	SF4	QD	302	-	-	-	0/6/5/5
57	PAR	XA	1794	-	-	3/18/94/94	0/4/4/4
57	PAR	QA	1821	-	-	4/18/94/94	0/4/4/4

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	QA	1821	PAR	C44-C34-C24	5.00	119.30	110.99
57	XA	1794	PAR	C13-O52-C52	-3.49	109.70	117.98
57	QA	1821	PAR	C13-O52-C52	-3.48	109.73	117.98
57	XA	1794	PAR	C14-O33-C33	-3.03	110.79	117.98
57	XA	1794	PAR	C11-O51-C51	2.74	119.07	113.72
57	QA	1821	PAR	O62-C62-C12	-2.58	105.07	109.90
57	QA	1821	PAR	C14-C24-N24	-2.54	105.63	110.20
57	QA	1821	PAR	O11-C42-C32	-2.44	103.35	109.18
57	QA	1821	PAR	C62-C12-N12	-2.41	106.19	110.94
57	QA	1821	PAR	O34-C34-C44	-2.38	104.77	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	QA	1821	PAR	C14-O33-C33	-2.36	112.38	117.98
57	QA	1821	PAR	O52-C13-O43	-2.31	109.00	111.37
57	XA	1794	PAR	O11-C42-C32	-2.21	103.90	109.18
57	XA	1794	PAR	O33-C33-C23	-2.18	104.30	111.32
57	QA	1821	PAR	O54-C14-C24	-2.18	105.26	110.08
57	XA	1794	PAR	O33-C14-O54	-2.12	105.11	110.69
57	XA	1794	PAR	O11-C11-C21	-2.12	104.61	108.08

There are no chirality outliers.

All (7) torsion outliers are listed below:

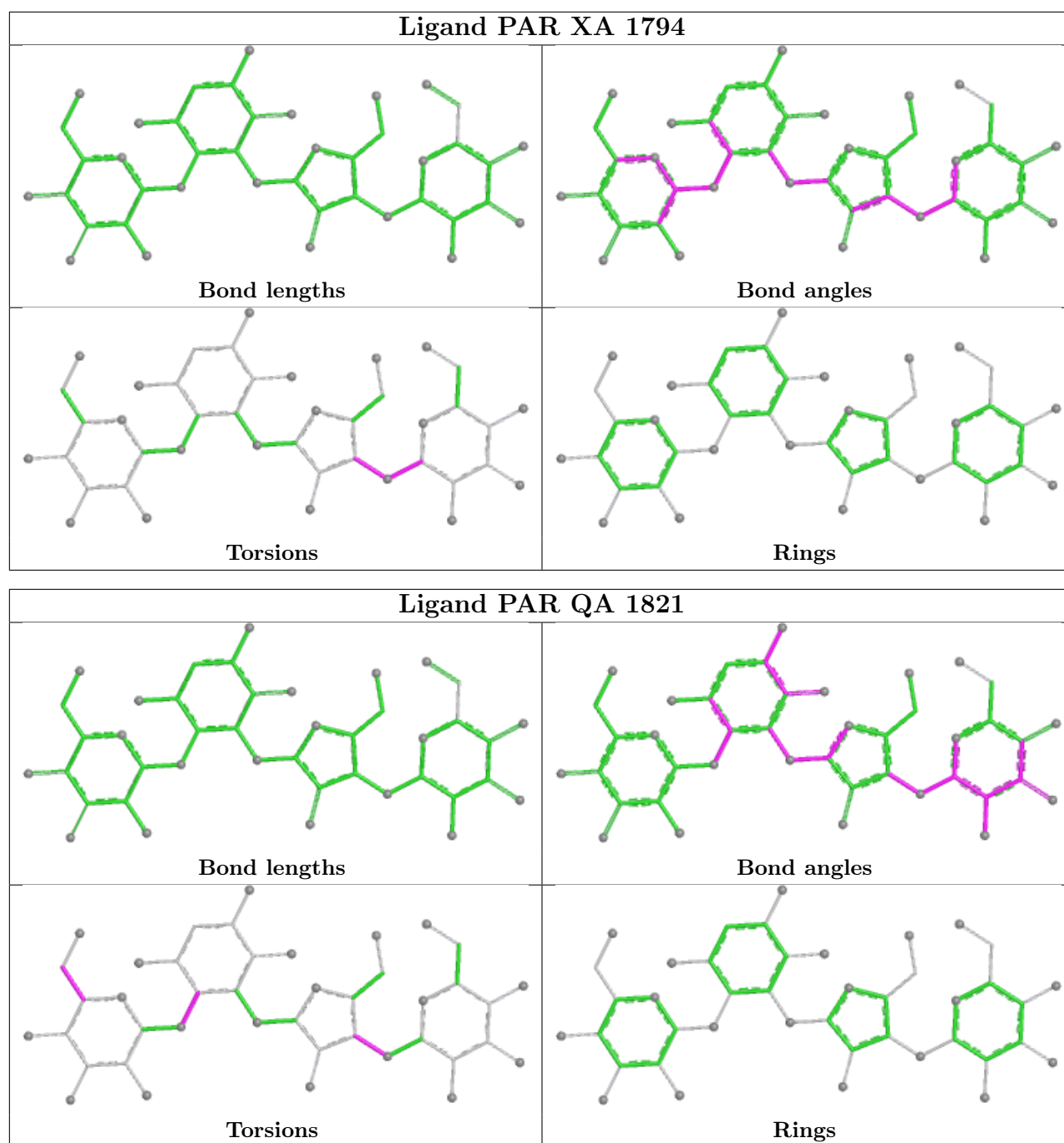
Mol	Chain	Res	Type	Atoms
57	QA	1821	PAR	O51-C51-C61-O61
57	QA	1821	PAR	C41-C51-C61-O61
57	XA	1794	PAR	O54-C14-O33-C33
57	QA	1821	PAR	C23-C33-O33-C14
57	QA	1821	PAR	C52-C42-O11-C11
57	XA	1794	PAR	C23-C33-O33-C14
57	XA	1794	PAR	C43-C33-O33-C14

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	XD	301	SF4	1	0
57	XA	1794	PAR	2	0
57	QA	1821	PAR	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1488/1522 (97%)	0.05	19 (1%) 75 56	59, 101, 188, 338	0
1	XA	1492/1522 (98%)	-0.12	11 (0%) 84 68	47, 90, 177, 328	0
2	QB	231/256 (90%)	0.54	12 (5%) 33 17	76, 130, 166, 190	0
2	XB	231/256 (90%)	0.45	8 (3%) 47 27	65, 117, 160, 194	0
3	QC	206/239 (86%)	0.42	11 (5%) 32 17	100, 135, 171, 196	0
3	XC	206/239 (86%)	0.33	11 (5%) 32 17	51, 105, 146, 163	0
4	QD	208/209 (99%)	0.59	14 (6%) 24 13	58, 102, 144, 164	0
4	XD	208/209 (99%)	0.70	19 (9%) 15 8	63, 99, 137, 171	0
5	QE	148/162 (91%)	0.38	4 (2%) 56 35	70, 104, 141, 172	0
5	XE	148/162 (91%)	0.30	2 (1%) 73 53	56, 91, 122, 138	0
6	QF	100/101 (99%)	0.12	0 100 100	63, 92, 129, 145	0
6	XF	100/101 (99%)	0.08	1 (1%) 79 61	64, 96, 127, 158	0
7	QG	155/156 (99%)	0.46	7 (4%) 38 20	88, 124, 155, 209	0
7	XG	155/156 (99%)	0.48	6 (3%) 43 24	75, 107, 147, 184	0
8	QH	137/138 (99%)	0.53	6 (4%) 39 21	67, 104, 135, 156	0
8	XH	137/138 (99%)	0.41	6 (4%) 39 21	59, 92, 127, 154	0
9	QI	127/128 (99%)	1.16	26 (20%) 2 1	94, 141, 174, 200	0
9	XI	126/128 (98%)	0.78	12 (9%) 14 7	70, 113, 147, 186	0
10	QJ	97/105 (92%)	1.00	11 (11%) 10 5	94, 140, 188, 200	0
10	XJ	96/105 (91%)	1.06	13 (13%) 7 4	87, 123, 160, 175	0
11	QK	114/129 (88%)	0.32	5 (4%) 39 21	70, 100, 132, 154	0
11	XK	114/129 (88%)	0.50	8 (7%) 22 12	58, 96, 141, 167	0
12	QL	121/132 (91%)	0.81	13 (10%) 11 6	55, 92, 120, 149	0
12	XL	121/132 (91%)	0.75	16 (13%) 7 4	52, 75, 112, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	QM	116/126 (92%)	0.72	9 (7%)	19 10	88, 127, 162, 177	0
13	XM	114/126 (90%)	0.65	6 (5%)	32 17	75, 111, 156, 195	0
14	QN	60/61 (98%)	1.45	14 (23%)	2 1	81, 135, 179, 194	0
14	XN	60/61 (98%)	1.01	10 (16%)	4 2	76, 101, 135, 139	0
15	QO	88/89 (98%)	0.49	1 (1%)	78 59	64, 94, 137, 167	0
15	XO	88/89 (98%)	0.65	9 (10%)	12 6	58, 88, 136, 145	0
16	QP	82/88 (93%)	0.89	6 (7%)	21 11	53, 94, 123, 156	0
16	XP	82/88 (93%)	0.86	7 (8%)	16 9	65, 94, 138, 174	0
17	QQ	99/105 (94%)	0.84	8 (8%)	18 10	71, 99, 140, 152	0
17	XQ	99/105 (94%)	0.86	10 (10%)	12 6	63, 93, 128, 153	0
18	QR	68/88 (77%)	0.25	0	100 100	75, 97, 130, 163	0
18	XR	68/88 (77%)	0.48	3 (4%)	39 21	62, 93, 139, 161	0
19	QS	83/93 (89%)	0.86	10 (12%)	9 5	101, 136, 184, 192	0
19	XS	83/93 (89%)	0.74	10 (12%)	9 5	75, 118, 155, 172	0
20	QT	96/106 (90%)	1.02	10 (10%)	11 6	65, 95, 144, 161	0
20	XT	98/106 (92%)	0.82	9 (9%)	14 8	75, 97, 152, 165	0
21	QU	23/27 (85%)	2.40	13 (56%)	0 0	91, 122, 147, 158	0
21	XU	23/27 (85%)	1.33	4 (17%)	4 2	90, 108, 124, 144	0
22	QV	77/77 (100%)	0.10	1 (1%)	75 56	86, 122, 172, 240	0
22	XV	77/77 (100%)	0.05	3 (3%)	43 24	58, 105, 164, 210	0
23	QX	18/19 (94%)	1.03	4 (22%)	2 1	71, 163, 230, 231	0
23	XX	18/19 (94%)	1.00	6 (33%)	1 0	64, 153, 241, 253	0
24	QY	76/76 (100%)	0.80	9 (11%)	9 5	105, 192, 252, 287	0
24	XY	76/76 (100%)	0.89	10 (13%)	7 4	85, 162, 243, 269	0
25	R0	77/85 (90%)	0.58	4 (5%)	33 17	54, 81, 100, 143	0
25	Y0	77/85 (90%)	0.17	0	100 100	21, 55, 85, 93	0
26	R1	97/98 (98%)	0.57	2 (2%)	63 42	52, 76, 116, 133	0
26	Y1	97/98 (98%)	0.56	7 (7%)	21 11	30, 63, 106, 133	0
27	R2	70/72 (97%)	0.42	2 (2%)	53 32	61, 93, 137, 159	0
27	Y2	70/72 (97%)	0.36	4 (5%)	29 16	38, 69, 100, 154	0
28	R3	59/60 (98%)	0.37	3 (5%)	33 18	50, 81, 129, 176	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
28	Y3	59/60 (98%)	0.25	4 (6%)	23 12	28, 51, 104, 137	0
29	R4	69/71 (97%)	0.57	1 (1%)	73 53	104, 149, 191, 208	0
29	Y4	69/71 (97%)	0.60	9 (13%)	7 4	85, 126, 184, 223	0
30	R5	59/60 (98%)	0.14	0	100 100	39, 73, 97, 152	0
30	Y5	59/60 (98%)	0.13	1 (1%)	69 48	32, 57, 102, 184	0
31	R6	53/54 (98%)	0.27	1 (1%)	66 45	60, 82, 120, 148	0
31	Y6	53/54 (98%)	-0.05	0	100 100	45, 65, 89, 92	0
32	R7	48/49 (97%)	0.43	4 (8%)	17 9	32, 58, 82, 117	0
32	Y7	48/49 (97%)	0.30	3 (6%)	26 14	34, 49, 74, 131	0
33	R8	64/65 (98%)	0.81	6 (9%)	14 8	46, 70, 96, 129	0
33	Y8	64/65 (98%)	0.48	6 (9%)	14 8	37, 51, 86, 111	0
34	R9	37/37 (100%)	1.11	5 (13%)	7 4	68, 96, 127, 185	0
34	Y9	37/37 (100%)	0.58	1 (2%)	56 35	46, 60, 78, 101	0
35	RA	2856/2915 (97%)	-0.01	64 (2%)	62 41	45, 74, 216, 308	0
35	YA	2856/2915 (97%)	-0.32	55 (1%)	66 45	31, 53, 205, 329	0
36	RB	120/122 (98%)	-0.08	1 (0%)	82 65	79, 108, 141, 171	0
36	YB	120/122 (98%)	-0.25	1 (0%)	82 65	54, 75, 101, 137	0
37	RD	275/276 (99%)	0.49	14 (5%)	33 18	40, 64, 104, 121	0
37	YD	275/276 (99%)	0.23	6 (2%)	62 41	33, 55, 86, 155	0
38	RE	204/206 (99%)	0.40	9 (4%)	39 21	46, 76, 113, 157	0
38	YE	204/206 (99%)	0.24	6 (2%)	53 32	35, 58, 96, 128	0
39	RF	202/210 (96%)	0.29	4 (1%)	65 44	39, 81, 129, 184	0
39	YF	202/210 (96%)	0.12	3 (1%)	72 52	27, 58, 111, 141	0
40	RG	181/182 (99%)	0.48	7 (3%)	43 24	84, 121, 157, 203	0
40	YG	181/182 (99%)	0.38	4 (2%)	62 41	63, 91, 139, 182	0
41	RH	174/180 (96%)	0.54	3 (1%)	69 48	80, 124, 159, 185	0
41	YH	173/180 (96%)	0.18	4 (2%)	61 39	38, 72, 108, 145	0
42	RI	147/148 (99%)	0.31	3 (2%)	65 44	57, 106, 145, 165	0
42	YI	146/148 (98%)	0.16	3 (2%)	63 42	55, 96, 141, 167	0
43	RN	140/140 (100%)	0.45	6 (4%)	40 22	48, 83, 128, 153	0
43	YN	140/140 (100%)	0.23	3 (2%)	63 42	35, 59, 97, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RO	122/122 (100%)	0.31	3 (2%) 58 37	43, 76, 104, 123	0
44	YO	122/122 (100%)	0.21	2 (1%) 70 49	27, 57, 93, 108	0
45	RP	149/150 (99%)	0.59	8 (5%) 31 17	38, 90, 138, 163	0
45	YP	149/150 (99%)	0.45	8 (5%) 31 17	33, 65, 104, 133	0
46	RQ	141/141 (100%)	0.76	15 (10%) 11 6	57, 89, 128, 180	0
46	YQ	141/141 (100%)	0.42	4 (2%) 55 34	31, 60, 94, 157	0
47	RR	118/118 (100%)	0.54	5 (4%) 40 22	45, 69, 103, 116	0
47	YR	118/118 (100%)	0.35	1 (0%) 82 65	37, 53, 89, 129	0
48	RS	110/112 (98%)	0.56	5 (4%) 38 20	61, 98, 132, 151	0
48	YS	110/112 (98%)	0.26	4 (3%) 46 26	40, 72, 106, 130	0
49	RT	131/146 (89%)	0.29	3 (2%) 61 39	49, 78, 130, 166	0
49	YT	131/146 (89%)	0.25	4 (3%) 51 30	42, 70, 116, 148	0
50	RU	116/118 (98%)	0.59	3 (2%) 57 36	44, 81, 123, 134	0
50	YU	116/118 (98%)	0.16	1 (0%) 81 63	29, 49, 79, 115	0
51	RV	101/101 (100%)	0.29	4 (3%) 42 23	55, 91, 130, 172	0
51	YV	101/101 (100%)	0.03	1 (0%) 79 61	37, 62, 101, 168	0
52	RW	112/113 (99%)	0.39	2 (1%) 67 47	36, 64, 105, 138	0
52	YW	112/113 (99%)	0.16	2 (1%) 67 47	32, 50, 89, 184	0
53	RX	95/96 (98%)	0.54	5 (5%) 32 17	42, 75, 116, 140	0
53	YX	95/96 (98%)	0.24	4 (4%) 40 22	28, 56, 104, 134	0
54	RY	107/110 (97%)	0.81	7 (6%) 25 13	59, 98, 129, 162	0
54	YY	107/110 (97%)	0.35	4 (3%) 45 25	41, 73, 109, 157	0
55	RZ	178/206 (86%)	0.86	18 (10%) 12 6	82, 136, 202, 263	0
55	YZ	177/206 (85%)	0.77	27 (15%) 5 3	53, 108, 209, 266	0
All	All	20859/21590 (96%)	0.23	812 (3%) 43 24	21, 84, 164, 338	0

All (812) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	RA	2602	A	8.1
20	QT	9	ASN	7.8
35	YA	1091	G	7.2
20	XT	6	PRO	6.6
9	QI	126	SER	6.0

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Mol	Chain	Res	Type	RSRZ
26	R1	2	SER	5.9
21	QU	15	ARG	5.9
9	QI	105	ASP	5.8
55	RZ	176	PRO	5.8
10	XJ	46	ARG	5.6
3	XC	158	GLY	5.5
54	YY	1	MET	5.5
9	QI	106	ALA	5.5
22	QV	1	C	5.5
38	YE	146	THR	5.3
22	XV	1	C	5.3
34	R9	28	GLU	5.2
21	QU	14	TRP	5.2
12	XL	21	LYS	5.2
26	Y1	2	SER	5.2
51	RV	73	SER	5.1
35	YA	1092	C	5.0
21	QU	6	ARG	5.0
45	RP	15	ARG	5.0
11	XK	117	ASN	4.9
4	QD	24	GLU	4.9
9	QI	102	LEU	4.9
1	XA	1397	C	4.9
55	YZ	120	ILE	4.8
54	RY	1	MET	4.8
35	YA	1075	C	4.8
10	QJ	47	PHE	4.8
12	QL	32	PHE	4.8
48	RS	32	LEU	4.7
35	YA	1090	U	4.7
35	RA	2155	G	4.7
9	XI	125	TYR	4.7
10	XJ	64	GLU	4.6
35	YA	1077	A	4.6
3	QC	160	ALA	4.6
7	QG	84	ASN	4.6
11	XK	126	ARG	4.5
47	YR	7	GLY	4.5
21	QU	2	GLY	4.4
16	QP	22	THR	4.3
16	QP	68	ASP	4.3
35	RA	2319	G	4.3

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Mol	Chain	Res	Type	RSRZ
20	QT	70	SER	4.3
55	YZ	177	PRO	4.3
55	YZ	166	SER	4.3
8	QH	99	GLU	4.3
55	RZ	115	GLY	4.2
10	QJ	76	ASN	4.2
35	YA	1067	A	4.2
35	YA	1093	G	4.2
32	R7	48	LYS	4.2
55	RZ	141	VAL	4.1
21	QU	5	ASP	4.1
35	RA	1171	G	4.1
12	QL	17	LYS	4.1
14	XN	2	ALA	4.1
46	RQ	22	LYS	4.1
12	XL	89	ARG	4.1
55	RZ	175	VAL	4.1
14	QN	35	ARG	4.0
17	QQ	24	GLU	4.0
7	XG	42	ILE	4.0
16	XP	28	ARG	4.0
35	YA	1078	U	4.0
17	XQ	24	GLU	4.0
21	QU	4	GLY	4.0
2	QB	101	MET	4.0
16	XP	68	ASP	4.0
35	RA	2062	A	4.0
55	RZ	113	ALA	3.9
1	QA	79	G	3.9
3	QC	157	ILE	3.9
10	XJ	73	ASP	3.8
55	RZ	117	LEU	3.8
12	QL	18	VAL	3.8
19	QS	9	VAL	3.8
37	RD	237	GLU	3.8
45	YP	70	GLN	3.8
9	XI	126	SER	3.8
1	XA	630	G	3.8
1	QA	1531	A	3.8
35	YA	1066	U	3.8
4	XD	2	GLY	3.7
45	RP	32	THR	3.7

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Mol	Chain	Res	Type	RSRZ
48	YS	3	ARG	3.7
1	QA	1030(C)	C	3.7
11	QK	117	ASN	3.7
4	XD	24	GLU	3.6
40	YG	35	GLU	3.6
29	Y4	63	TYR	3.6
46	RQ	10	ARG	3.6
24	XY	54	U	3.6
32	Y7	48	LYS	3.6
55	RZ	120	ILE	3.6
14	XN	14	PRO	3.6
12	QL	16	GLU	3.6
3	QC	158	GLY	3.6
4	XD	23	GLY	3.5
43	RN	68	GLU	3.5
4	QD	4	TYR	3.5
19	QS	84	GLY	3.5
55	YZ	172	ALA	3.5
54	RY	62	GLU	3.5
14	QN	3	ARG	3.5
12	XL	62	SER	3.5
46	YQ	113	GLN	3.5
1	QA	90	U	3.5
37	RD	217	ARG	3.5
14	QN	18	VAL	3.5
55	YZ	174	VAL	3.4
41	YH	4	ILE	3.4
33	Y8	65	GLU	3.4
4	QD	154	ASN	3.4
20	XT	18	GLN	3.4
38	RE	146	THR	3.4
20	XT	73	HIS	3.4
26	Y1	38	SER	3.4
13	QM	117	VAL	3.4
55	YZ	117	LEU	3.4
44	RO	1	MET	3.4
9	QI	64	THR	3.4
14	QN	7	ILE	3.4
11	XK	13	GLN	3.4
15	XO	37	ASN	3.4
35	RA	2804	C	3.4
55	RZ	116	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
35	RA	1046	A	3.3
33	R8	65	GLU	3.3
34	R9	37	GLY	3.3
35	RA	1091	G	3.3
35	RA	2182	G	3.3
20	QT	17	ARG	3.3
5	XE	81	GLU	3.3
4	XD	166	LYS	3.3
14	XN	22	THR	3.3
12	XL	19	ARG	3.3
24	XY	17	U	3.3
14	QN	16	PHE	3.3
51	YV	49	THR	3.3
54	RY	12	THR	3.3
11	QK	14	VAL	3.3
14	XN	18	VAL	3.3
46	RQ	112	GLU	3.3
14	QN	21	TYR	3.2
20	XT	74	LYS	3.2
37	RD	276	LYS	3.2
35	RA	1090	U	3.2
23	QX	12	A	3.2
24	QY	76	A	3.2
4	XD	120	LEU	3.2
14	QN	15	LYS	3.2
13	QM	9	ILE	3.2
55	RZ	98	MET	3.2
8	XH	136	GLU	3.2
9	QI	110	GLU	3.2
55	RZ	178	GLU	3.2
23	QX	23	A	3.2
46	RQ	104	PHE	3.2
31	R6	54	ILE	3.2
26	Y1	23	LYS	3.2
4	XD	73	ARG	3.2
42	RI	20	ASP	3.2
46	RQ	59	ARG	3.2
35	YA	1068	G	3.2
35	RA	2803	C	3.2
35	YA	1072	C	3.2
35	YA	1536	C	3.2
7	QG	4	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
19	XS	39	THR	3.2
1	XA	88	A	3.1
1	XA	1531	A	3.1
38	RE	121	ASN	3.1
48	YS	12	PHE	3.1
35	RA	1043	C	3.1
55	YZ	144	LEU	3.1
10	XJ	47	PHE	3.1
14	XN	16	PHE	3.1
55	YZ	176	PRO	3.1
11	XK	53	SER	3.1
12	XL	63	GLY	3.1
33	Y8	56	GLU	3.1
4	XD	3	ARG	3.1
24	XY	55	U	3.1
55	YZ	109	ALA	3.1
4	XD	134	ASP	3.1
9	QI	18	PHE	3.1
35	YA	34	C	3.1
17	XQ	37	LYS	3.1
3	QC	159	GLY	3.1
32	Y7	47	ARG	3.1
14	XN	15	LYS	3.1
26	Y1	27	GLU	3.1
23	XX	23	A	3.1
41	YH	175	LYS	3.1
46	RQ	1	MET	3.1
50	YU	117	GLN	3.0
13	QM	100	GLY	3.0
28	R3	55	ARG	3.0
24	QY	17	U	3.0
27	Y2	11	GLU	3.0
46	YQ	112	GLU	3.0
16	XP	29	ASP	3.0
29	Y4	67	TYR	3.0
10	QJ	62	HIS	3.0
55	YZ	81	ARG	3.0
35	RA	1092	C	3.0
35	YA	2803	C	3.0
55	RZ	114	GLY	3.0
11	XK	42	TRP	3.0
53	YX	1	MET	3.0

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Mol	Chain	Res	Type	RSRZ
8	QH	91	ARG	3.0
16	QP	21	VAL	3.0
9	XI	12	GLU	3.0
41	RH	155	SER	3.0
3	XC	162	GLN	3.0
35	RA	363(A)	G	3.0
35	RA	1042	G	3.0
4	QD	181	MET	3.0
35	YA	1046	A	3.0
35	YA	1095	A	3.0
55	YZ	173	ALA	3.0
24	QY	61	C	3.0
14	QN	38	GLY	3.0
27	Y2	70	GLN	3.0
16	QP	19	ILE	3.0
33	Y8	40	GLU	2.9
35	RA	2156	G	2.9
35	RA	2805	G	2.9
46	RQ	61	GLY	2.9
35	YA	1076	C	2.9
12	XL	85	ILE	2.9
15	XO	64	ARG	2.9
4	QD	98	GLU	2.9
9	QI	127	LYS	2.9
17	QQ	96	GLU	2.9
40	RG	46	ALA	2.9
11	QK	13	GLN	2.9
20	QT	14	LYS	2.9
21	QU	17	THR	2.9
9	XI	106	ALA	2.9
9	XI	36	TYR	2.9
26	Y1	36	GLY	2.9
37	RD	231	HIS	2.9
37	RD	268	ARG	2.9
43	RN	26	LEU	2.9
46	RQ	113	GLN	2.9
9	XI	105	ASP	2.9
21	QU	3	LYS	2.9
38	RE	17	ASP	2.9
43	RN	83	LYS	2.9
24	XY	15	G	2.9
35	RA	2140	C	2.9

