



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:42 PM EDT

PDB ID : 6OPE / pdb_00006ope
Title : Crystal structure of tRNA^{Ala}(GGC) U32-A38 bound to near-cognate 70S A site
Authors : Nguyen, H.A.; Sunita, S.; Dunham, C.M.
Deposited on : 2019-04-24
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

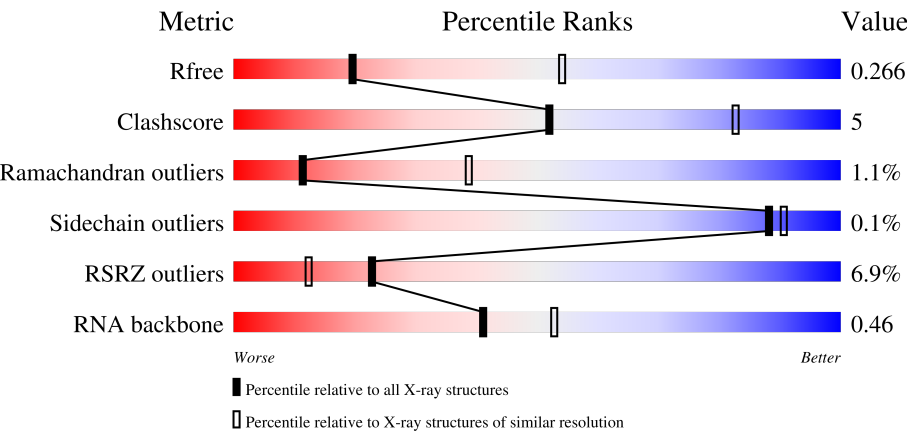
1 Overall quality at a glance i

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	2% 66% 28%
1	XA	1522	% 68% 27%
2	QB	256	8% 71% 20% 7%
2	XB	256	4% 72% 20% 7%

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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	131	
12	XL	131	
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	1601	-	-	-	X
56	MG	QA	1612	-	-	-	X
56	MG	QA	1618	-	-	-	X
56	MG	QA	1625	-	-	-	X
56	MG	QA	1628	-	-	-	X
56	MG	QA	1632	-	-	-	X
56	MG	QA	1638	-	-	-	X
56	MG	QA	1643	-	-	-	X
56	MG	QA	1658	-	-	-	X
56	MG	QX	102	-	-	-	X
56	MG	R9	101	-	-	-	X
56	MG	RA	3003	-	-	-	X
56	MG	RA	3011	-	-	-	X
56	MG	RA	3012	-	-	-	X
56	MG	RA	3013	-	-	-	X
56	MG	RA	3035	-	-	-	X
56	MG	RA	3051	-	-	-	X
56	MG	RA	3057	-	-	-	X
56	MG	RA	3067	-	-	-	X
56	MG	RA	3073	-	-	-	X
56	MG	RA	3112	-	-	-	X
56	MG	RA	3118	-	-	-	X
56	MG	RA	3120	-	-	-	X
56	MG	RA	3122	-	-	-	X
56	MG	RA	3126	-	-	-	X
56	MG	RA	3139	-	-	-	X
56	MG	RA	3142	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3146	-	-	-	X
56	MG	RA	3148	-	-	-	X
56	MG	RA	3149	-	-	-	X
56	MG	RA	3151	-	-	-	X
56	MG	RA	3159	-	-	-	X
56	MG	RA	3164	-	-	-	X
56	MG	RA	3166	-	-	-	X
56	MG	RA	3170	-	-	-	X
56	MG	RA	3173	-	-	-	X
56	MG	RA	3178	-	-	-	X
56	MG	RA	3180	-	-	-	X
56	MG	RA	3199	-	-	-	X
56	MG	RA	3202	-	-	-	X
56	MG	RA	3203	-	-	-	X
56	MG	RA	3206	-	-	-	X
56	MG	RA	3215	-	-	-	X
56	MG	RA	3217	-	-	-	X
56	MG	RA	3218	-	-	-	X
56	MG	RA	3223	-	-	-	X
56	MG	RA	3233	-	-	-	X
56	MG	RA	3236	-	-	-	X
56	MG	RA	3244	-	-	-	X
56	MG	RA	3249	-	-	-	X
56	MG	RA	3250	-	-	-	X
56	MG	RA	3252	-	-	-	X
56	MG	RA	3256	-	-	-	X
56	MG	RA	3262	-	-	-	X
56	MG	RA	3266	-	-	-	X
56	MG	RA	3277	-	-	-	X
56	MG	RA	3279	-	-	-	X
56	MG	XA	1607	-	-	-	X
56	MG	XA	1614	-	-	-	X
56	MG	XA	1619	-	-	-	X
56	MG	XA	1632	-	-	-	X
56	MG	XA	1646	-	-	-	X
56	MG	XA	1648	-	-	-	X
56	MG	XA	1654	-	-	-	X
56	MG	XA	1655	-	-	-	X
56	MG	XA	1660	-	-	-	X
56	MG	XA	1662	-	-	-	X
56	MG	XA	1667	-	-	-	X
56	MG	XA	1668	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	XA	1671	-	-	-	X
56	MG	XA	1687	-	-	-	X
56	MG	XA	1691	-	-	-	X
56	MG	XA	1692	-	-	-	X
56	MG	XX	101	-	-	-	X
56	MG	YA	3035	-	-	-	X
56	MG	YA	3106	-	-	-	X
56	MG	YA	3111	-	-	-	X
56	MG	YA	3154	-	-	-	X
56	MG	YA	3155	-	-	-	X
56	MG	YA	3162	-	-	-	X
56	MG	YA	3163	-	-	-	X
56	MG	YA	3168	-	-	-	X
56	MG	YA	3172	-	-	-	X
56	MG	YA	3181	-	-	-	X
56	MG	YA	3182	-	-	-	X
56	MG	YA	3191	-	-	-	X
56	MG	YA	3193	-	-	-	X
56	MG	YA	3197	-	-	-	X
56	MG	YA	3202	-	-	-	X
56	MG	YA	3205	-	-	-	X
56	MG	YA	3206	-	-	-	X
56	MG	YA	3220	-	-	-	X
56	MG	YA	3233	-	-	-	X
56	MG	YA	3239	-	-	-	X
56	MG	YA	3246	-	-	-	X
56	MG	YA	3286	-	-	-	X
56	MG	YA	3288	-	-	-	X
56	MG	YA	3294	-	-	-	X
56	MG	YA	3313	-	-	-	X
56	MG	YA	3321	-	-	-	X
56	MG	YA	3323	-	-	-	X
56	MG	YA	3333	-	-	-	X
56	MG	YA	3337	-	-	-	X
56	MG	YA	3338	-	-	-	X
56	MG	YA	3340	-	-	-	X
56	MG	YA	3346	-	-	-	X
56	MG	YB	201	-	-	-	X
56	MG	YP	201	-	-	-	X
56	MG	YQ	203	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 294981 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
			32247	14353	5981	10414	1499			
1	XA	1500	Total	C	N	O	P	0	0	0
			32249	14354	5984	10412	1499			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
2	XB	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	QC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	XC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	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
			1674	1050	333	284	7			
4	XD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	XE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	QF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	XF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	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
			1257	781	252	218	6			
7	XG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	XH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- 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
			1010	639	197	174				
9	XI	127	Total	C	N	O		0	0	0
			1010	639	197	174				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	QJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	XJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	XK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	QL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	XL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	121	Total	C	N	O	S	0	0	0
			964	597	199	166	2			
13	XM	121	Total	C	N	O	S	0	0	0
			964	597	199	166	2			

- 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	0	0	0
			492	312	104	72	4			
14	XN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- 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	0	0	0
			734	459	147	126	2			
15	XO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	QP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	XP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	QQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	XQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	XR	70	Total	C	N	O	0	0	0
			574	367	112	95			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			
19	XS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	XT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	QU	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	XU	25	Total	C	N	O	0	0	0
			217	134	52	31			

- 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
			396	177	82	119	18			
23	XX	18	Total	C	N	O	P	0	0	0
			396	177	82	119	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	75	Total	C	N	O	P	0	0	0
			1602	714	288	525	75			
24	XY	75	Total	C	N	O	P	0	0	0
			1602	714	288	525	75			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			
25	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	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
			763	481	150	131	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
27	Y2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- 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
			469	298	90	81			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	R4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			
29	Y4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	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
			459	288	90	76	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	R6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			
31	Y6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	R7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
32	Y7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	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	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			
35	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- 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
			2573	1146	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	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
37	YD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
38	YE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	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
			1585	1011	297	275	2			
39	YF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	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
			1474	942	268	260	4			
40	YG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
41	YH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
43	YN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	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	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
45	YP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	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	111	Total	C	N	O	0	0	0
			882	556	176	150			
48	YS	111	Total	C	N	O	0	0	0
			882	556	176	150			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	RT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
49	YT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	RU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
50	YU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	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
			779	501	142	135	1			
51	YV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	RW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
52	YW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	RX	92	Total	C	N	O	0	0	0
			725	471	131	123			
53	YX	92	Total	C	N	O	0	0	0
			725	471	131	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
54	YY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			
55	YZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	73	Total	Mg	0	0
			73	73		
56	QF	1	Total	Mg	0	0
			1	1		
56	QM	1	Total	Mg	0	0
			1	1		
56	QV	1	Total	Mg	0	0
			1	1		
56	QX	2	Total	Mg	0	0
			2	2		
56	R0	1	Total	Mg	0	0
			1	1		
56	R5	1	Total	Mg	0	0
			1	1		
56	R8	1	Total	Mg	0	0
			1	1		
56	R9	1	Total	Mg	0	0
			1	1		

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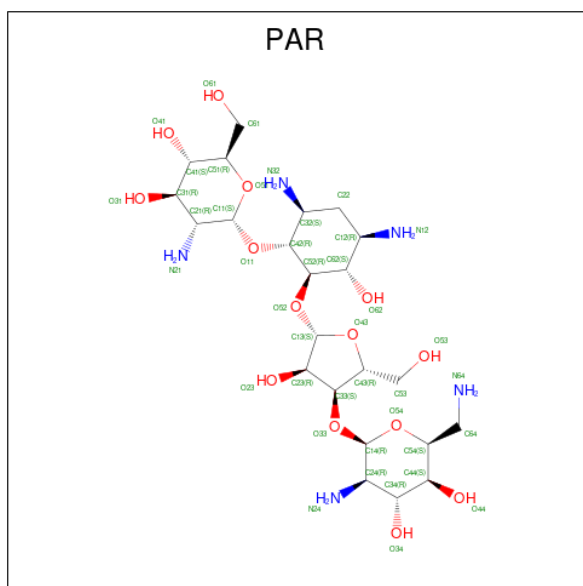
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	RA	281	Total 281	Mg 281	0	0
56	RB	4	Total 4	Mg 4	0	0
56	RD	1	Total 1	Mg 1	0	0
56	RE	4	Total 4	Mg 4	0	0
56	RF	1	Total 1	Mg 1	0	0
56	RP	3	Total 3	Mg 3	0	0
56	RR	1	Total 1	Mg 1	0	0
56	RU	1	Total 1	Mg 1	0	0
56	XA	91	Total 91	Mg 91	0	0
56	XF	1	Total 1	Mg 1	0	0
56	XM	1	Total 1	Mg 1	0	0
56	XV	2	Total 2	Mg 2	0	0
56	XX	1	Total 1	Mg 1	0	0
56	Y0	1	Total 1	Mg 1	0	0
56	Y1	1	Total 1	Mg 1	0	0
56	Y2	1	Total 1	Mg 1	0	0
56	Y5	1	Total 1	Mg 1	0	0
56	Y6	2	Total 2	Mg 2	0	0
56	Y8	1	Total 1	Mg 1	0	0
56	Y9	1	Total 1	Mg 1	0	0
56	YA	347	Total 347	Mg 347	0	0

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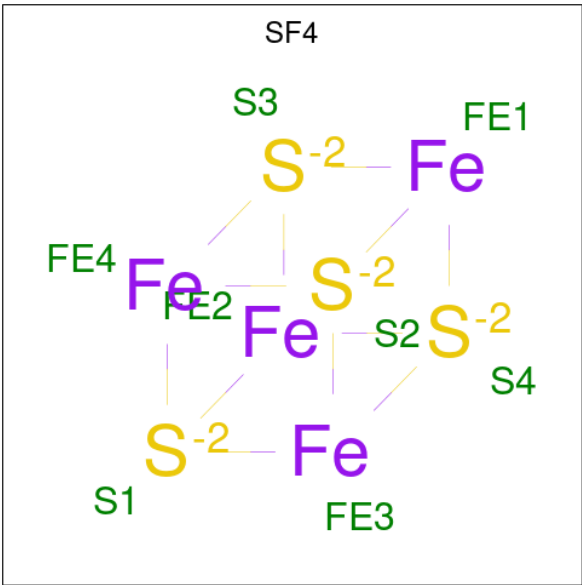
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	YB	6	Total Mg 6 6	0	0
56	YE	3	Total Mg 3 3	0	0
56	YN	1	Total Mg 1 1	0	0
56	YP	3	Total Mg 3 3	0	0
56	YQ	3	Total Mg 3 3	0	0
56	YR	1	Total Mg 1 1	0	0
56	YX	1	Total Mg 1 1	0	0

- Molecule 57 is PAROMOMYCIN (CCD ID: PAR) (formula: $\text{C}_{23}\text{H}_{45}\text{N}_5\text{O}_{14}$).



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

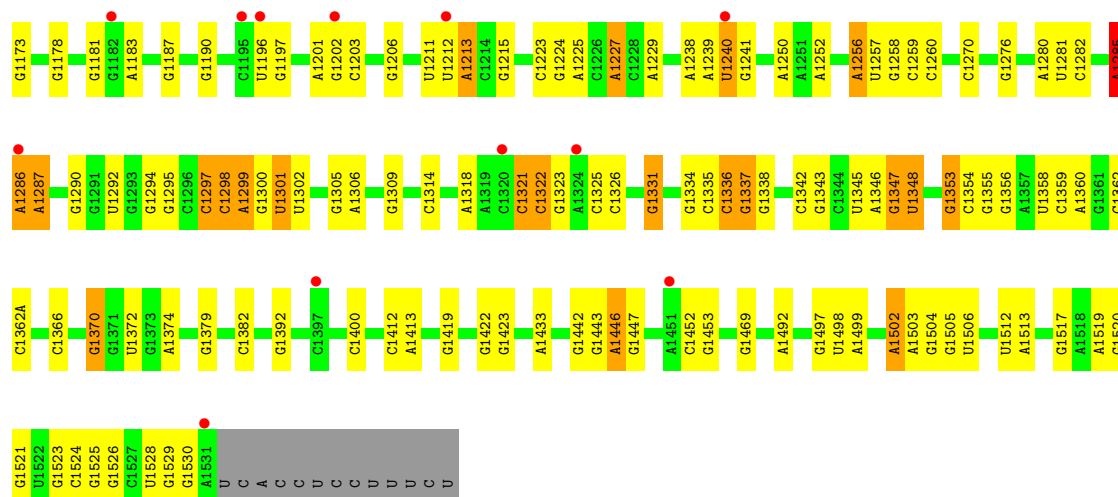
- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



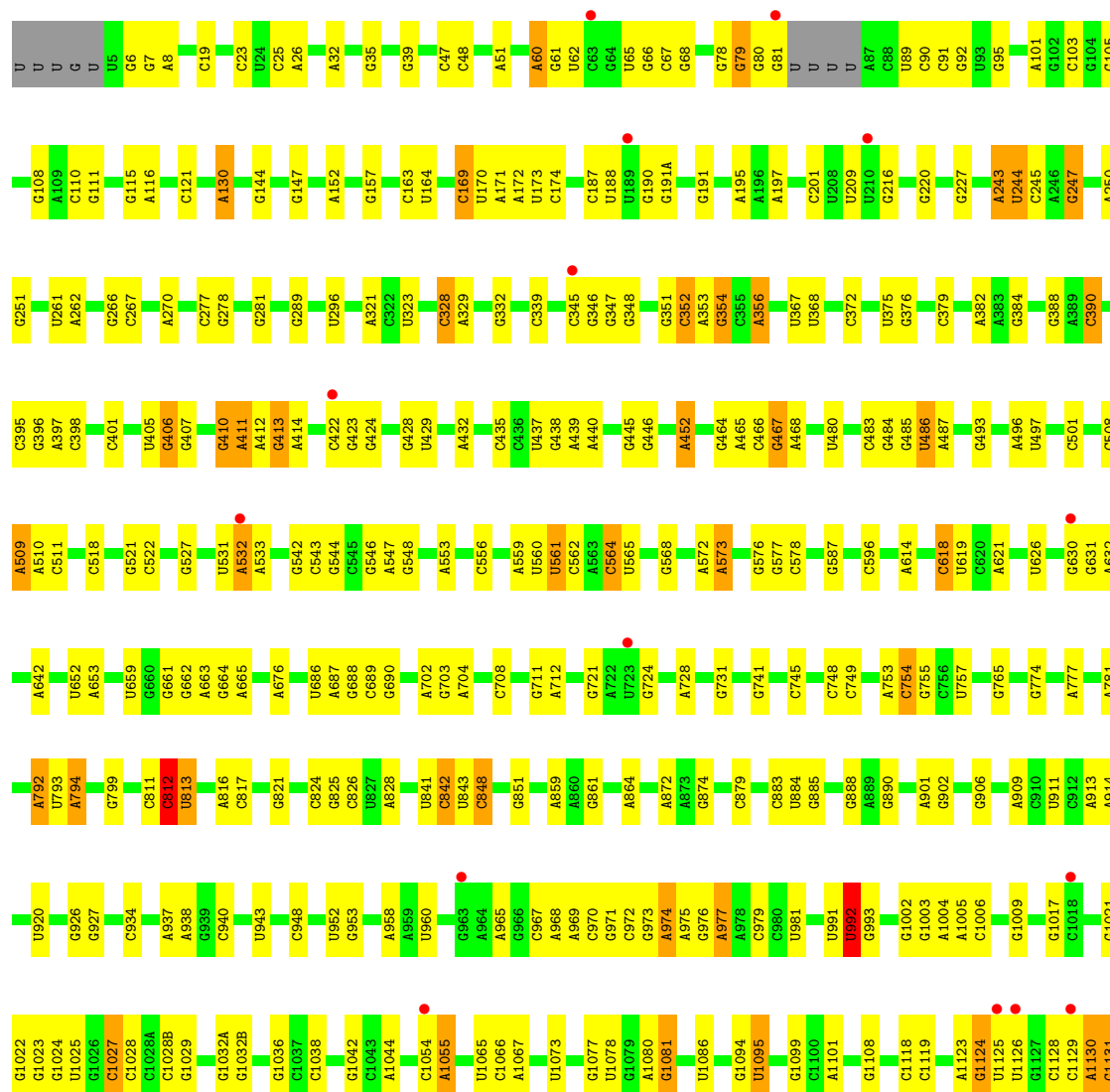
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	QD	1	Total	Fe	S	0	0
			8	4	4		
58	XD	1	Total	Fe	S	0	0
			8	4	4		

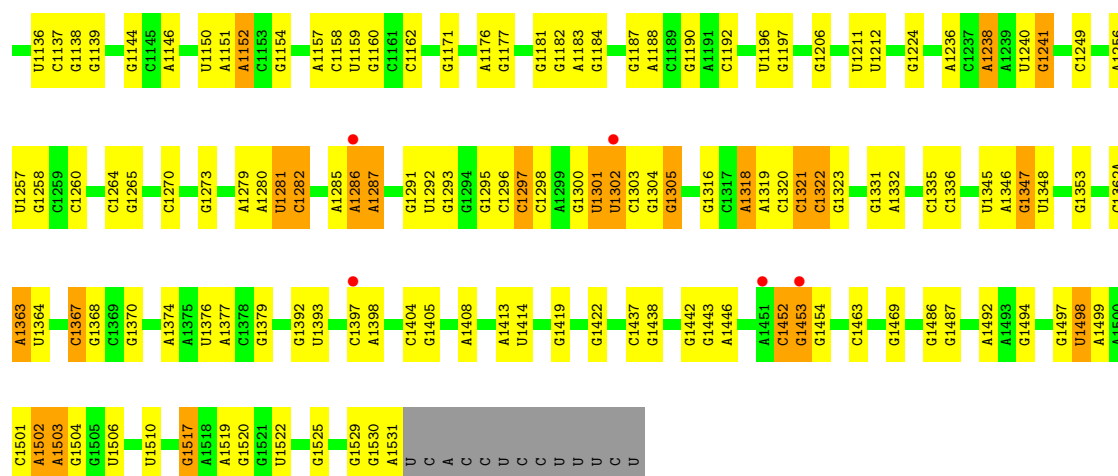
- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	QN	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		
59	Y9	1	Total	Zn	0	0
			1	1		

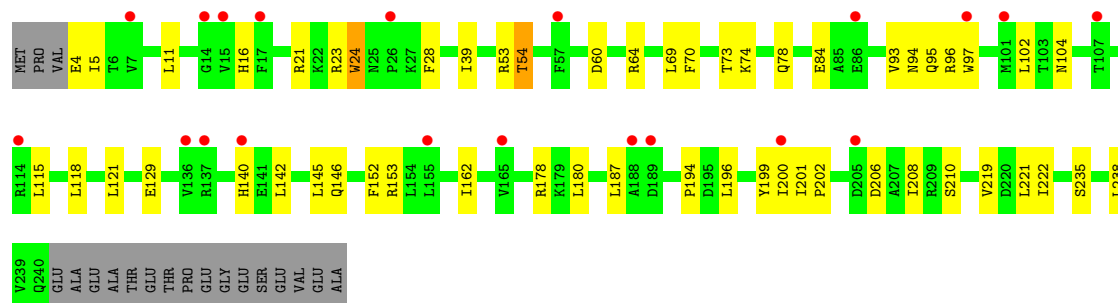
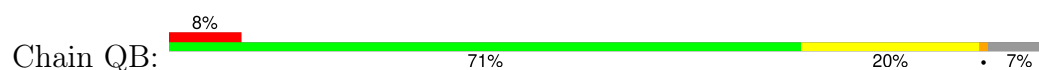