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Mol	Chain	Res	Type	RSRZ
8	QH	84	ARG	2.9
52	RW	92	ARG	2.9
10	QJ	59	SER	2.9
16	XP	19	ILE	2.9
4	XD	76	ARG	2.9
10	QJ	63	PHE	2.9
12	QL	29	GLY	2.9
34	R9	22	ARG	2.9
12	XL	23	LYS	2.9
38	RE	203	LYS	2.9
26	R1	8	SER	2.8
35	RA	1053	C	2.8
12	XL	30	ALA	2.8
37	YD	276	LYS	2.8
9	QI	36	TYR	2.8
35	RA	1087	G	2.8
5	QE	81	GLU	2.8
20	XT	8	ARG	2.8
35	RA	2139	C	2.8
35	RA	2142	C	2.8
35	YA	277	C	2.8
39	RF	161	GLU	2.8
17	XQ	100	LYS	2.8
3	XC	2	GLY	2.8
54	RY	5	MET	2.8
9	QI	62	TYR	2.8
3	QC	174	PRO	2.8
14	QN	29	ARG	2.8
20	XT	7	LYS	2.8
44	RO	81	ASP	2.8
45	RP	76	LYS	2.8
1	QA	1364	U	2.8
9	QI	115	GLY	2.8
12	QL	64	TYR	2.8
35	RA	2151	G	2.8
35	YA	1071	G	2.8
35	YA	2178	C	2.8
35	YA	2805	G	2.8
13	QM	92	HIS	2.8
12	XL	104	VAL	2.8
29	Y4	66	SER	2.8
34	R9	16	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
37	RD	265	PRO	2.8
45	YP	42	SER	2.8
21	QU	8	THR	2.8
1	QA	1363(B)	A	2.8
9	QI	125	TYR	2.8
35	RA	1103	A	2.8
36	YB	1	U	2.8
14	QN	2	ALA	2.8
14	XN	12	ARG	2.8
9	QI	11	LYS	2.8
10	QJ	33	GLN	2.8
35	RA	34	C	2.8
55	YZ	113	ALA	2.8
15	XO	60	VAL	2.8
55	YZ	116	VAL	2.8
14	QN	13	THR	2.8
37	RD	188	GLU	2.8
12	XL	29	GLY	2.7
15	XO	89	GLY	2.7
17	QQ	91	ARG	2.7
47	RR	68	ARG	2.7
4	QD	166	LYS	2.7
1	QA	1447	A	2.7
19	QS	11	VAL	2.7
24	QY	54	U	2.7
3	QC	166	GLU	2.7
14	XN	7	ILE	2.7
19	XS	38	SER	2.7
48	RS	8	GLU	2.7
13	XM	6	GLY	2.7
19	XS	68	GLY	2.7
4	QD	134	ASP	2.7
27	R2	52	ASP	2.7
35	YA	2318	G	2.7
9	QI	119	ALA	2.7
9	QI	14	VAL	2.7
19	XS	9	VAL	2.7
4	QD	165	MET	2.7
47	RR	1	MET	2.7
2	QB	12	GLU	2.7
38	YE	71	GLY	2.7
53	RX	68	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
35	YA	2174	C	2.7
4	XD	188	LEU	2.7
33	R8	56	GLU	2.7
13	QM	102	ARG	2.7
21	XU	6	ARG	2.7
37	YD	267	SER	2.7
35	YA	1097	U	2.7
1	QA	532	A	2.7
35	YA	2602	A	2.7
20	QT	64	ASP	2.7
49	RT	131	ALA	2.7
2	XB	7	VAL	2.7
7	XG	38	LEU	2.7
17	XQ	35	VAL	2.7
19	QS	5	LEU	2.7
12	QL	95	GLY	2.7
12	XL	47	LYS	2.7
55	YZ	170	THR	2.7
1	QA	1202	G	2.7
35	RA	2894	G	2.7
35	YA	2807	G	2.7
35	YA	1101	U	2.7
37	RD	84	TYR	2.7
38	RE	25	VAL	2.7
35	RA	2117	A	2.6
55	RZ	146	ILE	2.6
55	YZ	118	GLN	2.6
33	Y8	15	LYS	2.6
38	RE	145	LYS	2.6
35	RA	1076	C	2.6
9	XI	102	LEU	2.6
10	QJ	20	ALA	2.6
2	QB	70	PHE	2.6
14	QN	12	ARG	2.6
21	XU	15	ARG	2.6
24	QY	15	G	2.6
35	RA	2100	G	2.6
35	RA	2154	G	2.6
39	RF	78	ILE	2.6
28	R3	60	GLU	2.6
12	XL	120	TYR	2.6
40	RG	39	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
43	RN	84	LYS	2.6
21	XU	16	GLY	2.6
53	RX	61	GLY	2.6
17	XQ	5	VAL	2.6
41	YH	113	VAL	2.6
9	XI	71	SER	2.6
28	Y3	38	GLU	2.6
28	Y3	60	GLU	2.6
55	YZ	175	VAL	2.6
7	XG	5	ARG	2.6
10	XJ	100	THR	2.6
23	XX	11	U	2.6
27	Y2	69	ARG	2.6
37	YD	27	THR	2.6
32	R7	1	MET	2.6
35	RA	171	G	2.6
35	RA	2116	G	2.6
35	YA	1533	G	2.6
35	YA	2792	G	2.6
55	YZ	104	PHE	2.6
40	YG	2	PRO	2.6
35	YA	1098	A	2.6
4	QD	23	GLY	2.6
10	XJ	10	GLY	2.6
10	QJ	40	LEU	2.6
42	YI	116	LEU	2.6
4	XD	122	ARG	2.6
53	YX	60	ARG	2.6
54	RY	19	LYS	2.6
3	XC	192	THR	2.6
17	XQ	15	MET	2.5
20	QT	73	HIS	2.5
3	QC	13	GLY	2.5
19	XS	84	GLY	2.5
32	R7	47	ARG	2.5
9	QI	15	ALA	2.5
19	XS	73	GLU	2.5
1	XA	89	C	2.5
24	QY	16	C	2.5
35	RA	2755	C	2.5
12	QL	31	PRO	2.5
33	R8	45	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
13	XM	88	ARG	2.5
15	XO	65	ARG	2.5
33	Y8	46	ARG	2.5
37	RD	262	ARG	2.5
43	RN	74	ARG	2.5
14	QN	25	VAL	2.5
55	RZ	174	VAL	2.5
9	XI	110	GLU	2.5
17	XQ	27	PHE	2.5
24	XY	1	G	2.5
3	QC	12	LEU	2.5
1	QA	1397	C	2.5
4	XD	159	ARG	2.5
25	R0	74	ARG	2.5
45	RP	45	LEU	2.5
9	QI	100	GLY	2.5
19	QS	68	GLY	2.5
35	RA	1052	C	2.5
35	YA	1102	C	2.5
51	RV	48	GLY	2.5
45	YP	117	GLU	2.5
46	RQ	48	GLU	2.5
9	XI	64	THR	2.5
2	XB	175	ARG	2.5
10	XJ	62	HIS	2.5
51	RV	50	PRO	2.5
26	Y1	98	LEU	2.5
55	RZ	70	LEU	2.5
37	YD	238	GLY	2.5
7	XG	80	VAL	2.5
2	XB	200	ILE	2.5
10	XJ	76	ASN	2.5
52	RW	94	ASP	2.5
55	YZ	123	ASP	2.5
10	XJ	60	ARG	2.5
45	YP	16	ARG	2.5
55	YZ	108	PRO	2.5
48	YS	8	GLU	2.4
9	XI	9	ARG	2.4
12	XL	20	LYS	2.4
35	RA	273(K)	C	2.4
35	RA	2146	C	2.4

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Mol	Chain	Res	Type	RSRZ
55	YZ	157	LEU	2.4
1	XA	1532	U	2.4
3	XC	206	GLU	2.4
15	XO	41	GLU	2.4
43	YN	68	GLU	2.4
45	RP	74	GLU	2.4
8	QH	107	LEU	2.4
48	RS	16	ASN	2.4
35	YA	887	A	2.4
55	RZ	107	THR	2.4
7	XG	85	TYR	2.4
19	QS	41	VAL	2.4
24	QY	74	C	2.4
35	RA	1051	G	2.4
35	RA	1115	G	2.4
35	YA	1087	G	2.4
42	RI	1	MET	2.4
9	QI	128	ARG	2.4
14	XN	3	ARG	2.4
19	XS	78	ARG	2.4
28	Y3	55	ARG	2.4
42	YI	10	GLU	2.4
4	XD	27	TYR	2.4
9	QI	10	ARG	2.4
47	RR	2	ARG	2.4
2	XB	17	PHE	2.4
1	QA	723	U	2.4
4	XD	135	LEU	2.4
22	XV	47	U	2.4
35	RA	2150	U	2.4
46	YQ	41	TRP	2.4
4	XD	4	TYR	2.4
6	XF	55	ASP	2.4
28	R3	39	ASP	2.4
46	RQ	28	ALA	2.4
53	RX	63	LYS	2.4
19	XS	56	GLN	2.4
55	YZ	136	PHE	2.4
35	RA	1460	A	2.4
35	YA	1070	A	2.4
35	YA	9	U	2.4
35	RA	1100	C	2.3

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Mol	Chain	Res	Type	RSRZ
55	YZ	143	GLY	2.3
11	QK	123	LYS	2.3
4	QD	122	ARG	2.3
11	QK	126	ARG	2.3
15	XO	3	ILE	2.3
21	QU	20	LYS	2.3
21	QU	18	TYR	2.3
37	RD	54	ARG	2.3
14	QN	36	PHE	2.3
16	XP	34	GLU	2.3
40	YG	5	VAL	2.3
19	QS	38	SER	2.3
12	QL	13	LYS	2.3
23	QX	14	A	2.3
23	XX	12	A	2.3
23	XX	14	A	2.3
2	XB	172	ILE	2.3
3	XC	5	ILE	2.3
18	XR	82	THR	2.3
25	R0	19	LYS	2.3
33	R8	11	LYS	2.3
54	YY	80	GLY	2.3
49	YT	131	ALA	2.3
52	YW	111	HIS	2.3
13	XM	16	ASP	2.3
35	RA	2183	C	2.3
5	QE	20	GLN	2.3
7	QG	74	GLU	2.3
1	QA	1310	G	2.3
23	XX	9	G	2.3
35	YA	1074	G	2.3
40	RG	74	LYS	2.3
19	XS	2	PRO	2.3
37	RD	211	ARG	2.3
45	RP	21	ARG	2.3
48	RS	3	ARG	2.3
37	RD	224	ALA	2.3
7	QG	148	ASN	2.3
8	QH	112	LEU	2.3
20	XT	10	LEU	2.3
23	XX	13	A	2.3
29	Y4	59	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
10	QJ	58	ASP	2.3
34	R9	12	ASP	2.3
35	RA	273(B)	U	2.3
35	YA	1065	U	2.3
53	YX	38	GLU	2.3
13	XM	98	VAL	2.3
32	R7	46	VAL	2.3
37	RD	153	ALA	2.3
2	QB	187	LEU	2.3
13	XM	90	LEU	2.3
17	QQ	98	LEU	2.3
18	XR	78	LEU	2.3
23	QX	10	G	2.3
35	RA	11	G	2.3
35	RA	2807	G	2.3
4	XD	77	ASN	2.3
8	XH	4	ASP	2.3
33	Y8	26	LYS	2.3
7	QG	80	VAL	2.3
29	Y4	64	GLY	2.3
4	XD	33	MET	2.3
53	RX	91	ALA	2.3
55	RZ	172	ALA	2.3
35	YA	1178	C	2.3
12	QL	47	LYS	2.3
3	XC	179	ARG	2.3
33	R8	35	GLN	2.3
2	QB	93	VAL	2.3
8	QH	136	GLU	2.2
37	YD	237	GLU	2.2
44	YO	120	GLU	2.2
54	YY	64	GLU	2.2
1	QA	1117	G	2.2
35	RA	2141	G	2.2
35	YA	1089	G	2.2
20	QT	101	GLY	2.2
21	XU	11	GLY	2.2
54	RY	16	ALA	2.2
1	XA	60	A	2.2
5	QE	12	LEU	2.2
24	XY	76	A	2.2
35	RA	362	U	2.2

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Mol	Chain	Res	Type	RSRZ
35	RA	2585	U	2.2
20	XT	19	SER	2.2
1	XA	63	C	2.2
3	QC	164	ARG	2.2
24	QY	60	C	2.2
24	XY	16	C	2.2
35	RA	2789	C	2.2
55	RZ	80	ARG	2.2
15	XO	62	GLN	2.2
45	YP	71	VAL	2.2
4	XD	80	GLU	2.2
18	XR	62	GLU	2.2
27	R2	11	GLU	2.2
45	YP	74	GLU	2.2
15	XO	87	ILE	2.2
12	QL	48	PRO	2.2
42	RI	84	GLY	2.2
46	YQ	15	GLY	2.2
3	QC	4	LYS	2.2
13	QM	103	THR	2.2
24	XY	57	G	2.2
35	YA	1171	G	2.2
40	RG	165	THR	2.2
4	XD	209	ARG	2.2
1	XA	1447	A	2.2
19	QS	4	SER	2.2
49	RT	28	VAL	2.2
7	QG	37	ASN	2.2
13	QM	78	ILE	2.2
1	QA	1195	C	2.2
2	XB	18	GLY	2.2
9	QI	8	GLY	2.2
20	XT	103	GLY	2.2
39	RF	81	PRO	2.2
49	YT	93	ARG	2.2
12	XL	42	THR	2.2
9	QI	65	VAL	2.2
53	YX	59	VAL	2.2
1	QA	1065	U	2.2
1	QA	485	G	2.2
1	XA	324	G	2.2
2	QB	118	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
7	QG	73	MET	2.2
22	XV	38	A	2.2
24	XY	3	G	2.2
54	YY	40	GLU	2.2
55	YZ	119	GLU	2.2
55	YZ	150	LEU	2.2
8	XH	28	ALA	2.2
11	XK	118	GLY	2.2
17	XQ	33	GLY	2.2
48	RS	37	ALA	2.2
49	RT	130	ALA	2.2
39	YF	62	ARG	2.2
53	RX	60	ARG	2.2
2	QB	164	VAL	2.2
17	XQ	23	VAL	2.2
12	XL	116	SER	2.2
9	QI	99	LEU	2.2
3	XC	3	ASN	2.2
16	XP	54	GLU	2.2
41	RH	167	GLU	2.2
43	RN	92	ALA	2.2
4	QD	2	GLY	2.2
7	XG	81	GLY	2.2
13	QM	97	PRO	2.2
26	Y1	21	ARG	2.2
39	YF	74	ARG	2.2
9	XI	37	PHE	2.2
19	QS	12	ASP	2.2
35	RA	1088	A	2.2
35	RA	2802	G	2.2
35	YA	2141	G	2.2
9	QI	7	THR	2.1
24	XY	61	C	2.1
35	YA	2804	C	2.1
3	XC	188	LEU	2.1
10	XJ	33	GLN	2.1
13	QM	67	GLU	2.1
17	QQ	75	ARG	2.1
28	Y3	2	PRO	2.1
29	Y4	17	GLY	2.1
39	RF	85	GLY	2.1
11	XK	36	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
37	YD	71	ASP	2.1
42	YI	20	ASP	2.1
50	RU	56	ASP	2.1
1	QA	1286	A	2.1
35	RA	896	A	2.1
35	YA	2062	A	2.1
35	YA	2117	A	2.1
15	QO	31	LEU	2.1
20	QT	74	LYS	2.1
35	YA	545	G	2.1
35	YA	2190	G	2.1
46	RQ	103	MET	2.1
14	XN	35	ARG	2.1
48	YS	15	ARG	2.1
52	YW	93	ALA	2.1
3	XC	161	GLU	2.1
5	XE	23	GLY	2.1
38	YE	163	GLU	2.1
38	YE	193	GLY	2.1
41	YH	58	GLU	2.1
35	RA	1102	C	2.1
36	RB	12	C	2.1
10	XJ	58	ASP	2.1
2	QB	102	LEU	2.1
10	QJ	75	ILE	2.1
38	RE	152	LYS	2.1
10	XJ	43	ARG	2.1
43	YN	124	ALA	2.1
44	RO	41	ALA	2.1
29	Y4	54	GLY	2.1
29	Y4	57	GLU	2.1
35	RA	1098	A	2.1
40	RG	35	GLU	2.1
40	YG	164	GLU	2.1
2	QB	55	PHE	2.1
9	QI	108	VAL	2.1
30	Y5	60	VAL	2.1
35	YA	2319	G	2.1
35	YA	2793	G	2.1
50	RU	90	VAL	2.1
35	RA	1075	C	2.1
35	RA	1886	C	2.1