- Molecule 1: 16S rRNA

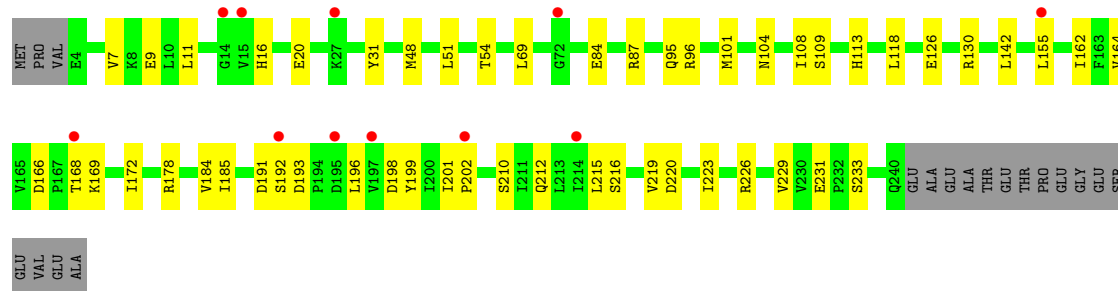
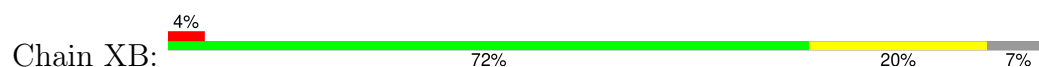




• Molecule 2: 30S ribosomal protein S2

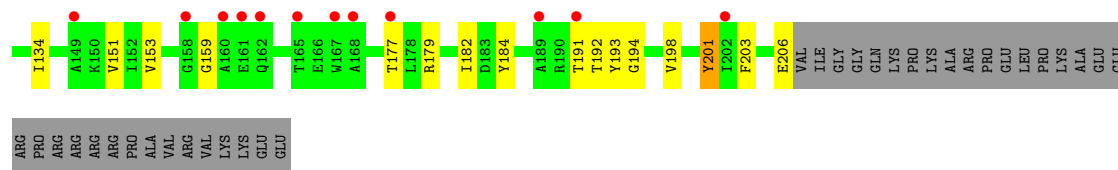


• Molecule 2: 30S ribosomal protein S2

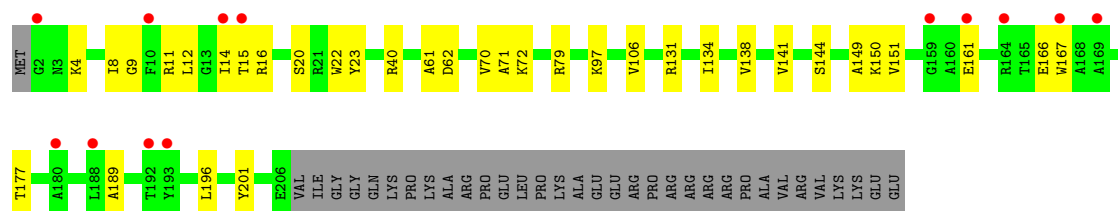
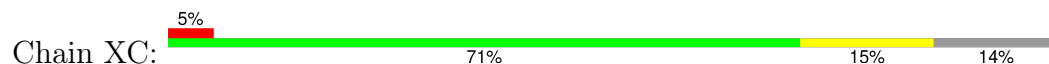


• Molecule 3: 30S ribosomal protein S3

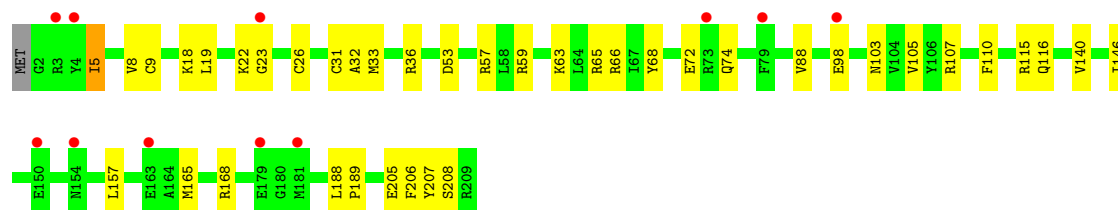
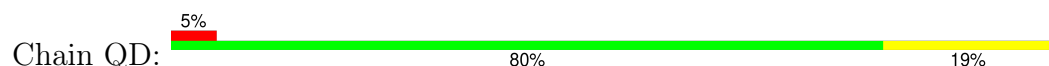




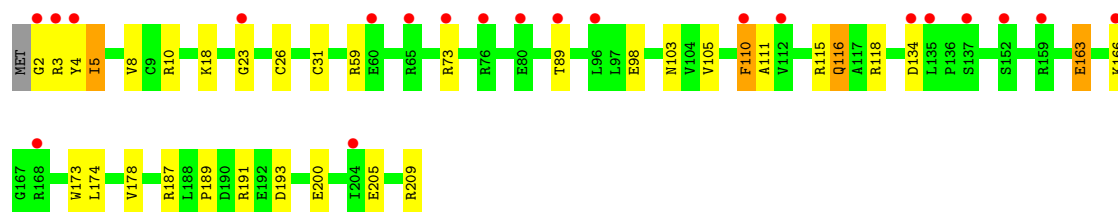
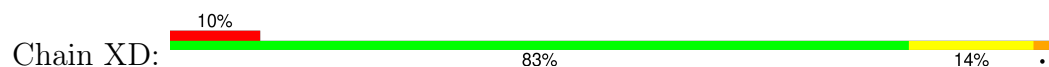
• Molecule 3: 30S ribosomal protein S3



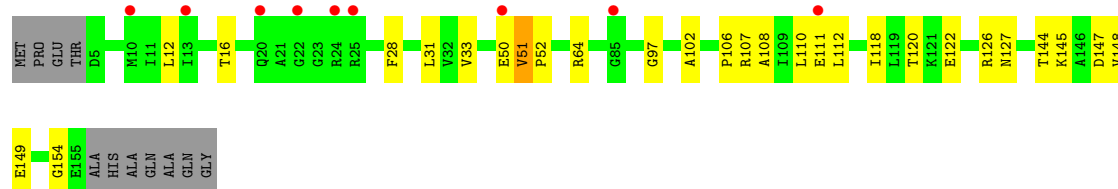
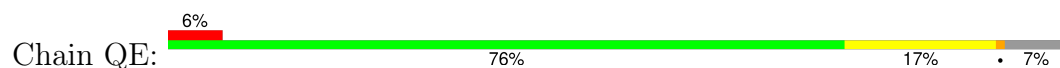
• Molecule 4: 30S ribosomal protein S4

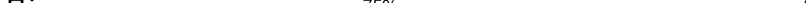


• Molecule 4: 30S ribosomal protein S4



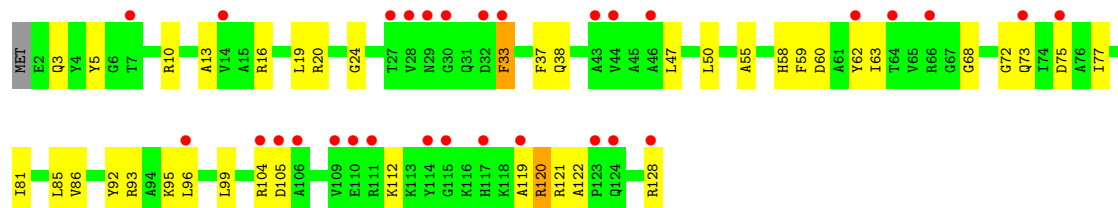
• Molecule 5: 30S ribosomal protein S5



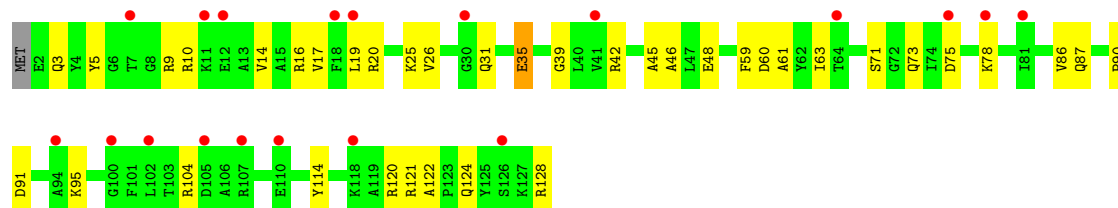
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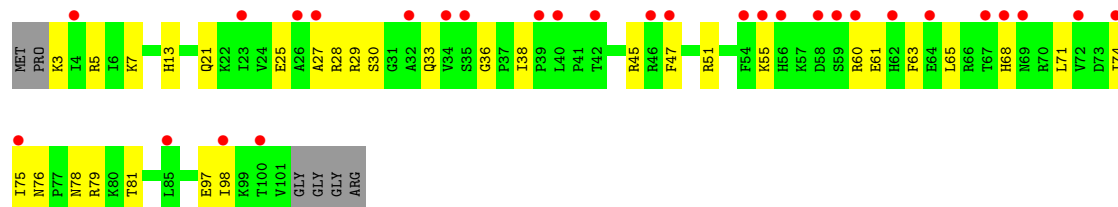
• Molecule 9: 30S ribosomal protein S9



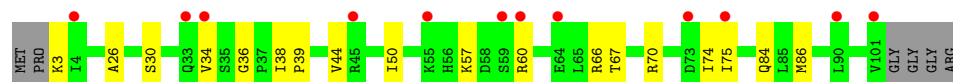
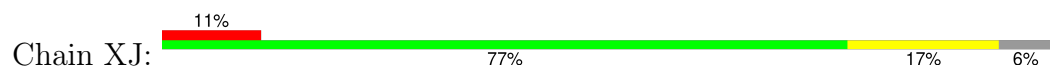
• Molecule 9: 30S ribosomal protein S9



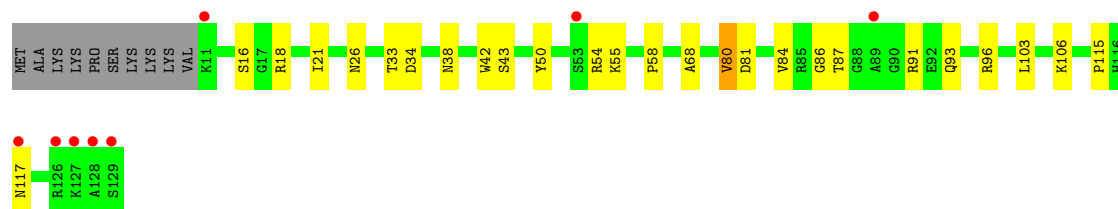
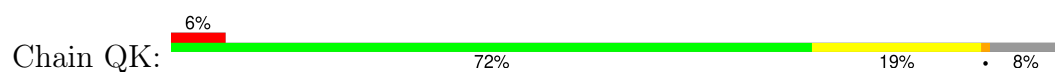
• Molecule 10: 30S ribosomal protein S10



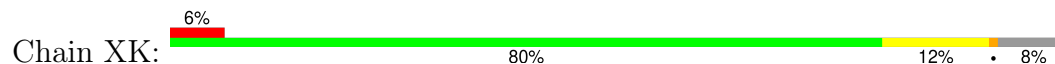
• Molecule 10: 30S ribosomal protein S10



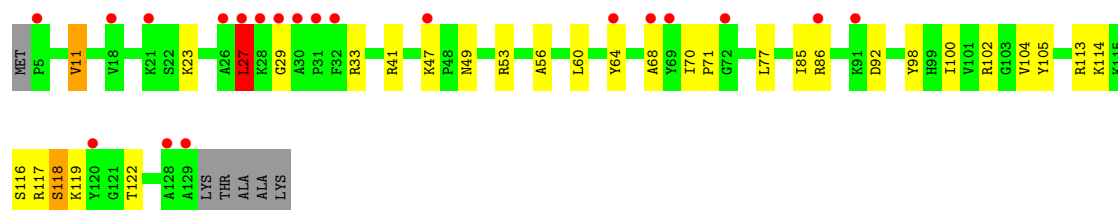
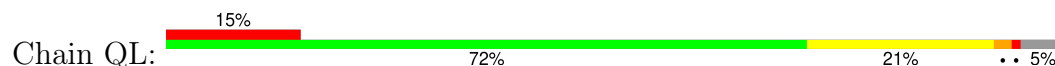
• Molecule 11: 30S ribosomal protein S11



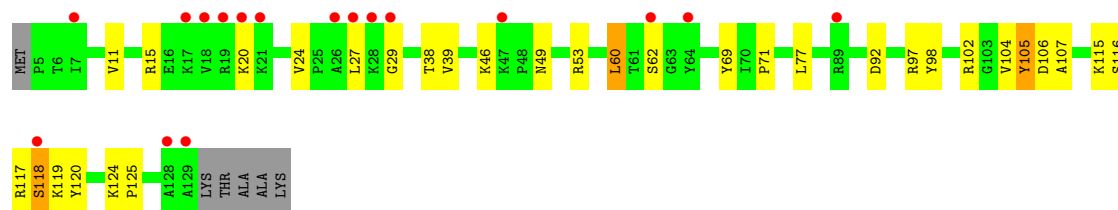
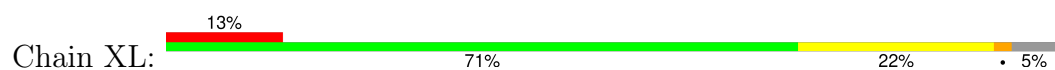
- Molecule 11: 30S ribosomal protein S11



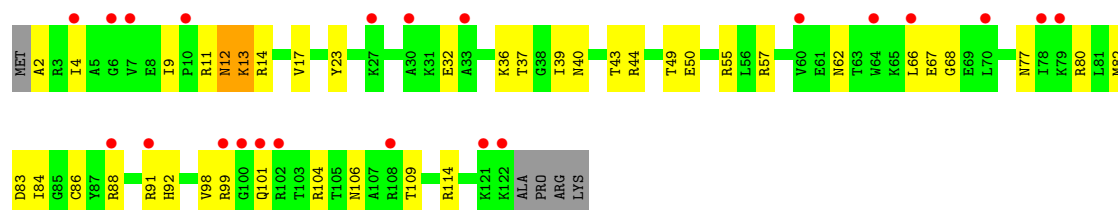
- Molecule 12: 30S ribosomal protein S12



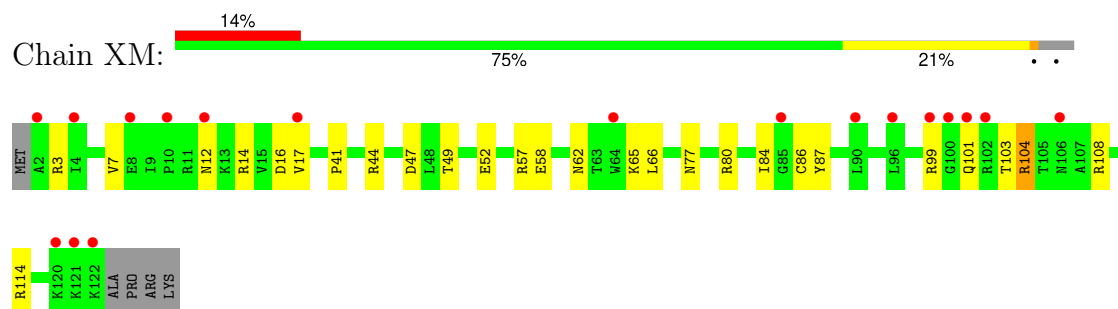
- Molecule 12: 30S ribosomal protein S12



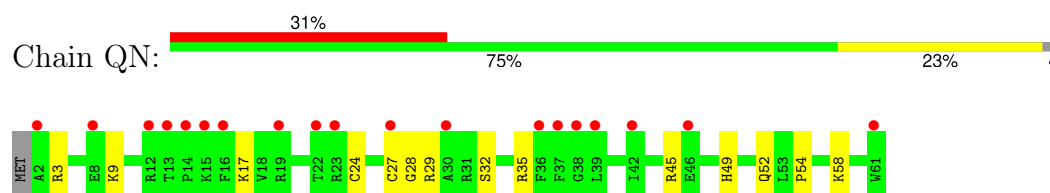
- Molecule 13: 30S ribosomal protein S13



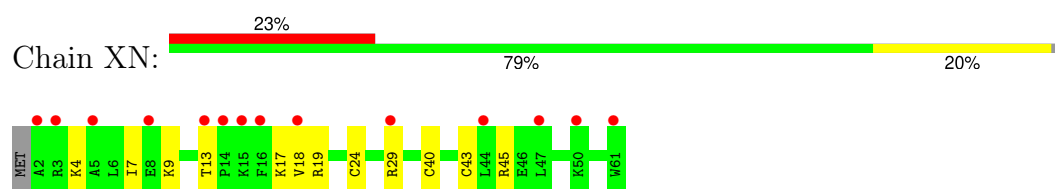
- Molecule 13: 30S ribosomal protein S13



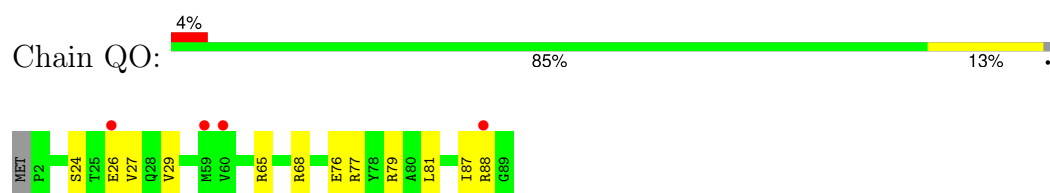
- Molecule 14: 30S ribosomal protein S14 type Z



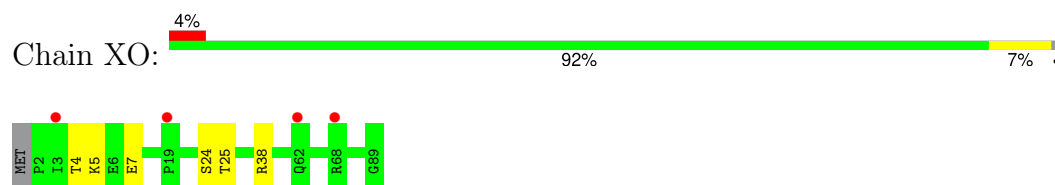
- Molecule 14: 30S ribosomal protein S14 type Z



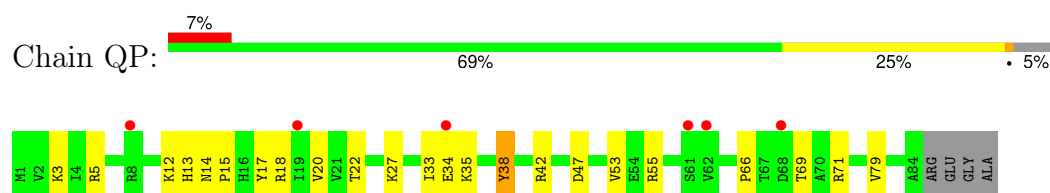
- Molecule 15: 30S ribosomal protein S15



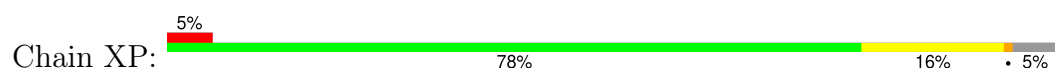
- Molecule 15: 30S ribosomal protein S15



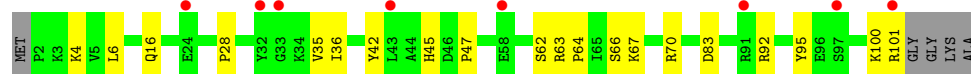
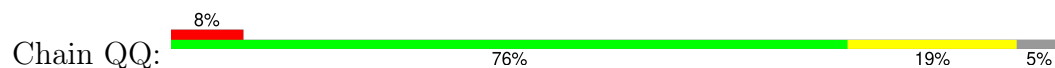
- Molecule 16: 30S ribosomal protein S16



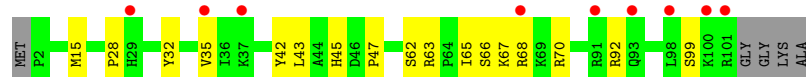
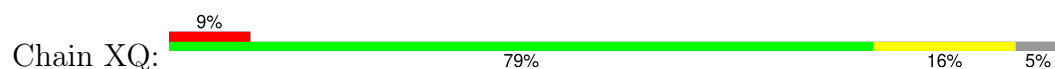
- Molecule 16: 30S ribosomal protein S16



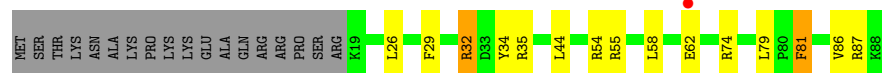
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



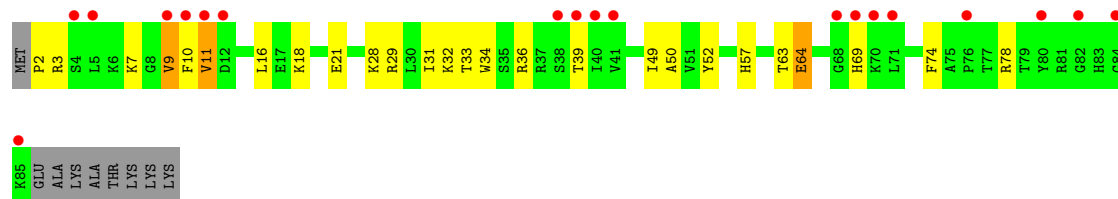
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18

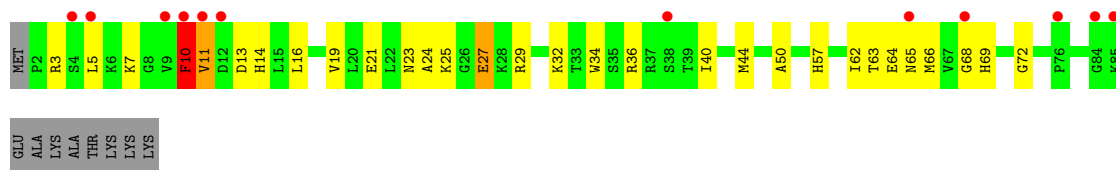


- Molecule 19: 30S ribosomal protein S19

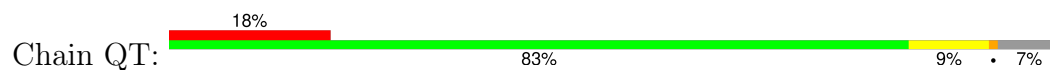


- Molecule 19: 30S ribosomal protein S19

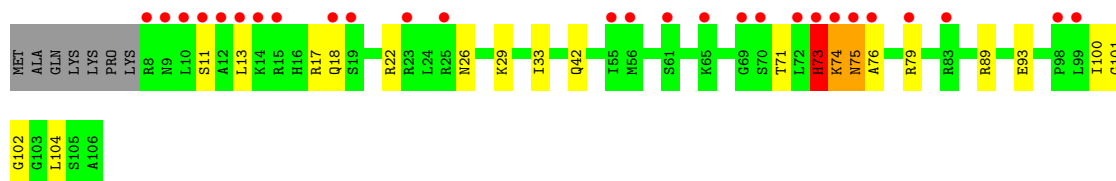
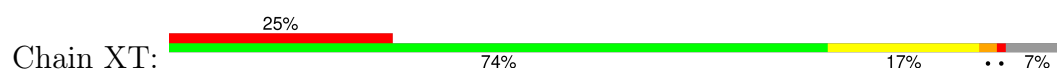




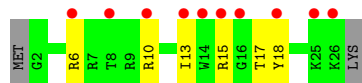
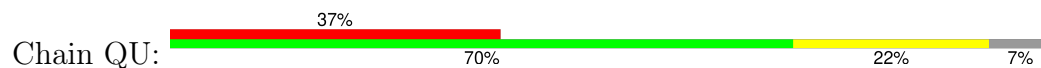
- Molecule 20: 30S ribosomal protein S20



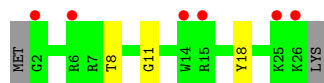
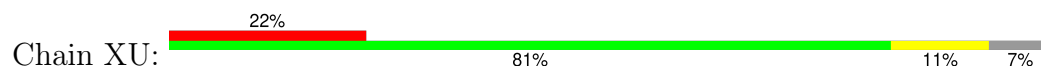
- Molecule 20: 30S ribosomal protein S20



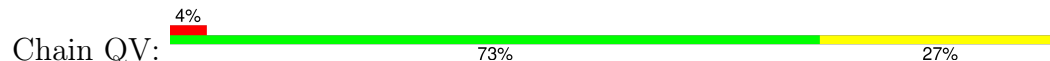
- Molecule 21: 30S ribosomal protein Thx



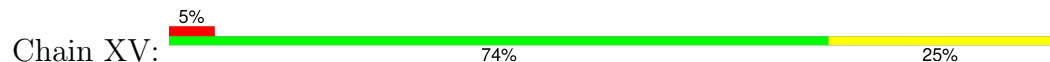
- Molecule 21: 30S ribosomal protein Thx

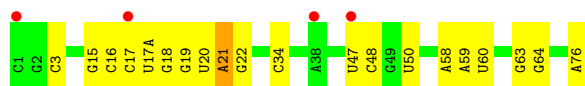


- Molecule 22: P-site tRNA^{fMet}

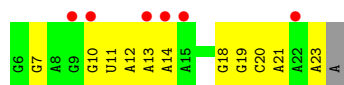


- Molecule 22: P-site tRNA^{fMet}

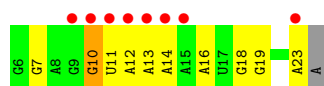




- Molecule 23: mRNA



- Molecule 23: mRNA



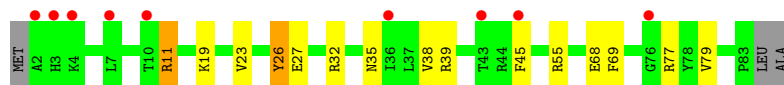
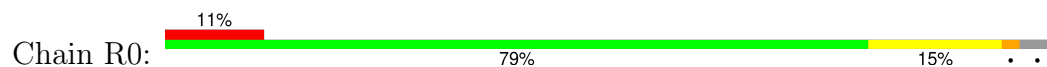
- Molecule 24: A-site tRNAAla(GGC) U32-A38



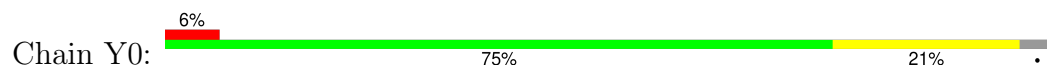
- Molecule 24: A-site tRNAAla(GGC) U32-A38



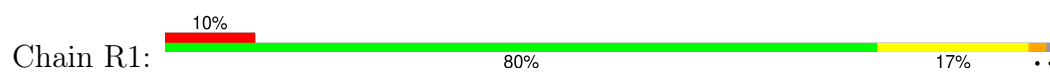
- Molecule 25: 50S ribosomal protein L27



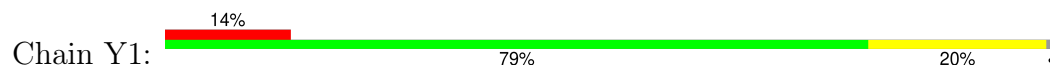
- Molecule 25: 50S ribosomal protein L27



- Molecule 26: 50S ribosomal protein L28



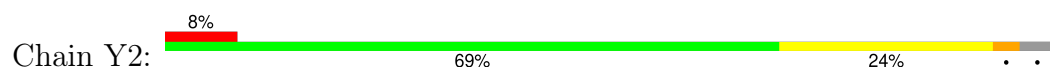
- Molecule 26: 50S ribosomal protein L28



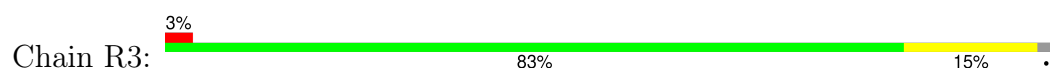
- Molecule 27: 50S ribosomal protein L29



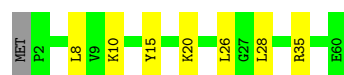
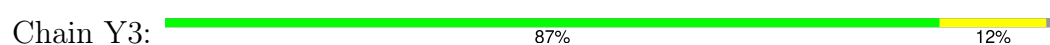
- Molecule 27: 50S ribosomal protein L29



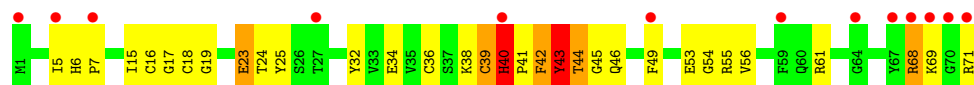
- Molecule 28: 50S ribosomal protein L30



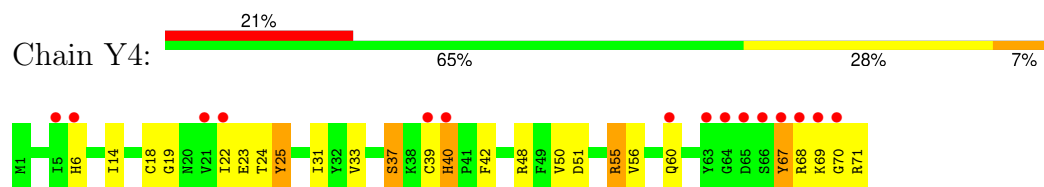
- Molecule 28: 50S ribosomal protein L30



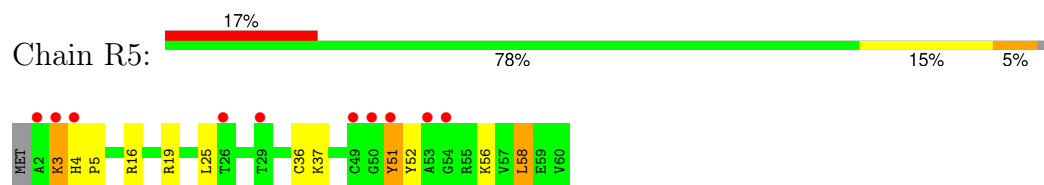
- Molecule 29: 50S ribosomal protein L31



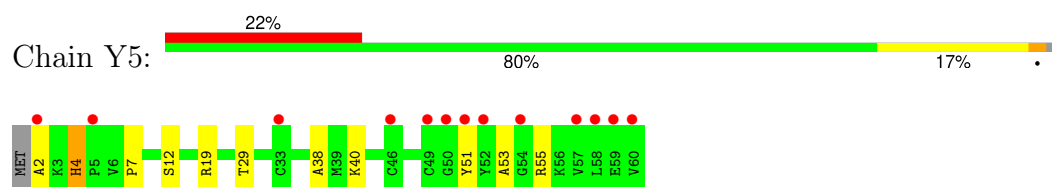
• Molecule 29: 50S ribosomal protein L31



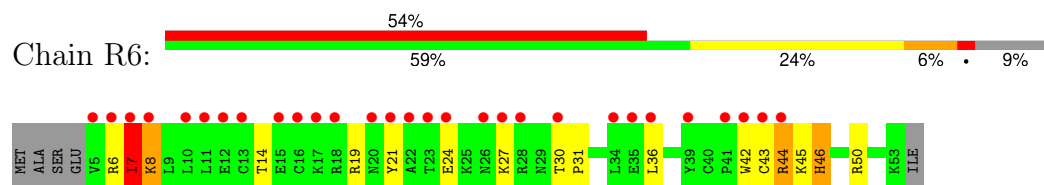
• Molecule 30: 50S ribosomal protein L32



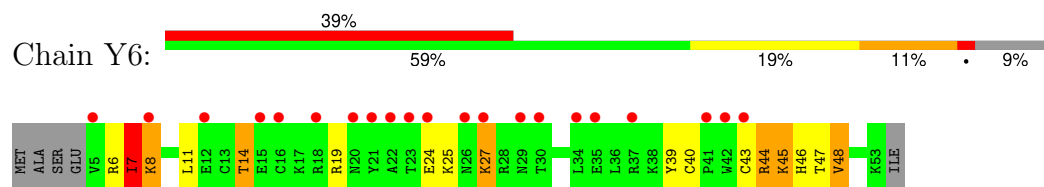
• Molecule 30: 50S ribosomal protein L32



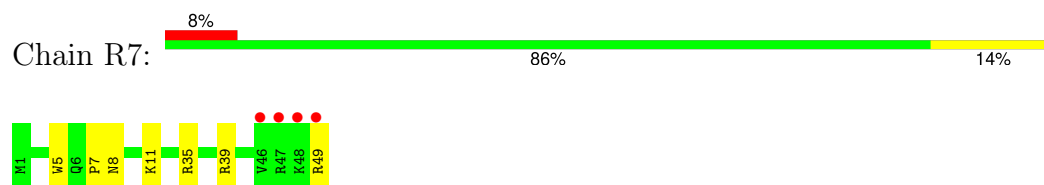
• Molecule 31: 50S ribosomal protein L33



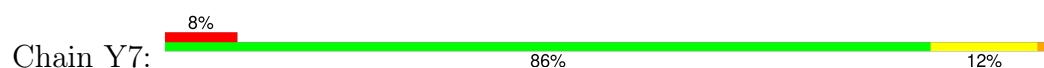
• Molecule 31: 50S ribosomal protein L33



• Molecule 32: 50S ribosomal protein L34

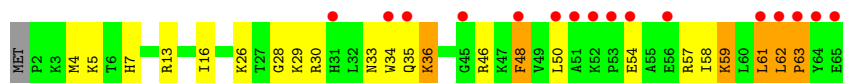


• Molecule 32: 50S ribosomal protein L34





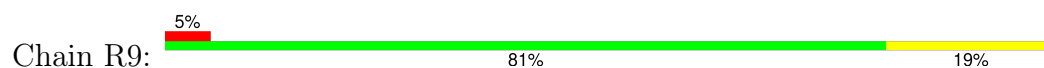
- Molecule 33: 50S ribosomal protein L35



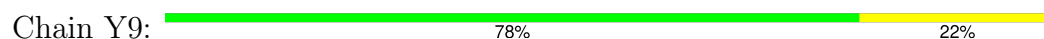
- Molecule 33: 50S ribosomal protein L35



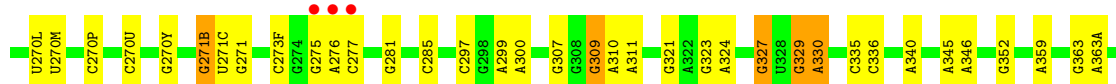
- Molecule 34: 50S ribosomal protein L36



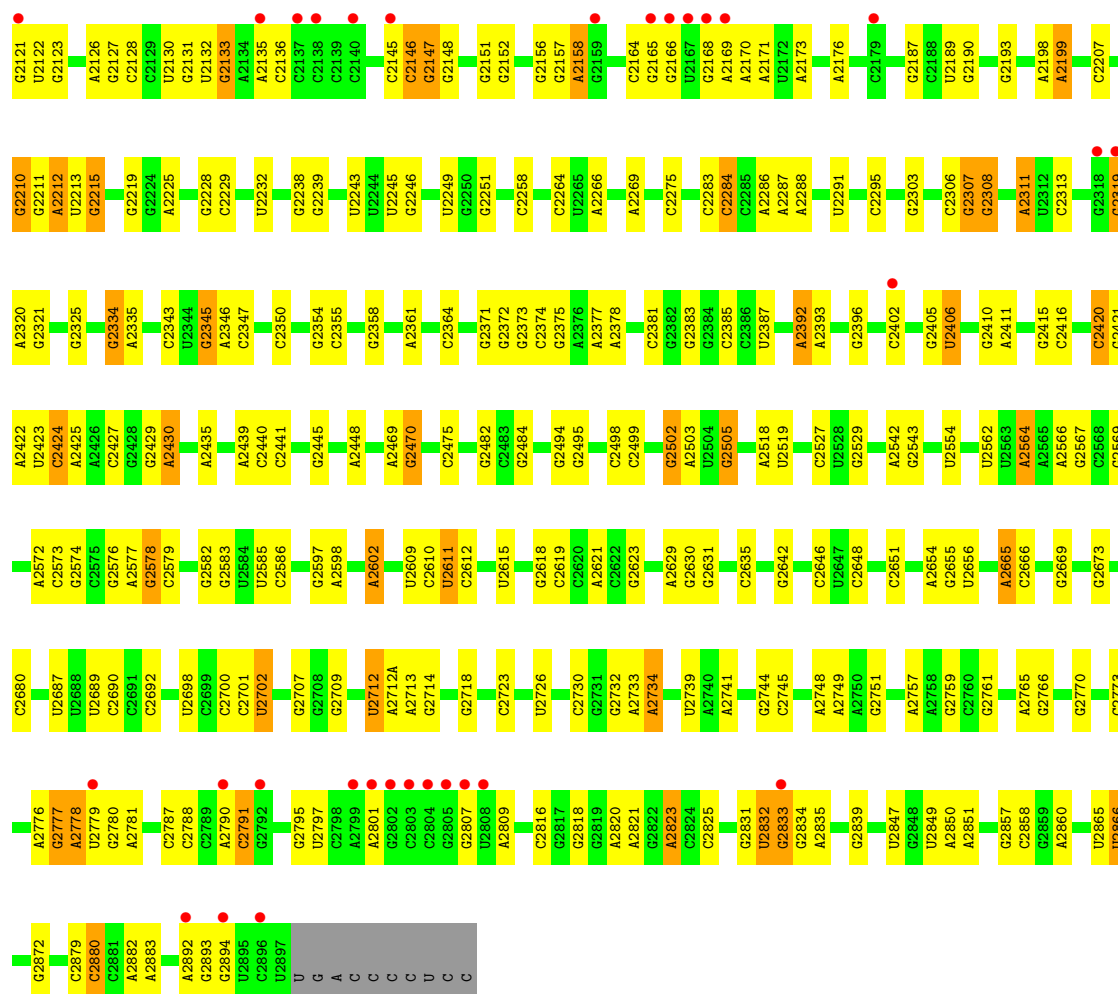
- Molecule 34: 50S ribosomal protein L36



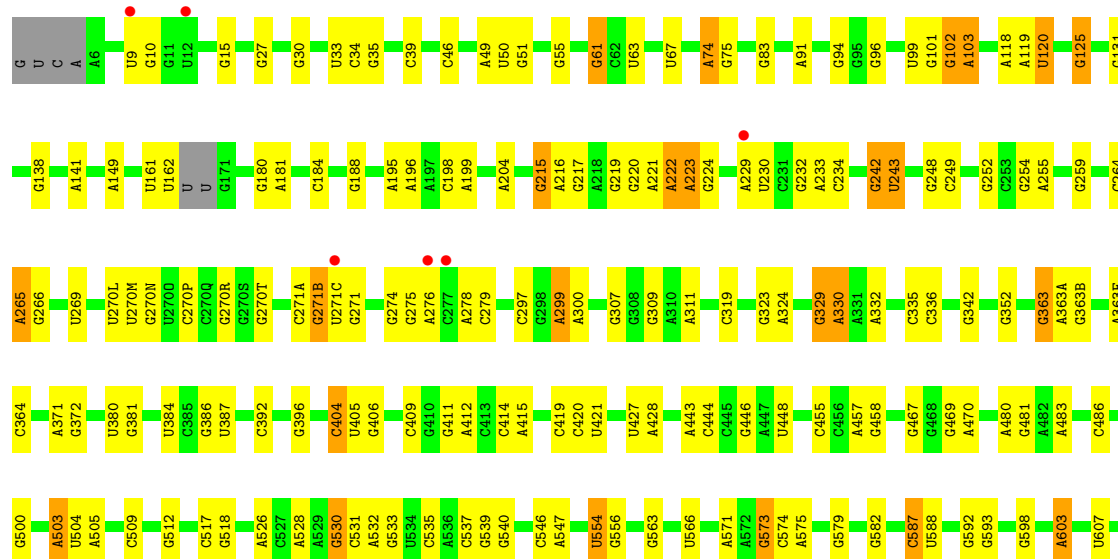
- Molecule 35: 23S rRNA



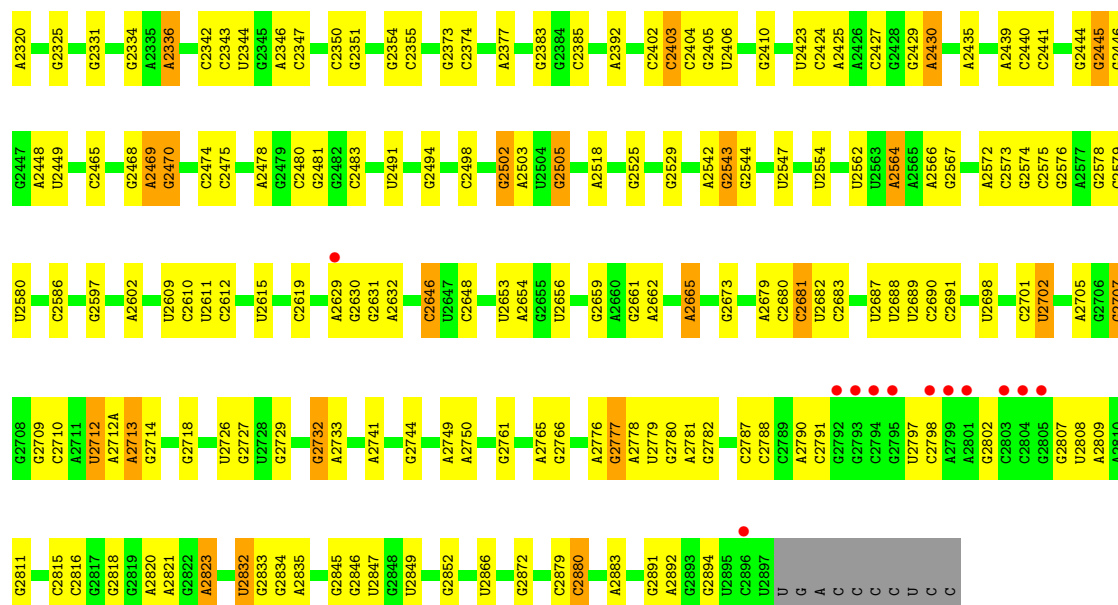




• Molecule 35: 23S rRNA



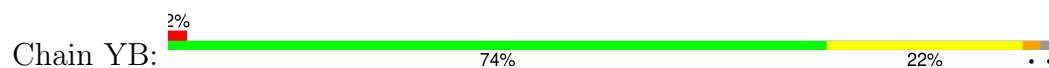
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G2210	U2113	C1996	G1858	G1567	G1449	A1301	C1140	U1060	G956	C846	G693	G614
G2114	A2114	C2006	A1859	A1569	G1449A	A1424	U1141	G1061	U957	U847	U694	A616
U2213	G2115	G2010	G1859	U1578	U1454	C1306	C1153	G1062	U958	C856	G695	G618
G2215	A2117	G2011	G1878	A1579	G1455	G1309	G1173	U1065	A959	C857	G701	A621
A2225	U2118	G2012	G1878	G1581	U1729	G1310	A1173	A960	C961	U859	G702	G622
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G2234	G2121	A2014	C1881	G1459	G1459	G1328	U1175	A1069	A973	A861	A722	A627
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G2238	G2123	A2019	G1883	G1595	G1461	C1178	A1177	G1071	C974A	A866	A722	G629
G2239	U2124	G2020	A1884	C1598	C1467	G1338	C1179	G1074	A983	C867	G729	G630
G2243	G2125	C2021	G1888	C1598	A1471	U1341	G1187	C1075	A984	U868	C730	A633
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G2253	G2131	G2032	G1896	C1612	G1483	A1349	G1195	U1082	C994	G879	G743	G638
G2258	U2132	U2033	G1896	G1617	G1484	A1352	G1203	U1083	C995	G880	U747	G639
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C2294	G2168	G2069	C1957	G1654	U1523	C1386	G1239	U1105	C1013	C897	A782	G654
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	G2191	G2101	U1991	G1695	A1559	A1428	C1291	G1136	G1055	G946	A820	A655
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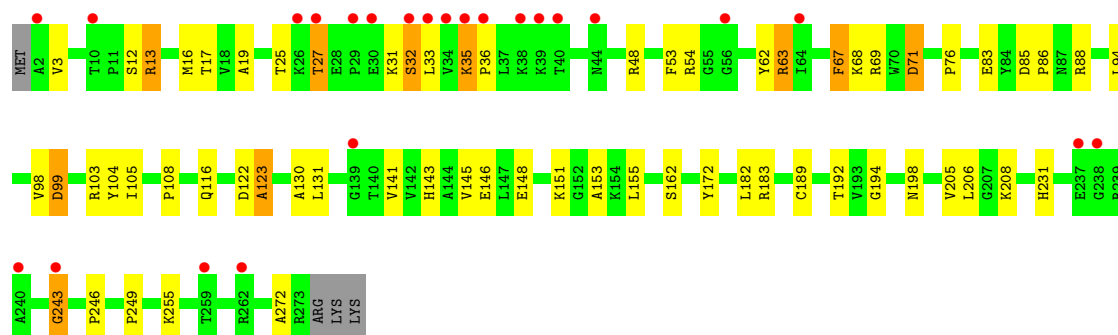
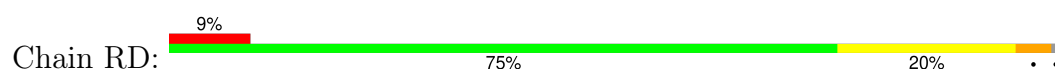
• Molecule 36: 5S rRNA