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Mol	Chain	Res	Type	RSRZ
35	YA	2179	C	2.1
27	Y2	15	LYS	2.1
50	RU	13	LYS	2.1
16	XP	73	LEU	2.1
19	XS	15	LEU	2.1
29	R4	22	ILE	2.1
40	RG	52	ILE	2.1
21	QU	22	ARG	2.1
16	QP	82	GLN	2.1
17	XQ	26	GLN	2.1
24	QY	55	U	2.1
35	RA	1101	U	2.1
38	RE	139	GLY	2.1
9	QI	123	PRO	2.1
47	RR	43	GLU	2.1
49	YT	45	PHE	2.1
49	YT	46	GLU	2.1
35	RA	1445(A)	A	2.1
35	RA	1847	A	2.1
35	YA	2169	A	2.1
43	YN	83	LYS	2.1
3	QC	5	ILE	2.1
8	XH	133	LEU	2.1
9	QI	96	LEU	2.1
10	QJ	8	LEU	2.1
45	RP	79	ARG	2.1
55	YZ	125	LEU	2.1
55	YZ	155	LEU	2.1
19	QS	44	MET	2.1
17	QQ	42	TYR	2.1
54	RY	35	TYR	2.1
35	RA	1536	C	2.1
35	YA	1100	C	2.1
1	QA	630	G	2.1
1	QA	1030(B)	G	2.1
35	RA	2318	G	2.1
3	XC	159	GLY	2.1
2	QB	163	PHE	2.1
5	QE	79	GLU	2.1
1	XA	1196	U	2.0
12	QL	91	LYS	2.0
45	RP	71	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
37	RD	22	SER	2.0
17	QQ	36	ILE	2.0
21	QU	13	ILE	2.0
40	RG	29	TRP	2.0
33	R8	25	MET	2.0
38	YE	1	MET	2.0
2	XB	237	ALA	2.0
16	QP	32	TYR	2.0
35	RA	1073	A	2.0
35	YA	529	A	2.0
35	YA	2135	A	2.0
38	YE	151	TYR	2.0
46	RQ	75	THR	2.0
32	Y7	26	GLY	2.0
45	YP	68	GLN	2.0
12	QL	94	PRO	2.0
17	QQ	69	LYS	2.0
20	QT	29	LYS	2.0
44	YO	108	GLU	2.0
35	YA	645	C	2.0
45	YP	76	LYS	2.0
46	RQ	85	LYS	2.0
2	XB	165	VAL	2.0
12	XL	18	VAL	2.0
41	RH	169	VAL	2.0
55	RZ	139	VAL	2.0
10	XJ	45	ARG	2.0
11	XK	98	LEU	2.0
35	RA	275	G	2.0
35	YA	2334	G	2.0
46	RQ	114	ALA	2.0
4	QD	54	TYR	2.0
8	XH	20	TYR	2.0
13	XM	21	TYR	2.0
25	R0	71	ASP	2.0
29	Y4	18	CYS	2.0
2	QB	131	PRO	2.0
4	QD	7	PRO	2.0
34	Y9	30	PRO	2.0
46	RQ	12	GLN	2.0
4	QD	73	ARG	2.0
8	XH	93	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
38	RE	188	VAL	2.0
39	YF	35	GLU	2.0
20	QT	22	ARG	2.0
25	R0	77	ARG	2.0
51	RV	72	VAL	2.0
55	YZ	161	VAL	2.0
2	QB	11	LEU	2.0
47	RR	18	LEU	2.0
35	RA	1072	C	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
35	5MU	RA	1915	21/22	0.86	0.10	86,101,109,111	0
1	PSU	QA	516	20/21	0.87	0.10	94,102,120,123	0
1	PSU	XA	516	20/21	0.87	0.10	78,89,96,97	0
1	2MG	QA	1207	24/25	0.87	0.11	126,135,147,148	0
12	0TD	XL	92	10/11	0.87	0.14	65,73,88,113	0
1	5MC	QA	967	21/22	0.89	0.12	97,98,105,116	0
1	2MG	XA	1207	24/25	0.90	0.11	91,102,107,114	0
1	G7M	XA	527	24/25	0.90	0.12	64,72,87,114	0
35	PSU	RA	1911	20/21	0.91	0.09	72,85,93,99	0
1	M2G	QA	966	25/26	0.91	0.13	96,100,111,116	0
35	5MU	YA	1915	21/22	0.91	0.09	60,70,89,93	0
35	OMC	RA	1920	21/22	0.91	0.10	67,70,77,83	0
12	0TD	QL	92	10/11	0.92	0.21	131,143,166,185	0
35	PSU	RA	1917	20/21	0.92	0.08	84,91,97,106	0
1	5MC	XA	1404	21/22	0.92	0.12	51,52,66,72	0
35	PSU	YA	1917	20/21	0.93	0.08	59,70,97,100	0
1	G7M	QA	527	24/25	0.93	0.12	79,88,104,109	0
35	5MC	RA	1962	21/22	0.93	0.10	57,64,94,105	0
35	OMU	RA	2552	21/22	0.93	0.11	48,49,71,96	0
35	PSU	YA	1911	20/21	0.94	0.08	58,71,82,84	0
1	5MC	XA	967	21/22	0.94	0.11	86,94,104,108	0
35	5MU	YA	1939	21/22	0.94	0.10	37,44,55,61	0
35	5MC	RA	1942	21/22	0.94	0.08	61,74,92,94	0
1	5MC	QA	1407	21/22	0.94	0.10	68,70,78,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	4OC	QA	1402	22/23	0.94	0.10	77,82,90,101	0
1	UR3	QA	1498	21/22	0.95	0.10	68,69,75,86	0
1	UR3	XA	1498	21/22	0.95	0.10	55,57,75,88	0
1	MA6	XA	1518	24/25	0.95	0.11	52,59,86,88	0
35	5MU	RA	1939	21/22	0.95	0.10	53,61,75,83	0
1	5MC	QA	1404	21/22	0.95	0.09	67,68,69,70	0
1	5MC	XA	1400	21/22	0.95	0.09	65,75,89,94	0
1	5MC	QA	1400	21/22	0.95	0.09	78,79,92,100	0
35	2MA	RA	2503	23/24	0.95	0.12	45,46,50,65	0
1	5MC	XA	1407	21/22	0.95	0.09	50,51,62,70	0
35	OMU	YA	2552	21/22	0.95	0.09	35,43,55,65	0
35	PSU	RA	2605	20/21	0.95	0.10	47,48,65,66	0
35	PSU	YA	2605	20/21	0.95	0.09	35,38,53,57	0
1	M2G	XA	966	25/26	0.96	0.11	73,82,100,102	0
35	5MC	YA	1962	21/22	0.96	0.08	37,38,52,72	0
35	OMG	RA	2251	24/25	0.96	0.09	47,49,65,68	0
35	OMG	YA	2251	24/25	0.96	0.09	34,35,41,43	0
35	OMC	YA	1920	21/22	0.96	0.08	59,67,75,79	0
1	MA6	XA	1519	24/25	0.96	0.10	55,60,73,80	0
1	4OC	XA	1402	22/23	0.96	0.10	62,72,90,95	0
1	MA6	QA	1518	24/25	0.96	0.09	64,65,71,75	0
35	5MC	YA	1942	21/22	0.96	0.07	43,53,69,74	0
1	MA6	QA	1519	24/25	0.97	0.11	65,66,70,80	0
35	2MA	YA	2503	23/24	0.97	0.08	36,39,50,79	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
56	MG	RA	3424	1/1	-0.12	0.53	121,121,121,121	0
56	MG	RA	3256	1/1	-0.02	0.52	96,96,96,96	0
56	MG	RA	3301	1/1	0.10	0.30	98,98,98,98	0
56	MG	RA	3189	1/1	0.11	0.24	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3309	1/1	0.13	0.20	99,99,99,99	0
56	MG	RA	3205	1/1	0.19	0.43	136,136,136,136	0
56	MG	QA	1737	1/1	0.24	0.36	78,78,78,78	0
56	MG	RA	3666	1/1	0.25	0.28	116,116,116,116	0
56	MG	RA	3579	1/1	0.26	0.19	87,87,87,87	0
56	MG	RA	3369	1/1	0.26	0.34	119,119,119,119	0
56	MG	RA	3536	1/1	0.33	0.22	114,114,114,114	0
56	MG	RA	3450	1/1	0.34	0.55	94,94,94,94	0
56	MG	RB	205	1/1	0.34	0.17	75,75,75,75	0
56	MG	QA	1607	1/1	0.35	0.37	73,73,73,73	0
56	MG	QA	1658	1/1	0.36	0.24	91,91,91,91	0
56	MG	QA	1796	1/1	0.36	0.34	111,111,111,111	0
56	MG	XR	101	1/1	0.36	0.27	89,89,89,89	0
56	MG	YA	3607	1/1	0.36	0.31	105,105,105,105	0
56	MG	RA	3159	1/1	0.37	0.63	97,97,97,97	0
56	MG	QE	201	1/1	0.37	0.39	114,114,114,114	0
56	MG	RA	3058	1/1	0.37	0.23	83,83,83,83	0
56	MG	RA	3400	1/1	0.37	0.36	88,88,88,88	0
56	MG	RA	3083	1/1	0.37	0.16	72,72,72,72	0
56	MG	RA	3272	1/1	0.37	0.19	51,51,51,51	0
56	MG	RA	3221	1/1	0.39	0.41	89,89,89,89	0
56	MG	RA	3381	1/1	0.40	0.43	87,87,87,87	0
56	MG	RA	3513	1/1	0.40	0.27	73,73,73,73	0
56	MG	RA	3053	1/1	0.40	0.51	108,108,108,108	0
56	MG	RA	3213	1/1	0.40	0.30	105,105,105,105	0
56	MG	RA	3214	1/1	0.41	0.36	105,105,105,105	0
56	MG	RA	3155	1/1	0.41	0.18	72,72,72,72	0
56	MG	RA	3153	1/1	0.42	0.61	127,127,127,127	0
56	MG	XA	1671	1/1	0.42	0.17	96,96,96,96	0
56	MG	QO	101	1/1	0.42	0.63	113,113,113,113	0
56	MG	YA	3024	1/1	0.42	0.23	102,102,102,102	0
56	MG	RA	3322	1/1	0.42	0.42	79,79,79,79	0
56	MG	RA	3069	1/1	0.43	0.71	144,144,144,144	0
56	MG	QA	1705	1/1	0.43	0.21	103,103,103,103	0
56	MG	RA	3096	1/1	0.43	0.28	102,102,102,102	0
56	MG	RA	3350	1/1	0.44	0.56	127,127,127,127	0
56	MG	RA	3591	1/1	0.47	0.42	74,74,74,74	0
56	MG	RA	3163	1/1	0.47	0.28	80,80,80,80	0
56	MG	XA	1718	1/1	0.47	0.42	116,116,116,116	0
56	MG	RA	3460	1/1	0.48	0.47	89,89,89,89	0
56	MG	XA	1723	1/1	0.48	0.26	72,72,72,72	0
56	MG	RA	3152	1/1	0.48	0.78	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3011	1/1	0.48	0.41	106,106,106,106	0
56	MG	YA	3480	1/1	0.48	0.32	74,74,74,74	0
56	MG	QG	202	1/1	0.48	0.17	133,133,133,133	0
56	MG	XA	1781	1/1	0.49	0.36	92,92,92,92	0
56	MG	RA	3507	1/1	0.49	0.33	76,76,76,76	0
56	MG	RA	3100	1/1	0.49	0.25	144,144,144,144	0
56	MG	RA	3484	1/1	0.49	0.26	71,71,71,71	0
56	MG	RA	3673	1/1	0.49	0.49	91,91,91,91	0
56	MG	QA	1695	1/1	0.50	0.23	65,65,65,65	0
56	MG	RA	3138	1/1	0.50	0.27	96,96,96,96	0
56	MG	RA	3382	1/1	0.50	0.21	57,57,57,57	0
56	MG	XA	1670	1/1	0.51	0.22	90,90,90,90	0
56	MG	QA	1762	1/1	0.52	0.13	66,66,66,66	0
56	MG	RA	3482	1/1	0.52	0.76	127,127,127,127	0
56	MG	RA	3103	1/1	0.52	0.19	59,59,59,59	0
56	MG	YA	3097	1/1	0.52	0.20	72,72,72,72	0
56	MG	RA	3182	1/1	0.52	0.23	94,94,94,94	0
56	MG	QV	102	1/1	0.52	0.19	92,92,92,92	0
56	MG	RA	3093	1/1	0.53	0.29	92,92,92,92	0
56	MG	RA	3326	1/1	0.53	0.22	67,67,67,67	0
56	MG	RA	3175	1/1	0.53	0.45	79,79,79,79	0
56	MG	QA	1618	1/1	0.53	0.28	86,86,86,86	0
56	MG	RA	3049	1/1	0.53	0.24	61,61,61,61	0
56	MG	RA	3405	1/1	0.54	0.16	71,71,71,71	0
56	MG	Y1	101	1/1	0.54	0.19	76,76,76,76	0
56	MG	RA	3682	1/1	0.54	0.27	84,84,84,84	0
56	MG	RA	3376	1/1	0.54	0.21	98,98,98,98	0
56	MG	RA	3104	1/1	0.54	0.46	89,89,89,89	0
56	MG	XJ	201	1/1	0.54	0.20	81,81,81,81	0
56	MG	RA	3178	1/1	0.55	0.20	97,97,97,97	0
56	MG	RB	204	1/1	0.55	0.17	140,140,140,140	0
56	MG	QA	1813	1/1	0.55	0.14	86,86,86,86	0
56	MG	RA	3458	1/1	0.55	0.23	97,97,97,97	0
56	MG	RA	3571	1/1	0.55	0.15	89,89,89,89	0
56	MG	RB	202	1/1	0.56	0.14	107,107,107,107	0
56	MG	RA	3110	1/1	0.56	0.12	83,83,83,83	0
56	MG	RA	3347	1/1	0.56	0.26	99,99,99,99	0
56	MG	RA	3403	1/1	0.57	0.36	84,84,84,84	0
56	MG	XA	1778	1/1	0.57	0.74	127,127,127,127	0
56	MG	QA	1676	1/1	0.57	0.31	81,81,81,81	0
56	MG	RA	3123	1/1	0.57	0.31	71,71,71,71	0
56	MG	RA	3080	1/1	0.57	0.48	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3140	1/1	0.57	0.19	67,67,67,67	0
56	MG	QA	1659	1/1	0.57	0.17	95,95,95,95	0
56	MG	QA	1660	1/1	0.57	0.18	120,120,120,120	0
56	MG	RA	3631	1/1	0.57	0.35	69,69,69,69	0
56	MG	RA	3654	1/1	0.57	0.55	90,90,90,90	0
56	MG	YA	3668	1/1	0.57	0.29	109,109,109,109	0
56	MG	RA	3219	1/1	0.58	0.37	101,101,101,101	0
56	MG	RA	3072	1/1	0.58	0.82	109,109,109,109	0
56	MG	RA	3323	1/1	0.58	0.11	76,76,76,76	0
56	MG	QA	1728	1/1	0.58	0.19	90,90,90,90	0
56	MG	RA	3397	1/1	0.58	0.35	96,96,96,96	0
56	MG	RA	3589	1/1	0.58	0.33	117,117,117,117	0
56	MG	RA	3469	1/1	0.58	0.74	114,114,114,114	0
56	MG	YA	3412	1/1	0.58	0.60	82,82,82,82	0
56	MG	YA	3426	1/1	0.58	0.14	67,67,67,67	0
56	MG	RA	3045	1/1	0.58	0.23	79,79,79,79	0
56	MG	RA	3647	1/1	0.58	0.70	121,121,121,121	0
56	MG	YA	3652	1/1	0.58	0.16	67,67,67,67	0
56	MG	QA	1787	1/1	0.58	0.18	140,140,140,140	0
56	MG	RA	3009	1/1	0.59	0.34	98,98,98,98	0
56	MG	QN	102	1/1	0.59	0.39	82,82,82,82	0
56	MG	YA	3253	1/1	0.59	0.26	41,41,41,41	0
56	MG	YG	201	1/1	0.59	0.15	111,111,111,111	0
56	MG	RA	3201	1/1	0.60	0.50	83,83,83,83	0
56	MG	QA	1646	1/1	0.60	0.11	80,80,80,80	0
56	MG	RA	3039	1/1	0.60	0.35	85,85,85,85	0
56	MG	RA	3392	1/1	0.60	0.18	103,103,103,103	0
56	MG	RA	3091	1/1	0.60	0.14	78,78,78,78	0
56	MG	RA	3134	1/1	0.61	0.21	63,63,63,63	0
56	MG	RA	3374	1/1	0.61	0.12	55,55,55,55	0
56	MG	QA	1770	1/1	0.61	0.21	68,68,68,68	0
56	MG	RA	3606	1/1	0.61	0.22	77,77,77,77	0
56	MG	RA	3060	1/1	0.61	0.23	84,84,84,84	0
56	MG	RA	3161	1/1	0.61	0.16	72,72,72,72	0
56	MG	RA	3143	1/1	0.61	0.20	94,94,94,94	0
56	MG	RA	3064	1/1	0.61	0.27	80,80,80,80	0
56	MG	RA	3481	1/1	0.62	0.38	102,102,102,102	0
56	MG	RA	3363	1/1	0.62	0.41	74,74,74,74	0
56	MG	RA	3313	1/1	0.62	0.16	84,84,84,84	0
56	MG	RA	3037	1/1	0.62	0.25	52,52,52,52	0
56	MG	RA	3029	1/1	0.62	0.19	99,99,99,99	0
56	MG	XA	1624	1/1	0.62	0.23	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	YA	3387	1/1	0.62	0.38	90,90,90,90	0
56	MG	RA	3461	1/1	0.63	0.39	104,104,104,104	0
56	MG	RA	3462	1/1	0.63	0.23	44,44,44,44	0
56	MG	RA	3173	1/1	0.63	0.52	142,142,142,142	0
56	MG	RA	3477	1/1	0.63	0.33	100,100,100,100	0
56	MG	RA	3059	1/1	0.63	0.15	61,61,61,61	0
56	MG	QA	1633	1/1	0.63	0.19	104,104,104,104	0
56	MG	QA	1601	1/1	0.63	0.25	94,94,94,94	0
56	MG	RA	3055	1/1	0.63	0.14	91,91,91,91	0
56	MG	RA	3224	1/1	0.63	0.16	111,111,111,111	0
56	MG	XA	1782	1/1	0.63	0.16	73,73,73,73	0
56	MG	RA	3250	1/1	0.63	0.37	97,97,97,97	0
56	MG	QA	1718	1/1	0.63	0.21	64,64,64,64	0
56	MG	RA	3454	1/1	0.64	0.11	51,51,51,51	0
56	MG	RA	3479	1/1	0.64	0.23	75,75,75,75	0
56	MG	XA	1700	1/1	0.64	0.26	90,90,90,90	0
56	MG	RA	3209	1/1	0.64	0.23	103,103,103,103	0
56	MG	QA	1694	1/1	0.64	0.23	87,87,87,87	0
56	MG	QA	1643	1/1	0.64	0.31	86,86,86,86	0
56	MG	RA	3497	1/1	0.64	0.13	56,56,56,56	0
56	MG	RA	3129	1/1	0.64	0.18	58,58,58,58	0
56	MG	RP	202	1/1	0.64	0.27	73,73,73,73	0
56	MG	RA	3015	1/1	0.64	0.28	70,70,70,70	0
56	MG	YB	207	1/1	0.64	0.34	77,77,77,77	0
56	MG	XA	1657	1/1	0.64	0.20	102,102,102,102	0
56	MG	QA	1662	1/1	0.65	0.15	42,42,42,42	0
56	MG	RA	3416	1/1	0.65	0.41	63,63,63,63	0
56	MG	RA	3330	1/1	0.65	0.16	57,57,57,57	0
56	MG	XA	1701	1/1	0.65	0.12	53,53,53,53	0
56	MG	QA	1688	1/1	0.65	0.30	98,98,98,98	0
56	MG	QA	1746	1/1	0.65	0.18	54,54,54,54	0
56	MG	RA	3237	1/1	0.65	0.19	111,111,111,111	0
56	MG	YA	3527	1/1	0.65	0.18	75,75,75,75	0
56	MG	QA	1791	1/1	0.65	0.11	83,83,83,83	0
56	MG	YA	3629	1/1	0.65	0.32	50,50,50,50	0
56	MG	XA	1607	1/1	0.65	0.19	95,95,95,95	0
56	MG	XA	1614	1/1	0.65	0.34	85,85,85,85	0
56	MG	RA	3401	1/1	0.65	0.52	124,124,124,124	0
56	MG	RA	3164	1/1	0.65	0.18	65,65,65,65	0
56	MG	RA	3677	1/1	0.66	0.14	47,47,47,47	0
56	MG	RA	3411	1/1	0.66	0.22	60,60,60,60	0
56	MG	QA	1673	1/1	0.66	0.16	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3601	1/1	0.66	0.30	88,88,88,88	0
56	MG	RA	3417	1/1	0.66	0.94	125,125,125,125	0
56	MG	RA	3463	1/1	0.66	0.35	104,104,104,104	0
56	MG	QA	1808	1/1	0.66	0.23	65,65,65,65	0
56	MG	RA	3128	1/1	0.66	0.13	69,69,69,69	0
56	MG	YA	3616	1/1	0.66	0.15	84,84,84,84	0
56	MG	RA	3665	1/1	0.66	0.24	63,63,63,63	0
56	MG	YA	3643	1/1	0.66	0.25	67,67,67,67	0
56	MG	XA	1634	1/1	0.66	0.17	40,40,40,40	0
56	MG	RA	3160	1/1	0.66	0.23	51,51,51,51	0
56	MG	RA	3226	1/1	0.66	0.17	72,72,72,72	0
56	MG	YA	3052	1/1	0.66	0.16	48,48,48,48	0
56	MG	RA	3471	1/1	0.67	0.21	98,98,98,98	0
56	MG	RQ	201	1/1	0.67	0.38	73,73,73,73	0
56	MG	RA	3218	1/1	0.67	0.15	79,79,79,79	0
56	MG	QH	202	1/1	0.67	0.11	82,82,82,82	0
56	MG	RA	3318	1/1	0.67	0.40	73,73,73,73	0
56	MG	YA	3483	1/1	0.67	0.29	83,83,83,83	0
56	MG	RA	3383	1/1	0.67	0.50	88,88,88,88	0
56	MG	RA	3198	1/1	0.67	0.24	97,97,97,97	0
56	MG	XY	101	1/1	0.67	0.25	72,72,72,72	0
56	MG	RA	3066	1/1	0.67	0.37	98,98,98,98	0
56	MG	RA	3421	1/1	0.67	0.26	59,59,59,59	0
56	MG	RA	3204	1/1	0.67	0.38	97,97,97,97	0
56	MG	RB	209	1/1	0.67	0.13	63,63,63,63	0
56	MG	YA	3152	1/1	0.67	0.31	81,81,81,81	0
56	MG	YA	3160	1/1	0.67	0.36	102,102,102,102	0
56	MG	XA	1649	1/1	0.68	0.26	96,96,96,96	0
56	MG	XA	1653	1/1	0.68	0.21	93,93,93,93	0
56	MG	RA	3483	1/1	0.68	0.25	69,69,69,69	0
56	MG	YA	3547	1/1	0.68	0.44	74,74,74,74	0
56	MG	RA	3192	1/1	0.68	0.48	85,85,85,85	0
56	MG	QA	1616	1/1	0.68	0.14	58,58,58,58	0
56	MG	RA	3514	1/1	0.69	0.42	108,108,108,108	0
56	MG	RA	3526	1/1	0.69	0.51	110,110,110,110	0
56	MG	RA	3113	1/1	0.69	0.26	69,69,69,69	0
56	MG	RA	3657	1/1	0.69	0.32	65,65,65,65	0
56	MG	YA	3027	1/1	0.69	0.17	70,70,70,70	0
56	MG	RA	3395	1/1	0.69	0.41	85,85,85,85	0
56	MG	RA	3026	1/1	0.69	0.15	63,63,63,63	0
56	MG	QA	1665	1/1	0.69	0.10	65,65,65,65	0
56	MG	RA	3499	1/1	0.69	0.53	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1754	1/1	0.69	0.23	89,89,89,89	0
56	MG	YA	3310	1/1	0.69	0.13	5,5,5,5	0
56	MG	RA	3706	1/1	0.69	0.23	94,94,94,94	0
56	MG	QA	1792	1/1	0.69	0.20	74,74,74,74	0
56	MG	RA	3391	1/1	0.70	0.10	55,55,55,55	0
56	MG	RA	3360	1/1	0.70	0.18	67,67,67,67	0
56	MG	RA	3592	1/1	0.70	0.22	58,58,58,58	0
56	MG	YA	3444	1/1	0.70	0.30	54,54,54,54	0
56	MG	RA	3474	1/1	0.70	0.26	71,71,71,71	0
56	MG	QA	1627	1/1	0.70	0.10	54,54,54,54	0
56	MG	QA	1804	1/1	0.70	0.21	85,85,85,85	0
56	MG	RA	3075	1/1	0.70	0.33	55,55,55,55	0
56	MG	RA	3119	1/1	0.71	0.12	62,62,62,62	0
56	MG	RA	3707	1/1	0.71	0.12	49,49,49,49	0
56	MG	XA	1623	1/1	0.71	0.12	71,71,71,71	0
56	MG	RA	3170	1/1	0.71	0.20	78,78,78,78	0
56	MG	RA	3184	1/1	0.71	0.22	78,78,78,78	0
56	MG	RA	3448	1/1	0.71	0.19	75,75,75,75	0
56	MG	RA	3186	1/1	0.71	0.13	50,50,50,50	0
56	MG	YA	3348	1/1	0.71	0.21	75,75,75,75	0
56	MG	RA	3642	1/1	0.71	0.16	84,84,84,84	0
56	MG	RP	203	1/1	0.71	0.20	60,60,60,60	0
56	MG	RA	3387	1/1	0.71	0.15	43,43,43,43	0
56	MG	RV	201	1/1	0.71	0.13	68,68,68,68	0
56	MG	YA	3186	1/1	0.72	0.14	62,62,62,62	0
56	MG	XA	1673	1/1	0.72	0.22	77,77,77,77	0
56	MG	RA	3057	1/1	0.72	0.23	75,75,75,75	0
56	MG	RA	3051	1/1	0.72	0.10	109,109,109,109	0
56	MG	XA	1706	1/1	0.72	0.32	87,87,87,87	0
56	MG	QA	1715	1/1	0.72	0.35	82,82,82,82	0
56	MG	RA	3639	1/1	0.72	0.21	55,55,55,55	0
56	MG	RA	3509	1/1	0.72	0.33	77,77,77,77	0
56	MG	RA	3426	1/1	0.72	0.19	78,78,78,78	0
56	MG	RA	3441	1/1	0.72	0.29	89,89,89,89	0
56	MG	RA	3139	1/1	0.72	0.20	62,62,62,62	0
56	MG	RA	3662	1/1	0.72	0.36	70,70,70,70	0
56	MG	RA	3087	1/1	0.72	0.25	88,88,88,88	0
56	MG	RA	3545	1/1	0.72	0.34	90,90,90,90	0
56	MG	RA	3566	1/1	0.72	0.20	46,46,46,46	0
56	MG	RA	3408	1/1	0.72	0.34	74,74,74,74	0
56	MG	RA	3455	1/1	0.72	0.31	82,82,82,82	0
56	MG	RA	3457	1/1	0.72	0.13	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1689	1/1	0.72	0.20	52,52,52,52	0
56	MG	RA	3380	1/1	0.72	0.20	62,62,62,62	0
56	MG	QA	1630	1/1	0.73	0.13	92,92,92,92	0
56	MG	QA	1812	1/1	0.73	0.09	73,73,73,73	0
56	MG	RA	3126	1/1	0.73	0.12	75,75,75,75	0
56	MG	RA	3106	1/1	0.73	0.11	51,51,51,51	0
56	MG	YA	3017	1/1	0.73	0.14	68,68,68,68	0
56	MG	YA	3365	1/1	0.73	0.24	78,78,78,78	0
56	MG	RA	3151	1/1	0.73	0.12	58,58,58,58	0
56	MG	QA	1703	1/1	0.73	0.73	82,82,82,82	0
56	MG	RA	3644	1/1	0.73	0.20	67,67,67,67	0
56	MG	YA	3697	1/1	0.73	0.42	66,66,66,66	0
56	MG	RA	3007	1/1	0.73	0.37	99,99,99,99	0
56	MG	RA	3249	1/1	0.73	0.32	84,84,84,84	0
56	MG	RA	3609	1/1	0.74	0.22	69,69,69,69	0
56	MG	QA	1773	1/1	0.74	0.14	51,51,51,51	0
56	MG	RA	3632	1/1	0.74	0.24	48,48,48,48	0
56	MG	RA	3032	1/1	0.74	0.30	95,95,95,95	0
56	MG	XA	1714	1/1	0.74	0.14	45,45,45,45	0
56	MG	YA	3051	1/1	0.74	0.35	58,58,58,58	0
56	MG	XA	1625	1/1	0.74	0.24	79,79,79,79	0
56	MG	YA	3514	1/1	0.74	0.35	85,85,85,85	0
56	MG	YA	3074	1/1	0.74	0.15	39,39,39,39	0
56	MG	QA	1649	1/1	0.74	0.19	115,115,115,115	0
56	MG	YA	3131	1/1	0.74	0.28	87,87,87,87	0
56	MG	XA	1770	1/1	0.74	0.26	87,87,87,87	0
56	MG	YA	3159	1/1	0.74	0.18	75,75,75,75	0
56	MG	RA	3560	1/1	0.74	0.26	72,72,72,72	0
56	MG	YA	3165	1/1	0.74	0.13	54,54,54,54	0
56	MG	RA	3414	1/1	0.74	0.40	91,91,91,91	0
56	MG	YA	3678	1/1	0.74	0.16	70,70,70,70	0
56	MG	RA	3689	1/1	0.74	0.18	66,66,66,66	0
56	MG	RA	3377	1/1	0.74	0.24	73,73,73,73	0
56	MG	YB	215	1/1	0.74	0.12	42,42,42,42	0
56	MG	XA	1604	1/1	0.74	0.19	91,91,91,91	0
56	MG	RA	3542	1/1	0.75	0.13	27,27,27,27	0
56	MG	RA	3242	1/1	0.75	0.15	34,34,34,34	0
56	MG	RA	3246	1/1	0.75	0.38	65,65,65,65	0
56	MG	QA	1655	1/1	0.75	0.22	90,90,90,90	0
56	MG	XE	201	1/1	0.75	0.15	51,51,51,51	0
56	MG	YA	3383	1/1	0.75	0.14	51,51,51,51	0
56	MG	RA	3393	1/1	0.75	0.31	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3054	1/1	0.75	0.19	72,72,72,72	0
56	MG	QE	203	1/1	0.75	0.17	71,71,71,71	0
56	MG	YA	3432	1/1	0.75	0.32	79,79,79,79	0
56	MG	QA	1636	1/1	0.75	0.10	70,70,70,70	0
56	MG	YA	3470	1/1	0.75	0.39	93,93,93,93	0
56	MG	YA	3014	1/1	0.75	0.21	48,48,48,48	0
56	MG	RA	3183	1/1	0.75	0.36	99,99,99,99	0
56	MG	RA	3597	1/1	0.75	0.16	46,46,46,46	0
56	MG	QA	1795	1/1	0.75	0.40	84,84,84,84	0
56	MG	RA	3404	1/1	0.75	0.08	47,47,47,47	0
56	MG	RA	3135	1/1	0.75	0.20	98,98,98,98	0
56	MG	YA	3066	1/1	0.75	0.43	103,103,103,103	0
56	MG	QA	1632	1/1	0.75	0.11	81,81,81,81	0
56	MG	YA	3633	1/1	0.75	0.31	41,41,41,41	0
56	MG	RA	3410	1/1	0.75	0.32	68,68,68,68	0
56	MG	YA	3111	1/1	0.75	0.22	58,58,58,58	0
56	MG	YA	3119	1/1	0.75	0.43	90,90,90,90	0
56	MG	XA	1702	1/1	0.75	0.23	67,67,67,67	0
56	MG	RA	3085	1/1	0.75	0.14	81,81,81,81	0
56	MG	RA	3518	1/1	0.75	0.23	53,53,53,53	0
56	MG	QA	1820	1/1	0.75	0.13	81,81,81,81	0
56	MG	RA	3027	1/1	0.75	0.68	92,92,92,92	0
56	MG	YR	202	1/1	0.75	0.14	44,44,44,44	0
56	MG	XA	1660	1/1	0.76	0.22	96,96,96,96	0
56	MG	XA	1787	1/1	0.76	0.11	94,94,94,94	0
56	MG	QA	1642	1/1	0.76	0.31	68,68,68,68	0
56	MG	YA	3499	1/1	0.76	0.41	78,78,78,78	0
56	MG	RA	3442	1/1	0.76	0.19	67,67,67,67	0
56	MG	XA	1602	1/1	0.76	0.20	66,66,66,66	0
56	MG	R5	103	1/1	0.76	0.13	63,63,63,63	0
56	MG	QE	204	1/1	0.76	0.10	60,60,60,60	0
56	MG	YA	3177	1/1	0.76	0.15	42,42,42,42	0
56	MG	RA	3625	1/1	0.76	0.31	59,59,59,59	0
56	MG	RA	3534	1/1	0.76	0.34	64,64,64,64	0
56	MG	RA	3535	1/1	0.76	0.21	47,47,47,47	0
56	MG	YA	3649	1/1	0.76	0.26	46,46,46,46	0
56	MG	RA	3670	1/1	0.76	0.10	60,60,60,60	0
56	MG	YA	3664	1/1	0.76	0.32	85,85,85,85	0
56	MG	RF	304	1/1	0.76	0.20	55,55,55,55	0
56	MG	XA	1745	1/1	0.76	0.35	74,74,74,74	0
56	MG	RP	201	1/1	0.76	0.28	60,60,60,60	0
56	MG	RA	3094	1/1	0.76	0.17	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YB	212	1/1	0.76	0.16	38,38,38,38	0
56	MG	YA	3082	1/1	0.76	0.09	73,73,73,73	0
56	MG	YA	3092	1/1	0.76	0.19	65,65,65,65	0
56	MG	RA	3511	1/1	0.76	0.78	87,87,87,87	0
56	MG	RA	3298	1/1	0.77	0.11	49,49,49,49	0
56	MG	RA	3473	1/1	0.77	0.36	87,87,87,87	0
56	MG	RA	3187	1/1	0.77	0.24	93,93,93,93	0
56	MG	RA	3303	1/1	0.77	0.30	79,79,79,79	0
56	MG	RA	3220	1/1	0.77	0.09	54,54,54,54	0
56	MG	RA	3480	1/1	0.77	0.29	65,65,65,65	0
56	MG	QA	1771	1/1	0.77	0.16	43,43,43,43	0
56	MG	RA	3063	1/1	0.77	0.41	101,101,101,101	0
56	MG	XA	1661	1/1	0.77	0.30	76,76,76,76	0
56	MG	YA	3029	1/1	0.77	0.20	47,47,47,47	0
56	MG	RA	3052	1/1	0.77	0.11	78,78,78,78	0
56	MG	YA	3490	1/1	0.77	0.25	37,37,37,37	0
56	MG	RA	3227	1/1	0.77	0.16	71,71,71,71	0
56	MG	RA	3228	1/1	0.77	0.18	75,75,75,75	0
56	MG	XA	1696	1/1	0.77	0.12	42,42,42,42	0
56	MG	R9	102	1/1	0.77	0.11	64,64,64,64	0
56	MG	YA	3555	1/1	0.77	0.14	47,47,47,47	0
56	MG	RA	3239	1/1	0.77	0.21	66,66,66,66	0
56	MG	RA	3620	1/1	0.77	0.31	33,33,33,33	0
56	MG	QA	1656	1/1	0.77	0.27	134,134,134,134	0
56	MG	RA	3351	1/1	0.77	0.20	41,41,41,41	0
56	MG	QK	201	1/1	0.77	0.11	73,73,73,73	0
56	MG	YA	3648	1/1	0.77	0.39	80,80,80,80	0
56	MG	YA	3151	1/1	0.77	0.18	70,70,70,70	0
56	MG	QA	1617	1/1	0.77	0.12	73,73,73,73	0
56	MG	RA	3640	1/1	0.77	0.12	50,50,50,50	0
56	MG	XA	1758	1/1	0.77	0.17	52,52,52,52	0
56	MG	RA	3077	1/1	0.77	0.16	50,50,50,50	0
56	MG	RA	3373	1/1	0.77	0.24	73,73,73,73	0
56	MG	QA	1608	1/1	0.77	0.12	87,87,87,87	0
56	MG	YA	3211	1/1	0.77	0.14	66,66,66,66	0
56	MG	YA	3247	1/1	0.77	0.33	77,77,77,77	0
56	MG	RA	3468	1/1	0.77	0.22	39,39,39,39	0
56	MG	QA	1740	1/1	0.77	0.30	100,100,100,100	0
56	MG	RA	3041	1/1	0.78	0.23	85,85,85,85	0
56	MG	YA	3080	1/1	0.78	0.11	65,65,65,65	0
56	MG	RA	3353	1/1	0.78	0.19	38,38,38,38	0
56	MG	RH	202	1/1	0.78	0.13	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1772	1/1	0.78	0.20	71,71,71,71	0
56	MG	XA	1656	1/1	0.78	0.13	67,67,67,67	0
56	MG	RN	202	1/1	0.78	0.26	89,89,89,89	0
56	MG	RA	3311	1/1	0.78	0.54	71,71,71,71	0
56	MG	YA	3147	1/1	0.78	0.13	59,59,59,59	0
56	MG	RA	3611	1/1	0.78	0.31	58,58,58,58	0
56	MG	RA	3208	1/1	0.78	0.12	73,73,73,73	0
56	MG	RA	3472	1/1	0.78	0.16	77,77,77,77	0
56	MG	R0	103	1/1	0.78	0.27	96,96,96,96	0
56	MG	XA	1680	1/1	0.78	0.26	65,65,65,65	0
56	MG	YA	3625	1/1	0.78	0.21	40,40,40,40	0
56	MG	QA	1774	1/1	0.78	0.15	108,108,108,108	0
56	MG	Y7	101	1/1	0.78	0.26	81,81,81,81	0
56	MG	YA	3201	1/1	0.78	0.44	89,89,89,89	0
56	MG	RA	3259	1/1	0.78	0.11	102,102,102,102	0
56	MG	RA	3181	1/1	0.78	0.11	51,51,51,51	0
56	MG	RA	3012	1/1	0.78	0.14	65,65,65,65	0
56	MG	YA	3288	1/1	0.78	0.13	56,56,56,56	0
56	MG	XA	1618	1/1	0.78	0.09	104,104,104,104	0
56	MG	QP	101	1/1	0.78	0.22	88,88,88,88	0
56	MG	XA	1717	1/1	0.78	0.15	70,70,70,70	0
56	MG	YA	3703	1/1	0.78	0.18	56,56,56,56	0
56	MG	RA	3594	1/1	0.78	0.14	43,43,43,43	0
56	MG	YA	3058	1/1	0.78	0.19	63,63,63,63	0
56	MG	YB	214	1/1	0.78	0.21	51,51,51,51	0
56	MG	YA	3396	1/1	0.78	0.16	74,74,74,74	0
56	MG	YD	301	1/1	0.78	0.12	78,78,78,78	0
56	MG	YA	3400	1/1	0.78	0.44	113,113,113,113	0
56	MG	YQ	201	1/1	0.78	0.40	65,65,65,65	0
56	MG	QA	1631	1/1	0.78	0.08	122,122,122,122	0
56	MG	RA	3390	1/1	0.79	0.21	68,68,68,68	0
56	MG	RA	3690	1/1	0.79	0.20	47,47,47,47	0
56	MG	QA	1641	1/1	0.79	0.11	78,78,78,78	0
56	MG	RA	3359	1/1	0.79	0.14	64,64,64,64	0
56	MG	QA	1644	1/1	0.79	0.30	150,150,150,150	0
56	MG	QA	1698	1/1	0.79	0.21	71,71,71,71	0
56	MG	RA	3365	1/1	0.79	0.13	66,66,66,66	0
56	MG	QA	1805	1/1	0.79	0.23	70,70,70,70	0
56	MG	RB	215	1/1	0.79	0.13	58,58,58,58	0
56	MG	QA	1747	1/1	0.79	0.22	65,65,65,65	0
56	MG	RA	3641	1/1	0.79	0.47	110,110,110,110	0
56	MG	RA	3084	1/1	0.79	0.25	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3205	1/1	0.79	0.09	52,52,52,52	0
56	MG	XA	1678	1/1	0.79	0.22	91,91,91,91	0
56	MG	QA	1749	1/1	0.79	0.15	113,113,113,113	0
56	MG	XA	1682	1/1	0.79	0.29	85,85,85,85	0