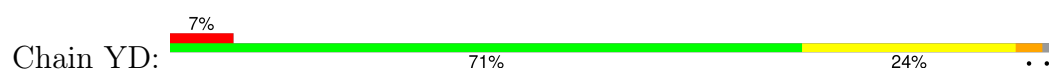
• Molecule 36: 5S rRNA

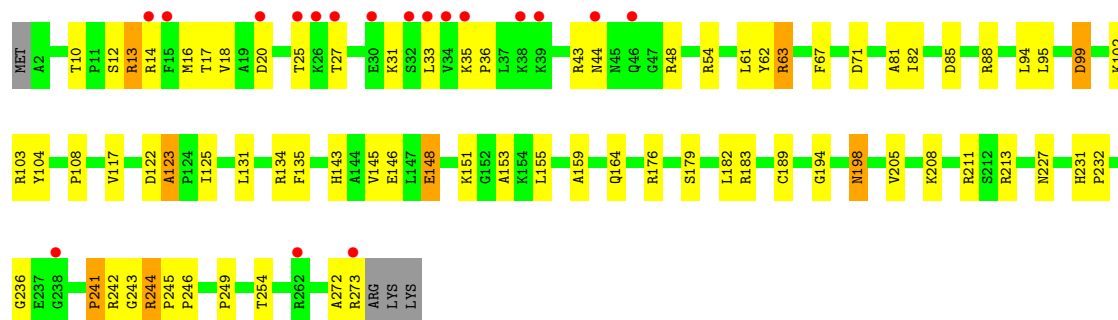


• Molecule 37: 50S ribosomal protein L2

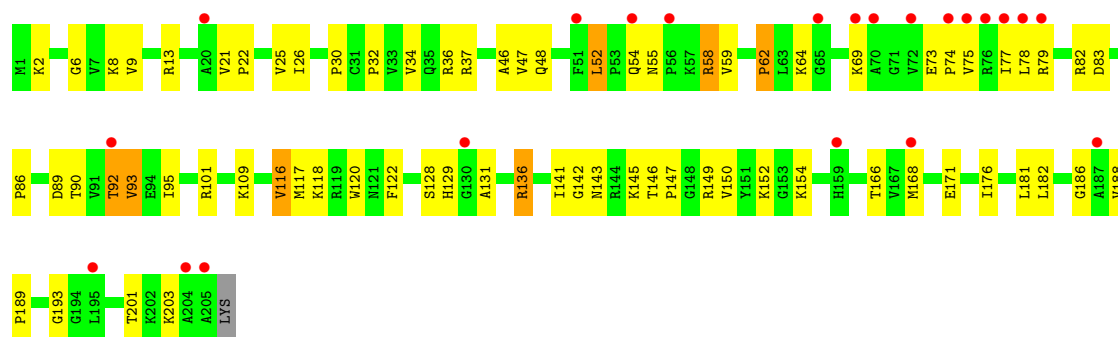


• Molecule 37: 50S ribosomal protein L2

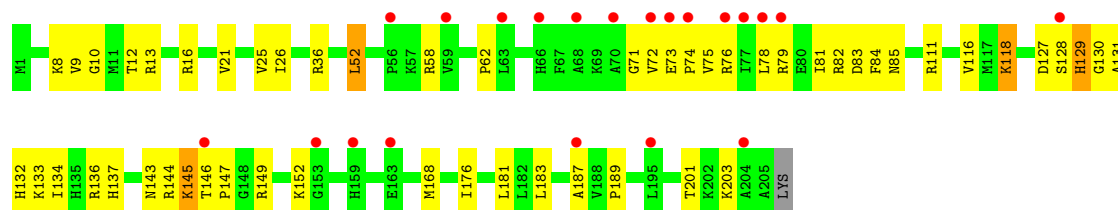
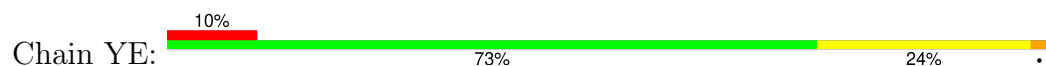




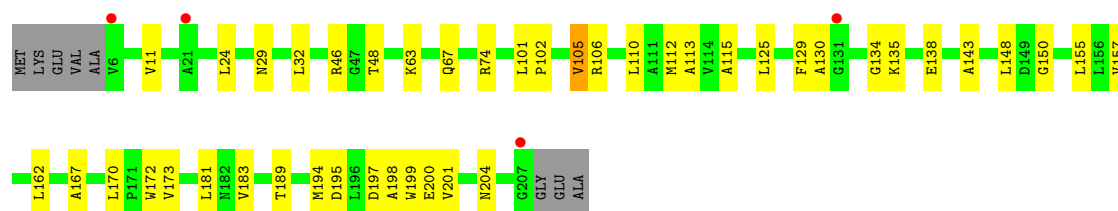
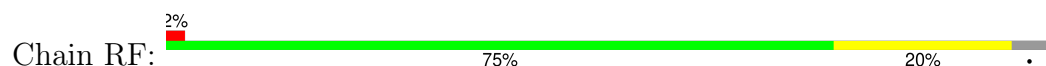
• Molecule 38: 50S ribosomal protein L3



• Molecule 38: 50S ribosomal protein L3

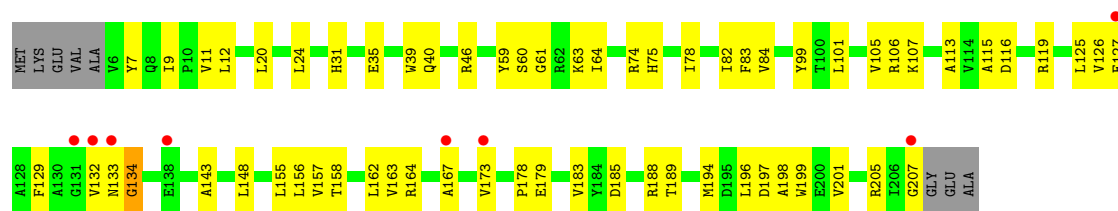


• Molecule 39: 50S ribosomal protein L4

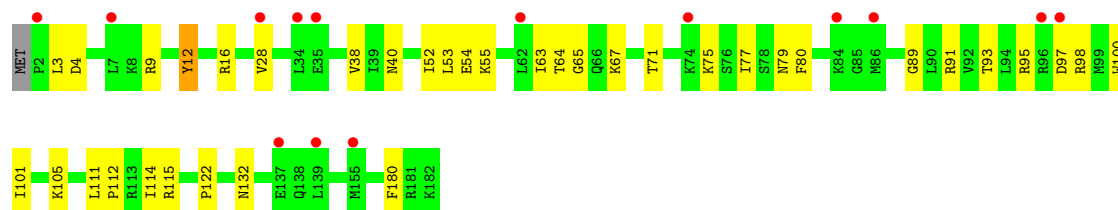
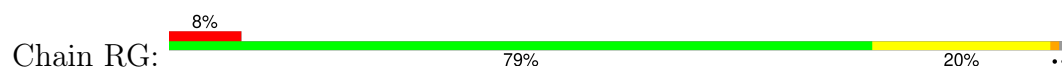


• Molecule 39: 50S ribosomal protein L4

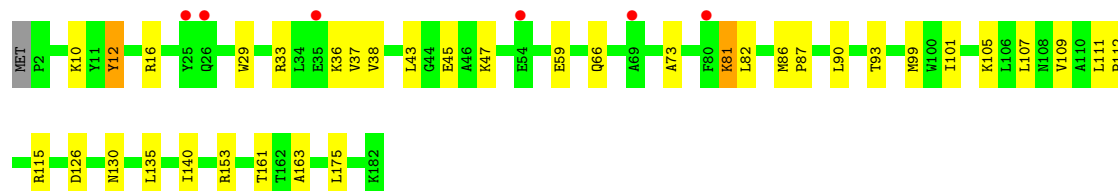
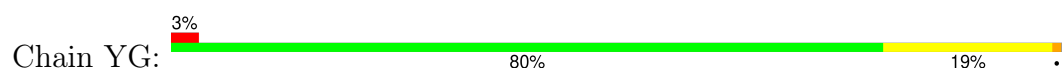




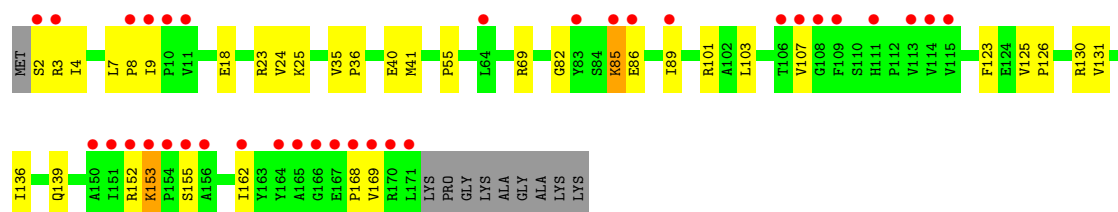
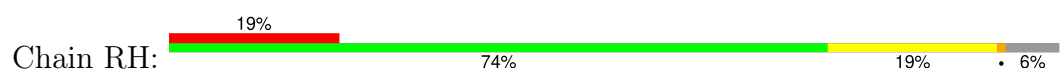
• Molecule 40: 50S ribosomal protein L5



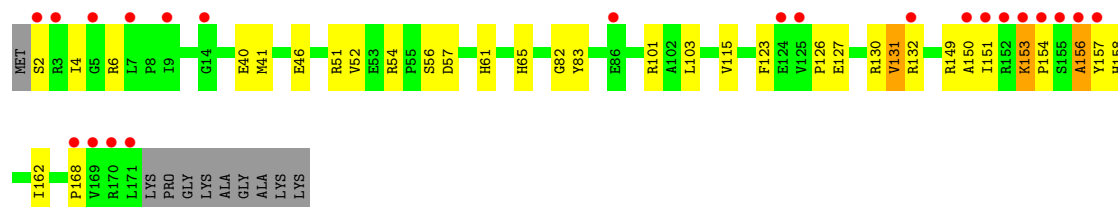
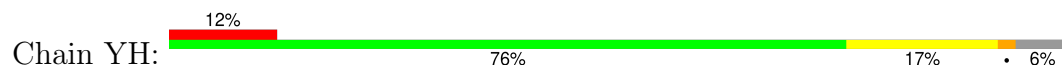
• Molecule 40: 50S ribosomal protein L5



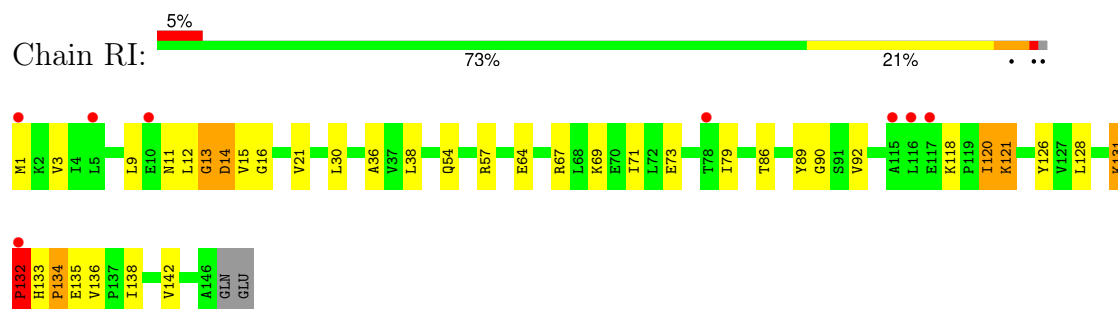
• Molecule 41: 50S ribosomal protein L6



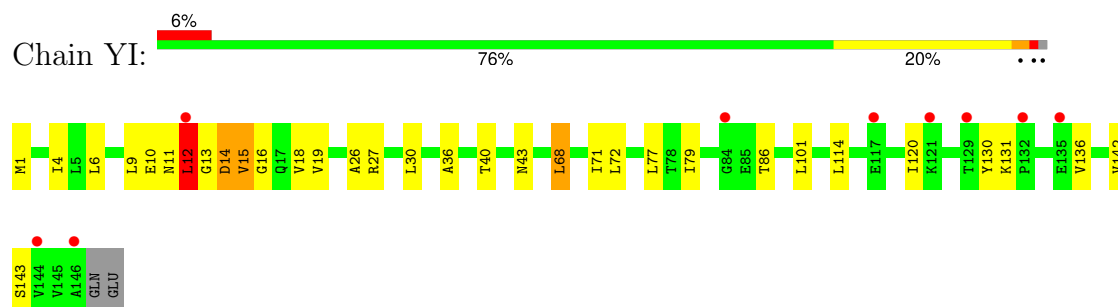
• Molecule 41: 50S ribosomal protein L6



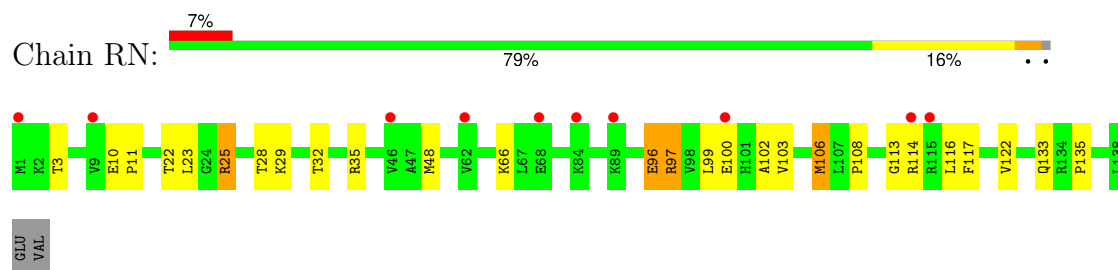
- Molecule 42: 50S ribosomal protein L9



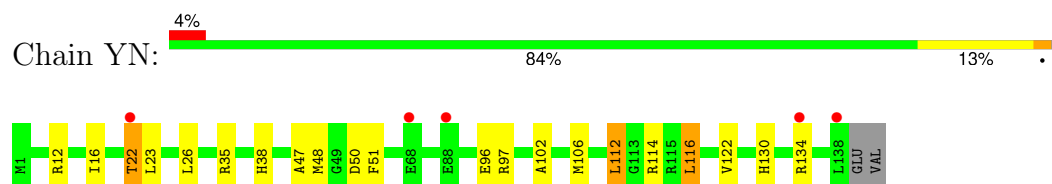
- Molecule 42: 50S ribosomal protein L9



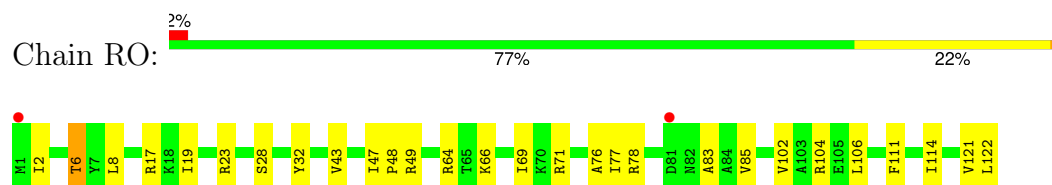
- Molecule 43: 50S ribosomal protein L13



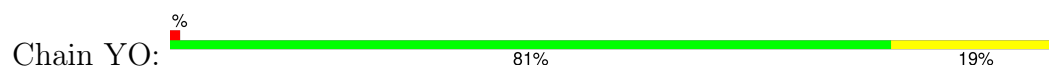
- Molecule 43: 50S ribosomal protein L13



- Molecule 44: 50S ribosomal protein L14

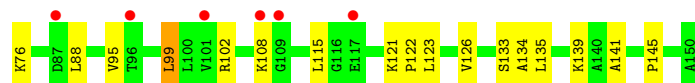
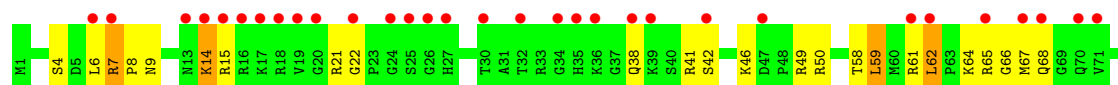
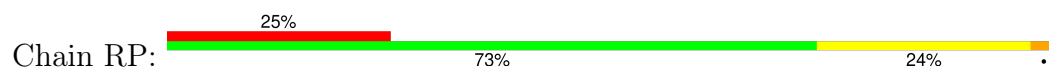


- Molecule 44: 50S ribosomal protein L14

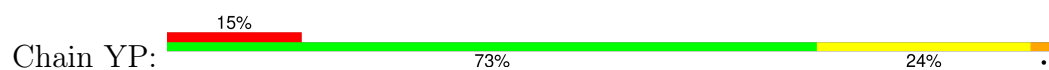




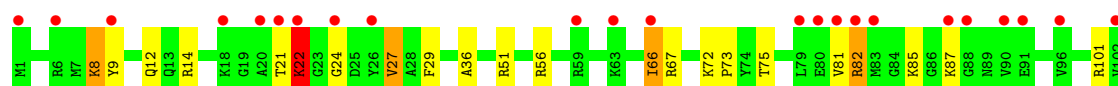
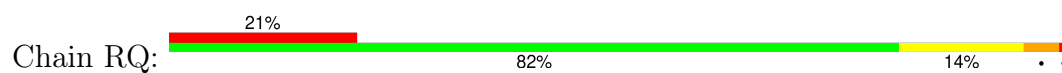
- Molecule 45: 50S ribosomal protein L15



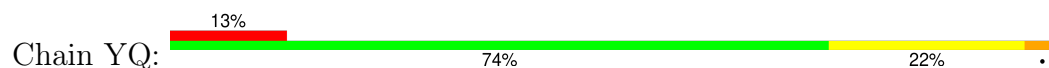
- Molecule 45: 50S ribosomal protein L15



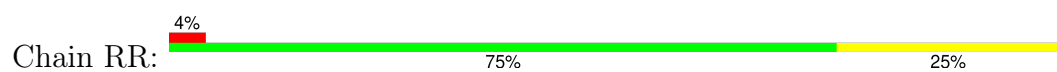
- Molecule 46: 50S ribosomal protein L16



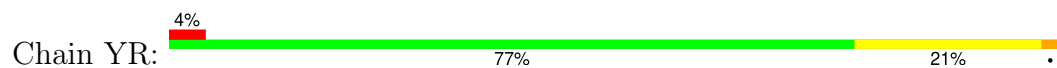
- Molecule 46: 50S ribosomal protein L16



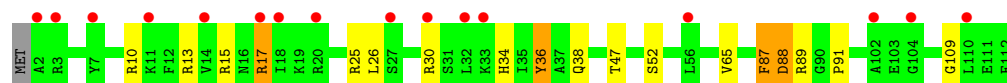
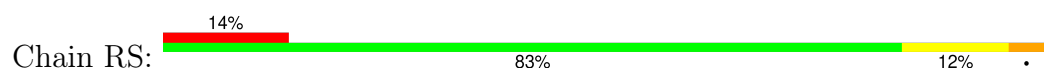
- Molecule 47: 50S ribosomal protein L17



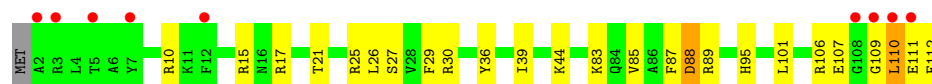
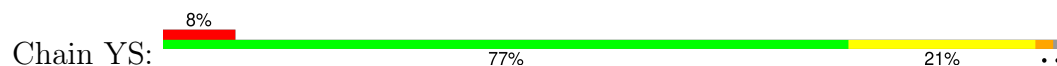
- Molecule 47: 50S ribosomal protein L17



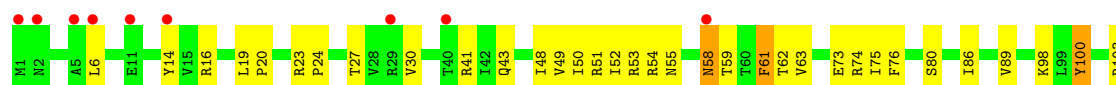
- Molecule 48: 50S ribosomal protein L18



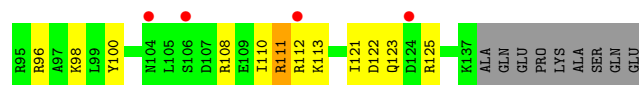
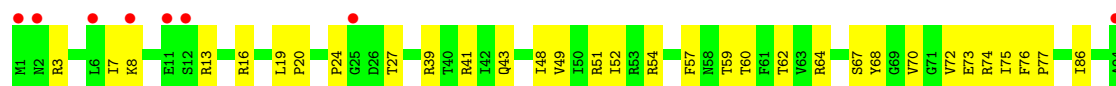
- Molecule 48: 50S ribosomal protein L18



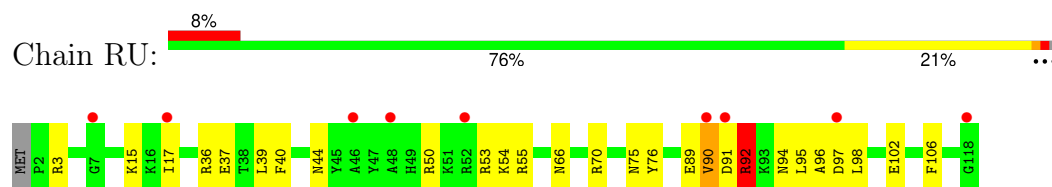
- Molecule 49: 50S ribosomal protein L19



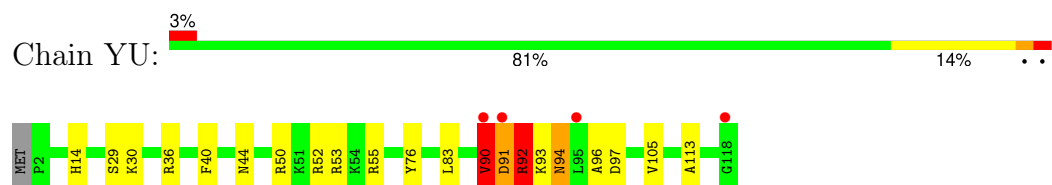
- Molecule 49: 50S ribosomal protein L19



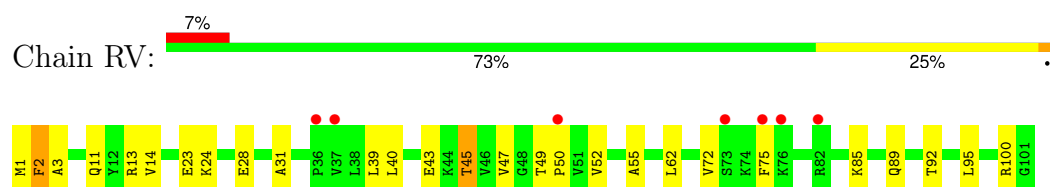
- Molecule 50: 50S ribosomal protein L20



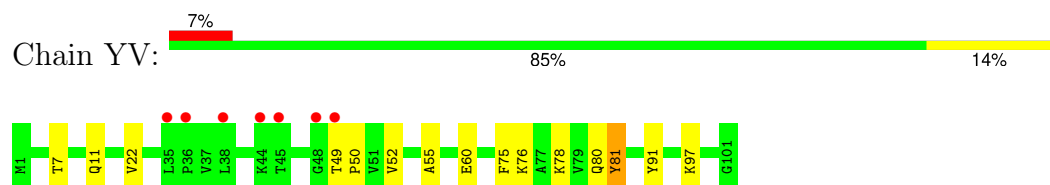
- Molecule 50: 50S ribosomal protein L20



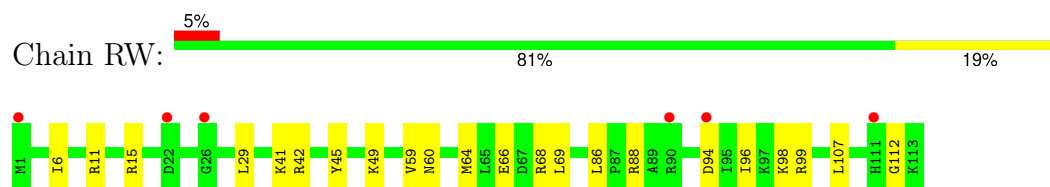
- Molecule 51: 50S ribosomal protein L21



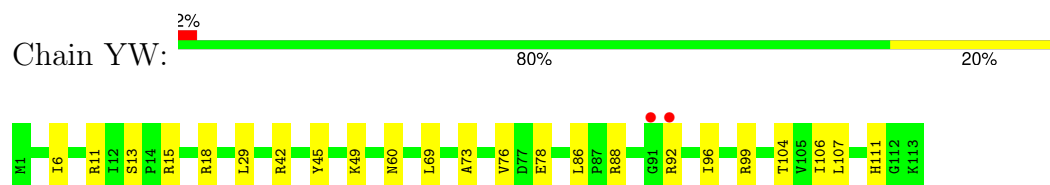
- Molecule 51: 50S ribosomal protein L21



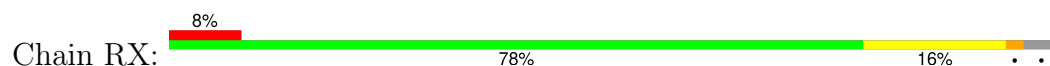
- Molecule 52: 50S ribosomal protein L22

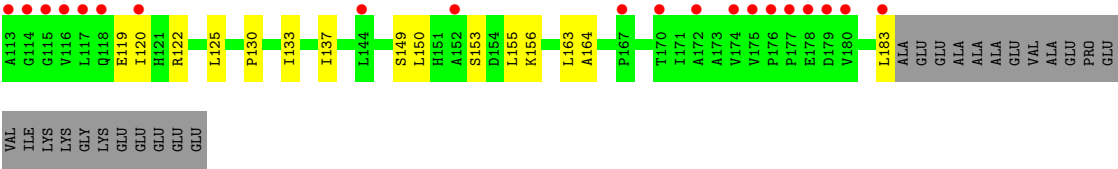


- Molecule 52: 50S ribosomal protein L22



- Molecule 53: 50S ribosomal protein L23





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 449.76Å 619.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 3.10 49.74 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.74-3.10) 97.1 (49.74-3.10)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.225 , 0.266 0.225 , 0.266	Depositor DCC
R_{free} test set	52649 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	294981	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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: PAR, ZN, MG, SF4

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	0.53	0/36098	0.49	7/56341 (0.0%)
1	XA	0.57	0/36101	0.50	6/56346 (0.0%)
2	QB	0.44	0/1959	0.96	9/2642 (0.3%)
2	XB	0.49	0/1959	0.94	3/2642 (0.1%)
3	QC	0.45	0/1629	0.89	4/2195 (0.2%)
3	XC	0.48	0/1629	0.83	3/2195 (0.1%)
4	QD	0.54	0/1704	0.87	5/2284 (0.2%)
4	XD	0.55	0/1704	0.90	9/2284 (0.4%)
5	QE	0.50	0/1171	0.91	3/1576 (0.2%)
5	XE	0.52	0/1171	0.84	2/1576 (0.1%)
6	QF	0.53	0/856	0.81	0/1154
6	XF	0.52	0/856	0.83	1/1154 (0.1%)
7	QG	0.45	0/1276	0.96	7/1709 (0.4%)
7	XG	0.47	0/1276	0.93	4/1709 (0.2%)
8	QH	0.46	0/1136	0.89	3/1527 (0.2%)
8	XH	0.53	0/1136	0.86	3/1527 (0.2%)
9	QI	0.50	0/1029	1.14	10/1379 (0.7%)
9	XI	0.49	0/1029	1.03	6/1379 (0.4%)
10	QJ	0.43	0/814	0.98	3/1095 (0.3%)
10	XJ	0.50	0/814	0.87	1/1095 (0.1%)
11	QK	0.51	0/900	0.86	1/1213 (0.1%)
11	XK	0.52	0/900	0.90	4/1213 (0.3%)
12	QL	0.54	0/991	1.05	12/1327 (0.9%)
12	XL	0.59	0/991	1.02	9/1327 (0.7%)
13	QM	0.50	0/974	1.10	6/1303 (0.5%)
13	XM	0.47	0/974	1.07	7/1303 (0.5%)
14	QN	0.49	0/501	0.90	0/664
14	XN	0.55	0/501	1.05	4/664 (0.6%)
15	QO	0.53	0/745	0.81	0/992
15	XO	0.49	0/745	0.81	0/992
16	QP	0.54	0/721	0.95	3/970 (0.3%)
16	XP	0.51	0/721	1.01	2/970 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.53	0/847	0.91	3/1131 (0.3%)
17	XQ	0.51	0/847	0.86	3/1131 (0.3%)
18	QR	0.57	0/579	1.05	2/768 (0.3%)
18	XR	0.56	0/579	0.95	3/768 (0.4%)
19	QS	0.46	0/689	1.06	5/926 (0.5%)
19	XS	0.56	0/689	1.25	12/926 (1.3%)
20	QT	0.52	0/765	0.99	3/1007 (0.3%)
20	XT	0.47	0/765	1.06	4/1007 (0.4%)
21	QU	0.52	0/221	0.82	0/288
21	XU	0.60	0/221	0.93	1/288 (0.3%)
22	QV	0.48	0/1832	0.46	0/2855
22	XV	0.55	0/1832	0.43	0/2855
23	QX	0.41	0/446	0.54	0/695
23	XX	0.45	0/446	0.55	0/695
24	QY	0.38	0/1790	0.47	0/2789
24	XY	0.39	0/1790	0.46	0/2789
25	R0	0.58	0/657	0.89	2/874 (0.2%)
25	Y0	0.64	0/657	0.94	2/874 (0.2%)
26	R1	0.61	0/770	1.06	4/1022 (0.4%)
26	Y1	0.64	0/770	0.98	3/1022 (0.3%)
27	R2	0.56	0/583	0.98	2/771 (0.3%)
27	Y2	0.58	0/583	1.04	4/771 (0.5%)
28	R3	0.45	0/474	0.81	0/635
28	Y3	0.56	0/474	0.82	0/635
29	R4	0.57	0/594	1.44	10/795 (1.3%)
29	Y4	0.50	0/594	1.55	14/795 (1.8%)
30	R5	0.60	0/473	1.25	6/639 (0.9%)
30	Y5	0.68	0/473	1.01	2/639 (0.3%)
31	R6	0.68	0/431	1.60	7/575 (1.2%)
31	Y6	0.67	0/431	1.57	9/575 (1.6%)
32	R7	0.68	0/438	0.86	0/575
32	Y7	0.71	0/438	0.98	3/575 (0.5%)
33	R8	0.66	0/525	1.21	9/691 (1.3%)
33	Y8	0.80	1/525 (0.2%)	1.22	8/691 (1.2%)
34	R9	0.57	0/310	0.71	0/407
34	Y9	0.62	0/310	0.81	0/407
35	RA	0.62	0/69521	0.52	15/108529 (0.0%)
35	YA	0.70	0/69543	0.54	17/108563 (0.0%)
36	RB	0.50	0/2878	0.49	0/4490
36	YB	0.62	0/2878	0.51	0/4490
37	RD	0.67	0/2165	1.03	12/2919 (0.4%)
37	YD	0.74	0/2165	1.03	12/2919 (0.4%)
38	RE	0.62	1/1601 (0.1%)	1.14	16/2160 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YE	0.69	0/1601	1.17	12/2160 (0.6%)
39	RF	0.59	0/1620	0.95	4/2194 (0.2%)
39	YF	0.65	0/1620	0.98	7/2194 (0.3%)
40	RG	0.49	0/1499	1.02	10/2016 (0.5%)
40	YG	0.55	0/1499	0.97	4/2016 (0.2%)
41	RH	0.45	0/1332	1.13	9/1802 (0.5%)
41	YH	0.59	0/1332	1.12	14/1802 (0.8%)
42	RI	0.57	2/1151 (0.2%)	1.32	21/1558 (1.3%)
42	YI	0.50	0/1151	1.16	14/1558 (0.9%)
43	RN	0.57	0/1131	1.05	7/1525 (0.5%)
43	YN	0.62	0/1131	1.02	8/1525 (0.5%)
44	RO	0.60	0/943	0.86	1/1269 (0.1%)
44	YO	0.67	0/943	0.98	1/1269 (0.1%)
45	RP	0.59	0/1162	1.20	7/1544 (0.5%)
45	YP	0.65	0/1162	1.18	12/1544 (0.8%)
46	RQ	0.59	0/1143	1.14	9/1527 (0.6%)
46	YQ	0.65	0/1143	1.18	10/1527 (0.7%)
47	RR	0.63	0/982	0.95	4/1312 (0.3%)
47	YR	0.65	0/982	1.02	5/1312 (0.4%)
48	RS	0.54	0/892	1.21	10/1187 (0.8%)
48	YS	0.58	0/892	1.12	6/1187 (0.5%)
49	RT	0.60	0/1155	1.06	13/1542 (0.8%)
49	YT	0.62	0/1155	1.14	11/1542 (0.7%)
50	RU	0.59	0/982	1.11	10/1306 (0.8%)
50	YU	0.66	0/982	1.05	8/1306 (0.6%)
51	RV	0.54	0/790	1.04	3/1057 (0.3%)
51	YV	0.67	0/790	1.10	4/1057 (0.4%)
52	RW	0.62	0/911	0.92	1/1220 (0.1%)
52	YW	0.63	0/911	0.88	1/1220 (0.1%)
53	RX	0.59	0/739	0.96	4/993 (0.4%)
53	YX	0.65	0/739	0.91	2/993 (0.2%)
54	RY	0.53	0/798	0.97	3/1064 (0.3%)
54	YY	0.63	0/798	1.02	4/1064 (0.4%)
55	RZ	0.46	0/1493	1.07	12/2026 (0.6%)
55	YZ	0.53	0/1493	1.08	8/2026 (0.4%)
All	All	0.61	4/319657 (0.0%)	0.69	589/478147 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
48	RS	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	RI	133	HIS	C-N	5.84	1.47	1.33
38	RE	136	ARG	C-N	-5.40	1.23	1.33
42	RI	134	PRO	N-CD	-5.12	1.40	1.47
33	Y8	23	VAL	CB-CG1	-5.00	1.36	1.52