56	MG	XA	1685	1/1	0.79	0.12	77,77,77,77	0
56	MG	YA	3657	1/1	0.79	0.30	76,76,76,76	0
56	MG	XA	1689	1/1	0.79	0.23	59,59,59,59	0
56	MG	QA	1675	1/1	0.79	0.11	45,45,45,45	0
56	MG	RA	3485	1/1	0.79	0.12	59,59,59,59	0
56	MG	RA	3378	1/1	0.79	0.15	43,43,43,43	0
56	MG	QA	1736	1/1	0.79	0.25	39,39,39,39	0
56	MG	RA	3503	1/1	0.79	0.17	63,63,63,63	0
56	MG	YA	3073	1/1	0.79	0.25	73,73,73,73	0
56	MG	RA	3222	1/1	0.79	0.12	69,69,69,69	0
56	MG	YA	3414	1/1	0.79	0.13	49,49,49,49	0
56	MG	RA	3596	1/1	0.79	0.21	52,52,52,52	0
56	MG	RA	3269	1/1	0.79	0.50	80,80,80,80	0
56	MG	RA	3120	1/1	0.79	0.10	57,57,57,57	0
56	MG	RA	3070	1/1	0.79	0.12	66,66,66,66	0
56	MG	QA	1640	1/1	0.80	0.19	104,104,104,104	0
56	MG	RA	3697	1/1	0.80	0.34	74,74,74,74	0
56	MG	XA	1750	1/1	0.80	0.27	82,82,82,82	0
56	MG	YA	3103	1/1	0.80	0.12	59,59,59,59	0
56	MG	YA	3478	1/1	0.80	0.41	89,89,89,89	0
56	MG	RA	3528	1/1	0.80	0.18	34,34,34,34	0
56	MG	RA	3533	1/1	0.80	0.16	35,35,35,35	0
56	MG	YA	3128	1/1	0.80	0.23	69,69,69,69	0
56	MG	RA	3628	1/1	0.80	0.19	40,40,40,40	0
56	MG	YA	3512	1/1	0.80	0.44	69,69,69,69	0
56	MG	QA	1776	1/1	0.80	0.22	47,47,47,47	0
56	MG	RA	3197	1/1	0.80	0.15	83,83,83,83	0
56	MG	RB	207	1/1	0.80	0.18	67,67,67,67	0
56	MG	RA	3034	1/1	0.80	0.09	35,35,35,35	0
56	MG	XA	1668	1/1	0.80	0.30	87,87,87,87	0
56	MG	RB	214	1/1	0.80	0.14	63,63,63,63	0
56	MG	RA	3001	1/1	0.80	0.20	43,43,43,43	0
56	MG	YA	3179	1/1	0.80	0.24	47,47,47,47	0
56	MG	RA	3145	1/1	0.80	0.09	68,68,68,68	0
56	MG	YA	3197	1/1	0.80	0.19	58,58,58,58	0
56	MG	RA	3453	1/1	0.80	0.16	50,50,50,50	0
56	MG	RA	3375	1/1	0.80	0.39	71,71,71,71	0
56	MG	RA	3132	1/1	0.80	0.15	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3226	1/1	0.80	0.28	79,79,79,79	0
56	MG	RA	3268	1/1	0.80	0.18	80,80,80,80	0
56	MG	YA	3666	1/1	0.80	0.28	86,86,86,86	0
56	MG	RA	3333	1/1	0.80	0.17	32,32,32,32	0
56	MG	YA	3265	1/1	0.80	0.36	58,58,58,58	0
56	MG	RA	3406	1/1	0.80	0.20	35,35,35,35	0
56	MG	RA	3379	1/1	0.80	0.11	44,44,44,44	0
56	MG	RA	3341	1/1	0.80	0.20	39,39,39,39	0
56	MG	RA	3185	1/1	0.80	0.23	70,70,70,70	0
56	MG	QA	1693	1/1	0.80	0.12	59,59,59,59	0
56	MG	RA	3210	1/1	0.80	0.25	115,115,115,115	0
56	MG	YA	3070	1/1	0.80	0.15	67,67,67,67	0
56	MG	YF	301	1/1	0.80	0.23	62,62,62,62	0
56	MG	RA	3229	1/1	0.80	0.19	77,77,77,77	0
56	MG	YI	201	1/1	0.80	0.09	83,83,83,83	0
56	MG	QA	1668	1/1	0.80	0.17	70,70,70,70	0
56	MG	XA	1721	1/1	0.80	0.30	64,64,64,64	0
56	MG	QA	1663	1/1	0.81	0.15	61,61,61,61	0
56	MG	YA	3032	1/1	0.81	0.13	24,24,24,24	0
56	MG	YA	3399	1/1	0.81	0.15	50,50,50,50	0
56	MG	YA	3045	1/1	0.81	0.07	38,38,38,38	0
56	MG	YA	3406	1/1	0.81	0.17	43,43,43,43	0
56	MG	RA	3547	1/1	0.81	0.28	57,57,57,57	0
56	MG	RA	3554	1/1	0.81	0.21	52,52,52,52	0
56	MG	YA	3420	1/1	0.81	0.18	54,54,54,54	0
56	MG	YA	3057	1/1	0.81	0.17	48,48,48,48	0
56	MG	QA	1619	1/1	0.81	0.23	77,77,77,77	0
56	MG	XA	1692	1/1	0.81	0.12	58,58,58,58	0
56	MG	YA	3456	1/1	0.81	0.10	47,47,47,47	0
56	MG	QA	1816	1/1	0.81	0.16	108,108,108,108	0
56	MG	QA	1605	1/1	0.81	0.13	48,48,48,48	0
56	MG	RA	3174	1/1	0.81	0.16	102,102,102,102	0
56	MG	QD	303	1/1	0.81	0.22	90,90,90,90	0
56	MG	RA	3024	1/1	0.81	0.10	44,44,44,44	0
56	MG	YA	3498	1/1	0.81	0.10	23,23,23,23	0
56	MG	RA	3510	1/1	0.81	0.20	80,80,80,80	0
56	MG	XA	1606	1/1	0.81	0.15	50,50,50,50	0
56	MG	RA	3025	1/1	0.81	0.38	109,109,109,109	0
56	MG	RA	3671	1/1	0.81	0.32	79,79,79,79	0
56	MG	QA	1786	1/1	0.81	0.12	45,45,45,45	0
56	MG	XA	1740	1/1	0.81	0.33	69,69,69,69	0
56	MG	XA	1621	1/1	0.81	0.12	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1622	1/1	0.81	0.38	88,88,88,88	0
56	MG	RA	3429	1/1	0.81	0.15	39,39,39,39	0
56	MG	RA	3438	1/1	0.81	0.31	91,91,91,91	0
56	MG	RA	3245	1/1	0.81	0.14	57,57,57,57	0
56	MG	YA	3642	1/1	0.81	0.22	54,54,54,54	0
56	MG	XA	1628	1/1	0.81	0.34	111,111,111,111	0
56	MG	XA	1780	1/1	0.81	0.30	57,57,57,57	0
56	MG	QA	1678	1/1	0.81	0.10	70,70,70,70	0
56	MG	XA	1636	1/1	0.81	0.09	53,53,53,53	0
56	MG	RA	3531	1/1	0.81	0.11	35,35,35,35	0
56	MG	YA	3660	1/1	0.81	0.20	52,52,52,52	0
56	MG	RA	3615	1/1	0.81	0.23	125,125,125,125	0
56	MG	XE	202	1/1	0.81	0.16	63,63,63,63	0
56	MG	RA	3532	1/1	0.81	0.41	69,69,69,69	0
56	MG	RA	3622	1/1	0.81	0.18	58,58,58,58	0
56	MG	R3	101	1/1	0.81	0.12	78,78,78,78	0
56	MG	R5	102	1/1	0.81	0.23	80,80,80,80	0
56	MG	QA	1671	1/1	0.81	0.08	48,48,48,48	0
56	MG	YA	3010	1/1	0.81	0.16	54,54,54,54	0
56	MG	YA	3276	1/1	0.81	0.17	45,45,45,45	0
56	MG	YA	3012	1/1	0.81	0.18	47,47,47,47	0
56	MG	YB	219	1/1	0.81	0.21	52,52,52,52	0
56	MG	QG	201	1/1	0.81	0.12	65,65,65,65	0
56	MG	YA	3331	1/1	0.81	0.21	50,50,50,50	0
56	MG	RA	3638	1/1	0.81	0.25	70,70,70,70	0
56	MG	YA	3360	1/1	0.81	0.20	32,32,32,32	0
56	MG	QA	1811	1/1	0.81	0.14	54,54,54,54	0
56	MG	RE	301	1/1	0.81	0.38	95,95,95,95	0
56	MG	YA	3068	1/1	0.82	0.51	98,98,98,98	0
56	MG	XA	1615	1/1	0.82	0.09	56,56,56,56	0
56	MG	QA	1803	1/1	0.82	0.17	75,75,75,75	0
56	MG	RA	3399	1/1	0.82	0.18	51,51,51,51	0
56	MG	QA	1652	1/1	0.82	0.41	115,115,115,115	0
56	MG	XA	1736	1/1	0.82	0.12	52,52,52,52	0
56	MG	YA	3428	1/1	0.82	0.28	87,87,87,87	0
56	MG	YA	3085	1/1	0.82	0.30	56,56,56,56	0
56	MG	QA	1653	1/1	0.82	0.10	99,99,99,99	0
56	MG	QA	1733	1/1	0.82	0.11	41,41,41,41	0
56	MG	RA	3372	1/1	0.82	0.22	40,40,40,40	0
56	MG	XA	1627	1/1	0.82	0.19	61,61,61,61	0
56	MG	QH	201	1/1	0.82	0.30	54,54,54,54	0
56	MG	RA	3223	1/1	0.82	0.18	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1773	1/1	0.82	0.27	51,51,51,51	0
56	MG	YA	3496	1/1	0.82	0.10	45,45,45,45	0
56	MG	QA	1750	1/1	0.82	0.08	43,43,43,43	0
56	MG	XA	1638	1/1	0.82	0.07	82,82,82,82	0
56	MG	XA	1643	1/1	0.82	0.21	51,51,51,51	0
56	MG	RA	3225	1/1	0.82	0.10	64,64,64,64	0
56	MG	RA	3188	1/1	0.82	0.28	90,90,90,90	0
56	MG	YA	3531	1/1	0.82	0.11	52,52,52,52	0
56	MG	YA	3164	1/1	0.82	0.16	76,76,76,76	0
56	MG	RA	3038	1/1	0.82	0.36	95,95,95,95	0
56	MG	RA	3415	1/1	0.82	0.41	80,80,80,80	0
56	MG	QA	1691	1/1	0.82	0.11	60,60,60,60	0
56	MG	YA	3623	1/1	0.82	0.29	54,54,54,54	0
56	MG	RA	3133	1/1	0.82	0.12	58,58,58,58	0
56	MG	YA	3189	1/1	0.82	0.17	74,74,74,74	0
56	MG	RD	306	1/1	0.82	0.15	64,64,64,64	0
56	MG	RA	3420	1/1	0.82	0.40	116,116,116,116	0
56	MG	QA	1789	1/1	0.82	0.20	70,70,70,70	0
56	MG	YA	3006	1/1	0.82	0.26	47,47,47,47	0
56	MG	YA	3215	1/1	0.82	0.16	65,65,65,65	0
56	MG	RA	3165	1/1	0.82	0.24	56,56,56,56	0
56	MG	RN	201	1/1	0.82	0.10	86,86,86,86	0
56	MG	XA	1679	1/1	0.82	0.27	55,55,55,55	0
56	MG	RA	3168	1/1	0.82	0.18	71,71,71,71	0
56	MG	QA	1761	1/1	0.82	0.31	79,79,79,79	0
56	MG	RA	3650	1/1	0.82	0.28	55,55,55,55	0
56	MG	YA	3674	1/1	0.82	0.23	63,63,63,63	0
56	MG	YA	3289	1/1	0.82	0.26	44,44,44,44	0
56	MG	YA	3687	1/1	0.82	0.22	107,107,107,107	0
56	MG	YA	3689	1/1	0.82	0.12	59,59,59,59	0
56	MG	RA	3653	1/1	0.82	0.25	57,57,57,57	0
56	MG	YA	3702	1/1	0.82	0.20	27,27,27,27	0
56	MG	YA	3313	1/1	0.82	0.16	78,78,78,78	0
56	MG	RA	3137	1/1	0.82	0.18	52,52,52,52	0
56	MG	RA	3014	1/1	0.82	0.24	88,88,88,88	0
56	MG	QA	1637	1/1	0.82	0.08	45,45,45,45	0
56	MG	RA	3495	1/1	0.82	0.18	69,69,69,69	0
56	MG	YA	3372	1/1	0.82	0.12	63,63,63,63	0
56	MG	YA	3375	1/1	0.82	0.10	23,23,23,23	0
56	MG	YA	3377	1/1	0.82	0.34	65,65,65,65	0
56	MG	YA	3056	1/1	0.82	0.21	85,85,85,85	0
56	MG	YG	202	1/1	0.82	0.15	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1602	1/1	0.82	0.44	84,84,84,84	0
56	MG	QA	1741	1/1	0.82	0.09	36,36,36,36	0
56	MG	RA	3451	1/1	0.82	0.29	54,54,54,54	0
56	MG	RA	3629	1/1	0.83	0.15	33,33,33,33	0
56	MG	RA	3294	1/1	0.83	0.11	54,54,54,54	0
56	MG	RA	3446	1/1	0.83	0.27	62,62,62,62	0
56	MG	YA	3492	1/1	0.83	0.28	42,42,42,42	0
56	MG	RA	3633	1/1	0.83	0.23	32,32,32,32	0
56	MG	RA	3162	1/1	0.83	0.35	67,67,67,67	0
56	MG	R7	103	1/1	0.83	0.15	59,59,59,59	0
56	MG	RA	3056	1/1	0.83	0.11	67,67,67,67	0
56	MG	RA	3452	1/1	0.83	0.29	107,107,107,107	0
56	MG	RA	3238	1/1	0.83	0.27	52,52,52,52	0
56	MG	RA	3028	1/1	0.83	0.28	119,119,119,119	0
56	MG	YA	3064	1/1	0.83	0.13	64,64,64,64	0
56	MG	RA	3074	1/1	0.83	0.10	54,54,54,54	0
56	MG	RA	3648	1/1	0.83	0.21	55,55,55,55	0
56	MG	RA	3586	1/1	0.83	0.17	64,64,64,64	0
56	MG	RA	3149	1/1	0.83	0.13	40,40,40,40	0
56	MG	RO	201	1/1	0.83	0.13	45,45,45,45	0
56	MG	QA	1625	1/1	0.83	0.08	38,38,38,38	0
56	MG	RA	3459	1/1	0.83	0.13	57,57,57,57	0
56	MG	YA	3634	1/1	0.83	0.14	11,11,11,11	0
56	MG	YA	3084	1/1	0.83	0.28	87,87,87,87	0
56	MG	YA	3354	1/1	0.83	0.30	47,47,47,47	0
56	MG	YA	3358	1/1	0.83	0.19	44,44,44,44	0
56	MG	RA	3195	1/1	0.83	0.17	64,64,64,64	0
56	MG	QA	1685	1/1	0.83	0.22	36,36,36,36	0
56	MG	YA	3656	1/1	0.83	0.22	34,34,34,34	0
56	MG	RA	3251	1/1	0.83	0.15	47,47,47,47	0
56	MG	YA	3373	1/1	0.83	0.26	47,47,47,47	0
56	MG	RA	3254	1/1	0.83	0.26	50,50,50,50	0
56	MG	YA	3104	1/1	0.83	0.21	50,50,50,50	0
56	MG	YA	3106	1/1	0.83	0.09	52,52,52,52	0
56	MG	QA	1677	1/1	0.83	0.19	37,37,37,37	0
56	MG	YA	3388	1/1	0.83	0.27	86,86,86,86	0
56	MG	YA	3684	1/1	0.83	0.28	70,70,70,70	0
56	MG	YA	3115	1/1	0.83	0.11	69,69,69,69	0
56	MG	RA	3061	1/1	0.83	0.14	49,49,49,49	0
56	MG	XT	201	1/1	0.83	0.13	55,55,55,55	0
56	MG	XA	1683	1/1	0.83	0.16	67,67,67,67	0
56	MG	RA	3264	1/1	0.83	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3148	1/1	0.83	0.10	35,35,35,35	0
56	MG	Y6	102	1/1	0.83	0.35	54,54,54,54	0
56	MG	XA	1610	1/1	0.83	0.10	73,73,73,73	0
56	MG	RA	3035	1/1	0.83	0.29	75,75,75,75	0
56	MG	QD	305	1/1	0.83	0.15	67,67,67,67	0
56	MG	YA	3436	1/1	0.83	0.31	59,59,59,59	0
56	MG	YA	3439	1/1	0.83	0.11	64,64,64,64	0
56	MG	QA	1815	1/1	0.83	0.07	75,75,75,75	0
56	MG	RA	3285	1/1	0.83	0.12	70,70,70,70	0
56	MG	YA	3457	1/1	0.83	0.08	47,47,47,47	0
56	MG	YA	3174	1/1	0.83	0.07	64,64,64,64	0
56	MG	RA	3290	1/1	0.83	0.10	59,59,59,59	0
56	MG	RV	202	1/1	0.84	0.08	37,37,37,37	0
56	MG	RA	3604	1/1	0.84	0.13	67,67,67,67	0
56	MG	YA	3185	1/1	0.84	0.14	50,50,50,50	0
56	MG	RA	3669	1/1	0.84	0.26	82,82,82,82	0
56	MG	QA	1766	1/1	0.84	0.06	63,63,63,63	0
56	MG	YA	3488	1/1	0.84	0.23	26,26,26,26	0
56	MG	YA	3192	1/1	0.84	0.10	49,49,49,49	0
56	MG	RA	3608	1/1	0.84	0.13	57,57,57,57	0
56	MG	RA	3130	1/1	0.84	0.12	54,54,54,54	0
56	MG	YA	3043	1/1	0.84	0.20	37,37,37,37	0
56	MG	R3	102	1/1	0.84	0.19	83,83,83,83	0
56	MG	XA	1710	1/1	0.84	0.20	51,51,51,51	0
56	MG	YA	3221	1/1	0.84	0.12	34,34,34,34	0
56	MG	QA	1680	1/1	0.84	0.16	58,58,58,58	0
56	MG	RA	3686	1/1	0.84	0.10	65,65,65,65	0
56	MG	RA	3619	1/1	0.84	0.22	38,38,38,38	0
56	MG	RA	3315	1/1	0.84	0.19	74,74,74,74	0
56	MG	YA	3271	1/1	0.84	0.08	28,28,28,28	0
56	MG	RA	3018	1/1	0.84	0.12	43,43,43,43	0
56	MG	XA	1724	1/1	0.84	0.25	55,55,55,55	0
56	MG	QA	1782	1/1	0.84	0.58	80,80,80,80	0
56	MG	YA	3307	1/1	0.84	0.11	41,41,41,41	0
56	MG	RA	3252	1/1	0.84	0.21	33,33,33,33	0
56	MG	RA	3708	1/1	0.84	0.41	56,56,56,56	0
56	MG	RA	3105	1/1	0.84	0.09	41,41,41,41	0
56	MG	YA	3336	1/1	0.84	0.15	25,25,25,25	0
56	MG	YA	3343	1/1	0.84	0.17	32,32,32,32	0
56	MG	QL	202	1/1	0.84	0.13	54,54,54,54	0
56	MG	RA	3044	1/1	0.84	0.12	55,55,55,55	0
56	MG	RA	3498	1/1	0.84	0.33	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3563	1/1	0.84	0.27	43,43,43,43	0
56	MG	XA	1774	1/1	0.84	0.21	51,51,51,51	0
56	MG	QA	1744	1/1	0.84	0.23	68,68,68,68	0
56	MG	QA	1817	1/1	0.84	0.15	52,52,52,52	0
56	MG	RA	3385	1/1	0.84	0.15	42,42,42,42	0
56	MG	RA	3584	1/1	0.84	0.26	107,107,107,107	0
56	MG	QF	202	1/1	0.84	0.24	82,82,82,82	0
56	MG	RG	204	1/1	0.84	0.07	74,74,74,74	0
56	MG	RA	3588	1/1	0.84	0.15	40,40,40,40	0
56	MG	XF	201	1/1	0.84	0.19	80,80,80,80	0
56	MG	QA	1818	1/1	0.84	0.34	71,71,71,71	0
56	MG	YA	3146	1/1	0.84	0.09	18,18,18,18	0
56	MG	RA	3177	1/1	0.84	0.13	51,51,51,51	0
56	MG	YA	3408	1/1	0.84	0.10	35,35,35,35	0
56	MG	XA	1672	1/1	0.84	0.20	108,108,108,108	0
56	MG	RA	3512	1/1	0.84	0.10	38,38,38,38	0
56	MG	RA	3233	1/1	0.84	0.36	83,83,83,83	0
56	MG	RA	3092	1/1	0.84	0.10	76,76,76,76	0
56	MG	RA	3658	1/1	0.84	0.19	49,49,49,49	0
56	MG	RA	3127	1/1	0.84	0.08	53,53,53,53	0
56	MG	RU	202	1/1	0.84	0.53	63,63,63,63	0
56	MG	YA	3169	1/1	0.84	0.22	65,65,65,65	0
56	MG	YA	3170	1/1	0.84	0.14	77,77,77,77	0
56	MG	YA	3451	1/1	0.84	0.14	45,45,45,45	0
56	MG	QA	1614	1/1	0.84	0.09	82,82,82,82	0
56	MG	YA	3244	1/1	0.85	0.24	47,47,47,47	0
56	MG	RH	201	1/1	0.85	0.06	68,68,68,68	0
56	MG	RA	3443	1/1	0.85	0.31	49,49,49,49	0
56	MG	YA	3256	1/1	0.85	0.16	47,47,47,47	0
56	MG	YA	3263	1/1	0.85	0.18	43,43,43,43	0
56	MG	QA	1764	1/1	0.85	0.09	41,41,41,41	0
56	MG	RA	3111	1/1	0.85	0.23	97,97,97,97	0
56	MG	XA	1663	1/1	0.85	0.20	50,50,50,50	0
56	MG	RA	3663	1/1	0.85	0.45	90,90,90,90	0
56	MG	QV	105	1/1	0.85	0.19	80,80,80,80	0
56	MG	YA	3301	1/1	0.85	0.38	58,58,58,58	0
56	MG	RA	3262	1/1	0.85	0.09	54,54,54,54	0
56	MG	YA	3096	1/1	0.85	0.06	40,40,40,40	0
56	MG	XA	1783	1/1	0.85	0.12	46,46,46,46	0
56	MG	YA	3321	1/1	0.85	0.18	66,66,66,66	0
56	MG	RA	3031	1/1	0.85	0.13	53,53,53,53	0
56	MG	RA	3265	1/1	0.85	0.18	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1677	1/1	0.85	0.06	41,41,41,41	0
56	MG	QA	1650	1/1	0.85	0.07	60,60,60,60	0
56	MG	QA	1711	1/1	0.85	0.25	49,49,49,49	0
56	MG	RA	3546	1/1	0.85	0.30	81,81,81,81	0
56	MG	YA	3639	1/1	0.85	0.17	45,45,45,45	0
56	MG	XA	1681	1/1	0.85	0.29	43,43,43,43	0
56	MG	XV	101	1/1	0.85	0.17	41,41,41,41	0
56	MG	RA	3680	1/1	0.85	0.22	59,59,59,59	0
56	MG	RA	3335	1/1	0.85	0.31	41,41,41,41	0
56	MG	QA	1634	1/1	0.85	0.13	70,70,70,70	0
56	MG	RA	3278	1/1	0.85	0.08	37,37,37,37	0
56	MG	QA	1696	1/1	0.85	0.20	49,49,49,49	0
56	MG	RA	3505	1/1	0.85	0.34	60,60,60,60	0
56	MG	YA	3011	1/1	0.85	0.23	75,75,75,75	0
56	MG	RA	3506	1/1	0.85	0.12	39,39,39,39	0
56	MG	RA	3575	1/1	0.85	0.23	51,51,51,51	0
56	MG	YA	3670	1/1	0.85	0.30	101,101,101,101	0
56	MG	XA	1620	1/1	0.85	0.14	46,46,46,46	0
56	MG	RA	3635	1/1	0.85	0.10	45,45,45,45	0
56	MG	YA	3407	1/1	0.85	0.14	44,44,44,44	0
56	MG	YA	3171	1/1	0.85	0.20	61,61,61,61	0
56	MG	RA	3288	1/1	0.85	0.20	74,74,74,74	0
56	MG	RA	3581	1/1	0.85	0.20	54,54,54,54	0
56	MG	YA	3418	1/1	0.85	0.26	55,55,55,55	0
56	MG	RA	3389	1/1	0.85	0.27	72,72,72,72	0
56	MG	YA	3423	1/1	0.85	0.21	29,29,29,29	0
56	MG	RA	3585	1/1	0.85	0.23	53,53,53,53	0
56	MG	RA	3243	1/1	0.85	0.24	51,51,51,51	0
56	MG	RB	212	1/1	0.85	0.08	53,53,53,53	0
56	MG	QA	1692	1/1	0.85	0.21	71,71,71,71	0
56	MG	R7	101	1/1	0.85	0.20	68,68,68,68	0
56	MG	YE	302	1/1	0.85	0.39	82,82,82,82	0
56	MG	QA	1775	1/1	0.85	0.10	82,82,82,82	0
56	MG	QA	1679	1/1	0.85	0.13	35,35,35,35	0
56	MG	YA	3059	1/1	0.85	0.18	42,42,42,42	0
56	MG	QA	1801	1/1	0.85	0.11	66,66,66,66	0
56	MG	YP	201	1/1	0.85	0.14	32,32,32,32	0
56	MG	RA	3108	1/1	0.85	0.11	60,60,60,60	0
56	MG	XA	1759	1/1	0.85	0.11	71,71,71,71	0
56	MG	QA	1667	1/1	0.86	0.13	55,55,55,55	0
56	MG	YA	3429	1/1	0.86	0.11	43,43,43,43	0
56	MG	RA	3434	1/1	0.86	0.12	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3437	1/1	0.86	0.30	42,42,42,42	0
56	MG	YA	3193	1/1	0.86	0.12	44,44,44,44	0
56	MG	YA	3443	1/1	0.86	0.14	43,43,43,43	0
56	MG	RA	3260	1/1	0.86	0.13	47,47,47,47	0
56	MG	RA	3386	1/1	0.86	0.12	44,44,44,44	0
56	MG	YA	3046	1/1	0.86	0.28	51,51,51,51	0
56	MG	YA	3210	1/1	0.86	0.15	77,77,77,77	0
56	MG	XA	1603	1/1	0.86	0.16	92,92,92,92	0
56	MG	YA	3474	1/1	0.86	0.23	42,42,42,42	0
56	MG	RA	3043	1/1	0.86	0.17	52,52,52,52	0
56	MG	RA	3082	1/1	0.86	0.42	86,86,86,86	0
56	MG	YA	3225	1/1	0.86	0.15	48,48,48,48	0
56	MG	RA	3444	1/1	0.86	0.08	63,63,63,63	0
56	MG	YA	3235	1/1	0.86	0.15	30,30,30,30	0
56	MG	QD	301	1/1	0.86	0.23	56,56,56,56	0
56	MG	QA	1806	1/1	0.86	0.31	85,85,85,85	0
56	MG	YA	3252	1/1	0.86	0.19	22,22,22,22	0
56	MG	RA	3046	1/1	0.86	0.10	38,38,38,38	0
56	MG	YA	3507	1/1	0.86	0.20	81,81,81,81	0
56	MG	YA	3508	1/1	0.86	0.18	38,38,38,38	0
56	MG	YA	3254	1/1	0.86	0.13	40,40,40,40	0
56	MG	RA	3598	1/1	0.86	0.13	30,30,30,30	0
56	MG	YA	3522	1/1	0.86	0.30	31,31,31,31	0
56	MG	RA	3048	1/1	0.86	0.11	46,46,46,46	0
56	MG	RA	3357	1/1	0.86	0.22	47,47,47,47	0
56	MG	YA	3542	1/1	0.86	0.15	28,28,28,28	0
56	MG	YA	3546	1/1	0.86	0.31	73,73,73,73	0
56	MG	YA	3267	1/1	0.86	0.22	37,37,37,37	0
56	MG	RA	3169	1/1	0.86	0.15	93,93,93,93	0
56	MG	YA	3577	1/1	0.86	0.17	29,29,29,29	0
56	MG	YA	3595	1/1	0.86	0.16	52,52,52,52	0
56	MG	RA	3398	1/1	0.86	0.41	97,97,97,97	0
56	MG	RA	3199	1/1	0.86	0.17	45,45,45,45	0
56	MG	YA	3622	1/1	0.86	0.12	18,18,18,18	0
56	MG	RA	3699	1/1	0.86	0.31	96,96,96,96	0
56	MG	XA	1762	1/1	0.86	0.29	36,36,36,36	0
56	MG	YA	3627	1/1	0.86	0.19	37,37,37,37	0
56	MG	YA	3306	1/1	0.86	0.25	37,37,37,37	0
56	MG	RA	3700	1/1	0.86	0.17	72,72,72,72	0
56	MG	RA	3704	1/1	0.86	0.18	40,40,40,40	0
56	MG	RA	3456	1/1	0.86	0.31	63,63,63,63	0
56	MG	RA	3115	1/1	0.86	0.08	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3364	1/1	0.86	0.20	37,37,37,37	0
56	MG	RA	3203	1/1	0.86	0.41	95,95,95,95	0
56	MG	YA	3338	1/1	0.86	0.29	33,33,33,33	0
56	MG	RA	3529	1/1	0.86	0.23	34,34,34,34	0
56	MG	RA	3367	1/1	0.86	0.15	69,69,69,69	0
56	MG	RA	3118	1/1	0.86	0.23	98,98,98,98	0
56	MG	RA	3371	1/1	0.86	0.29	117,117,117,117	0
56	MG	YA	3126	1/1	0.86	0.30	72,72,72,72	0
56	MG	YA	3364	1/1	0.86	0.20	34,34,34,34	0
56	MG	RA	3141	1/1	0.86	0.20	49,49,49,49	0
56	MG	YA	3367	1/1	0.86	0.12	61,61,61,61	0
56	MG	RA	3466	1/1	0.86	0.12	29,29,29,29	0
56	MG	YA	3140	1/1	0.86	0.18	41,41,41,41	0
56	MG	YA	3374	1/1	0.86	0.16	84,84,84,84	0
56	MG	RA	3206	1/1	0.86	0.31	89,89,89,89	0
56	MG	XA	1665	1/1	0.86	0.15	81,81,81,81	0
56	MG	QD	304	1/1	0.86	0.13	73,73,73,73	0
56	MG	RD	307	1/1	0.86	0.08	73,73,73,73	0
56	MG	RD	308	1/1	0.86	0.19	75,75,75,75	0
56	MG	QA	1726	1/1	0.86	0.14	61,61,61,61	0
56	MG	RA	3122	1/1	0.86	0.16	90,90,90,90	0
56	MG	RA	3212	1/1	0.86	0.27	70,70,70,70	0
56	MG	QA	1727	1/1	0.86	0.17	46,46,46,46	0
56	MG	YB	216	1/1	0.86	0.21	46,46,46,46	0
56	MG	RA	3418	1/1	0.86	0.21	56,56,56,56	0
56	MG	RA	3478	1/1	0.86	0.21	32,32,32,32	0
56	MG	RA	3006	1/1	0.86	0.13	72,72,72,72	0
56	MG	RA	3569	1/1	0.86	0.41	72,72,72,72	0
56	MG	YA	3415	1/1	0.86	0.70	84,84,84,84	0
56	MG	YA	3416	1/1	0.86	0.12	43,43,43,43	0
56	MG	QE	202	1/1	0.86	0.21	109,109,109,109	0
56	MG	QA	1638	1/1	0.86	0.39	103,103,103,103	0
56	MG	YA	3181	1/1	0.86	0.15	47,47,47,47	0
56	MG	RA	3040	1/1	0.86	0.10	40,40,40,40	0
59	ZN	R4	101	1/1	0.86	0.11	285,285,285,285	0
56	MG	RA	3236	1/1	0.87	0.26	80,80,80,80	0
56	MG	YA	3100	1/1	0.87	0.09	41,41,41,41	0
56	MG	RA	3270	1/1	0.87	0.26	73,73,73,73	0
56	MG	RA	3530	1/1	0.87	0.12	101,101,101,101	0
56	MG	XA	1792	1/1	0.87	0.16	70,70,70,70	0
56	MG	YA	3280	1/1	0.87	0.20	15,15,15,15	0
56	MG	QA	1710	1/1	0.87	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3432	1/1	0.87	0.22	88,88,88,88	0
56	MG	YA	3500	1/1	0.87	0.23	30,30,30,30	0
56	MG	QA	1735	1/1	0.87	0.17	34,34,34,34	0
56	MG	RA	3354	1/1	0.87	0.23	56,56,56,56	0
56	MG	RR	201	1/1	0.87	0.22	74,74,74,74	0
56	MG	YA	3129	1/1	0.87	0.16	47,47,47,47	0
56	MG	RT	202	1/1	0.87	0.15	82,82,82,82	0
56	MG	QA	1639	1/1	0.87	0.18	57,57,57,57	0
56	MG	YA	3327	1/1	0.87	0.31	39,39,39,39	0
56	MG	YA	3533	1/1	0.87	0.12	40,40,40,40	0
56	MG	YA	3534	1/1	0.87	0.11	18,18,18,18	0
56	MG	QA	1697	1/1	0.87	0.25	58,58,58,58	0
56	MG	RA	3047	1/1	0.87	0.18	65,65,65,65	0
56	MG	Y3	101	1/1	0.87	0.24	38,38,38,38	0
56	MG	YA	3149	1/1	0.87	0.42	77,77,77,77	0
56	MG	RA	3097	1/1	0.87	0.35	77,77,77,77	0
56	MG	YA	3582	1/1	0.87	0.27	59,59,59,59	0
56	MG	YA	3586	1/1	0.87	0.08	44,44,44,44	0
56	MG	YA	3349	1/1	0.87	0.29	70,70,70,70	0
56	MG	RA	3297	1/1	0.87	0.16	38,38,38,38	0
56	MG	YA	3154	1/1	0.87	0.20	57,57,57,57	0
56	MG	YA	3157	1/1	0.87	0.13	39,39,39,39	0
56	MG	YA	3361	1/1	0.87	0.12	53,53,53,53	0
56	MG	RA	3693	1/1	0.87	0.32	77,77,77,77	0
56	MG	QA	1654	1/1	0.87	0.12	92,92,92,92	0
56	MG	RA	3550	1/1	0.87	0.33	70,70,70,70	0
56	MG	RA	3248	1/1	0.87	0.25	38,38,38,38	0
56	MG	RA	3702	1/1	0.87	0.11	41,41,41,41	0
56	MG	RA	3193	1/1	0.87	0.17	90,90,90,90	0
56	MG	YA	3023	1/1	0.87	0.47	90,90,90,90	0
56	MG	RA	3308	1/1	0.87	0.12	25,25,25,25	0
56	MG	YA	3644	1/1	0.87	0.22	38,38,38,38	0
56	MG	YA	3647	1/1	0.87	0.41	54,54,54,54	0
56	MG	RA	3101	1/1	0.87	0.32	60,60,60,60	0
56	MG	RA	3102	1/1	0.87	0.18	48,48,48,48	0
56	MG	QA	1701	1/1	0.87	0.17	67,67,67,67	0
56	MG	QA	1622	1/1	0.87	0.11	60,60,60,60	0
56	MG	YA	3398	1/1	0.87	0.13	43,43,43,43	0
56	MG	YA	3658	1/1	0.87	0.24	36,36,36,36	0
56	MG	QA	1670	1/1	0.87	0.13	37,37,37,37	0
56	MG	YA	3662	1/1	0.87	0.22	39,39,39,39	0
56	MG	YA	3188	1/1	0.87	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1768	1/1	0.87	0.23	51,51,51,51	0
56	MG	RA	3643	1/1	0.87	0.11	44,44,44,44	0
56	MG	RA	3413	1/1	0.87	0.32	72,72,72,72	0
56	MG	YA	3194	1/1	0.87	0.21	50,50,50,50	0
56	MG	YA	3413	1/1	0.87	0.24	46,46,46,46	0
56	MG	YA	3679	1/1	0.87	0.15	49,49,49,49	0
56	MG	XA	1633	1/1	0.87	0.06	45,45,45,45	0
56	MG	XA	1744	1/1	0.87	0.17	72,72,72,72	0
56	MG	RA	3508	1/1	0.87	0.13	50,50,50,50	0
56	MG	QA	1769	1/1	0.87	0.12	68,68,68,68	0
56	MG	XA	1752	1/1	0.87	0.12	38,38,38,38	0
56	MG	YA	3214	1/1	0.87	0.25	66,66,66,66	0
56	MG	YB	202	1/1	0.87	0.14	91,91,91,91	0
56	MG	YB	204	1/1	0.87	0.10	46,46,46,46	0
56	MG	YA	3424	1/1	0.87	0.30	70,70,70,70	0
56	MG	YB	210	1/1	0.87	0.20	44,44,44,44	0
56	MG	XA	1755	1/1	0.87	0.14	45,45,45,45	0
56	MG	YA	3216	1/1	0.87	0.07	38,38,38,38	0
56	MG	RA	3156	1/1	0.87	0.14	76,76,76,76	0
56	MG	RA	3328	1/1	0.87	0.25	40,40,40,40	0
56	MG	XA	1646	1/1	0.87	0.21	92,92,92,92	0
56	MG	YA	3234	1/1	0.87	0.12	60,60,60,60	0
56	MG	RA	3158	1/1	0.87	0.05	63,63,63,63	0
56	MG	YA	3243	1/1	0.87	0.15	48,48,48,48	0
56	MG	RA	3231	1/1	0.87	0.30	91,91,91,91	0
56	MG	RA	3464	1/1	0.87	0.35	118,118,118,118	0
56	MG	RG	201	1/1	0.87	0.07	79,79,79,79	0
56	MG	YA	3460	1/1	0.87	0.24	48,48,48,48	0
56	MG	RA	3660	1/1	0.87	0.39	62,62,62,62	0
56	MG	RA	3267	1/1	0.87	0.26	45,45,45,45	0
56	MG	RA	3089	1/1	0.87	0.07	35,35,35,35	0
56	MG	YA	3316	1/1	0.88	0.31	44,44,44,44	0
56	MG	YA	3510	1/1	0.88	0.21	49,49,49,49	0
56	MG	YA	3026	1/1	0.88	0.14	43,43,43,43	0
56	MG	YA	3513	1/1	0.88	0.09	38,38,38,38	0
56	MG	QA	1651	1/1	0.88	0.26	91,91,91,91	0
56	MG	YA	3519	1/1	0.88	0.14	48,48,48,48	0
56	MG	XA	1650	1/1	0.88	0.08	54,54,54,54	0
56	MG	YA	3031	1/1	0.88	0.24	58,58,58,58	0
56	MG	YA	3528	1/1	0.88	0.16	18,18,18,18	0
56	MG	YA	3161	1/1	0.88	0.13	65,65,65,65	0
56	MG	RA	3445	1/1	0.88	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3034	1/1	0.88	0.19	41,41,41,41	0
56	MG	YA	3167	1/1	0.88	0.33	51,51,51,51	0
56	MG	QA	1664	1/1	0.88	0.15	60,60,60,60	0
56	MG	RA	3261	1/1	0.88	0.07	36,36,36,36	0
56	MG	YA	3552	1/1	0.88	0.19	16,16,16,16	0
56	MG	RA	3307	1/1	0.88	0.12	35,35,35,35	0
56	MG	RA	3131	1/1	0.88	0.23	58,58,58,58	0
56	MG	YA	3579	1/1	0.88	0.13	43,43,43,43	0
56	MG	RA	3645	1/1	0.88	0.20	42,42,42,42	0
56	MG	YA	3585	1/1	0.88	0.14	45,45,45,45	0
56	MG	RA	3202	1/1	0.88	0.13	49,49,49,49	0
56	MG	YA	3180	1/1	0.88	0.20	57,57,57,57	0
56	MG	RW	201	1/1	0.88	0.07	57,57,57,57	0
56	MG	YA	3611	1/1	0.88	0.15	49,49,49,49	0
56	MG	RA	3065	1/1	0.88	0.15	66,66,66,66	0
56	MG	RA	3709	1/1	0.88	0.37	120,120,120,120	0
56	MG	QA	1729	1/1	0.88	0.27	36,36,36,36	0
56	MG	QA	1788	1/1	0.88	0.11	51,51,51,51	0
56	MG	YA	3378	1/1	0.88	0.12	95,95,95,95	0
56	MG	QA	1763	1/1	0.88	0.11	41,41,41,41	0
56	MG	XA	1608	1/1	0.88	0.40	71,71,71,71	0
56	MG	RA	3321	1/1	0.88	0.23	54,54,54,54	0
56	MG	YA	3196	1/1	0.88	0.14	70,70,70,70	0
56	MG	RA	3366	1/1	0.88	0.68	98,98,98,98	0
56	MG	YA	3077	1/1	0.88	0.21	69,69,69,69	0
56	MG	RA	3422	1/1	0.88	0.17	46,46,46,46	0
56	MG	YA	3206	1/1	0.88	0.26	77,77,77,77	0
56	MG	QA	1748	1/1	0.88	0.13	38,38,38,38	0
56	MG	RA	3073	1/1	0.88	0.26	104,104,104,104	0