All (589) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y4	39	CYS	N-CA-C	-12.70	95.90	112.41
13	XM	7	VAL	N-CA-C	-12.60	101.18	113.53
26	R1	75	GLU	N-CA-C	-11.51	100.25	114.75
39	RF	199	TRP	N-CA-C	-11.32	99.96	113.88
35	RA	1992	G	C2'-C3'-O3'	11.15	126.23	109.50
29	R4	43	TYR	CA-CB-CG	10.95	133.61	113.90
49	YT	125	ARG	N-CA-C	-10.94	99.44	113.12
45	YP	59	LEU	N-CA-C	-10.77	96.17	113.19
14	XN	45	ARG	N-CA-C	-10.76	99.99	113.55
47	YR	76	VAL	N-CA-C	-10.67	100.27	111.58
45	YP	99	LEU	N-CA-C	-10.56	100.52	113.41
40	RG	53	LEU	N-CA-C	-10.34	102.83	114.62
43	YN	114	ARG	N-CA-C	-10.05	94.33	110.32
46	YQ	5	ARG	CG-CD-NE	-10.03	89.94	112.00
31	Y6	7	ILE	CA-C-N	10.01	140.66	121.54
31	Y6	7	ILE	C-N-CA	10.01	140.66	121.54
31	R6	7	ILE	CA-C-N	10.01	140.65	121.54
31	R6	7	ILE	C-N-CA	10.01	140.65	121.54
41	RH	153	LYS	N-CA-C	9.98	125.75	112.17
29	Y4	39	CYS	CA-C-N	9.94	146.06	121.80
29	Y4	39	CYS	C-N-CA	9.94	146.06	121.80
48	YS	21	THR	N-CA-C	-9.84	101.37	113.97
42	RI	14	ASP	N-CA-C	9.67	124.39	109.60
31	Y6	11	LEU	N-CA-C	9.37	123.10	109.14
43	YN	116	LEU	N-CA-C	-9.36	101.98	113.50
9	XI	86	VAL	N-CA-C	-9.29	101.80	113.22
37	YD	13	ARG	N-CA-C	-9.26	101.68	113.72
42	RI	135	GLU	N-CA-C	9.21	124.14	109.86
50	RU	98	LEU	N-CA-C	-9.02	102.68	114.31
39	YF	199	TRP	N-CA-C	-8.95	101.17	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	R5	3	LYS	CA-C-N	8.92	143.58	121.80
30	R5	3	LYS	C-N-CA	8.92	143.58	121.80
20	XT	73	HIS	CA-C-N	8.85	138.44	121.54
20	XT	73	HIS	C-N-CA	8.85	138.44	121.54
10	QJ	98	ILE	N-CA-C	8.81	115.63	106.21
29	R4	39	CYS	N-CA-C	-8.79	97.41	111.04
42	YI	131	LYS	N-CA-C	8.79	124.97	108.97
48	RS	88	ASP	CA-C-N	8.75	138.25	121.54
48	RS	88	ASP	C-N-CA	8.75	138.25	121.54
42	RI	134	PRO	CA-C-N	8.72	137.46	122.12
42	RI	134	PRO	C-N-CA	8.72	137.46	122.12
20	QT	13	LEU	N-CA-C	-8.69	102.67	113.28
9	QI	99	LEU	N-CA-C	-8.66	102.88	113.97
49	YT	111	ARG	N-CA-C	-8.66	96.56	110.32
48	RS	17	ARG	CG-CD-NE	8.63	130.99	112.00
51	YV	81	TYR	CA-CB-CG	8.57	129.33	113.90
12	QL	118	SER	N-CA-C	-8.52	101.21	111.69
48	YS	44	LYS	N-CA-C	-8.49	103.78	114.56
43	RN	116	LEU	N-CA-C	-8.46	103.10	113.50
37	RD	67	PHE	N-CA-C	-8.34	103.97	114.56
12	QL	105	TYR	CA-CB-CG	8.24	128.73	113.90
46	YQ	66	ILE	N-CA-C	8.20	119.97	110.62
44	YO	71	ARG	CG-CD-NE	8.20	130.03	112.00
43	YN	97	ARG	N-CA-C	-8.19	103.08	113.23
39	YF	64	ILE	N-CA-C	8.18	118.96	110.62
55	YZ	120	ILE	N-CA-C	-8.18	103.84	111.45
10	XJ	86	MET	N-CA-C	-8.17	104.45	114.75
49	YT	13	ARG	N-CA-C	-8.08	102.47	113.30
43	RN	114	ARG	N-CA-C	-8.06	98.52	110.46
13	QM	9	ILE	N-CA-C	8.02	120.38	107.71
45	YP	64	LYS	N-CA-C	-7.99	102.44	112.90
45	RP	59	LEU	N-CA-C	-7.96	100.61	113.19
39	RF	197	ASP	N-CA-C	-7.96	100.26	110.53
31	Y6	48	VAL	N-CA-C	7.94	118.74	110.72
5	QE	51	VAL	CB-CA-C	-7.92	105.95	114.35
9	QI	33	PHE	CA-CB-CG	7.92	121.72	113.80
42	YI	11	ASN	CA-C-N	7.89	136.61	121.54
42	YI	11	ASN	C-N-CA	7.89	136.61	121.54
5	QE	51	VAL	N-CA-C	7.88	124.04	112.61
38	YE	73	GLU	N-CA-C	7.88	118.67	109.60
29	R4	36	CYS	N-CA-C	-7.88	100.04	111.30
39	YF	197	ASP	N-CA-C	-7.84	99.96	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	YH	153	LYS	N-CA-C	7.84	127.14	109.81
42	RI	131	LYS	N-CA-C	7.84	123.98	107.91
42	RI	11	ASN	CA-C-N	7.76	136.36	121.54
42	RI	11	ASN	C-N-CA	7.76	136.36	121.54
41	YH	127	GLU	N-CA-C	-7.72	98.81	110.39
19	XS	23	ASN	N-CA-C	-7.72	102.47	111.03
37	RD	13	ARG	N-CA-C	-7.71	102.97	113.30
29	Y4	40	HIS	N-CA-C	7.71	126.84	109.81
7	XG	69	VAL	N-CA-C	-7.70	105.04	113.43
43	RN	97	ARG	N-CA-C	-7.68	104.05	113.50
38	YE	58	ARG	N-CA-C	-7.66	103.52	113.17
41	RH	136	ILE	N-CA-C	-7.65	105.69	112.12
12	QL	119	LYS	N-CA-C	-7.64	100.23	110.55
50	RU	97	ASP	N-CA-C	-7.63	103.86	113.02
33	R8	61	LEU	CA-C-N	7.56	140.26	121.80
33	R8	61	LEU	C-N-CA	7.56	140.26	121.80
12	QL	27	LEU	CA-C-N	7.56	135.98	121.54
12	QL	27	LEU	C-N-CA	7.56	135.98	121.54
10	QJ	21	GLN	N-CA-C	-7.54	103.88	113.23
50	YU	94	ASN	N-CA-C	-7.54	102.74	112.23
49	RT	113	LYS	N-CA-C	-7.52	104.07	113.55
43	RN	25	ARG	N-CA-C	-7.50	102.78	112.23
49	YT	57	PHE	N-CA-C	-7.49	100.44	110.55
38	RE	69	LYS	N-CA-C	-7.48	101.69	111.71
7	QG	69	VAL	N-CA-C	-7.43	106.25	113.53
9	QI	120	ARG	N-CA-C	-7.42	106.16	114.62
18	XR	87	ARG	N-CA-C	7.39	119.56	110.91
33	R8	59	LYS	N-CA-C	-7.39	104.29	113.38
41	YH	131	VAL	N-CA-C	7.36	118.55	108.84
3	QC	23	TYR	CA-CB-CG	7.36	127.14	113.90
46	YQ	21	THR	N-CA-C	7.33	118.19	108.07
9	QI	86	VAL	N-CA-C	-7.32	102.63	113.39
31	R6	21	TYR	N-CA-C	7.30	119.45	110.91
35	YA	2712	U	P-O3'-C3'	7.29	128.45	119.70
30	Y5	51	TYR	N-CA-C	7.26	119.10	108.86
50	YU	96	ALA	N-CA-C	-7.25	102.73	113.61
37	RD	35	LYS	N-CA-C	7.24	125.80	109.81
29	Y4	70	GLY	N-CA-C	7.22	123.98	111.78
14	XN	43	CYS	N-CA-C	-7.21	100.82	110.55
48	RS	36	TYR	CA-CB-CG	7.18	126.83	113.90
42	RI	14	ASP	CA-C-N	7.16	134.86	121.97
42	RI	14	ASP	C-N-CA	7.16	134.86	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	QQ	62	SER	N-CA-C	7.15	117.70	108.34
37	YD	198	ASN	N-CA-C	-7.14	102.11	111.74
19	XS	69	HIS	N-CA-C	7.13	119.77	110.43
48	RS	17	ARG	CD-NE-CZ	7.10	134.34	124.40
45	YP	25	SER	N-CA-C	-7.09	102.97	113.61
16	XP	38	TYR	CA-CB-CG	7.08	126.64	113.90
42	RI	120	ILE	N-CA-C	7.05	118.53	109.30
19	XS	13	ASP	N-CA-C	7.04	118.95	111.28
38	RE	58	ARG	N-CA-C	-7.04	104.69	113.28
42	YI	9	LEU	N-CA-C	7.02	121.12	111.71
49	RT	111	ARG	N-CA-C	-7.01	100.08	110.46
48	YS	111	GLU	N-CA-C	7.01	119.79	111.02
12	QL	104	VAL	CA-C-N	7.01	134.92	121.54
12	QL	104	VAL	C-N-CA	7.01	134.92	121.54
52	YW	111	HIS	N-CA-C	7.00	119.56	111.02
5	XE	72	GLN	CA-C-N	6.98	134.88	121.54
5	XE	72	GLN	C-N-CA	6.98	134.88	121.54
39	YF	7	TYR	CA-CB-CG	6.97	126.45	113.90
30	R5	3	LYS	N-CA-C	6.94	121.48	108.65
52	RW	64	MET	N-CA-C	6.93	121.04	112.59
50	YU	97	ASP	N-CA-C	-6.93	103.81	111.36
41	YH	150	ALA	CA-C-N	-6.88	115.18	121.65
41	YH	150	ALA	C-N-CA	-6.88	115.18	121.65
53	YX	5	TYR	N-CA-C	-6.88	104.00	112.88
21	XU	18	TYR	CA-CB-CG	6.87	126.27	113.90
19	XS	10	PHE	CA-CB-CG	6.85	120.65	113.80
46	RQ	66	ILE	N-CA-C	6.84	120.61	111.17
31	Y6	46	HIS	N-CA-C	6.83	125.34	110.80
13	XM	104	ARG	N-CA-C	-6.81	104.44	112.89
46	RQ	22	LYS	N-CA-C	6.80	119.87	110.35
38	RE	118	LYS	N-CA-C	-6.79	104.88	113.43
16	QP	38	TYR	CA-CB-CG	6.78	126.11	113.90
16	XP	53	VAL	N-CA-C	6.77	117.56	110.72
26	R1	53	VAL	N-CA-C	-6.76	100.22	109.55
41	YH	83	TYR	N-CA-C	6.76	125.20	110.80
50	RU	90	VAL	CA-C-N	6.75	134.44	121.54
50	RU	90	VAL	C-N-CA	6.75	134.44	121.54
46	YQ	89	ASN	N-CA-C	-6.74	102.68	111.71
19	XS	11	VAL	N-CA-C	6.73	119.49	112.83
41	YH	151	ILE	N-CA-C	6.73	113.41	106.21
47	RR	77	ARG	N-CA-C	-6.72	104.03	111.82
45	YP	35	HIS	N-CA-C	-6.71	104.22	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	YE	71	GLY	CA-C-N	6.71	134.04	121.97
38	YE	71	GLY	C-N-CA	6.71	134.04	121.97
38	RE	82	ARG	CA-C-N	6.70	134.34	121.54
38	RE	82	ARG	C-N-CA	6.70	134.34	121.54
45	RP	62	LEU	N-CA-C	6.70	119.09	110.39
9	QI	93	ARG	N-CA-C	-6.68	106.08	114.56
55	RZ	4	ARG	CA-C-N	-6.66	112.79	121.79
55	RZ	4	ARG	C-N-CA	-6.66	112.79	121.79
49	YT	110	ILE	N-CA-C	-6.66	102.52	111.44
46	YQ	82	ARG	N-CA-C	6.66	118.93	107.28
50	YU	92	ARG	CA-C-N	6.65	134.24	121.54
50	YU	92	ARG	C-N-CA	6.65	134.24	121.54
13	QM	13	LYS	N-CA-C	6.65	124.96	110.80
2	QB	121	LEU	N-CA-C	-6.63	104.77	112.92
51	RV	45	THR	N-CA-C	6.61	124.89	110.80
1	XA	812	C	C2'-C3'-O3'	6.61	119.42	109.50
4	XD	89	THR	N-CA-C	6.61	119.31	111.71
18	XR	81	PHE	N-CA-C	-6.61	104.24	112.90
7	QG	45	ASP	N-CA-C	-6.60	105.04	113.23
46	RQ	9	TYR	CA-CB-CG	6.60	125.79	113.90
35	RA	2712	U	P-O3'-C3'	6.59	127.60	119.70
29	R4	68	ARG	CA-C-N	6.58	132.04	122.36
29	R4	68	ARG	C-N-CA	6.58	132.04	122.36
1	XA	812	C	P-O3'-C3'	6.57	130.06	120.20
17	XQ	65	ILE	N-CA-C	-6.57	104.61	111.58
48	RS	34	HIS	N-CA-C	6.56	119.39	109.41
38	YE	116	VAL	N-CA-C	-6.56	102.90	110.05
40	RG	12	TYR	N-CA-C	6.55	119.24	111.71
42	YI	14	ASP	CA-C-N	6.54	133.75	121.97
42	YI	14	ASP	C-N-CA	6.54	133.75	121.97
49	RT	14	TYR	N-CA-C	-6.54	104.44	112.88
12	XL	118	SER	N-CA-C	-6.54	104.24	111.36
49	RT	6	LEU	N-CA-C	-6.53	104.00	112.23
7	QG	153	HIS	N-CA-C	-6.52	103.83	113.61
12	XL	120	TYR	CA-CB-CG	6.51	125.62	113.90
43	RN	35	ARG	N-CA-C	-6.50	99.13	109.59
49	YT	100	TYR	CA-CB-CG	6.48	125.57	113.90
26	Y1	53	VAL	N-CA-C	-6.47	102.99	110.05
8	XH	19	VAL	N-CA-C	-6.47	106.69	112.90
35	YA	271(B)	G	P-O3'-C3'	6.47	127.46	119.70
40	YG	12	TYR	N-CA-C	6.47	120.27	112.38
46	RQ	82	ARG	N-CA-C	6.45	118.57	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	XT	93	GLU	N-CA-C	-6.45	104.89	112.89
37	RD	198	ASN	N-CA-C	-6.45	102.49	111.52
19	XS	14	HIS	N-CA-C	6.44	119.13	111.33
38	YE	52	LEU	N-CA-C	6.43	117.76	109.65
41	YH	82	GLY	N-CA-C	6.43	128.43	113.18
43	YN	35	ARG	N-CA-C	-6.43	98.73	108.96
25	R0	11	ARG	N-CA-C	-6.40	105.22	114.12
31	R6	46	HIS	N-CA-C	6.39	124.41	110.80
13	XM	12	ASN	N-CA-C	6.39	124.41	110.80
45	RP	46	LYS	N-CA-C	-6.38	99.92	109.94
9	XI	91	ASP	N-CA-C	-6.38	105.50	113.28
50	RU	92	ARG	CA-C-N	6.38	133.72	121.54
50	RU	92	ARG	C-N-CA	6.38	133.72	121.54
19	XS	25	LYS	N-CA-C	-6.38	103.45	110.91
29	Y4	55	ARG	N-CA-C	-6.36	105.56	113.38
55	YZ	53	ILE	N-CA-C	6.36	122.57	109.34
33	R8	62	LEU	N-CA-C	6.34	123.82	109.81
29	Y4	22	ILE	CA-C-N	6.33	133.64	121.54
29	Y4	22	ILE	C-N-CA	6.33	133.64	121.54
19	XS	34	TRP	N-CA-C	-6.33	104.11	113.61
2	QB	73	THR	N-CA-C	-6.33	107.41	114.62
51	RV	2	PHE	CA-CB-CG	6.31	120.11	113.80
37	YD	244	ARG	N-CA-C	-6.31	102.46	108.07
49	RT	110	ILE	N-CA-C	-6.30	103.74	112.50
4	XD	8	VAL	N-CA-C	6.28	117.21	111.81
8	QH	79	VAL	N-CA-C	-6.28	103.81	113.16
42	YI	72	LEU	N-CA-C	-6.28	106.59	114.56
40	RG	98	ARG	N-CA-C	-6.26	104.69	112.90
29	R4	23	GLU	CA-C-N	6.24	133.46	121.54
29	R4	23	GLU	C-N-CA	6.24	133.46	121.54
55	YZ	9	TYR	CA-CB-CG	6.24	125.13	113.90
7	XG	7	ALA	CA-C-N	6.23	130.59	121.31
7	XG	7	ALA	C-N-CA	6.23	130.59	121.31
46	YQ	79	LEU	N-CA-C	-6.22	104.95	114.16
31	R6	44	ARG	CA-C-N	6.21	133.41	121.54
31	R6	44	ARG	C-N-CA	6.21	133.41	121.54
3	QC	8	ILE	N-CA-C	-6.21	106.47	111.81
20	QT	14	LYS	N-CA-C	-6.21	104.59	111.36
38	RE	75	VAL	N-CA-C	-6.21	104.69	110.53
49	YT	113	LYS	N-CA-C	-6.21	106.35	114.04
49	RT	89	VAL	N-CA-C	-6.20	105.78	111.67
31	Y6	44	ARG	CA-C-N	6.20	133.38	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Y6	44	ARG	C-N-CA	6.20	133.38	121.54
38	RE	188	VAL	N-CA-C	6.20	115.72	108.96
41	RH	82	GLY	N-CA-C	6.18	127.84	113.18
7	QG	61	VAL	N-CA-C	-6.18	104.30	113.39
7	XG	87	VAL	N-CA-C	6.18	115.70	108.96
27	Y2	5	GLU	N-CA-C	-6.16	105.59	113.23
43	RN	117	PHE	N-CA-C	-6.15	105.26	112.89
45	YP	116	GLY	N-CA-C	6.15	120.78	112.17
39	YF	84	VAL	N-CA-C	-6.13	101.09	109.55
43	RN	32	THR	N-CA-C	-6.12	105.30	112.89
29	Y4	22	ILE	N-CA-C	6.12	116.92	108.84
43	YN	51	PHE	N-CA-C	-6.12	99.69	109.96
18	QR	81	PHE	N-CA-C	-6.10	103.97	112.45
37	YD	10	THR	N-CA-C	-6.10	99.03	108.55
45	YP	21	ARG	N-CA-C	6.10	120.56	111.96
46	RQ	27	VAL	N-CA-C	-6.09	96.67	109.34
55	RZ	53	ILE	N-CA-C	6.09	122.00	109.34
50	RU	89	GLU	N-CA-C	-6.08	105.51	113.17
42	YI	143	SER	N-CA-C	6.08	116.46	108.07
9	XI	95	LYS	N-CA-C	-6.08	105.82	113.72
11	XK	34	ASP	N-CA-C	-6.07	103.15	110.13
50	RU	106	PHE	N-CA-C	-6.07	104.22	111.69
37	YD	241	PRO	CA-C-N	6.07	133.13	121.54
37	YD	241	PRO	C-N-CA	6.07	133.13	121.54
41	RH	85	LYS	N-CA-C	6.06	119.10	109.65
55	YZ	153	SER	N-CA-C	6.05	118.28	110.65
13	XM	103	THR	N-CA-C	6.04	119.40	112.57
12	QL	104	VAL	N-CA-C	6.04	116.71	107.77
12	XL	119	LYS	N-CA-C	-6.01	101.63	110.52
53	YX	6	ASP	N-CA-C	-6.01	106.11	113.50
11	XK	36	ASP	N-CA-C	-6.00	104.31	111.69
29	R4	15	ILE	N-CA-C	6.00	118.84	108.95
42	RI	133	HIS	N-CA-C	-5.99	96.56	109.81
37	YD	63	ARG	N-CA-C	-5.99	95.65	107.69
54	YY	83	THR	N-CA-C	5.99	118.07	109.14
19	XS	5	LEU	N-CA-C	-5.98	106.31	113.97
46	YQ	90	VAL	N-CA-C	5.98	119.42	111.17
3	QC	201	TYR	CA-CB-CG	5.97	124.64	113.90
37	RD	27	THR	N-CA-C	-5.96	101.54	110.06
41	RH	101	ARG	N-CA-C	-5.96	106.02	113.28
47	RR	14	SER	N-CA-C	5.95	118.28	111.02
13	QM	12	ASN	N-CA-C	5.95	123.46	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Y2	47	ASN	N-CA-C	5.94	123.45	110.80
53	RX	12	VAL	N-CA-C	-5.94	101.36	109.55
9	QI	95	LYS	N-CA-C	-5.93	104.91	114.09
55	RZ	61	LEU	N-CA-C	5.92	122.90	109.81
55	RZ	49	ARG	N-CA-C	-5.92	105.89	113.23
33	Y8	63	PRO	N-CA-C	-5.92	100.28	112.47
48	YS	101	LEU	N-CA-C	-5.91	104.92	111.36
2	QB	129	GLU	N-CA-C	-5.90	105.58	112.89
27	Y2	14	ARG	N-CA-C	-5.89	101.76	110.48
31	R6	42	TRP	N-CA-C	-5.87	106.16	113.38
45	RP	38	GLN	N-CA-C	5.87	119.27	111.75
55	RZ	3	TYR	CA-CB-CG	5.87	124.46	113.90
50	RU	76	TYR	N-CA-C	-5.87	105.79	113.12
42	YI	14	ASP	N-CA-C	5.85	123.27	110.80
49	YT	121	ILE	N-CA-C	-5.85	105.38	111.58
43	YN	112	LEU	N-CA-C	-5.84	106.49	113.97
33	Y8	54	GLU	N-CA-C	-5.83	105.01	111.36
35	YA	2832	U	P-O3'-C3'	5.82	128.93	120.20
37	YD	48	ARG	N-CA-C	5.82	118.22	110.53
51	YV	91	TYR	CA-CB-CG	5.82	124.37	113.90
49	RT	58	ASN	CA-CB-CG	5.81	118.41	112.60
4	XD	163	GLU	N-CA-C	-5.81	105.08	111.82
49	RT	55	ASN	N-CA-C	-5.81	103.64	112.99
55	RZ	8	TYR	CA-CB-CG	5.81	124.35	113.90
38	YE	168	MET	N-CA-C	5.80	119.14	110.14
8	QH	134	ILE	N-CA-C	5.79	115.87	110.42
26	R1	43	TYR	CA-CB-CG	5.79	124.32	113.90
37	RD	71	ASP	N-CA-C	-5.79	104.57	111.69
49	YT	112	ARG	N-CA-C	-5.76	104.75	113.51
17	XQ	42	TYR	CA-CB-CG	5.76	124.27	113.90
2	QB	140	HIS	N-CA-C	-5.74	104.99	112.23
54	YY	84	ARG	N-CA-C	-5.73	100.94	110.17
12	XL	27	LEU	N-CA-C	5.73	118.38	110.35
7	QG	38	LEU	N-CA-C	-5.73	104.49	112.45
55	YZ	61	LEU	N-CA-C	5.72	122.46	109.81
16	QP	47	ASP	N-CA-C	-5.72	104.71	112.26
2	QB	23	ARG	N-CA-C	-5.72	103.44	110.65
33	Y8	36	LYS	N-CA-C	-5.72	100.57	109.72
2	QB	11	LEU	N-CA-C	-5.71	106.31	113.28
40	RG	80	PHE	N-CA-C	-5.71	99.12	108.76
27	Y2	51	ARG	N-CA-C	-5.71	105.14	111.36
54	YY	94	LYS	N-CA-C	-5.71	101.58	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	QR	32	ARG	N-CA-C	-5.70	106.37	113.38
35	RA	271(B)	G	P-O3'-C3'	5.68	126.52	119.70
55	YZ	98	MET	N-CA-C	5.68	117.42	108.96
38	RE	62	PRO	CA-C-N	5.68	128.67	120.38
38	RE	62	PRO	C-N-CA	5.68	128.67	120.38
37	YD	236	GLY	N-CA-C	-5.68	104.52	112.13
45	RP	14	LYS	N-CA-C	-5.67	106.12	113.16
46	YQ	5	ARG	N-CA-C	-5.67	100.44	109.96
35	RA	222	A	C2'-C3'-O3'	5.67	118.00	109.50
49	RT	76	PHE	CA-CB-CG	5.66	119.46	113.80
35	RA	856	C	C2'-C3'-O3'	5.66	122.19	113.70
9	QI	63	ILE	N-CA-C	5.65	116.08	108.17
41	YH	82	GLY	CA-C-N	5.65	132.32	121.54
41	YH	82	GLY	C-N-CA	5.65	132.32	121.54
12	QL	11	VAL	N-CA-C	-5.64	104.86	111.00
50	YU	90	VAL	CA-C-N	5.64	132.31	121.54
50	YU	90	VAL	C-N-CA	5.64	132.31	121.54
37	RD	53	PHE	N-CA-C	5.64	119.41	111.52
13	QM	17	VAL	N-CA-C	-5.63	104.77	113.16
31	Y6	14	THR	N-CA-C	5.63	118.66	109.59
2	XB	155	LEU	N-CA-C	5.63	118.06	111.02
46	YQ	9	TYR	CA-CB-CG	5.63	124.03	113.90
29	Y4	25	TYR	N-CA-C	5.62	119.09	111.17
33	Y8	58	ILE	N-CA-C	-5.61	104.80	113.16
42	YI	120	ILE	N-CA-C	5.61	121.01	109.34
19	QS	28	LYS	N-CA-C	5.60	119.06	111.17
33	R8	36	LYS	N-CA-C	-5.59	101.01	109.85
47	YR	9	LYS	N-CA-C	-5.59	100.18	109.46
45	RP	22	GLY	N-CA-C	5.59	123.74	112.34
12	XL	11	VAL	N-CA-C	-5.59	104.91	111.00
46	YQ	82	ARG	CB-CA-C	-5.58	103.80	111.51
42	YI	12	LEU	N-CA-C	-5.58	98.91	110.80
38	RE	52	LEU	N-CA-C	5.58	116.68	109.65
41	RH	9	ILE	N-CA-C	5.57	114.24	107.61
39	RF	195	ASP	CA-CB-CG	5.57	118.17	112.60
1	QA	1297	C	P-O3'-C3'	5.57	128.56	120.20
3	XC	79	ARG	N-CA-C	5.57	119.02	111.17
8	QH	44	PHE	N-CA-C	-5.57	107.13	114.31
47	RR	117	VAL	N-CA-C	5.56	115.58	108.12
35	RA	227	A	C2'-C3'-O3'	5.56	117.84	109.50
48	RS	65	VAL	N-CA-C	-5.56	105.11	110.72
39	YF	105	VAL	N-CA-C	-5.55	105.11	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1558	A	P-O3'-C3'	5.55	128.52	120.20
4	XD	178	VAL	N-CA-C	5.55	116.32	110.72
54	YY	85	VAL	N-CA-C	5.54	117.32	108.89
1	XA	328	C	P-O3'-C3'	5.54	128.52	120.20
35	RA	227	A	P-O3'-C3'	5.54	128.51	120.20
20	QT	86	ARG	N-CA-C	-5.54	105.25	112.23
55	RZ	115	GLY	N-CA-C	5.53	126.29	113.18
45	RP	99	LEU	N-CA-C	-5.53	106.90	113.97
55	RZ	29	TYR	N-CA-C	5.53	117.47	109.07
2	XB	172	ILE	N-CA-C	-5.53	105.14	110.72
55	RZ	111	VAL	N-CA-C	-5.52	97.86	109.34
6	XF	60	PHE	N-CA-C	5.52	118.47	109.59
35	YA	222	A	C2'-C3'-O3'	5.52	117.77	109.50
32	Y7	47	ARG	N-CA-C	5.51	117.13	109.31
39	YF	132	VAL	N-CA-C	-5.51	104.05	110.05
33	Y8	29	LYS	N-CA-C	-5.50	99.08	110.80
35	RA	1022	G	C2'-C3'-O3'	5.49	117.74	109.50
32	Y7	47	ARG	CA-C-N	5.49	132.03	121.54
32	Y7	47	ARG	C-N-CA	5.49	132.03	121.54
9	XI	35	GLU	N-CA-C	-5.49	107.23	114.31
55	YZ	3	TYR	CA-CB-CG	5.49	123.78	113.90
53	RX	38	GLU	N-CA-C	-5.49	105.71	112.90
4	XD	110	PHE	N-CA-C	-5.49	106.08	112.89
47	RR	9	LYS	N-CA-C	-5.48	100.24	108.96
4	QD	188	LEU	N-CA-C	-5.48	103.14	109.93
14	XN	9	LYS	N-CA-C	-5.48	106.10	112.89
40	RG	79	ASN	N-CA-C	-5.48	105.39	111.36
19	QS	21	GLU	N-CA-C	-5.47	106.10	112.89
38	YE	82	ARG	CA-C-N	5.47	131.99	121.54
38	YE	82	ARG	C-N-CA	5.47	131.99	121.54
26	Y1	43	TYR	CA-CB-CG	5.46	123.74	113.90
37	RD	98	VAL	N-CA-C	-5.46	105.64	113.07
35	YA	2681	C	C2'-C3'-O3'	5.45	117.68	109.50
35	YA	1026	U	P-O3'-C3'	5.45	128.38	120.20
17	QQ	42	TYR	CA-CB-CG	5.45	123.70	113.90
9	QI	85	LEU	N-CA-C	-5.44	106.23	112.92
11	QK	80	VAL	N-CA-C	5.43	115.45	108.82
4	XD	116	GLN	N-CA-C	-5.42	105.45	111.36
55	YZ	50	GLN	N-CA-C	-5.42	104.92	112.45
51	YV	49	THR	CA-C-N	-5.42	113.06	119.84
51	YV	49	THR	C-N-CA	-5.42	113.06	119.84
29	Y4	37	SER	CA-C-N	5.42	131.89	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y4	37	SER	C-N-CA	5.42	131.89	121.54
13	QM	4	ILE	N-CA-C	5.42	120.60	109.34
14	XN	13	THR	N-CA-C	5.41	121.77	109.81
2	QB	54	THR	N-CA-C	5.40	118.08	111.82
40	YG	115	ARG	CA-C-N	5.40	131.85	121.54
40	YG	115	ARG	C-N-CA	5.40	131.85	121.54
41	RH	7	LEU	N-CA-C	5.40	121.73	109.81
42	RI	126	TYR	CA-CB-CG	5.40	123.61	113.90
49	RT	100	TYR	CA-CB-CG	5.40	123.61	113.90
12	XL	60	LEU	N-CA-C	5.39	118.06	109.65
4	XD	73	ARG	N-CA-C	-5.39	105.32	111.14
18	XR	46	GLU	N-CA-C	-5.39	106.20	112.89
45	YP	28	GLY	CA-C-N	5.39	131.83	121.54
45	YP	28	GLY	C-N-CA	5.39	131.83	121.54
4	XD	4	TYR	CA-C-N	5.38	131.66	121.97
4	XD	4	TYR	C-N-CA	5.38	131.66	121.97
17	XQ	62	SER	N-CA-C	5.38	115.39	108.34
16	QP	17	TYR	CA-CB-CG	5.38	123.59	113.90
8	XH	127	LEU	N-CA-C	-5.38	106.71	113.28
40	RG	115	ARG	CA-C-N	5.38	131.81	121.54
40	RG	115	ARG	C-N-CA	5.38	131.81	121.54
38	RE	89	ASP	N-CA-C	5.38	116.69	108.52
42	RI	71	ILE	N-CA-C	-5.38	106.61	113.22
35	YA	2681	C	P-O3'-C3'	5.38	128.26	120.20
38	RE	186	GLY	N-CA-C	5.37	125.91	113.18
55	RZ	50	GLN	N-CA-C	-5.37	107.27	113.88
42	YI	15	VAL	N-CA-C	5.37	120.51	109.34
1	QA	328	C	P-O3'-C3'	5.37	128.26	120.20
26	R1	56	GLN	N-CA-C	5.37	115.12	108.19
33	R8	50	LEU	CA-C-N	5.36	131.78	121.54
33	R8	50	LEU	C-N-CA	5.36	131.78	121.54
11	XK	106	LYS	N-CA-C	-5.36	107.39	114.04
2	QB	24	TRP	N-CA-C	5.36	118.67	110.36
2	XB	226	ARG	N-CA-C	-5.36	106.87	113.41
48	YS	88	ASP	CA-C-N	5.36	131.77	121.54
48	YS	88	ASP	C-N-CA	5.36	131.77	121.54
35	RA	1022	G	P-O3'-C3'	5.35	128.23	120.20
51	RV	14	VAL	N-CA-C	5.35	117.03	108.89
35	YA	271(B)	G	OP2-P-O3'	5.35	116.97	105.20
37	YD	148	GLU	N-CA-C	-5.35	101.92	110.10
53	RX	23	GLU	N-CA-C	-5.34	101.55	109.94
10	QJ	29	ARG	N-CA-C	-5.33	106.28	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	R5	58	LEU	N-CA-C	5.33	117.17	110.24
29	R4	40	HIS	N-CA-C	5.33	121.59	109.81
48	RS	109	GLY	CA-C-N	5.33	131.72	121.54
48	RS	109	GLY	C-N-CA	5.33	131.72	121.54
12	XL	46	LYS	CA-C-N	5.32	129.98	121.62
12	XL	46	LYS	C-N-CA	5.32	129.98	121.62
38	YE	118	LYS	N-CA-C	-5.32	106.10	113.18
42	RI	13	GLY	N-CA-C	5.32	125.79	113.18
40	RG	54	GLU	N-CA-C	-5.32	106.64	113.23
19	QS	64	GLU	N-CA-C	5.32	119.52	113.19
37	YD	20	ASP	N-CA-C	-5.32	101.03	109.96
50	RU	96	ALA	N-CA-C	-5.31	106.47	113.17
45	YP	108	LYS	N-CA-C	5.31	122.12	110.80
12	QL	41	ARG	N-CA-C	5.31	115.24	108.24
35	RA	229	A	P-O3'-C3'	5.31	128.16	120.20
35	RA	271(B)	G	OP2-P-O3'	5.29	116.85	105.20
35	YA	856	C	C2'-C3'-O3'	5.29	121.64	113.70
42	RI	57	ARG	N-CA-C	-5.29	106.33	112.89
38	RE	116	VAL	CA-C-N	5.29	135.44	125.66
38	RE	116	VAL	C-N-CA	5.29	135.44	125.66
54	RY	83	THR	N-CA-C	5.28	116.68	109.18
1	QA	410	G	C4'-C3'-O3'	5.28	120.92	113.00
9	QI	73	GLN	N-CA-C	-5.28	106.69	113.23
2	QB	152	PHE	N-CA-C	-5.28	106.52	113.17
26	Y1	3	LYS	N-CA-C	-5.27	99.58	110.80
1	QA	1285	A	P-O3'-C3'	5.26	128.10	120.20
5	QE	148	VAL	N-CA-C	-5.26	105.26	111.00
43	YN	48	MET	CG-SD-CE	-5.26	89.32	100.90
47	YR	80	PHE	N-CA-C	5.26	117.76	111.71
41	RH	85	LYS	CA-C-N	5.26	131.59	121.54
41	RH	85	LYS	C-N-CA	5.26	131.59	121.54
25	Y0	56	ASP	N-CA-C	-5.26	106.72	112.72
46	RQ	82	ARG	CB-CA-C	-5.26	104.25	111.51
40	RG	114	ILE	N-CA-C	-5.26	100.81	109.12
47	YR	14	SER	N-CA-C	5.25	116.70	110.97
37	YD	99	ASP	N-CA-C	-5.25	105.61	112.23
33	R8	48	PHE	CA-CB-CG	5.25	119.05	113.80
4	QD	19	LEU	CA-C-N	-5.25	116.02	122.84
4	QD	19	LEU	C-N-CA	-5.25	116.02	122.84
29	R4	49	PHE	N-CA-C	5.25	119.16	112.87
4	QD	208	SER	N-CA-C	-5.24	106.88	113.28
37	RD	94	LEU	N-CA-C	-5.24	101.92	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	XH	79	VAL	N-CA-C	-5.24	104.42	111.44
31	Y6	27	LYS	N-CA-C	5.24	119.37	112.25
4	QD	63	LYS	N-CA-C	-5.23	105.49	111.14
37	RD	99	ASP	N-CA-C	-5.22	106.42	112.89
9	XI	48	GLU	N-CA-C	5.22	120.77	113.57
1	QA	792	A	P-O3'-C3'	5.22	128.03	120.20
13	QM	62	ASN	N-CA-C	5.22	119.13	112.87
3	QC	90	GLU	N-CA-C	-5.21	106.76	113.23
38	YE	127	ASP	N-CA-C	-5.21	105.17	112.25
49	YT	122	ASP	N-CA-C	-5.21	105.69	111.36
7	QG	22	LEU	N-CA-C	-5.20	105.67	112.23
19	XS	10	PHE	CB-CG-CD1	5.19	129.52	120.70
35	YA	1558	A	P-O3'-C3'	5.18	127.98	120.20
41	YH	101	ARG	N-CA-C	-5.18	106.64	113.12
13	XM	66	LEU	CA-C-N	5.18	131.44	121.54
13	XM	66	LEU	C-N-CA	5.18	131.44	121.54
12	XL	20	LYS	N-CA-C	5.18	117.40	110.35
46	RQ	103	MET	CA-C-N	5.17	131.43	121.54
46	RQ	103	MET	C-N-CA	5.17	131.43	121.54
42	RI	132	PRO	CA-C-N	5.17	134.40	121.80
42	RI	132	PRO	C-N-CA	5.17	134.40	121.80
12	QL	47	LYS	N-CA-C	5.16	120.49	113.16
1	QA	1065	U	P-O3'-C3'	5.16	127.94	120.20
42	RI	121	LYS	N-CA-C	-5.16	99.81	110.80
19	QS	36	ARG	N-CA-C	-5.16	106.67	113.17
53	RX	28	PHE	CA-CB-CG	5.15	118.95	113.80
45	YP	30	THR	N-CA-C	-5.15	106.81	114.64
39	RF	105	VAL	N-CA-C	-5.15	104.54	111.44
13	XM	84	ILE	N-CA-C	-5.15	108.27	113.47
45	YP	71	VAL	N-CA-C	5.15	120.00	108.88
42	YI	86	THR	N-CA-C	5.14	118.69	111.90
12	QL	23	LYS	N-CA-C	-5.13	106.42	113.30
27	R2	47	ASN	CA-C-N	5.13	131.35	121.54
27	R2	47	ASN	C-N-CA	5.13	131.35	121.54
49	RT	136	GLN	N-CA-C	-5.13	105.74	112.41
47	YR	74	LYS	N-CA-C	-5.13	103.91	110.53
17	QQ	92	ARG	N-CA-C	-5.13	106.87	113.23
54	RY	40	GLU	N-CA-C	5.13	117.78	110.24
19	XS	21	GLU	N-CA-C	-5.13	106.61	112.92
35	YA	1022	G	P-O3'-C3'	5.13	127.89	120.20
40	RG	111	LEU	N-CA-C	5.12	120.57	113.45
35	YA	1022	G	C2'-C3'-O3'	5.12	117.18	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	R8	63	PRO	N-CA-C	-5.12	101.93	112.47
25	R0	26	TYR	CA-CB-CG	5.11	123.10	113.90
35	RA	1178	C	C2'-C3'-O3'	5.11	121.36	113.70
44	RO	32	TYR	CA-CB-CG	5.10	123.08	113.90
20	XT	42	GLN	N-CA-C	-5.10	105.36	112.45
33	Y8	50	LEU	CA-C-N	5.10	131.28	121.54
33	Y8	50	LEU	C-N-CA	5.10	131.28	121.54
35	YA	404	C	P-O3'-C3'	5.10	127.84	120.20
37	RD	48	ARG	N-CA-C	5.09	118.42	110.32
11	XK	103	LEU	N-CA-C	5.09	117.39	111.02
1	QA	812	C	P-O3'-C3'	5.08	127.83	120.20
9	QI	50	LEU	N-CA-C	-5.08	106.59	112.89
35	YA	587	C	C4'-C3'-O3'	5.08	117.02	109.40
35	YA	846	C	P-O3'-C3'	5.08	127.82	120.20
40	YG	45	GLU	N-CA-C	-5.08	107.08	113.28
54	RY	55	TYR	N-CA-C	5.08	117.39	108.75
41	YH	40	GLU	N-CA-C	-5.08	103.23	110.59
38	RE	142	GLY	CA-C-N	5.07	131.23	121.54
38	RE	142	GLY	C-N-CA	5.07	131.23	121.54
1	XA	1297	C	P-O3'-C3'	5.07	127.81	120.20
50	YU	105	VAL	N-CA-C	-5.07	105.20	112.35
49	YT	123	GLN	N-CA-C	-5.07	102.97	110.48
1	XA	1027	C	P-O3'-C3'	5.07	127.80	120.20
35	YA	752	A	C4'-C3'-O3'	5.07	117.00	109.40
49	RT	61	PHE	CA-CB-CG	5.07	118.87	113.80
33	Y8	33	ASN	N-CA-C	5.07	118.29	112.57
42	RI	89	TYR	N-CA-C	-5.06	105.85	112.23
41	YH	156	ALA	CA-C-N	5.06	131.21	121.54
41	YH	156	ALA	C-N-CA	5.06	131.21	121.54
49	RT	58	ASN	CB-CA-C	5.06	118.91	111.73
42	RI	9	LEU	N-CA-C	5.05	118.48	111.71
48	RS	17	ARG	CB-CG-CD	5.05	122.91	111.30
9	XI	87	GLN	N-CA-C	-5.05	105.48	111.69
35	RA	1045	A	P-O3'-C3'	5.04	127.77	120.20
38	YE	145	LYS	N-CA-C	5.04	118.20	111.75
29	Y4	67	TYR	CA-C-N	5.04	131.17	121.54
29	Y4	67	TYR	C-N-CA	5.04	131.17	121.54
30	R5	51	TYR	CA-C-N	5.04	134.85	123.16
30	R5	51	TYR	C-N-CA	5.04	134.85	123.16
35	RA	846	C	P-O3'-C3'	5.04	127.76	120.20
19	XS	24	ALA	N-CA-C	-5.04	102.24	110.20
43	YN	38	HIS	N-CA-C	-5.04	107.19	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	QS	7	LYS	N-CA-C	-5.03	100.97	109.07
35	YA	222	A	P-O3'-C3'	5.03	127.74	120.20
37	RD	63	ARG	N-CA-C	-5.03	97.72	107.62
46	RQ	8	LYS	N-CA-C	-5.03	105.27	111.40
3	XC	61	ALA	CA-C-N	5.02	131.13	121.54
3	XC	61	ALA	C-N-CA	5.02	131.13	121.54
42	RI	54	GLN	N-CA-C	-5.02	107.71	113.88
55	RZ	5	LEU	N-CA-C	5.02	116.13	108.30
25	Y0	62	LEU	N-CA-C	-5.01	107.72	113.88
42	YI	68	LEU	N-CA-C	-5.01	107.12	113.18
7	QG	114	ARG	N-CA-C	5.00	116.58	111.03
1	XA	992	U	P-O3'-C3'	5.00	127.71	120.20
30	Y5	4	HIS	N-CA-C	5.00	120.87	109.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	RS	17	ARG	Sidechain