56	MG	R3	103	1/1	0.88	0.41	111,111,111,111	0
56	MG	RA	3327	1/1	0.88	0.29	68,68,68,68	0
56	MG	XA	1691	1/1	0.88	0.32	51,51,51,51	0
56	MG	QA	1730	1/1	0.88	0.30	73,73,73,73	0
56	MG	YA	3659	1/1	0.88	0.10	39,39,39,39	0
56	MG	RA	3564	1/1	0.88	0.12	41,41,41,41	0
56	MG	RA	3230	1/1	0.88	0.27	41,41,41,41	0
56	MG	YA	3228	1/1	0.88	0.28	63,63,63,63	0
56	MG	RA	3467	1/1	0.88	0.12	55,55,55,55	0
56	MG	QA	1714	1/1	0.88	0.19	76,76,76,76	0
56	MG	YA	3669	1/1	0.88	0.12	56,56,56,56	0
56	MG	YA	3109	1/1	0.88	0.06	54,54,54,54	0
56	MG	YA	3427	1/1	0.88	0.16	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1703	1/1	0.88	0.21	55,55,55,55	0
56	MG	XA	1705	1/1	0.88	0.18	50,50,50,50	0
56	MG	YA	3680	1/1	0.88	0.20	133,133,133,133	0
56	MG	YA	3248	1/1	0.88	0.32	52,52,52,52	0
56	MG	YA	3118	1/1	0.88	0.12	34,34,34,34	0
56	MG	YA	3688	1/1	0.88	0.15	51,51,51,51	0
56	MG	XA	1629	1/1	0.88	0.23	71,71,71,71	0
56	MG	YA	3002	1/1	0.88	0.13	45,45,45,45	0
56	MG	RA	3255	1/1	0.88	0.29	35,35,35,35	0
56	MG	YA	3447	1/1	0.88	0.15	42,42,42,42	0
56	MG	YA	3706	1/1	0.88	0.19	82,82,82,82	0
56	MG	YA	3259	1/1	0.88	0.06	24,24,24,24	0
56	MG	YA	3262	1/1	0.88	0.06	32,32,32,32	0
56	MG	YA	3008	1/1	0.88	0.07	67,67,67,67	0
56	MG	YA	3130	1/1	0.88	0.07	28,28,28,28	0
56	MG	RA	3470	1/1	0.88	0.31	88,88,88,88	0
56	MG	YA	3473	1/1	0.88	0.12	66,66,66,66	0
56	MG	RA	3179	1/1	0.88	0.14	51,51,51,51	0
56	MG	YA	3475	1/1	0.88	0.27	47,47,47,47	0
56	MG	YA	3142	1/1	0.88	0.14	39,39,39,39	0
56	MG	RA	3687	1/1	0.88	0.38	148,148,148,148	0
56	MG	YD	307	1/1	0.88	0.19	40,40,40,40	0
56	MG	RA	3583	1/1	0.88	0.07	44,44,44,44	0
56	MG	XA	1645	1/1	0.88	0.16	67,67,67,67	0
56	MG	YA	3296	1/1	0.88	0.08	39,39,39,39	0
56	MG	YA	3019	1/1	0.88	0.19	67,67,67,67	0
56	MG	YA	3150	1/1	0.88	0.11	50,50,50,50	0
56	MG	RA	3344	1/1	0.88	0.24	41,41,41,41	0
56	MG	XA	1648	1/1	0.88	0.08	67,67,67,67	0
56	MG	YA	3311	1/1	0.88	0.22	55,55,55,55	0
56	MG	YA	3153	1/1	0.88	0.10	52,52,52,52	0
59	ZN	Y4	101	1/1	0.88	0.07	284,284,284,284	0
56	MG	YA	3342	1/1	0.89	0.29	23,23,23,23	0
56	MG	QA	1819	1/1	0.89	0.19	46,46,46,46	0
56	MG	RQ	202	1/1	0.89	0.11	45,45,45,45	0
56	MG	XA	1756	1/1	0.89	0.09	35,35,35,35	0
56	MG	RQ	204	1/1	0.89	0.08	49,49,49,49	0
56	MG	XA	1659	1/1	0.89	0.08	40,40,40,40	0
56	MG	YA	3359	1/1	0.89	0.28	31,31,31,31	0
56	MG	YA	3183	1/1	0.89	0.08	39,39,39,39	0
56	MG	RA	3296	1/1	0.89	0.21	45,45,45,45	0
56	MG	QI	201	1/1	0.89	0.11	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RT	204	1/1	0.89	0.08	57,57,57,57	0
56	MG	RU	201	1/1	0.89	0.07	43,43,43,43	0
56	MG	YA	3565	1/1	0.89	0.15	45,45,45,45	0
56	MG	YA	3191	1/1	0.89	0.13	38,38,38,38	0
56	MG	XA	1666	1/1	0.89	0.07	59,59,59,59	0
56	MG	RA	3099	1/1	0.89	0.06	40,40,40,40	0
56	MG	RA	3425	1/1	0.89	0.17	53,53,53,53	0
56	MG	QA	1778	1/1	0.89	0.08	50,50,50,50	0
56	MG	YA	3588	1/1	0.89	0.17	45,45,45,45	0
56	MG	RV	203	1/1	0.89	0.18	56,56,56,56	0
56	MG	YA	3596	1/1	0.89	0.24	50,50,50,50	0
56	MG	YA	3605	1/1	0.89	0.23	74,74,74,74	0
56	MG	YA	3198	1/1	0.89	0.10	43,43,43,43	0
56	MG	YA	3385	1/1	0.89	0.35	62,62,62,62	0
56	MG	YA	3199	1/1	0.89	0.19	84,84,84,84	0
56	MG	RA	3427	1/1	0.89	0.16	39,39,39,39	0
56	MG	XA	1784	1/1	0.89	0.20	33,33,33,33	0
56	MG	XA	1785	1/1	0.89	0.20	38,38,38,38	0
56	MG	XA	1674	1/1	0.89	0.15	28,28,28,28	0
56	MG	RA	3346	1/1	0.89	0.20	65,65,65,65	0
56	MG	YA	3401	1/1	0.89	0.16	41,41,41,41	0
56	MG	YA	3403	1/1	0.89	0.09	53,53,53,53	0
56	MG	QA	1780	1/1	0.89	0.08	43,43,43,43	0
56	MG	RA	3537	1/1	0.89	0.10	23,23,23,23	0
56	MG	RA	3539	1/1	0.89	0.13	26,26,26,26	0
56	MG	RA	3541	1/1	0.89	0.16	30,30,30,30	0
56	MG	YA	3223	1/1	0.89	0.17	34,34,34,34	0
56	MG	RB	203	1/1	0.89	0.07	68,68,68,68	0
56	MG	RA	3602	1/1	0.89	0.37	66,66,66,66	0
56	MG	YA	3651	1/1	0.89	0.27	43,43,43,43	0
56	MG	RA	3656	1/1	0.89	0.27	57,57,57,57	0
56	MG	YA	3113	1/1	0.89	0.25	72,72,72,72	0
56	MG	XV	103	1/1	0.89	0.11	40,40,40,40	0
56	MG	QA	1687	1/1	0.89	0.06	40,40,40,40	0
56	MG	RA	3501	1/1	0.89	0.12	41,41,41,41	0
56	MG	RA	3247	1/1	0.89	0.09	46,46,46,46	0
56	MG	RA	3088	1/1	0.89	0.08	77,77,77,77	0
56	MG	QA	1623	1/1	0.89	0.54	86,86,86,86	0
56	MG	RA	3407	1/1	0.89	0.11	59,59,59,59	0
56	MG	RA	3090	1/1	0.89	0.10	52,52,52,52	0
56	MG	YA	3135	1/1	0.89	0.27	56,56,56,56	0
56	MG	YA	3139	1/1	0.89	0.08	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3261	1/1	0.89	0.20	67,67,67,67	0
56	MG	RA	3076	1/1	0.89	0.18	72,72,72,72	0
56	MG	YA	3445	1/1	0.89	0.06	67,67,67,67	0
56	MG	YA	3141	1/1	0.89	0.10	58,58,58,58	0
56	MG	RA	3232	1/1	0.89	0.24	69,69,69,69	0
56	MG	RF	301	1/1	0.89	0.23	72,72,72,72	0
56	MG	YA	3268	1/1	0.89	0.25	77,77,77,77	0
56	MG	RA	3282	1/1	0.89	0.24	25,25,25,25	0
56	MG	YA	3691	1/1	0.89	0.20	44,44,44,44	0
56	MG	XA	1711	1/1	0.89	0.16	46,46,46,46	0
56	MG	YA	3472	1/1	0.89	0.13	45,45,45,45	0
56	MG	XA	1632	1/1	0.89	0.14	34,34,34,34	0
56	MG	YA	3705	1/1	0.89	0.13	77,77,77,77	0
56	MG	YA	3284	1/1	0.89	0.25	15,15,15,15	0
56	MG	RA	3672	1/1	0.89	0.18	38,38,38,38	0
56	MG	RA	3283	1/1	0.89	0.21	41,41,41,41	0
56	MG	RA	3676	1/1	0.89	0.41	108,108,108,108	0
56	MG	YA	3298	1/1	0.89	0.20	13,13,13,13	0
56	MG	YA	3484	1/1	0.89	0.11	45,45,45,45	0
56	MG	XA	1722	1/1	0.89	0.32	58,58,58,58	0
56	MG	QA	1669	1/1	0.89	0.19	74,74,74,74	0
56	MG	YA	3491	1/1	0.89	0.20	28,28,28,28	0
56	MG	YB	218	1/1	0.89	0.10	38,38,38,38	0
56	MG	RA	3287	1/1	0.89	0.18	37,37,37,37	0
56	MG	YA	3030	1/1	0.89	0.18	48,48,48,48	0
56	MG	YD	303	1/1	0.89	0.23	44,44,44,44	0
56	MG	QA	1743	1/1	0.89	0.11	66,66,66,66	0
56	MG	RA	3685	1/1	0.89	0.09	58,58,58,58	0
56	MG	XA	1741	1/1	0.89	0.08	23,23,23,23	0
56	MG	YA	3320	1/1	0.89	0.27	54,54,54,54	0
56	MG	YA	3040	1/1	0.89	0.06	33,33,33,33	0
56	MG	YA	3509	1/1	0.89	0.07	3,3,3,3	0
56	MG	YN	201	1/1	0.89	0.07	36,36,36,36	0
56	MG	YA	3042	1/1	0.89	0.21	47,47,47,47	0
56	MG	YA	3511	1/1	0.89	0.08	39,39,39,39	0
56	MG	RA	3524	1/1	0.89	0.21	41,41,41,41	0
56	MG	YW	201	1/1	0.89	0.20	69,69,69,69	0
56	MG	RA	3081	1/1	0.89	0.05	63,63,63,63	0
56	MG	RA	3637	1/1	0.89	0.20	62,62,62,62	0
56	MG	YA	3569	1/1	0.90	0.26	48,48,48,48	0
56	MG	YA	3571	1/1	0.90	0.10	33,33,33,33	0
56	MG	XA	1720	1/1	0.90	0.20	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3242	1/1	0.90	0.23	43,43,43,43	0
56	MG	QV	104	1/1	0.90	0.17	71,71,71,71	0
56	MG	RA	3167	1/1	0.90	0.09	53,53,53,53	0
56	MG	RA	3684	1/1	0.90	0.14	44,44,44,44	0
56	MG	RA	3217	1/1	0.90	0.10	86,86,86,86	0
56	MG	YA	3591	1/1	0.90	0.21	37,37,37,37	0
56	MG	YA	3593	1/1	0.90	0.21	30,30,30,30	0
56	MG	YA	3020	1/1	0.90	0.12	44,44,44,44	0
56	MG	XA	1647	1/1	0.90	0.06	68,68,68,68	0
56	MG	RA	3142	1/1	0.90	0.28	59,59,59,59	0
56	MG	YA	3606	1/1	0.90	0.09	9,9,9,9	0
56	MG	QA	1681	1/1	0.90	0.23	34,34,34,34	0
56	MG	YA	3258	1/1	0.90	0.12	28,28,28,28	0
56	MG	YA	3143	1/1	0.90	0.20	51,51,51,51	0
56	MG	QA	1752	1/1	0.90	0.05	51,51,51,51	0
56	MG	RQ	203	1/1	0.90	0.13	67,67,67,67	0
56	MG	YA	3421	1/1	0.90	0.12	28,28,28,28	0
56	MG	YA	3626	1/1	0.90	0.12	27,27,27,27	0
56	MG	RA	3196	1/1	0.90	0.08	42,42,42,42	0
56	MG	QA	1682	1/1	0.90	0.15	66,66,66,66	0
56	MG	RA	3578	1/1	0.90	0.08	45,45,45,45	0
56	MG	RA	3368	1/1	0.90	0.31	52,52,52,52	0
56	MG	YA	3636	1/1	0.90	0.07	48,48,48,48	0
56	MG	YA	3269	1/1	0.90	0.16	54,54,54,54	0
56	MG	YA	3640	1/1	0.90	0.15	37,37,37,37	0
56	MG	YA	3641	1/1	0.90	0.09	46,46,46,46	0
56	MG	RA	3067	1/1	0.90	0.14	66,66,66,66	0
56	MG	RA	3516	1/1	0.90	0.13	35,35,35,35	0
56	MG	YA	3277	1/1	0.90	0.22	22,22,22,22	0
56	MG	RA	3703	1/1	0.90	0.14	55,55,55,55	0
56	MG	XA	1769	1/1	0.90	0.15	28,28,28,28	0
56	MG	QA	1809	1/1	0.90	0.06	43,43,43,43	0
56	MG	RA	3520	1/1	0.90	0.09	40,40,40,40	0
56	MG	QA	1777	1/1	0.90	0.22	46,46,46,46	0
56	MG	RZ	301	1/1	0.90	0.05	44,44,44,44	0
56	MG	YA	3452	1/1	0.90	0.17	42,42,42,42	0
56	MG	RA	3525	1/1	0.90	0.14	83,83,83,83	0
56	MG	RA	3286	1/1	0.90	0.25	25,25,25,25	0
56	MG	QA	1759	1/1	0.90	0.07	49,49,49,49	0
56	MG	YA	3462	1/1	0.90	0.18	44,44,44,44	0
56	MG	YA	3060	1/1	0.90	0.15	60,60,60,60	0
56	MG	RA	3016	1/1	0.90	0.25	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1725	1/1	0.90	0.08	51,51,51,51	0
56	MG	RA	3293	1/1	0.90	0.17	15,15,15,15	0
56	MG	QA	1781	1/1	0.90	0.12	48,48,48,48	0
56	MG	XA	1613	1/1	0.90	0.08	41,41,41,41	0
56	MG	YA	3479	1/1	0.90	0.13	53,53,53,53	0
56	MG	YA	3324	1/1	0.90	0.26	48,48,48,48	0
56	MG	YA	3482	1/1	0.90	0.16	72,72,72,72	0
56	MG	YA	3681	1/1	0.90	0.17	35,35,35,35	0
56	MG	XA	1790	1/1	0.90	0.12	56,56,56,56	0
56	MG	YA	3685	1/1	0.90	0.13	58,58,58,58	0
56	MG	XA	1791	1/1	0.90	0.34	67,67,67,67	0
56	MG	RA	3295	1/1	0.90	0.21	68,68,68,68	0
56	MG	RA	3659	1/1	0.90	0.41	81,81,81,81	0
56	MG	XA	1617	1/1	0.90	0.17	53,53,53,53	0
56	MG	YA	3696	1/1	0.90	0.25	145,145,145,145	0
56	MG	RA	3412	1/1	0.90	0.10	29,29,29,29	0
56	MG	YA	3493	1/1	0.90	0.15	41,41,41,41	0
56	MG	YA	3344	1/1	0.90	0.18	45,45,45,45	0
56	MG	YA	3088	1/1	0.90	0.12	39,39,39,39	0
56	MG	XA	1619	1/1	0.90	0.06	51,51,51,51	0
56	MG	YA	3093	1/1	0.90	0.15	38,38,38,38	0
56	MG	YA	3501	1/1	0.90	0.21	57,57,57,57	0
56	MG	YB	206	1/1	0.90	0.06	52,52,52,52	0
56	MG	YA	3095	1/1	0.90	0.14	33,33,33,33	0
56	MG	RA	3345	1/1	0.90	0.10	27,27,27,27	0
56	MG	RA	3114	1/1	0.90	0.29	50,50,50,50	0
56	MG	RA	3493	1/1	0.90	0.18	43,43,43,43	0
56	MG	R7	102	1/1	0.90	0.32	92,92,92,92	0
56	MG	QA	1657	1/1	0.90	0.09	50,50,50,50	0
56	MG	RA	3384	1/1	0.90	0.07	26,26,26,26	0
56	MG	YA	3369	1/1	0.90	0.10	54,54,54,54	0
56	MG	YA	3108	1/1	0.90	0.11	67,67,67,67	0
56	MG	RF	302	1/1	0.90	0.23	107,107,107,107	0
56	MG	RA	3544	1/1	0.90	0.09	36,36,36,36	0
56	MG	YA	3112	1/1	0.90	0.14	40,40,40,40	0
56	MG	QA	1784	1/1	0.90	0.11	53,53,53,53	0
56	MG	RA	3500	1/1	0.90	0.28	58,58,58,58	0
56	MG	YA	3117	1/1	0.90	0.13	50,50,50,50	0
56	MG	QA	1606	1/1	0.90	0.06	48,48,48,48	0
56	MG	RA	3305	1/1	0.90	0.17	30,30,30,30	0
56	MG	YA	3123	1/1	0.90	0.10	40,40,40,40	0
56	MG	YA	3551	1/1	0.90	0.09	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3395	1/1	0.90	0.29	30,30,30,30	0
56	MG	RA	3679	1/1	0.90	0.19	42,42,42,42	0
56	MG	YA	3564	1/1	0.90	0.20	46,46,46,46	0
56	MG	YA	3127	1/1	0.90	0.21	46,46,46,46	0
56	MG	RA	3630	1/1	0.91	0.20	39,39,39,39	0
56	MG	YA	3575	1/1	0.91	0.15	30,30,30,30	0
56	MG	RA	3570	1/1	0.91	0.08	40,40,40,40	0
56	MG	YA	3245	1/1	0.91	0.12	55,55,55,55	0
56	MG	QA	1798	1/1	0.91	0.24	52,52,52,52	0
56	MG	RA	3572	1/1	0.91	0.12	27,27,27,27	0
56	MG	YA	3138	1/1	0.91	0.22	50,50,50,50	0
56	MG	YA	3587	1/1	0.91	0.13	68,68,68,68	0
56	MG	RA	3125	1/1	0.91	0.27	94,94,94,94	0
56	MG	XA	1654	1/1	0.91	0.12	46,46,46,46	0
56	MG	RA	3692	1/1	0.91	0.29	56,56,56,56	0
56	MG	QA	1717	1/1	0.91	0.33	45,45,45,45	0
56	MG	RT	203	1/1	0.91	0.09	61,61,61,61	0
56	MG	YA	3598	1/1	0.91	0.20	50,50,50,50	0
56	MG	YA	3417	1/1	0.91	0.20	54,54,54,54	0
56	MG	YA	3144	1/1	0.91	0.12	38,38,38,38	0
56	MG	YA	3036	1/1	0.91	0.16	56,56,56,56	0
56	MG	QA	1802	1/1	0.91	0.30	61,61,61,61	0
56	MG	RA	3580	1/1	0.91	0.14	87,87,87,87	0
56	MG	QA	1757	1/1	0.91	0.05	54,54,54,54	0
56	MG	QA	1745	1/1	0.91	0.06	50,50,50,50	0
56	MG	RA	3349	1/1	0.91	0.14	14,14,14,14	0
56	MG	RA	3147	1/1	0.91	0.09	71,71,71,71	0
56	MG	RA	3095	1/1	0.91	0.15	43,43,43,43	0
56	MG	YA	3054	1/1	0.91	0.23	65,65,65,65	0
56	MG	R0	101	1/1	0.91	0.20	56,56,56,56	0
56	MG	YA	3438	1/1	0.91	0.15	32,32,32,32	0
56	MG	RA	3436	1/1	0.91	0.29	60,60,60,60	0
56	MG	RA	3590	1/1	0.91	0.12	22,22,22,22	0
56	MG	RA	3649	1/1	0.91	0.25	98,98,98,98	0
56	MG	YA	3163	1/1	0.91	0.12	63,63,63,63	0
56	MG	QA	1604	1/1	0.91	0.08	60,60,60,60	0
56	MG	YA	3062	1/1	0.91	0.11	43,43,43,43	0
56	MG	RA	3356	1/1	0.91	0.21	39,39,39,39	0
56	MG	QL	203	1/1	0.91	0.12	61,61,61,61	0
56	MG	XA	1609	1/1	0.91	0.28	55,55,55,55	0
56	MG	YA	3069	1/1	0.91	0.37	62,62,62,62	0
56	MG	YA	3173	1/1	0.91	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3358	1/1	0.91	0.32	54,54,54,54	0
56	MG	YA	3471	1/1	0.91	0.24	84,84,84,84	0
56	MG	YA	3319	1/1	0.91	0.12	36,36,36,36	0
56	MG	XA	1789	1/1	0.91	0.16	59,59,59,59	0
56	MG	RA	3154	1/1	0.91	0.06	39,39,39,39	0
56	MG	YA	3322	1/1	0.91	0.12	21,21,21,21	0
56	MG	RA	3289	1/1	0.91	0.19	39,39,39,39	0
56	MG	YA	3663	1/1	0.91	0.26	49,49,49,49	0
56	MG	RA	3599	1/1	0.91	0.25	29,29,29,29	0
56	MG	RA	3086	1/1	0.91	0.11	57,57,57,57	0
56	MG	YA	3481	1/1	0.91	0.29	80,80,80,80	0
56	MG	RB	216	1/1	0.91	0.09	74,74,74,74	0
56	MG	RD	301	1/1	0.91	0.13	50,50,50,50	0
56	MG	XA	1695	1/1	0.91	0.15	34,34,34,34	0
56	MG	RA	3019	1/1	0.91	0.12	37,37,37,37	0
56	MG	RA	3548	1/1	0.91	0.24	41,41,41,41	0
56	MG	YA	3347	1/1	0.91	0.14	8,8,8,8	0
56	MG	RA	3036	1/1	0.91	0.42	80,80,80,80	0
56	MG	RA	3553	1/1	0.91	0.20	22,22,22,22	0
56	MG	RE	302	1/1	0.91	0.16	35,35,35,35	0
56	MG	RA	3475	1/1	0.91	0.13	34,34,34,34	0
56	MG	RA	3449	1/1	0.91	0.08	39,39,39,39	0
56	MG	RA	3612	1/1	0.91	0.25	47,47,47,47	0
56	MG	RA	3562	1/1	0.91	0.15	23,23,23,23	0
56	MG	YA	3107	1/1	0.91	0.26	80,80,80,80	0
56	MG	YA	3202	1/1	0.91	0.24	48,48,48,48	0
56	MG	Y7	102	1/1	0.91	0.08	36,36,36,36	0
56	MG	YA	3368	1/1	0.91	0.14	21,21,21,21	0
56	MG	RA	3263	1/1	0.91	0.10	42,42,42,42	0
56	MG	YA	3370	1/1	0.91	0.20	30,30,30,30	0
56	MG	YB	201	1/1	0.91	0.21	55,55,55,55	0
56	MG	YA	3209	1/1	0.91	0.17	38,38,38,38	0
56	MG	YA	3110	1/1	0.91	0.29	42,42,42,42	0
56	MG	QA	1739	1/1	0.91	0.17	41,41,41,41	0
56	MG	YA	3007	1/1	0.91	0.07	66,66,66,66	0
56	MG	YB	208	1/1	0.91	0.07	44,44,44,44	0
56	MG	YB	209	1/1	0.91	0.15	92,92,92,92	0
56	MG	YA	3525	1/1	0.91	0.18	28,28,28,28	0
56	MG	YA	3376	1/1	0.91	0.11	48,48,48,48	0
56	MG	RA	3565	1/1	0.91	0.10	50,50,50,50	0
56	MG	YA	3530	1/1	0.91	0.16	2,2,2,2	0
56	MG	RA	3678	1/1	0.91	0.27	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3380	1/1	0.91	0.33	49,49,49,49	0
56	MG	YA	3116	1/1	0.91	0.11	49,49,49,49	0
56	MG	YA	3537	1/1	0.91	0.20	55,55,55,55	0
56	MG	YD	302	1/1	0.91	0.24	69,69,69,69	0
56	MG	YA	3540	1/1	0.91	0.14	33,33,33,33	0
56	MG	YD	305	1/1	0.91	0.14	42,42,42,42	0
56	MG	YA	3384	1/1	0.91	0.07	18,18,18,18	0
56	MG	YA	3543	1/1	0.91	0.12	16,16,16,16	0
56	MG	YE	303	1/1	0.91	0.27	33,33,33,33	0
56	MG	RA	3623	1/1	0.91	0.28	48,48,48,48	0
56	MG	RA	3180	1/1	0.91	0.11	36,36,36,36	0
56	MG	RA	3568	1/1	0.91	0.10	34,34,34,34	0
56	MG	YA	3393	1/1	0.91	0.17	64,64,64,64	0
56	MG	YA	3016	1/1	0.91	0.15	48,48,48,48	0
56	MG	YA	3557	1/1	0.91	0.09	42,42,42,42	0
56	MG	RA	3419	1/1	0.91	0.24	44,44,44,44	0
56	MG	XA	1728	1/1	0.91	0.26	44,44,44,44	0
56	MG	YA	3566	1/1	0.91	0.10	25,25,25,25	0
57	PAR	QA	1821	42/42	0.91	0.13	52,66,86,95	0
57	PAR	XA	1794	42/42	0.91	0.10	52,63,76,81	0
56	MG	XA	1735	1/1	0.91	0.08	19,19,19,19	0
56	MG	YA	3570	1/1	0.91	0.13	42,42,42,42	0
56	MG	YA	3231	1/1	0.92	0.13	37,37,37,37	0
56	MG	RA	3194	1/1	0.92	0.14	64,64,64,64	0
56	MG	YA	3567	1/1	0.92	0.14	27,27,27,27	0
56	MG	XA	1715	1/1	0.92	0.08	41,41,41,41	0
56	MG	YA	3237	1/1	0.92	0.10	38,38,38,38	0
56	MG	YA	3238	1/1	0.92	0.18	39,39,39,39	0
56	MG	YA	3574	1/1	0.92	0.17	24,24,24,24	0
56	MG	QA	1707	1/1	0.92	0.07	62,62,62,62	0
56	MG	YA	3576	1/1	0.92	0.14	46,46,46,46	0
56	MG	YA	3404	1/1	0.92	0.05	32,32,32,32	0
56	MG	YA	3120	1/1	0.92	0.32	102,102,102,102	0
56	MG	YA	3580	1/1	0.92	0.20	52,52,52,52	0
56	MG	YA	3581	1/1	0.92	0.31	41,41,41,41	0
56	MG	RA	3361	1/1	0.92	0.22	46,46,46,46	0
56	MG	YA	3013	1/1	0.92	0.14	63,63,63,63	0
56	MG	YA	3411	1/1	0.92	0.19	33,33,33,33	0
56	MG	XA	1719	1/1	0.92	0.08	35,35,35,35	0
56	MG	RA	3402	1/1	0.92	0.14	42,42,42,42	0
56	MG	YA	3590	1/1	0.92	0.11	47,47,47,47	0
56	MG	YA	3250	1/1	0.92	0.22	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3030	1/1	0.92	0.13	64,64,64,64	0
56	MG	RA	3603	1/1	0.92	0.17	56,56,56,56	0
56	MG	RA	3667	1/1	0.92	0.13	54,54,54,54	0
56	MG	YA	3255	1/1	0.92	0.13	28,28,28,28	0
56	MG	YA	3419	1/1	0.92	0.25	35,35,35,35	0
56	MG	YA	3132	1/1	0.92	0.08	48,48,48,48	0
56	MG	QA	1760	1/1	0.92	0.10	37,37,37,37	0
56	MG	YA	3136	1/1	0.92	0.16	43,43,43,43	0
56	MG	YA	3613	1/1	0.92	0.21	41,41,41,41	0
56	MG	YA	3615	1/1	0.92	0.14	22,22,22,22	0
56	MG	XA	1726	1/1	0.92	0.06	42,42,42,42	0
56	MG	YA	3425	1/1	0.92	0.20	55,55,55,55	0
56	MG	QA	1708	1/1	0.92	0.22	37,37,37,37	0
56	MG	YA	3624	1/1	0.92	0.14	17,17,17,17	0
56	MG	XA	1642	1/1	0.92	0.05	77,77,77,77	0
56	MG	YA	3264	1/1	0.92	0.15	21,21,21,21	0
56	MG	RG	203	1/1	0.92	0.13	59,59,59,59	0
56	MG	RA	3607	1/1	0.92	0.13	38,38,38,38	0
56	MG	YA	3631	1/1	0.92	0.13	40,40,40,40	0
56	MG	RA	3033	1/1	0.92	0.21	52,52,52,52	0
56	MG	QA	1779	1/1	0.92	0.18	38,38,38,38	0
56	MG	QA	1603	1/1	0.92	0.05	50,50,50,50	0
56	MG	YA	3442	1/1	0.92	0.23	86,86,86,86	0
56	MG	XA	1746	1/1	0.92	0.20	61,61,61,61	0
56	MG	YA	3037	1/1	0.92	0.21	45,45,45,45	0
56	MG	XA	1747	1/1	0.92	0.08	28,28,28,28	0
56	MG	YA	3446	1/1	0.92	0.08	25,25,25,25	0
56	MG	RA	3320	1/1	0.92	0.50	93,93,93,93	0
56	MG	YA	3449	1/1	0.92	0.22	53,53,53,53	0
56	MG	YA	3450	1/1	0.92	0.16	40,40,40,40	0
56	MG	QA	1615	1/1	0.92	0.16	47,47,47,47	0
56	MG	QV	101	1/1	0.92	0.12	52,52,52,52	0
56	MG	YA	3454	1/1	0.92	0.06	31,31,31,31	0
56	MG	YA	3655	1/1	0.92	0.16	43,43,43,43	0
56	MG	QA	1629	1/1	0.92	0.08	75,75,75,75	0
56	MG	YA	3047	1/1	0.92	0.09	60,60,60,60	0
56	MG	RA	3281	1/1	0.92	0.14	26,26,26,26	0
56	MG	RA	3117	1/1	0.92	0.35	69,69,69,69	0
56	MG	YA	3467	1/1	0.92	0.12	51,51,51,51	0
56	MG	YA	3053	1/1	0.92	0.12	35,35,35,35	0
56	MG	YA	3309	1/1	0.92	0.32	54,54,54,54	0
56	MG	RA	3624	1/1	0.92	0.32	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1764	1/1	0.92	0.23	25,25,25,25	0
56	MG	XA	1765	1/1	0.92	0.09	31,31,31,31	0
56	MG	QA	1731	1/1	0.92	0.26	46,46,46,46	0
56	MG	YA	3477	1/1	0.92	0.29	98,98,98,98	0
56	MG	YA	3671	1/1	0.92	0.15	55,55,55,55	0
56	MG	YA	3672	1/1	0.92	0.18	68,68,68,68	0
56	MG	RA	3626	1/1	0.92	0.28	47,47,47,47	0
56	MG	YA	3675	1/1	0.92	0.19	40,40,40,40	0
56	MG	YA	3676	1/1	0.92	0.16	48,48,48,48	0
56	MG	YA	3168	1/1	0.92	0.10	41,41,41,41	0
56	MG	RA	3688	1/1	0.92	0.20	35,35,35,35	0
56	MG	RA	3146	1/1	0.92	0.08	44,44,44,44	0
56	MG	RA	3331	1/1	0.92	0.21	40,40,40,40	0
56	MG	YA	3683	1/1	0.92	0.12	24,24,24,24	0
56	MG	YA	3325	1/1	0.92	0.21	37,37,37,37	0
56	MG	RA	3332	1/1	0.92	0.20	42,42,42,42	0
56	MG	YA	3686	1/1	0.92	0.07	51,51,51,51	0
56	MG	YA	3329	1/1	0.92	0.28	51,51,51,51	0
56	MG	RA	3465	1/1	0.92	0.34	45,45,45,45	0
56	MG	RA	3696	1/1	0.92	0.25	57,57,57,57	0
56	MG	YA	3178	1/1	0.92	0.14	42,42,42,42	0
56	MG	YA	3339	1/1	0.92	0.18	34,34,34,34	0
56	MG	YA	3495	1/1	0.92	0.13	30,30,30,30	0
56	MG	QA	1621	1/1	0.92	0.36	100,100,100,100	0
56	MG	YA	3071	1/1	0.92	0.09	64,64,64,64	0
56	MG	YA	3704	1/1	0.92	0.27	30,30,30,30	0
56	MG	RA	3698	1/1	0.92	0.12	56,56,56,56	0
56	MG	YA	3182	1/1	0.92	0.07	40,40,40,40	0
56	MG	RA	3573	1/1	0.92	0.14	38,38,38,38	0
56	MG	YA	3504	1/1	0.92	0.17	51,51,51,51	0
56	MG	QA	1674	1/1	0.92	0.25	42,42,42,42	0
56	MG	YA	3078	1/1	0.92	0.06	66,66,66,66	0
56	MG	RA	3701	1/1	0.92	0.16	52,52,52,52	0
56	MG	RA	3576	1/1	0.92	0.12	31,31,31,31	0
56	MG	RA	3519	1/1	0.92	0.17	32,32,32,32	0
56	MG	RA	3150	1/1	0.92	0.09	35,35,35,35	0
56	MG	YA	3087	1/1	0.92	0.05	24,24,24,24	0
56	MG	RA	3121	1/1	0.92	0.07	47,47,47,47	0
56	MG	YA	3515	1/1	0.92	0.14	45,45,45,45	0
56	MG	R0	102	1/1	0.92	0.07	65,65,65,65	0
56	MG	RA	3582	1/1	0.92	0.32	49,49,49,49	0
56	MG	RA	3291	1/1	0.92	0.14	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RB	201	1/1	0.92	0.25	98,98,98,98	0
56	MG	QA	1609	1/1	0.92	0.09	34,34,34,34	0
56	MG	RA	3348	1/1	0.92	0.10	2,2,2,2	0
56	MG	QA	1719	1/1	0.92	0.06	43,43,43,43	0
56	MG	RA	3022	1/1	0.92	0.11	45,45,45,45	0
56	MG	QA	1720	1/1	0.92	0.08	46,46,46,46	0
56	MG	YA	3536	1/1	0.92	0.14	41,41,41,41	0
56	MG	QA	1814	1/1	0.92	0.32	64,64,64,64	0
56	MG	YF	302	1/1	0.92	0.19	67,67,67,67	0
56	MG	YA	3538	1/1	0.92	0.13	36,36,36,36	0
56	MG	QA	1755	1/1	0.92	0.09	47,47,47,47	0
56	MG	RA	3299	1/1	0.92	0.10	26,26,26,26	0
56	MG	YA	3382	1/1	0.92	0.20	50,50,50,50	0
56	MG	YA	3544	1/1	0.92	0.39	34,34,34,34	0
56	MG	YP	202	1/1	0.92	0.07	41,41,41,41	0
56	MG	RA	3593	1/1	0.92	0.19	52,52,52,52	0
56	MG	XA	1707	1/1	0.92	0.07	49,49,49,49	0
56	MG	XA	1709	1/1	0.92	0.19	42,42,42,42	0
56	MG	YA	3005	1/1	0.92	0.09	49,49,49,49	0
56	MG	YA	3114	1/1	0.92	0.15	60,60,60,60	0
56	MG	QA	1793	1/1	0.92	0.21	64,64,64,64	0
56	MG	QA	1612	1/1	0.92	0.08	43,43,43,43	0
56	MG	YA	3041	1/1	0.93	0.10	41,41,41,41	0
56	MG	YA	3257	1/1	0.93	0.05	38,38,38,38	0
56	MG	QA	1767	1/1	0.93	0.14	52,52,52,52	0
56	MG	XA	1675	1/1	0.93	0.17	39,39,39,39	0
56	MG	RA	3215	1/1	0.93	0.28	69,69,69,69	0
56	MG	RA	3486	1/1	0.93	0.17	50,50,50,50	0
56	MG	RA	3491	1/1	0.93	0.20	40,40,40,40	0
56	MG	XA	1766	1/1	0.93	0.23	53,53,53,53	0
56	MG	RA	3492	1/1	0.93	0.17	36,36,36,36	0
56	MG	YA	3266	1/1	0.93	0.09	37,37,37,37	0
56	MG	RA	3423	1/1	0.93	0.16	31,31,31,31	0
56	MG	RA	3216	1/1	0.93	0.24	52,52,52,52	0
56	MG	YA	3592	1/1	0.93	0.19	16,16,16,16	0
56	MG	RA	3496	1/1	0.93	0.19	43,43,43,43	0
56	MG	YA	3155	1/1	0.93	0.15	35,35,35,35	0
56	MG	YA	3274	1/1	0.93	0.23	67,67,67,67	0
56	MG	RA	3587	1/1	0.93	0.27	72,72,72,72	0
56	MG	YA	3604	1/1	0.93	0.18	43,43,43,43	0
56	MG	XA	1775	1/1	0.93	0.13	39,39,39,39	0
56	MG	YA	3430	1/1	0.93	0.08	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3431	1/1	0.93	0.19	10,10,10,10	0
56	MG	XA	1686	1/1	0.93	0.21	55,55,55,55	0
56	MG	YA	3612	1/1	0.93	0.24	41,41,41,41	0
56	MG	YA	3434	1/1	0.93	0.14	22,22,22,22	0
56	MG	YA	3281	1/1	0.93	0.16	23,23,23,23	0
56	MG	YA	3437	1/1	0.93	0.23	29,29,29,29	0
56	MG	XA	1779	1/1	0.93	0.15	42,42,42,42	0
56	MG	YA	3162	1/1	0.93	0.14	34,34,34,34	0
56	MG	XA	1688	1/1	0.93	0.28	55,55,55,55	0
56	MG	YA	3292	1/1	0.93	0.06	42,42,42,42	0
56	MG	RA	3157	1/1	0.93	0.10	59,59,59,59	0
56	MG	XA	1690	1/1	0.93	0.20	31,31,31,31	0
56	MG	YA	3299	1/1	0.93	0.17	43,43,43,43	0
56	MG	YA	3300	1/1	0.93	0.15	28,28,28,28	0
56	MG	RA	3071	1/1	0.93	0.38	102,102,102,102	0
56	MG	QF	201	1/1	0.93	0.07	29,29,29,29	0
56	MG	YA	3635	1/1	0.93	0.14	18,18,18,18	0
56	MG	XA	1694	1/1	0.93	0.08	27,27,27,27	0
56	MG	QA	1753	1/1	0.93	0.21	83,83,83,83	0
56	MG	YA	3072	1/1	0.93	0.12	7,7,7,7	0
56	MG	YA	3455	1/1	0.93	0.07	40,40,40,40	0
56	MG	XA	1788	1/1	0.93	0.05	48,48,48,48	0
56	MG	RA	3543	1/1	0.93	0.14	4,4,4,4	0
56	MG	YA	3175	1/1	0.93	0.13	41,41,41,41	0
56	MG	YA	3317	1/1	0.93	0.10	41,41,41,41	0
56	MG	YA	3464	1/1	0.93	0.10	39,39,39,39	0
56	MG	YA	3176	1/1	0.93	0.10	55,55,55,55	0
56	MG	YA	3468	1/1	0.93	0.10	57,57,57,57	0
56	MG	XA	1699	1/1	0.93	0.09	34,34,34,34	0
56	MG	RA	3694	1/1	0.93	0.35	39,39,39,39	0
56	MG	RA	3302	1/1	0.93	0.14	34,34,34,34	0
56	MG	RA	3502	1/1	0.93	0.10	30,30,30,30	0
56	MG	RA	3433	1/1	0.93	0.13	51,51,51,51	0
56	MG	QA	1684	1/1	0.93	0.33	60,60,60,60	0
56	MG	YA	3328	1/1	0.93	0.13	52,52,52,52	0
56	MG	XA	1641	1/1	0.93	0.17	52,52,52,52	0
56	MG	RA	3435	1/1	0.93	0.16	41,41,41,41	0
56	MG	YA	3335	1/1	0.93	0.05	32,32,32,32	0
56	MG	YA	3089	1/1	0.93	0.07	54,54,54,54	0
56	MG	YA	3667	1/1	0.93	0.19	67,67,67,67	0
56	MG	YA	3091	1/1	0.93	0.18	39,39,39,39	0
56	MG	XA	1708	1/1	0.93	0.24	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1635	1/1	0.93	0.10	43,43,43,43	0
56	MG	YA	3487	1/1	0.93	0.25	37,37,37,37	0
56	MG	XA	1644	1/1	0.93	0.10	71,71,71,71	0
56	MG	RA	3273	1/1	0.93	0.14	51,51,51,51	0
56	MG	YA	3345	1/1	0.93	0.07	28,28,28,28	0
56	MG	RA	3651	1/1	0.93	0.06	47,47,47,47	0
56	MG	YA	3195	1/1	0.93	0.09	72,72,72,72	0
56	MG	RA	3275	1/1	0.93	0.11	43,43,43,43	0
56	MG	YA	3350	1/1	0.93	0.12	24,24,24,24	0
56	MG	QA	1756	1/1	0.93	0.05	58,58,58,58	0
56	MG	YA	3682	1/1	0.93	0.21	63,63,63,63	0
56	MG	RA	3017	1/1	0.93	0.07	53,53,53,53	0
56	MG	QA	1772	1/1	0.93	0.05	37,37,37,37	0
56	MG	YA	3001	1/1	0.93	0.13	39,39,39,39	0
56	MG	YA	3502	1/1	0.93	0.24	60,60,60,60	0
56	MG	XA	1651	1/1	0.93	0.05	42,42,42,42	0
56	MG	YA	3505	1/1	0.93	0.10	35,35,35,35	0
56	MG	YA	3203	1/1	0.93	0.14	48,48,48,48	0
56	MG	YA	3003	1/1	0.93	0.13	52,52,52,52	0
56	MG	YA	3693	1/1	0.93	0.39	59,59,59,59	0
56	MG	YA	3694	1/1	0.93	0.30	65,65,65,65	0
56	MG	YA	3366	1/1	0.93	0.17	51,51,51,51	0
56	MG	XA	1652	1/1	0.93	0.06	35,35,35,35	0
56	MG	QA	1713	1/1	0.93	0.15	38,38,38,38	0
56	MG	RA	3317	1/1	0.93	0.13	7,7,7,7	0
56	MG	QA	1645	1/1	0.93	0.12	45,45,45,45	0
56	MG	RA	3610	1/1	0.93	0.10	62,62,62,62	0
56	MG	XA	1727	1/1	0.93	0.12	40,40,40,40	0
56	MG	YA	3516	1/1	0.93	0.13	36,36,36,36	0
56	MG	RA	3517	1/1	0.93	0.06	38,38,38,38	0
56	MG	XA	1730	1/1	0.93	0.08	41,41,41,41	0
56	MG	XA	1733	1/1	0.93	0.16	40,40,40,40	0
56	MG	YA	3224	1/1	0.93	0.16	44,44,44,44	0
56	MG	RA	3253	1/1	0.93	0.23	28,28,28,28	0
56	MG	YA	3379	1/1	0.93	0.19	37,37,37,37	0
56	MG	RB	206	1/1	0.93	0.21	39,39,39,39	0
56	MG	YA	3121	1/1	0.93	0.23	51,51,51,51	0
56	MG	YA	3230	1/1	0.93	0.20	50,50,50,50	0
56	MG	YA	3535	1/1	0.93	0.23	35,35,35,35	0
56	MG	XA	1738	1/1	0.93	0.12	38,38,38,38	0
56	MG	XA	1662	1/1	0.93	0.06	39,39,39,39	0
56	MG	RA	3613	1/1	0.93	0.15	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1742	1/1	0.93	0.34	40,40,40,40	0
56	MG	YA	3389	1/1	0.93	0.12	53,53,53,53	0
56	MG	YA	3391	1/1	0.93	0.06	43,43,43,43	0
56	MG	YA	3392	1/1	0.93	0.15	43,43,43,43	0
56	MG	YD	306	1/1	0.93	0.17	84,84,84,84	0
56	MG	XA	1743	1/1	0.93	0.15	33,33,33,33	0
56	MG	YA	3394	1/1	0.93	0.21	46,46,46,46	0
56	MG	YA	3239	1/1	0.93	0.08	14,14,14,14	0
56	MG	RA	3207	1/1	0.93	0.21	107,107,107,107	0
56	MG	YA	3554	1/1	0.93	0.15	7,7,7,7	0
56	MG	QL	201	1/1	0.93	0.16	103,103,103,103	0
56	MG	XA	1667	1/1	0.93	0.14	81,81,81,81	0
56	MG	YA	3134	1/1	0.93	0.08	35,35,35,35	0
56	MG	RA	3523	1/1	0.93	0.15	46,46,46,46	0
56	MG	YO	201	1/1	0.93	0.39	88,88,88,88	0
56	MG	QA	1783	1/1	0.93	0.12	42,42,42,42	0
56	MG	XA	1751	1/1	0.93	0.26	56,56,56,56	0
56	MG	YA	3405	1/1	0.93	0.33	32,32,32,32	0
56	MG	RA	3190	1/1	0.93	0.06	46,46,46,46	0
56	MG	YT	202	1/1	0.93	0.17	85,85,85,85	0
56	MG	YV	201	1/1	0.93	0.07	37,37,37,37	0
56	MG	RA	3068	1/1	0.93	0.09	49,49,49,49	0
56	MG	YA	3572	1/1	0.93	0.15	36,36,36,36	0
56	MG	YA	3573	1/1	0.93	0.10	24,24,24,24	0
56	MG	YA	3039	1/1	0.93	0.11	65,65,65,65	0
56	MG	R1	101	1/1	0.93	0.37	57,57,57,57	0
56	MG	YA	3610	1/1	0.94	0.19	39,39,39,39	0
56	MG	YA	3465	1/1	0.94	0.25	17,17,17,17	0
56	MG	YA	3212	1/1	0.94	0.18	45,45,45,45	0
56	MG	YA	3213	1/1	0.94	0.07	50,50,50,50	0
56	MG	RD	302	1/1	0.94	0.22	82,82,82,82	0
56	MG	YA	3028	1/1	0.94	0.10	40,40,40,40	0
56	MG	YA	3617	1/1	0.94	0.12	19,19,19,19	0
56	MG	YA	3620	1/1	0.94	0.08	33,33,33,33	0
56	MG	RD	303	1/1	0.94	0.23	91,91,91,91	0
56	MG	YA	3352	1/1	0.94	0.21	38,38,38,38	0
56	MG	YA	3219	1/1	0.94	0.07	35,35,35,35	0
56	MG	RA	3675	1/1	0.94	0.07	10,10,10,10	0
56	MG	RA	3021	1/1	0.94	0.14	60,60,60,60	0
56	MG	YA	3125	1/1	0.94	0.10	43,43,43,43	0
56	MG	RA	3487	1/1	0.94	0.09	14,14,14,14	0
56	MG	YA	3363	1/1	0.94	0.12	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3632	1/1	0.94	0.12	15,15,15,15	0
56	MG	RA	3003	1/1	0.94	0.18	19,19,19,19	0
56	MG	YA	3035	1/1	0.94	0.13	38,38,38,38	0
56	MG	YA	3229	1/1	0.94	0.20	34,34,34,34	0
56	MG	RA	3171	1/1	0.94	0.09	52,52,52,52	0
56	MG	YA	3486	1/1	0.94	0.09	31,31,31,31	0
56	MG	RA	3023	1/1	0.94	0.20	105,105,105,105	0
56	MG	YA	3233	1/1	0.94	0.11	38,38,38,38	0
56	MG	YA	3489	1/1	0.94	0.17	36,36,36,36	0
56	MG	XA	1626	1/1	0.94	0.06	31,31,31,31	0
56	MG	QA	1610	1/1	0.94	0.06	41,41,41,41	0
56	MG	YA	3645	1/1	0.94	0.09	36,36,36,36	0
56	MG	XA	1771	1/1	0.94	0.15	44,44,44,44	0
56	MG	RF	303	1/1	0.94	0.24	102,102,102,102	0
56	MG	RA	3109	1/1	0.94	0.16	37,37,37,37	0
56	MG	YA	3044	1/1	0.94	0.10	44,44,44,44	0
56	MG	XA	1630	1/1	0.94	0.09	55,55,55,55	0
56	MG	YA	3654	1/1	0.94	0.23	15,15,15,15	0
56	MG	QA	1704	1/1	0.94	0.11	41,41,41,41	0
56	MG	XA	1698	1/1	0.94	0.11	40,40,40,40	0
56	MG	YA	3049	1/1	0.94	0.25	48,48,48,48	0
56	MG	RG	202	1/1	0.94	0.05	56,56,56,56	0
56	MG	RA	3310	1/1	0.94	0.33	77,77,77,77	0
56	MG	XA	1635	1/1	0.94	0.05	55,55,55,55	0
56	MG	YA	3506	1/1	0.94	0.15	17,17,17,17	0
56	MG	RA	3540	1/1	0.94	0.23	29,29,29,29	0
56	MG	YA	3055	1/1	0.94	0.11	40,40,40,40	0
56	MG	XA	1637	1/1	0.94	0.21	78,78,78,78	0
56	MG	QA	1807	1/1	0.94	0.06	63,63,63,63	0
56	MG	QA	1797	1/1	0.94	0.21	51,51,51,51	0
56	MG	RA	3388	1/1	0.94	0.16	38,38,38,38	0
56	MG	RA	3314	1/1	0.94	0.23	51,51,51,51	0
56	MG	YA	3061	1/1	0.94	0.09	40,40,40,40	0
56	MG	QA	1723	1/1	0.94	0.06	39,39,39,39	0
56	MG	RA	3284	1/1	0.94	0.20	21,21,21,21	0
56	MG	YA	3397	1/1	0.94	0.21	59,59,59,59	0
56	MG	YA	3520	1/1	0.94	0.12	10,10,10,10	0
56	MG	YA	3158	1/1	0.94	0.07	44,44,44,44	0
56	MG	RA	3695	1/1	0.94	0.11	47,47,47,47	0
56	MG	YA	3067	1/1	0.94	0.06	33,33,33,33	0
56	MG	XA	1712	1/1	0.94	0.18	44,44,44,44	0
56	MG	RA	3013	1/1	0.94	0.11	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3078	1/1	0.94	0.08	55,55,55,55	0
56	MG	RA	3394	1/1	0.94	0.18	35,35,35,35	0
56	MG	RA	3079	1/1	0.94	0.18	56,56,56,56	0
56	MG	YA	3166	1/1	0.94	0.07	60,60,60,60	0
56	MG	XL	202	1/1	0.94	0.09	53,53,53,53	0
56	MG	YA	3409	1/1	0.94	0.13	26,26,26,26	0
56	MG	YA	3279	1/1	0.94	0.21	19,19,19,19	0
56	MG	YA	3690	1/1	0.94	0.24	126,126,126,126	0
56	MG	QA	1799	1/1	0.94	0.05	52,52,52,52	0
56	MG	YA	3075	1/1	0.94	0.15	52,52,52,52	0
56	MG	YA	3283	1/1	0.94	0.17	61,61,61,61	0
56	MG	RA	3555	1/1	0.94	0.37	55,55,55,55	0
56	MG	YA	3286	1/1	0.94	0.18	31,31,31,31	0
56	MG	YA	3699	1/1	0.94	0.17	48,48,48,48	0
56	MG	RA	3557	1/1	0.94	0.11	17,17,17,17	0
56	MG	YA	3550	1/1	0.94	0.20	21,21,21,21	0
56	MG	RA	3098	1/1	0.94	0.09	33,33,33,33	0
56	MG	YA	3081	1/1	0.94	0.21	41,41,41,41	0
56	MG	YA	3293	1/1	0.94	0.21	26,26,26,26	0
56	MG	YA	3707	1/1	0.94	0.25	98,98,98,98	0
56	MG	YA	3295	1/1	0.94	0.12	16,16,16,16	0
56	MG	RA	3605	1/1	0.94	0.16	23,23,23,23	0
56	MG	YA	3562	1/1	0.94	0.18	35,35,35,35	0
56	MG	YA	3563	1/1	0.94	0.22	22,22,22,22	0
56	MG	YA	3083	1/1	0.94	0.08	39,39,39,39	0
56	MG	RA	3705	1/1	0.94	0.17	54,54,54,54	0
56	MG	RA	3258	1/1	0.94	0.11	66,66,66,66	0
56	MG	YA	3086	1/1	0.94	0.13	38,38,38,38	0
56	MG	QA	1800	1/1	0.94	0.13	45,45,45,45	0
56	MG	RA	3292	1/1	0.94	0.22	56,56,56,56	0
56	MG	XA	1729	1/1	0.94	0.07	44,44,44,44	0
56	MG	QA	1790	1/1	0.94	0.06	73,73,73,73	0
56	MG	XA	1731	1/1	0.94	0.19	62,62,62,62	0
56	MG	YA	3312	1/1	0.94	0.22	42,42,42,42	0
56	MG	RA	3440	1/1	0.94	0.14	20,20,20,20	0
56	MG	RA	3661	1/1	0.94	0.28	46,46,46,46	0
56	MG	RA	3370	1/1	0.94	0.27	117,117,117,117	0
56	MG	YD	304	1/1	0.94	0.12	46,46,46,46	0
56	MG	YA	3318	1/1	0.94	0.11	32,32,32,32	0
56	MG	QA	1611	1/1	0.94	0.05	31,31,31,31	0
56	MG	XA	1739	1/1	0.94	0.27	39,39,39,39	0
56	MG	RA	3664	1/1	0.94	0.05	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3584	1/1	0.94	0.07	58,58,58,58	0
56	MG	YE	305	1/1	0.94	0.05	53,53,53,53	0
56	MG	RA	3234	1/1	0.94	0.13	60,60,60,60	0
56	MG	YA	3105	1/1	0.94	0.13	48,48,48,48	0
56	MG	RA	3235	1/1	0.94	0.16	18,18,18,18	0
56	MG	RA	3616	1/1	0.94	0.08	39,39,39,39	0
56	MG	RA	3334	1/1	0.94	0.19	24,24,24,24	0
56	MG	YA	3015	1/1	0.94	0.07	34,34,34,34	0
56	MG	RA	3166	1/1	0.94	0.12	68,68,68,68	0
56	MG	YA	3453	1/1	0.94	0.24	56,56,56,56	0
56	MG	YA	3594	1/1	0.94	0.12	30,30,30,30	0
56	MG	RA	3409	1/1	0.94	0.06	30,30,30,30	0
56	MG	XA	1676	1/1	0.94	0.10	35,35,35,35	0
56	MG	YT	201	1/1	0.94	0.12	50,50,50,50	0
56	MG	YA	3597	1/1	0.94	0.14	30,30,30,30	0
56	MG	YT	203	1/1	0.94	0.30	97,97,97,97	0
56	MG	QA	1738	1/1	0.94	0.14	40,40,40,40	0
56	MG	YA	3603	1/1	0.94	0.27	51,51,51,51	0
56	MG	RB	217	1/1	0.94	0.07	62,62,62,62	0
56	MG	QA	1648	1/1	0.94	0.08	69,69,69,69	0
56	MG	YA	3025	1/1	0.94	0.15	49,49,49,49	0
56	MG	XA	1753	1/1	0.94	0.16	38,38,38,38	0
56	MG	XA	1777	1/1	0.95	0.15	28,28,28,28	0
56	MG	RA	3200	1/1	0.95	0.07	45,45,45,45	0
56	MG	RA	3340	1/1	0.95	0.05	31,31,31,31	0
56	MG	XA	1669	1/1	0.95	0.05	55,55,55,55	0
56	MG	YA	3653	1/1	0.95	0.17	29,29,29,29	0
56	MG	RA	3002	1/1	0.95	0.04	55,55,55,55	0
56	MG	YA	3094	1/1	0.95	0.15	36,36,36,36	0
56	MG	RA	3342	1/1	0.95	0.15	19,19,19,19	0
56	MG	QO	102	1/1	0.95	0.14	73,73,73,73	0
56	MG	RA	3004	1/1	0.95	0.14	52,52,52,52	0
56	MG	YA	3440	1/1	0.95	0.17	23,23,23,23	0
56	MG	YA	3441	1/1	0.95	0.08	11,11,11,11	0
56	MG	YA	3098	1/1	0.95	0.26	41,41,41,41	0
56	MG	YA	3548	1/1	0.95	0.28	47,47,47,47	0
56	MG	YA	3351	1/1	0.95	0.15	12,12,12,12	0
56	MG	YA	3099	1/1	0.95	0.21	43,43,43,43	0
56	MG	XA	1725	1/1	0.95	0.16	30,30,30,30	0
56	MG	YA	3355	1/1	0.95	0.19	35,35,35,35	0
56	MG	XA	1786	1/1	0.95	0.11	44,44,44,44	0
56	MG	YA	3556	1/1	0.95	0.28	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	QA	1686	1/1	0.95	0.14	38,38,38,38	0
56	MG	YA	3561	1/1	0.95	0.09	37,37,37,37	0
56	MG	YA	3038	1/1	0.95	0.07	47,47,47,47	0
56	MG	QA	1702	1/1	0.95	0.05	48,48,48,48	0
56	MG	YA	3362	1/1	0.95	0.19	29,29,29,29	0
56	MG	YA	3677	1/1	0.95	0.08	2,2,2,2	0
56	MG	RA	3244	1/1	0.95	0.06	36,36,36,36	0
56	MG	RA	3428	1/1	0.95	0.15	53,53,53,53	0
56	MG	RA	3668	1/1	0.95	0.12	58,58,58,58	0
56	MG	RA	3551	1/1	0.95	0.14	11,11,11,11	0
56	MG	QA	1628	1/1	0.95	0.09	33,33,33,33	0
56	MG	QA	1613	1/1	0.95	0.05	97,97,97,97	0
56	MG	RA	3490	1/1	0.95	0.15	27,27,27,27	0
56	MG	RA	3556	1/1	0.95	0.05	37,37,37,37	0
56	MG	YA	3048	1/1	0.95	0.05	61,61,61,61	0
56	MG	RA	3319	1/1	0.95	0.12	38,38,38,38	0
56	MG	YA	3050	1/1	0.95	0.05	47,47,47,47	0
56	MG	YA	3469	1/1	0.95	0.18	12,12,12,12	0
56	MG	YA	3578	1/1	0.95	0.20	20,20,20,20	0
56	MG	R6	102	1/1	0.95	0.15	48,48,48,48	0
56	MG	YA	3278	1/1	0.95	0.19	22,22,22,22	0
56	MG	RA	3561	1/1	0.95	0.11	31,31,31,31	0
56	MG	RB	208	1/1	0.95	0.07	44,44,44,44	0
56	MG	YA	3583	1/1	0.95	0.19	39,39,39,39	0
56	MG	XV	102	1/1	0.95	0.06	43,43,43,43	0
56	MG	YA	3700	1/1	0.95	0.06	30,30,30,30	0
56	MG	YA	3282	1/1	0.95	0.12	17,17,17,17	0
56	MG	YA	3476	1/1	0.95	0.28	44,44,44,44	0
56	MG	RA	3124	1/1	0.95	0.18	90,90,90,90	0
56	MG	QA	1810	1/1	0.95	0.21	59,59,59,59	0
56	MG	Y0	101	1/1	0.95	0.07	14,14,14,14	0
56	MG	RB	213	1/1	0.95	0.10	28,28,28,28	0
56	MG	YA	3386	1/1	0.95	0.17	38,38,38,38	0
56	MG	RA	3211	1/1	0.95	0.12	43,43,43,43	0
56	MG	YB	203	1/1	0.95	0.04	48,48,48,48	0
56	MG	YA	3291	1/1	0.95	0.16	2,2,2,2	0
56	MG	YB	205	1/1	0.95	0.12	41,41,41,41	0
56	MG	YA	3200	1/1	0.95	0.08	42,42,42,42	0
56	MG	YA	3390	1/1	0.95	0.09	38,38,38,38	0
56	MG	QA	1721	1/1	0.95	0.09	50,50,50,50	0
56	MG	XA	1748	1/1	0.95	0.07	36,36,36,36	0
56	MG	XA	1749	1/1	0.95	0.08	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YB	211	1/1	0.95	0.21	38,38,38,38	0
56	MG	YA	3297	1/1	0.95	0.18	28,28,28,28	0
56	MG	YA	3063	1/1	0.95	0.06	35,35,35,35	0
56	MG	QA	1661	1/1	0.95	0.06	35,35,35,35	0
56	MG	RA	3300	1/1	0.95	0.14	17,17,17,17	0
56	MG	YA	3608	1/1	0.95	0.19	32,32,32,32	0
56	MG	XA	1601	1/1	0.95	0.06	40,40,40,40	0
56	MG	YA	3302	1/1	0.95	0.11	23,23,23,23	0
56	MG	YA	3303	1/1	0.95	0.17	25,25,25,25	0
56	MG	YA	3137	1/1	0.95	0.08	18,18,18,18	0
56	MG	RA	3329	1/1	0.95	0.13	43,43,43,43	0
56	MG	YA	3308	1/1	0.95	0.11	34,34,34,34	0
56	MG	RA	3646	1/1	0.95	0.26	39,39,39,39	0
56	MG	RA	3112	1/1	0.95	0.11	51,51,51,51	0
56	MG	YA	3621	1/1	0.95	0.18	11,11,11,11	0
56	MG	RD	305	1/1	0.95	0.08	35,35,35,35	0
56	MG	QA	1724	1/1	0.95	0.05	37,37,37,37	0
56	MG	XA	1655	1/1	0.95	0.05	38,38,38,38	0
56	MG	XA	1763	1/1	0.95	0.27	40,40,40,40	0
56	MG	YF	303	1/1	0.95	0.05	38,38,38,38	0
56	MG	YA	3145	1/1	0.95	0.15	28,28,28,28	0
56	MG	QA	1699	1/1	0.95	0.20	41,41,41,41	0
56	MG	YG	203	1/1	0.95	0.05	48,48,48,48	0
56	MG	YA	3628	1/1	0.95	0.10	30,30,30,30	0
56	MG	YA	3076	1/1	0.95	0.22	44,44,44,44	0
56	MG	RA	3691	1/1	0.95	0.22	89,89,89,89	0
56	MG	RA	3504	1/1	0.95	0.08	31,31,31,31	0
56	MG	YA	3079	1/1	0.95	0.23	64,64,64,64	0
56	MG	XA	1611	1/1	0.95	0.08	52,52,52,52	0
56	MG	YQ	202	1/1	0.95	0.08	30,30,30,30	0
56	MG	YR	201	1/1	0.95	0.20	50,50,50,50	0
56	MG	RA	3148	1/1	0.95	0.17	55,55,55,55	0
56	MG	YA	3517	1/1	0.95	0.12	24,24,24,24	0
56	MG	RA	3538	1/1	0.95	0.24	53,53,53,53	0
56	MG	XA	1713	1/1	0.95	0.18	42,42,42,42	0
56	MG	YA	3022	1/1	0.95	0.04	17,17,17,17	0
56	MG	YA	3330	1/1	0.95	0.19	32,32,32,32	0
56	MG	RA	3577	1/1	0.95	0.12	40,40,40,40	0
56	MG	YA	3332	1/1	0.95	0.18	31,31,31,31	0
56	MG	RA	3257	1/1	0.95	0.06	43,43,43,43	0
59	ZN	RY	201	1/1	0.95	0.10	197,197,197,197	0
56	MG	RA	3614	1/1	0.95	0.15	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1761	1/1	0.96	0.17	41,41,41,41	0
56	MG	XA	1605	1/1	0.96	0.05	64,64,64,64	0
56	MG	YA	3560	1/1	0.96	0.05	28,28,28,28	0
56	MG	YA	3459	1/1	0.96	0.05	37,37,37,37	0
56	MG	YA	3287	1/1	0.96	0.16	11,11,11,11	0
56	MG	YA	3461	1/1	0.96	0.08	46,46,46,46	0
56	MG	QA	1647	1/1	0.96	0.04	64,64,64,64	0
56	MG	RA	3274	1/1	0.96	0.13	19,19,19,19	0
56	MG	YA	3290	1/1	0.96	0.06	34,34,34,34	0
56	MG	YA	3466	1/1	0.96	0.10	21,21,21,21	0
56	MG	YA	3673	1/1	0.96	0.13	41,41,41,41	0
56	MG	QA	1666	1/1	0.96	0.09	52,52,52,52	0
56	MG	YA	3208	1/1	0.96	0.08	47,47,47,47	0
56	MG	RA	3324	1/1	0.96	0.18	37,37,37,37	0
56	MG	XA	1767	1/1	0.96	0.04	46,46,46,46	0
56	MG	XA	1768	1/1	0.96	0.18	33,33,33,33	0
56	MG	RA	3574	1/1	0.96	0.10	40,40,40,40	0
56	MG	RA	3277	1/1	0.96	0.14	32,32,32,32	0
56	MG	XA	1612	1/1	0.96	0.07	57,57,57,57	0
56	MG	RE	303	1/1	0.96	0.06	50,50,50,50	0
56	MG	RA	3008	1/1	0.96	0.05	45,45,45,45	0
56	MG	YA	3218	1/1	0.96	0.07	39,39,39,39	0
56	MG	XA	1664	1/1	0.96	0.21	64,64,64,64	0
56	MG	YA	3220	1/1	0.96	0.07	51,51,51,51	0
56	MG	XA	1716	1/1	0.96	0.18	52,52,52,52	0
56	MG	YA	3222	1/1	0.96	0.09	64,64,64,64	0
56	MG	RA	3655	1/1	0.96	0.11	18,18,18,18	0
56	MG	RA	3279	1/1	0.96	0.13	31,31,31,31	0
56	MG	QA	1700	1/1	0.96	0.06	47,47,47,47	0
56	MG	YA	3692	1/1	0.96	0.09	44,44,44,44	0
56	MG	RA	3172	1/1	0.96	0.18	72,72,72,72	0
56	MG	RA	3476	1/1	0.96	0.12	63,63,63,63	0
56	MG	YA	3695	1/1	0.96	0.12	39,39,39,39	0
56	MG	YA	3589	1/1	0.96	0.13	30,30,30,30	0
56	MG	RA	3617	1/1	0.96	0.10	15,15,15,15	0
56	MG	YA	3698	1/1	0.96	0.14	40,40,40,40	0
56	MG	YA	3156	1/1	0.96	0.18	39,39,39,39	0
56	MG	YA	3402	1/1	0.96	0.15	42,42,42,42	0
56	MG	RA	3116	1/1	0.96	0.09	57,57,57,57	0
56	MG	RA	3306	1/1	0.96	0.16	11,11,11,11	0
56	MG	RA	3050	1/1	0.96	0.08	49,49,49,49	0
56	MG	YA	3494	1/1	0.96	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3191	1/1	0.96	0.13	30,30,30,30	0
56	MG	RA	3010	1/1	0.96	0.13	58,58,58,58	0
56	MG	RA	3336	1/1	0.96	0.05	15,15,15,15	0
56	MG	RA	3515	1/1	0.96	0.06	38,38,38,38	0
56	MG	RA	3337	1/1	0.96	0.05	39,39,39,39	0
56	MG	YA	3101	1/1	0.96	0.14	49,49,49,49	0
56	MG	YA	3102	1/1	0.96	0.06	19,19,19,19	0
56	MG	YA	3503	1/1	0.96	0.05	13,13,13,13	0
56	MG	RA	3552	1/1	0.96	0.09	38,38,38,38	0
56	MG	RA	3339	1/1	0.96	0.17	38,38,38,38	0
56	MG	RA	3176	1/1	0.96	0.20	69,69,69,69	0
56	MG	YA	3249	1/1	0.96	0.18	31,31,31,31	0
56	MG	YA	3614	1/1	0.96	0.18	38,38,38,38	0
56	MG	RA	3062	1/1	0.96	0.19	46,46,46,46	0
56	MG	YB	213	1/1	0.96	0.10	34,34,34,34	0
56	MG	YA	3337	1/1	0.96	0.11	7,7,7,7	0
56	MG	XA	1737	1/1	0.96	0.04	38,38,38,38	0
56	MG	YA	3618	1/1	0.96	0.09	7,7,7,7	0
56	MG	RA	3107	1/1	0.96	0.26	83,83,83,83	0
56	MG	YA	3422	1/1	0.96	0.17	29,29,29,29	0
56	MG	XA	1684	1/1	0.96	0.10	35,35,35,35	0
56	MG	RA	3634	1/1	0.96	0.13	30,30,30,30	0
56	MG	RA	3343	1/1	0.96	0.10	34,34,34,34	0
56	MG	XA	1687	1/1	0.96	0.28	57,57,57,57	0
56	MG	RA	3595	1/1	0.96	0.11	39,39,39,39	0
56	MG	XA	1640	1/1	0.96	0.09	53,53,53,53	0
56	MG	RA	3042	1/1	0.96	0.04	45,45,45,45	0
56	MG	RB	210	1/1	0.96	0.17	43,43,43,43	0
56	MG	YA	3630	1/1	0.96	0.24	25,25,25,25	0
56	MG	YA	3523	1/1	0.96	0.17	4,4,4,4	0
56	MG	RA	3430	1/1	0.96	0.05	35,35,35,35	0
56	MG	YA	3526	1/1	0.96	0.12	18,18,18,18	0
56	MG	XA	1693	1/1	0.96	0.24	42,42,42,42	0
56	MG	YA	3433	1/1	0.96	0.09	32,32,32,32	0
56	MG	YA	3353	1/1	0.96	0.17	3,3,3,3	0
56	MG	YA	3184	1/1	0.96	0.10	56,56,56,56	0
56	MG	YA	3532	1/1	0.96	0.10	22,22,22,22	0
56	MG	QA	1716	1/1	0.96	0.05	73,73,73,73	0
56	MG	YA	3356	1/1	0.96	0.15	37,37,37,37	0
56	MG	YA	3357	1/1	0.96	0.12	66,66,66,66	0
56	MG	RA	3527	1/1	0.96	0.30	37,37,37,37	0
56	MG	RA	3683	1/1	0.96	0.06	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	Y8	101	1/1	0.96	0.17	34,34,34,34	0
56	MG	YA	3270	1/1	0.96	0.06	34,34,34,34	0
56	MG	YA	3124	1/1	0.96	0.13	22,22,22,22	0
56	MG	RA	3494	1/1	0.96	0.14	57,57,57,57	0
56	MG	RA	3136	1/1	0.96	0.03	45,45,45,45	0
56	MG	QV	103	1/1	0.96	0.08	58,58,58,58	0
56	MG	YA	3065	1/1	0.96	0.05	37,37,37,37	0
56	MG	YA	3004	1/1	0.96	0.29	39,39,39,39	0
56	MG	RA	3271	1/1	0.96	0.12	38,38,38,38	0
56	MG	XA	1757	1/1	0.96	0.17	50,50,50,50	0
56	MG	RA	3020	1/1	0.96	0.07	71,71,71,71	0
56	MG	YA	3371	1/1	0.96	0.20	29,29,29,29	0
56	MG	RD	304	1/1	0.96	0.26	131,131,131,131	0
56	MG	YA	3458	1/1	0.97	0.08	20,20,20,20	0
56	MG	QA	1706	1/1	0.97	0.12	57,57,57,57	0
56	MG	YA	3529	1/1	0.97	0.14	5,5,5,5	0
56	MG	YA	3326	1/1	0.97	0.11	11,11,11,11	0
56	MG	Y5	102	1/1	0.97	0.21	45,45,45,45	0
56	MG	RA	3355	1/1	0.97	0.19	30,30,30,30	0
56	MG	YA	3463	1/1	0.97	0.16	54,54,54,54	0
56	MG	RA	3652	1/1	0.97	0.10	29,29,29,29	0
56	MG	RA	3621	1/1	0.97	0.04	7,7,7,7	0
56	MG	QT	201	1/1	0.97	0.10	51,51,51,51	0
56	MG	RA	3266	1/1	0.97	0.17	31,31,31,31	0
56	MG	QA	1690	1/1	0.97	0.09	48,48,48,48	0
56	MG	YA	3539	1/1	0.97	0.14	32,32,32,32	0
56	MG	XA	1616	1/1	0.97	0.12	31,31,31,31	0
56	MG	RA	3144	1/1	0.97	0.12	38,38,38,38	0
56	MG	RA	3312	1/1	0.97	0.13	7,7,7,7	0
56	MG	YA	3207	1/1	0.97	0.14	23,23,23,23	0
56	MG	YA	3701	1/1	0.97	0.07	20,20,20,20	0
56	MG	RA	3627	1/1	0.97	0.18	44,44,44,44	0
56	MG	XA	1732	1/1	0.97	0.11	35,35,35,35	0
56	MG	QA	1624	1/1	0.97	0.06	63,63,63,63	0
56	MG	YA	3272	1/1	0.97	0.11	6,6,6,6	0
56	MG	YA	3273	1/1	0.97	0.07	16,16,16,16	0
56	MG	YA	3009	1/1	0.97	0.08	8,8,8,8	0
56	MG	XA	1734	1/1	0.97	0.18	46,46,46,46	0
56	MG	QA	1709	1/1	0.97	0.10	33,33,33,33	0
56	MG	XA	1658	1/1	0.97	0.06	47,47,47,47	0
56	MG	QA	1751	1/1	0.97	0.10	45,45,45,45	0
56	MG	XA	1697	1/1	0.97	0.10	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3217	1/1	0.97	0.12	37,37,37,37	0
56	MG	YA	3637	1/1	0.97	0.11	24,24,24,24	0
56	MG	YA	3638	1/1	0.97	0.05	32,32,32,32	0
56	MG	RR	202	1/1	0.97	0.05	39,39,39,39	0
56	MG	RT	201	1/1	0.97	0.13	47,47,47,47	0
56	MG	QA	1732	1/1	0.97	0.11	33,33,33,33	0
56	MG	RA	3488	1/1	0.97	0.15	24,24,24,24	0
56	MG	QA	1765	1/1	0.97	0.06	60,60,60,60	0
56	MG	YA	3021	1/1	0.97	0.18	87,87,87,87	0
56	MG	QB	301	1/1	0.97	0.06	69,69,69,69	0
56	MG	YA	3646	1/1	0.97	0.13	10,10,10,10	0
56	MG	XA	1704	1/1	0.97	0.08	59,59,59,59	0
56	MG	YA	3172	1/1	0.97	0.10	88,88,88,88	0
56	MG	YB	220	1/1	0.97	0.15	38,38,38,38	0
56	MG	YA	3227	1/1	0.97	0.10	16,16,16,16	0
56	MG	YA	3650	1/1	0.97	0.16	40,40,40,40	0
56	MG	QA	1742	1/1	0.97	0.14	10,10,10,10	0
56	MG	YA	3497	1/1	0.97	0.14	17,17,17,17	0
56	MG	QA	1794	1/1	0.97	0.16	43,43,43,43	0
56	MG	XA	1631	1/1	0.97	0.09	37,37,37,37	0
56	MG	XA	1793	1/1	0.97	0.13	57,57,57,57	0
56	MG	QA	1672	1/1	0.97	0.05	54,54,54,54	0
56	MG	QA	1734	1/1	0.97	0.05	46,46,46,46	0
56	MG	YE	304	1/1	0.97	0.07	43,43,43,43	0
56	MG	RA	3521	1/1	0.97	0.24	42,42,42,42	0
56	MG	XF	202	1/1	0.97	0.09	46,46,46,46	0
56	MG	RA	3549	1/1	0.97	0.15	21,21,21,21	0
56	MG	YA	3661	1/1	0.97	0.24	38,38,38,38	0
56	MG	XL	201	1/1	0.97	0.04	22,22,22,22	0
56	MG	YA	3240	1/1	0.97	0.15	2,2,2,2	0
56	MG	YA	3241	1/1	0.97	0.05	18,18,18,18	0
56	MG	YA	3665	1/1	0.97	0.10	26,26,26,26	0
56	MG	RA	3522	1/1	0.97	0.12	19,19,19,19	0
56	MG	RA	3240	1/1	0.97	0.11	2,2,2,2	0
56	MG	RA	3396	1/1	0.97	0.17	48,48,48,48	0
56	MG	XA	1639	1/1	0.97	0.12	34,34,34,34	0
56	MG	YA	3246	1/1	0.97	0.19	18,18,18,18	0
56	MG	YA	3187	1/1	0.97	0.09	19,19,19,19	0
56	MG	YA	3315	1/1	0.97	0.18	3,3,3,3	0
56	MG	RA	3325	1/1	0.97	0.11	9,9,9,9	0
56	MG	RA	3241	1/1	0.97	0.14	26,26,26,26	0
56	MG	YA	3190	1/1	0.97	0.17	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3251	1/1	0.97	0.14	16,16,16,16	0
56	MG	QA	1683	1/1	0.97	0.17	37,37,37,37	0
56	MG	QA	1712	1/1	0.97	0.07	44,44,44,44	0
56	MG	YW	202	1/1	0.97	0.04	35,35,35,35	0
56	MG	YA	3599	1/1	0.97	0.32	42,42,42,42	0
56	MG	YA	3600	1/1	0.97	0.19	2,2,2,2	0
58	SF4	QD	302	8/8	0.97	0.08	54,93,149,174	0
56	MG	YA	3524	1/1	0.97	0.08	6,6,6,6	0
56	MG	QA	1758	1/1	0.97	0.06	39,39,39,39	0
56	MG	Y1	102	1/1	0.97	0.07	35,35,35,35	0
59	ZN	YY	201	1/1	0.97	0.05	99,99,99,99	0
56	MG	YA	3260	1/1	0.98	0.06	2,2,2,2	0
56	MG	YA	3553	1/1	0.98	0.07	11,11,11,11	0
56	MG	YA	3204	1/1	0.98	0.07	49,49,49,49	0
56	MG	YA	3609	1/1	0.98	0.11	28,28,28,28	0
56	MG	YA	3294	1/1	0.98	0.10	13,13,13,13	0
56	MG	YA	3232	1/1	0.98	0.10	2,2,2,2	0
56	MG	YA	3333	1/1	0.98	0.10	4,4,4,4	0
56	MG	YA	3558	1/1	0.98	0.11	9,9,9,9	0
56	MG	YA	3334	1/1	0.98	0.08	14,14,14,14	0
56	MG	RA	3304	1/1	0.98	0.06	16,16,16,16	0
56	MG	RA	3489	1/1	0.98	0.05	4,4,4,4	0
56	MG	YB	217	1/1	0.98	0.10	8,8,8,8	0
56	MG	RA	3280	1/1	0.98	0.10	26,26,26,26	0
56	MG	YA	3236	1/1	0.98	0.15	40,40,40,40	0
56	MG	QA	1620	1/1	0.98	0.03	56,56,56,56	0
56	MG	YA	3340	1/1	0.98	0.10	15,15,15,15	0
56	MG	YA	3341	1/1	0.98	0.09	29,29,29,29	0
56	MG	YA	3568	1/1	0.98	0.09	21,21,21,21	0
56	MG	XA	1776	1/1	0.98	0.25	38,38,38,38	0
56	MG	RA	3439	1/1	0.98	0.12	25,25,25,25	0
56	MG	YA	3033	1/1	0.98	0.11	54,54,54,54	0
56	MG	YA	3305	1/1	0.98	0.06	2,2,2,2	0
56	MG	YA	3346	1/1	0.98	0.08	14,14,14,14	0
56	MG	YA	3521	1/1	0.98	0.10	12,12,12,12	0
56	MG	YA	3133	1/1	0.98	0.10	48,48,48,48	0
56	MG	XA	1754	1/1	0.98	0.11	22,22,22,22	0
56	MG	RA	3338	1/1	0.98	0.08	30,30,30,30	0
56	MG	RA	3276	1/1	0.98	0.16	32,32,32,32	0
56	MG	YA	3435	1/1	0.98	0.08	4,4,4,4	0
56	MG	YA	3275	1/1	0.98	0.09	8,8,8,8	0
56	MG	RA	3600	1/1	0.98	0.12	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3674	1/1	0.98	0.06	31,31,31,31	0
56	MG	RA	3636	1/1	0.98	0.14	42,42,42,42	0
56	MG	YA	3314	1/1	0.98	0.14	2,2,2,2	0
56	MG	YA	3485	1/1	0.98	0.12	18,18,18,18	0
56	MG	RA	3618	1/1	0.98	0.10	21,21,21,21	0
56	MG	QA	1722	1/1	0.98	0.14	25,25,25,25	0
56	MG	YA	3090	1/1	0.98	0.15	45,45,45,45	0
56	MG	RA	3431	1/1	0.98	0.25	17,17,17,17	0
56	MG	RA	3316	1/1	0.98	0.18	18,18,18,18	0
56	MG	RA	3005	1/1	0.98	0.21	36,36,36,36	0
56	MG	YA	3285	1/1	0.98	0.09	2,2,2,2	0
56	MG	YA	3448	1/1	0.98	0.13	2,2,2,2	0
56	MG	YA	3541	1/1	0.98	0.12	11,11,11,11	0
56	MG	RA	3681	1/1	0.98	0.05	12,12,12,12	0
56	MG	YA	3323	1/1	0.98	0.12	2,2,2,2	0
56	MG	RA	3352	1/1	0.98	0.04	20,20,20,20	0
56	MG	YA	3545	1/1	0.98	0.04	19,19,19,19	0
56	MG	RA	3447	1/1	0.98	0.13	11,11,11,11	0
56	MG	QA	1785	1/1	0.98	0.06	74,74,74,74	0
58	SF4	XD	301	8/8	0.98	0.07	64,74,104,108	0
59	ZN	QN	101	1/1	0.98	0.07	200,200,200,200	0
56	MG	YA	3602	1/1	0.98	0.26	40,40,40,40	0
56	MG	YA	3410	1/1	0.98	0.08	37,37,37,37	0
59	ZN	XN	101	1/1	0.98	0.06	114,114,114,114	0
56	MG	RA	3558	1/1	0.98	0.06	32,32,32,32	0
59	ZN	Y5	101	1/1	0.98	0.04	88,88,88,88	0
59	ZN	Y9	101	1/1	0.98	0.03	61,61,61,61	0
56	MG	RA	3559	1/1	0.98	0.04	38,38,38,38	0
56	MG	YA	3018	1/1	0.99	0.05	48,48,48,48	0
56	MG	YA	3304	1/1	0.99	0.21	14,14,14,14	0
56	MG	YA	3518	1/1	0.99	0.03	10,10,10,10	0
56	MG	RB	211	1/1	0.99	0.04	39,39,39,39	0
56	MG	QA	1822	1/1	0.99	0.03	62,62,62,62	0
56	MG	QA	1626	1/1	0.99	0.10	34,34,34,34	0
56	MG	YA	3601	1/1	0.99	0.19	12,12,12,12	0
56	MG	YA	3559	1/1	0.99	0.04	9,9,9,9	0
56	MG	RE	304	1/1	0.99	0.07	2,2,2,2	0
56	MG	YA	3619	1/1	0.99	0.05	9,9,9,9	0
56	MG	XA	1760	1/1	0.99	0.25	35,35,35,35	0
59	ZN	R5	101	1/1	0.99	0.05	126,126,126,126	0
59	ZN	R6	101	1/1	0.99	0.03	71,71,71,71	0
56	MG	RA	3362	1/1	0.99	0.06	17,17,17,17	0