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	32247	0	16277	208	0
1	XA	32249	0	16279	180	0
2	QB	1924	0	1975	28	0
2	XB	1924	0	1975	29	0
3	QC	1605	0	1668	37	0
3	XC	1605	0	1668	19	0
4	QD	1674	0	1718	29	0
4	XD	1674	0	1718	21	0
5	QE	1155	0	1213	20	0
5	XE	1155	0	1213	8	0
6	QF	843	0	857	11	0
6	XF	843	0	857	8	0
7	QG	1257	0	1296	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1296	8	0
8	QH	1116	0	1177	13	0
8	XH	1116	0	1177	20	0
9	QI	1010	0	1037	23	0
9	XI	1010	0	1037	24	0
10	QJ	801	0	849	19	0
10	XJ	801	0	849	15	0
11	QK	885	0	904	17	0
11	XK	885	0	904	9	0
12	QL	975	0	1062	17	0
12	XL	975	0	1062	16	0
13	QM	964	0	1034	35	0
13	XM	964	0	1034	16	0
14	QN	492	0	529	14	0
14	XN	492	0	529	5	0
15	QO	734	0	771	7	0
15	XO	734	0	771	4	0
16	QP	705	0	725	14	0
16	XP	705	0	725	12	0
17	QQ	834	0	904	12	0
17	XQ	834	0	904	10	0
18	QR	574	0	644	13	0
18	XR	574	0	644	8	0
19	QS	674	0	699	21	0
19	XS	674	0	699	14	0
20	QT	763	0	860	6	0
20	XT	763	0	861	17	0
21	QU	217	0	234	5	0
21	XU	217	0	234	1	0
22	QV	1640	0	837	5	0
22	XV	1640	0	837	4	0
23	QX	396	0	197	1	0
23	XX	396	0	197	3	0
24	QY	1602	0	811	23	0
24	XY	1602	0	811	10	0
25	R0	648	0	672	15	0
25	Y0	648	0	672	10	0
26	R1	763	0	848	12	0
26	Y1	763	0	848	11	0
27	R2	581	0	629	14	0
27	Y2	581	0	629	11	0
28	R3	469	0	518	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	Y3	469	0	518	4	0
29	R4	581	0	577	17	0
29	Y4	581	0	577	17	0
30	R5	459	0	480	9	0
30	Y5	459	0	480	11	0
31	R6	424	0	450	11	0
31	Y6	424	0	450	9	0
32	R7	430	0	480	7	0
32	Y7	430	0	480	7	0
33	R8	517	0	582	18	0
33	Y8	517	0	582	33	0
34	R9	307	0	335	5	0
34	Y9	307	0	335	6	0
35	RA	62071	0	31280	358	0
35	YA	62091	0	31290	306	0
36	RB	2573	0	1306	16	0
36	YB	2573	0	1306	13	0
37	RD	2115	0	2195	43	0
37	YD	2115	0	2195	53	0
38	RE	1568	0	1634	46	0
38	YE	1568	0	1634	32	0
39	RF	1585	0	1632	24	0
39	YF	1585	0	1632	32	0
40	RG	1474	0	1535	21	0
40	YG	1474	0	1535	19	0
41	RH	1307	0	1382	22	0
41	YH	1307	0	1382	20	0
42	RI	1136	0	1223	12	0
42	YI	1136	0	1223	12	0
43	RN	1104	0	1180	24	0
43	YN	1104	0	1180	9	0
44	RO	933	0	996	23	0
44	YO	933	0	996	19	0
45	RP	1145	0	1227	30	0
45	YP	1145	0	1227	28	0
46	RQ	1122	0	1179	25	0
46	YQ	1122	0	1177	22	0
47	RR	968	0	1033	19	0
47	YR	968	0	1033	17	0
48	RS	882	0	943	9	0
48	YS	882	0	943	16	0
49	RT	1141	0	1202	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	YT	1141	0	1202	24	0
50	RU	964	0	1022	22	0
50	YU	964	0	1022	20	0
51	RV	779	0	852	18	0
51	YV	779	0	852	12	0
52	RW	900	0	964	15	0
52	YW	900	0	964	18	0
53	RX	725	0	778	9	0
53	YX	725	0	778	9	0
54	RY	785	0	878	14	0
54	YY	785	0	878	9	0
55	RZ	1461	0	1493	28	0
55	YZ	1461	0	1493	32	0
56	QA	73	0	0	0	0
56	QF	1	0	0	0	0
56	QM	1	0	0	0	0
56	QV	1	0	0	0	0
56	QX	2	0	0	0	0
56	R0	1	0	0	0	0
56	R5	1	0	0	0	0
56	R8	1	0	0	0	0
56	R9	1	0	0	0	0
56	RA	281	0	0	0	0
56	RB	4	0	0	0	0
56	RD	1	0	0	0	0
56	RE	4	0	0	0	0
56	RF	1	0	0	0	0
56	RP	3	0	0	0	0
56	RR	1	0	0	0	0
56	RU	1	0	0	0	0
56	XA	91	0	0	0	0
56	XF	1	0	0	0	0
56	XM	1	0	0	0	0
56	XV	2	0	0	0	0
56	XX	1	0	0	0	0
56	Y0	1	0	0	0	0
56	Y1	1	0	0	0	0
56	Y2	1	0	0	0	0
56	Y5	1	0	0	0	0
56	Y6	2	0	0	0	0
56	Y8	1	0	0	0	0
56	Y9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	YA	347	0	0	0	0
56	YB	6	0	0	0	0
56	YE	3	0	0	0	0
56	YN	1	0	0	0	0
56	YP	3	0	0	0	0
56	YQ	3	0	0	0	0
56	YR	1	0	0	0	0
56	YX	1	0	0	0	0
57	QA	42	0	45	0	0
57	XA	42	0	45	4	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
59	QN	1	0	0	0	0
59	R9	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y9	1	0	0	0	0
All	All	294981	0	199667	2249	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 5.