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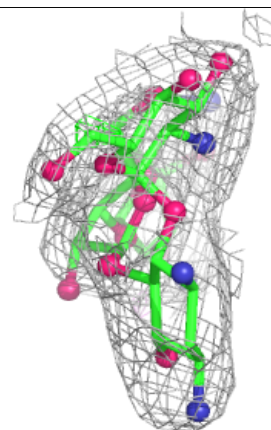
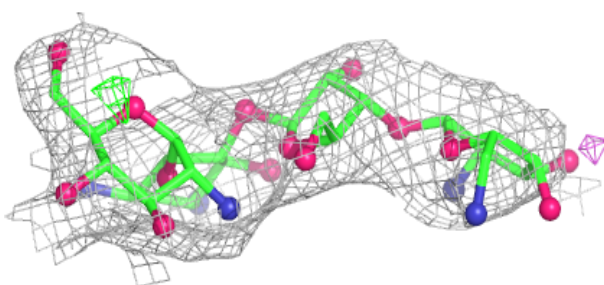
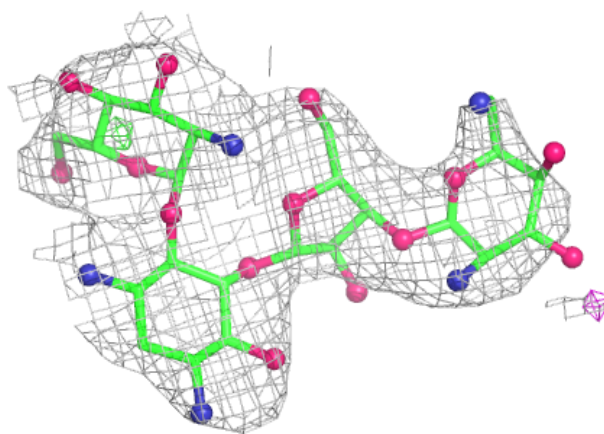
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3549	1/1	0.99	0.31	44,44,44,44	0
56	MG	YE	301	1/1	0.99	0.11	12,12,12,12	0
56	MG	YA	3381	1/1	0.99	0.03	26,26,26,26	0
59	ZN	Y6	101	1/1	0.99	0.03	52,52,52,52	0
56	MG	RA	3567	1/1	0.99	0.10	19,19,19,19	0
56	MG	YA	3122	1/1	0.99	0.04	36,36,36,36	0
59	ZN	R9	101	1/1	1.00	0.02	90,90,90,90	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

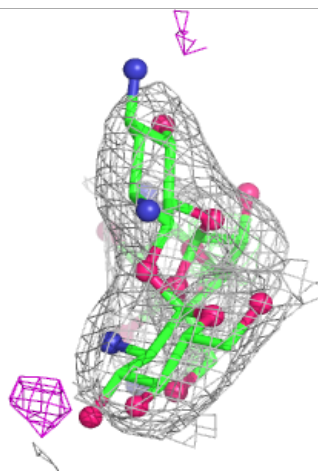
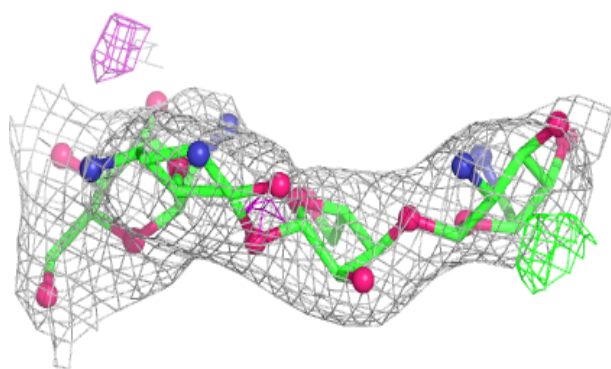
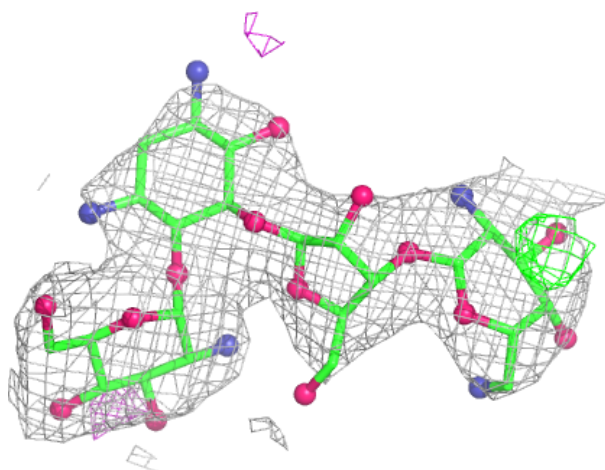
Electron density around PAR QA 1821:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PAR XA 1794:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.