All (2249) 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:YZ:94:GLU:CG	55:YZ:95:PRO:HD3	1.74	1.18
35:RA:1138:G:H21	43:RN:106:MET:HE1	1.05	1.09
35:RA:2055:C:H5'	35:RA:2056:G:H5''	1.35	1.07
55:YZ:94:GLU:HB3	55:YZ:95:PRO:CD	1.85	1.07
19:QS:10:PHE:HB2	19:QS:16:LEU:HD11	1.34	1.06
35:RA:1138:G:H21	43:RN:106:MET:CE	1.72	1.02
26:Y1:4:VAL:HG12	26:Y1:11:ARG:HD3	1.41	1.01
55:YZ:94:GLU:HG3	55:YZ:95:PRO:HD3	1.42	1.00
55:YZ:94:GLU:CB	55:YZ:95:PRO:HD3	1.90	1.00
35:RA:1138:G:N2	43:RN:106:MET:HE1	1.78	0.96
25:R0:69:PHE:CE2	25:R0:79:VAL:HG22	1.98	0.96
25:R0:69:PHE:CD2	25:R0:79:VAL:HG22	2.00	0.96
3:QC:159:GLY:CA	3:QC:193:TYR:HE2	1.78	0.96
3:QC:159:GLY:CA	3:QC:193:TYR:CE2	2.50	0.95
55:YZ:94:GLU:CB	55:YZ:95:PRO:CD	2.45	0.94
35:RA:1138:G:N3	43:RN:106:MET:HE3	1.83	0.94
49:RT:54:ARG:HA	49:RT:59:THR:HG23	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:QD:68:TYR:HE1	4:QD:103:ASN:ND2	1.70	0.90
24:QY:76:A:H2	35:RA:2583:G:H21	1.17	0.89
38:RE:13:ARG:HH21	49:RT:58:ASN:HB2	1.39	0.88
3:QC:159:GLY:HA2	3:QC:193:TYR:CE2	2.10	0.86
3:QC:159:GLY:HA2	3:QC:193:TYR:CD2	2.12	0.85
3:QC:159:GLY:N	3:QC:193:TYR:HE2	1.75	0.84
33:Y8:4:MET:CE	33:Y8:61:LEU:CD1	2.55	0.84
35:RA:1138:G:N3	43:RN:106:MET:CE	2.42	0.82
10:XJ:57:LYS:HD2	10:XJ:60:ARG:HH21	1.44	0.82
41:YH:103:LEU:HD22	41:YH:123:PHE:CE2	2.16	0.81
55:YZ:94:GLU:HB3	55:YZ:95:PRO:HD3	1.56	0.80
55:YZ:94:GLU:HB3	55:YZ:95:PRO:HD2	1.63	0.80
41:YH:103:LEU:HD22	41:YH:123:PHE:HE2	1.47	0.79
24:QY:76:A:C2	35:RA:2583:G:N2	2.48	0.79
33:Y8:4:MET:SD	33:Y8:61:LEU:HD12	2.23	0.78
3:XC:9:GLY:HA2	3:XC:12:LEU:HD23	1.65	0.78
35:RA:1043:C:H42	35:RA:1112:G:H1	1.30	0.77
18:QR:26:LEU:HD11	18:QR:29:PHE:CE2	2.20	0.77
38:RE:13:ARG:NH2	49:RT:58:ASN:HB2	2.00	0.76
26:Y1:11:ARG:HG3	26:Y1:12:PRO:HD2	1.69	0.75
35:YA:2102:U:H3	35:YA:2187:G:H1	1.35	0.75
26:Y1:4:VAL:CG1	26:Y1:11:ARG:HD3	2.15	0.75
35:RA:1138:G:N2	43:RN:106:MET:CE	2.42	0.75
1:XA:659:U:H5''	15:XO:5:LYS:HE3	1.67	0.75
35:RA:676:A:H8	35:RA:2069:G:H21	1.35	0.74
24:XY:5:C:H42	24:XY:68:G:H1	1.36	0.74
18:QR:26:LEU:HD11	18:QR:29:PHE:HE2	1.53	0.73
3:QC:20:SER:HB2	3:QC:40:ARG:HH22	1.54	0.72
38:YE:143:ASN:HD22	38:YE:147:PRO:HG2	1.54	0.72
13:QM:84:ILE:HD11	13:QM:86:CYS:HB2	1.72	0.72
32:Y7:9:ARG:NH1	35:YA:1310:G:OP2	2.22	0.72
35:RA:2056:G:H2'	35:RA:2056:G:N3	2.02	0.72
2:QB:178:ARG:HH22	8:QH:74:PRO:HB3	1.54	0.71
13:QM:80:ARG:O	13:QM:84:ILE:HG21	1.90	0.71
30:Y5:4:HIS:O	35:YA:2056:G:N2	2.23	0.71
5:QE:51:VAL:HG23	5:QE:52:PRO:HD3	1.71	0.71
30:Y5:38:ALA:HB3	30:Y5:40:LYS:HZ3	1.54	0.71
33:Y8:62:LEU:HD13	35:YA:242:G:H5''	1.73	0.71
39:YF:107:LYS:HD2	39:YF:207:GLY:H	1.56	0.71
35:RA:1006:C:O2	43:RN:106:MET:HE2	1.91	0.71
18:QR:54:ARG:HH21	18:QR:55:ARG:HH22	1.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1693:U:H1'	37:YD:14:ARG:HH22	1.56	0.71
33:Y8:65:GLU:H	33:Y8:65:GLU:CD	2.00	0.69
19:XS:10:PHE:HZ	19:XS:16:LEU:HB2	1.58	0.69
37:RD:35:LYS:NZ	37:RD:83:GLU:OE1	2.24	0.69
1:QA:1360:A:OP2	14:QN:35:ARG:NH2	2.26	0.69
31:Y6:14:THR:HG21	31:Y6:19:ARG:HH21	1.58	0.69
35:YA:2130:U:HO2'	35:YA:2133:G:HO2'	1.40	0.69
50:YU:92:ARG:NH1	51:YV:11:GLN:O	2.25	0.69
1:XA:544:G:OP1	4:XD:59:ARG:NH2	2.26	0.69
37:YD:182:LEU:H	37:YD:272:ALA:HB3	1.58	0.69
35:YA:1728:G:H8	35:YA:1732:A:H62	1.41	0.69
41:YH:130:ARG:HH12	41:YH:132:ARG:HH21	1.40	0.69
5:QE:154:GLY:HA2	8:QH:64:LYS:HD2	1.74	0.69
35:RA:1061:U:H5'	35:RA:1070:A:H1'	1.75	0.69
45:RP:58:THR:O	45:RP:61:ARG:NH2	2.26	0.69
54:RY:73:ARG:HD2	54:RY:82:PRO:HB2	1.75	0.69
30:R5:16:ARG:NH2	35:RA:517:C:OP1	2.26	0.68
35:RA:2055:C:H5'	35:RA:2056:G:C5'	2.19	0.68
35:RA:2100:G:H1	35:RA:2189:U:H3	1.39	0.68
36:YB:74:U:H1'	55:YZ:34:ASN:HD21	1.57	0.68
1:XA:1295:G:N2	1:XA:1302:U:O4	2.27	0.68
25:R0:69:PHE:CE2	25:R0:79:VAL:CG2	2.76	0.68
50:RU:44:ASN:HD21	51:RV:75:PHE:HB3	1.58	0.68
51:YV:76:LYS:HG3	51:YV:81:TYR:CD1	2.28	0.68
9:QI:10:ARG:HE	9:QI:105:ASP:HB2	1.58	0.68
7:XG:15:ASP:HB3	7:XG:19:GLY:H	1.57	0.68
35:RA:1607:C:N4	35:RA:1622:G:OP2	2.27	0.68
35:RA:2055:C:C5'	35:RA:2056:G:H5''	2.19	0.68
44:YO:104:ARG:NH2	49:YT:43:GLN:OE1	2.26	0.68
29:Y4:14:ILE:HG22	29:Y4:31:ILE:HB	1.75	0.68
10:QJ:61:GLU:OE1	14:QN:45:ARG:NH1	2.27	0.67
35:RA:2313:C:H4'	40:RG:91:ARG:HG3	1.76	0.67
35:YA:2068:U:H3	35:YA:2430:A:H2	1.42	0.67
36:RB:7:G:H21	48:RS:38:GLN:HE22	1.40	0.67
39:RF:143:ALA:HB1	39:RF:148:LEU:HB2	1.75	0.67
35:YA:39:C:O2	39:YF:46:ARG:NH2	2.26	0.67
49:YT:51:ARG:HG2	49:YT:98:LYS:HD2	1.75	0.67
30:Y5:29:THR:HG21	35:YA:2815:C:H5'	1.76	0.67
34:Y9:27:CYS:SG	34:Y9:28:GLU:N	2.67	0.67
1:QA:1009:G:H1	1:QA:1020:U:H3	1.43	0.67
13:XM:99:ARG:HB2	13:XM:101:GLN:HE22	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Y8:65:GLU:HB2	35:YA:628:G:OP1	1.94	0.67
37:RD:35:LYS:HD2	37:RD:63:ARG:HG3	1.77	0.66
10:XJ:50:ILE:HA	10:XJ:60:ARG:HB3	1.76	0.66
35:RA:1138:G:C2	43:RN:106:MET:CE	2.79	0.66
35:YA:1902:C:OP1	37:YD:242:ARG:NH1	2.28	0.66
54:YY:39:VAL:HG13	54:YY:42:VAL:HB	1.77	0.66
1:XA:1316:G:N7	19:XS:7:LYS:NZ	2.43	0.66
35:YA:2483:C:N3	46:YQ:124:LYS:NZ	2.40	0.66
50:YU:92:ARG:HD2	51:YV:11:GLN:HB2	1.78	0.66
37:RD:182:LEU:H	37:RD:272:ALA:HB3	1.59	0.66
1:QA:407:G:H5''	4:QD:115:ARG:HG2	1.77	0.66
35:RA:958:U:OP2	46:RQ:14:ARG:NH1	2.28	0.66
35:RA:2115:G:N2	35:RA:2165:G:N7	2.41	0.66
1:XA:8:A:N6	4:XD:205:GLU:O	2.29	0.66
1:XA:664:G:H22	1:XA:741:G:H1	1.42	0.66
34:R9:27:CYS:SG	34:R9:28:GLU:N	2.69	0.66
35:RA:2032:G:N2	38:RE:146:THR:OG1	2.29	0.66
27:Y2:47:ASN:ND2	35:YA:94:G:N3	2.44	0.66
1:QA:1073:U:O2	2:QB:104:ASN:ND2	2.29	0.65
10:QJ:3:LYS:N	10:QJ:74:ILE:O	2.30	0.65
49:RT:53:ARG:O	49:RT:59:THR:HG23	1.96	0.65
35:YA:2013:A:N3	52:YW:88:ARG:NH2	2.43	0.65
1:QA:1252:A:H61	1:QA:1285:A:H61	1.43	0.65
2:XB:168:THR:HB	2:XB:192:SER:HB2	1.79	0.65
3:QC:159:GLY:N	3:QC:193:TYR:CE2	2.63	0.65
17:QQ:66:SER:O	17:QQ:70:ARG:NH1	2.29	0.65
19:XS:50:ALA:HB1	19:XS:57:HIS:HB3	1.77	0.65
33:Y8:28:GLY:O	33:Y8:44:LYS:NZ	2.29	0.65
35:YA:265:A:N6	35:YA:427:U:O2'	2.30	0.65
50:RU:90:VAL:HG22	51:RV:39:LEU:HD12	1.78	0.65
1:XA:686:U:H1'	11:XK:42:TRP:HE1	1.62	0.65
10:XJ:57:LYS:HD2	10:XJ:60:ARG:NH2	2.10	0.65
35:YA:919:G:N2	35:YA:2269:A:OP2	2.29	0.65
1:QA:8:A:N6	4:QD:205:GLU:O	2.29	0.65
4:QD:68:TYR:CE1	4:QD:103:ASN:ND2	2.59	0.65
55:YZ:52:SER:O	55:YZ:54:HIS:N	2.30	0.65
15:QO:26:GLU:OE2	15:QO:77:ARG:NH1	2.30	0.65
38:RE:143:ASN:HD22	38:RE:147:PRO:HG2	1.61	0.65
18:XR:86:VAL:HG12	18:XR:87:ARG:HG2	1.78	0.65
38:YE:78:LEU:HG	38:YE:79:ARG:HG3	1.79	0.65
35:YA:960:A:H61	46:YQ:82:ARG:HH21	1.43	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:QC:47:LEU:HD11	3:QC:76:VAL:HG12	1.79	0.64
35:RA:27:G:N2	35:RA:513:A:OP2	2.30	0.64
2:XB:212:GLN:NE2	2:XB:216:SER:OG	2.30	0.64
38:RE:176:ILE:HB	38:RE:181:LEU:HB2	1.79	0.64
38:YE:36:ARG:NH1	38:YE:85:ASN:OD1	2.30	0.64
37:RD:13:ARG:NH1	37:RD:16:MET:SD	2.70	0.64
55:RZ:52:SER:O	55:RZ:54:HIS:N	2.31	0.64
5:XE:102:ALA:HB1	5:XE:106:PRO:HG2	1.80	0.64
3:QC:56:ASP:HB2	3:QC:67:THR:HB	1.79	0.64
35:RA:2751:G:N7	41:RH:2:SER:OG	2.28	0.64
29:R4:16:CYS:SG	29:R4:17:GLY:N	2.69	0.64
55:RZ:99:TYR:HB3	55:RZ:123:ASP:HB2	1.79	0.64
15:XO:7:GLU:OE2	15:XO:38:ARG:NH2	2.27	0.64
33:Y8:4:MET:HE1	33:Y8:61:LEU:CD1	2.26	0.64
35:YA:1113:U:H5'	41:YH:2:SER:HB3	1.79	0.64
35:RA:2651:C:H42	35:RA:2669:G:H1	1.42	0.64
41:RH:89:ILE:HG22	41:RH:162:ILE:HG12	1.78	0.64
54:YY:55:TYR:HE2	54:YY:61:ILE:HG21	1.61	0.64
39:RF:29:ASN:HD22	39:RF:32:LEU:HD23	1.63	0.64
2:XB:223:ILE:HG23	2:XB:229:VAL:HG22	1.78	0.64
12:XL:71:PRO:O	12:XL:102:ARG:NH1	2.30	0.64
19:QS:9:VAL:CG1	19:QS:39:THR:HB	2.28	0.64
37:YD:85:ASP:OD2	37:YD:88:ARG:NH1	2.31	0.64
35:YA:1693:U:O2	37:YD:14:ARG:NH1	2.30	0.63
19:QS:3:ARG:HH12	19:QS:11:VAL:HG11	1.63	0.63
2:XB:231:GLU:HG3	2:XB:233:SER:H	1.61	0.63
36:YB:9:G:OP1	48:YS:15:ARG:NH1	2.28	0.63
35:RA:2303:G:N3	40:RG:132:ASN:ND2	2.47	0.63
8:XH:18:ARG:NH2	8:XH:81:HIS:O	2.32	0.63
35:YA:1068:G:O2'	35:YA:1096:A:N3	2.31	0.63
45:YP:65:ARG:O	45:YP:68:GLN:NE2	2.32	0.63
16:XP:45:THR:HG22	16:XP:47:ASP:H	1.63	0.63
3:QC:7:PRO:O	3:QC:11:ARG:NE	2.31	0.63
4:QD:18:LYS:NZ	4:QD:31:CYS:SG	2.71	0.63
35:RA:67:U:H3	35:RA:74:A:H2	1.45	0.63
35:RA:321:G:O2'	35:RA:340:A:N3	2.32	0.63
37:YD:17:THR:HB	37:YD:205:VAL:H	1.63	0.63
52:RW:11:ARG:HH21	52:RW:98:LYS:HD2	1.64	0.63
1:QA:406:G:H5'	4:QD:5:ILE:HD11	1.80	0.63
35:RA:2701:C:H3'	35:RA:2702:U:H5''	1.79	0.63
35:RA:300:A:OP1	54:RY:86:ARG:NH2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:RO:2:ILE:HG23	44:RO:6:THR:HG21	1.79	0.63
4:XD:18:LYS:NZ	4:XD:31:CYS:SG	2.71	0.63
30:Y5:19:ARG:NH2	35:YA:1264:G:OP1	2.28	0.63
1:QA:878:G:H5'	8:QH:89:PRO:HG2	1.81	0.62
1:QA:1086:U:H3	1:QA:1099:G:H22	1.47	0.62
3:QC:64:VAL:HG22	3:QC:99:VAL:HA	1.81	0.62
35:RA:1667:G:H8	35:RA:1667:G:OP2	1.82	0.62
45:RP:65:ARG:O	45:RP:68:GLN:NE2	2.28	0.62
35:YA:2392:A:H2	35:YA:2424:C:H42	1.47	0.62
42:RI:90:GLY:O	42:RI:121:LYS:NZ	2.32	0.62
11:QK:86:GLY:O	11:QK:91:ARG:NH1	2.32	0.62
1:XA:992:U:H3	1:XA:1044:A:H62	1.46	0.62
35:YA:67:U:H3	35:YA:74:A:H2	1.48	0.62
55:YZ:7:ALA:HB2	55:YZ:59:LEU:HB3	1.80	0.62
3:QC:76:VAL:HG21	3:QC:103:VAL:HG21	1.81	0.62
49:RT:51:ARG:HG2	49:RT:98:LYS:HD2	1.81	0.62
17:XQ:66:SER:O	17:XQ:70:ARG:NH1	2.33	0.62
13:QM:2:ALA:HA	13:QM:11:ARG:HG2	1.82	0.62
29:R4:39:CYS:SG	29:R4:40:HIS:N	2.72	0.62
34:R9:36:GLN:NE2	35:RA:1124:C:O2	2.32	0.62
35:RA:1991:U:O5'	35:RA:1991:U:H6	1.82	0.62
35:YA:2292:C:OP1	48:YS:17:ARG:NH2	2.32	0.62
41:RH:107:VAL:O	41:RH:153:LYS:NZ	2.33	0.62
35:RA:1056:G:H21	35:RA:1103:A:H62	1.46	0.62
1:XA:765:G:N2	1:XA:813:U:OP2	2.33	0.62
37:YD:27:THR:HG21	37:YD:81:ALA:HB1	1.80	0.62
1:QA:979:C:OP1	1:QA:1223:C:N4	2.33	0.62
46:RQ:27:VAL:HG21	46:RQ:134:ARG:HA	1.82	0.62
1:XA:406:G:H5'	4:XD:5:ILE:HD11	1.79	0.62
1:XA:501:C:OP1	12:XL:117:ARG:NH2	2.33	0.62
42:YI:40:THR:HG23	42:YI:43:ASN:H	1.65	0.62
2:QB:178:ARG:NH1	2:QB:196:LEU:O	2.33	0.61
1:XA:1073:U:O2	2:XB:104:ASN:ND2	2.33	0.61
25:Y0:27:GLU:HG3	25:Y0:68:GLU:HA	1.82	0.61
35:YA:1138:G:H21	43:YN:106:MET:HE3	1.65	0.61
39:YF:116:ASP:OD1	39:YF:119:ARG:NH2	2.32	0.61
42:RI:30:LEU:HB3	42:RI:36:ALA:HB3	1.83	0.61
37:YD:148:GLU:HB2	37:YD:151:LYS:HD2	1.82	0.61
1:QA:544:G:OP1	4:QD:59:ARG:NH2	2.33	0.61
35:YA:987:G:O2'	35:YA:1000:A:N3	2.33	0.61
1:QA:1306:A:N6	1:QA:1331:G:O2'	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y0:77:ARG:NH2	35:YA:857:C:OP2	2.32	0.61
1:QA:686:U:H1'	11:QK:42:TRP:HE1	1.65	0.61
46:RQ:66:ILE:HA	46:RQ:104:PHE:HA	1.83	0.61
1:XA:1130:A:O2'	9:XI:3:GLN:NE2	2.34	0.61
29:Y4:68:ARG:HG2	29:Y4:69:LYS:HG2	1.82	0.61
38:YE:201:THR:HG22	38:YE:203:LYS:H	1.65	0.61
50:YU:44:ASN:HD21	51:YV:75:PHE:HB3	1.65	0.61
37:RD:143:HIS:ND1	37:RD:194:GLY:O	2.32	0.61
46:YQ:13:GLN:O	46:YQ:72:LYS:NZ	2.34	0.61
51:YV:7:THR:HG23	51:YV:22:VAL:HG11	1.83	0.61
8:QH:10:LEU:HD22	8:QH:83:ILE:HD11	1.82	0.61
19:QS:10:PHE:HB2	19:QS:16:LEU:CD1	2.22	0.61
30:Y5:2:ALA:N	35:YA:2015:A:N3	2.48	0.61
35:YA:573:G:N1	35:YA:2031:A:OP2	2.24	0.61
35:YA:807:U:O2	39:YF:74:ARG:NH2	2.34	0.61
5:QE:102:ALA:HB1	5:QE:106:PRO:HG2	1.83	0.60
9:QI:10:ARG:NH1	9:QI:75:ASP:OD2	2.34	0.60
11:QK:58:PRO:HB2	11:QK:93:GLN:HG3	1.82	0.60
35:RA:994:C:OP1	50:RU:53:ARG:NH2	2.33	0.60
35:RA:1059:G:O6	35:RA:1079:C:N4	2.34	0.60
52:YW:18:ARG:HD2	52:YW:76:VAL:HG13	1.82	0.60
11:QK:18:ARG:HG2	11:QK:81:ASP:HB2	1.83	0.60
27:R2:47:ASN:ND2	35:RA:94:G:N3	2.48	0.60
33:R8:58:ILE:HG13	45:RP:49:ARG:HD2	1.83	0.60
9:XI:31:GLN:HE21	9:XI:35:GLU:HG2	1.66	0.60
35:YA:948:G:N2	35:YA:985:C:OP2	2.35	0.60
35:RA:1130:U:O2	38:RE:149:ARG:NH2	2.34	0.60
35:RA:1800:C:OP2	37:RD:183:ARG:NH1	2.33	0.60
36:RB:52:A:O2'	36:RB:53:A:N7	2.34	0.60
1:XA:1123:A:H4'	10:XJ:36:GLY:HA3	1.83	0.60
3:XC:20:SER:HB2	3:XC:40:ARG:HH22	1.66	0.60
8:XH:34:GLU:OE1	8:XH:37:ARG:NH2	2.35	0.60
35:YA:996:A:OP2	50:YU:92:ARG:NH2	2.33	0.60
35:YA:2343:C:HO2'	35:YA:2373:G:HO2'	1.47	0.60
35:YA:2575:C:H5'	38:YE:144:ARG:HG2	1.82	0.60
39:YF:143:ALA:HB1	39:YF:148:LEU:HB2	1.84	0.60
26:R1:51:VAL:HG21	26:R1:74:VAL:HG11	1.84	0.60
33:Y8:62:LEU:N	33:Y8:63:PRO:HD3	2.15	0.60
35:YA:571:A:O2'	51:YV:78:LYS:NZ	2.35	0.60
55:YZ:94:GLU:HG3	55:YZ:95:PRO:CD	2.26	0.60
1:QA:1147:C:HO2'	9:QI:5:TYR:HH	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1901:A:OP2	37:RD:255:LYS:NZ	2.34	0.60
35:RA:1980:G:O2'	35:RA:1982:C:OP2	2.20	0.60
38:RE:26:ILE:HG23	38:RE:182:LEU:HB3	1.81	0.60
32:R7:39:ARG:NH2	35:RA:468:G:N7	2.49	0.60
38:RE:117:MET:HA	38:RE:122:PHE:H	1.67	0.60
1:XA:1348:U:H3	1:XA:1374:A:H2	1.48	0.60
21:XU:8:THR:HG23	21:XU:11:GLY:H	1.66	0.60
33:Y8:4:MET:SD	33:Y8:61:LEU:CD1	2.89	0.60
35:YA:336:C:HO2'	54:YY:35:TYR:HH	1.49	0.60
6:QF:3:ARG:NH1	6:QF:38:GLU:OE2	2.34	0.60
35:YA:2727:G:O2'	44:YO:70:LYS:NZ	2.34	0.60
39:YF:185:ASP:OD1	39:YF:188:ARG:NH1	2.35	0.60
1:QA:842:C:O2'	1:QA:848:C:N4	2.34	0.60
35:RA:693:C:O2'	35:RA:1353:A:N3	2.31	0.60
37:RD:85:ASP:OD2	37:RD:88:ARG:NH1	2.32	0.60
1:XA:1118:C:OP1	9:XI:104:ARG:NH1	2.35	0.60
35:RA:864:G:H1'	35:RA:914:C:H42	1.65	0.60
51:RV:52:VAL:HG21	51:RV:55:ALA:HB3	1.84	0.60
1:XA:1124:G:H1'	10:XJ:38:ILE:HD13	1.84	0.60
27:Y2:7:ARG:NH2	35:YA:102:G:OP1	2.35	0.60
1:XA:842:C:O2'	1:XA:848:C:N4	2.35	0.60
1:XA:970:C:N4	9:XI:128:ARG:OXT	2.35	0.60
35:YA:662:G:OP1	45:YP:15:ARG:NH1	2.35	0.60
35:YA:820:A:N3	35:YA:943:U:O2'	2.33	0.60
55:YZ:119:GLU:HG3	55:YZ:122:ARG:HB3	1.83	0.60
35:RA:309:G:N3	35:RA:329:G:O2'	2.34	0.59
38:RE:128:SER:OG	38:RE:129:HIS:N	2.35	0.59
55:RZ:69:THR:OG1	55:RZ:70:LEU:N	2.35	0.59
33:Y8:14:VAL:HG23	45:YP:61:ARG:HH21	1.67	0.59
33:Y8:46:ARG:NH1	35:YA:630:G:OP1	2.35	0.59
35:RA:2759:G:N2	41:RH:139:GLN:OE1	2.35	0.59
1:XA:375:U:H5''	16:XP:69:THR:HG21	1.83	0.59
6:XF:35:ALA:HB1	6:XF:65:VAL:HG11	1.84	0.59
35:YA:1689:A:H62	35:YA:1698:A:H2	1.50	0.59
52:YW:78:GLU:OE2	52:YW:99:ARG:NH1	2.34	0.59
1:QA:587:G:N2	1:QA:754:C:OP2	2.35	0.59
25:R0:77:ARG:NH2	35:RA:857:C:OP2	2.35	0.59
35:RA:910:A:H62	46:RQ:12:GLN:HA	1.68	0.59
1:QA:1347:G:N2	1:QA:1374:A:OP2	2.36	0.59
28:R3:6:VAL:HG12	28:R3:56:VAL:HG12	1.85	0.59
35:RA:141:A:H8	35:RA:1595:G:H21	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1112:G:HO2'	41:RH:2:SER:N	2.01	0.59
37:RD:31:LYS:NZ	37:RD:32:SER:OG	2.36	0.59
46:RQ:75:THR:HG21	46:RQ:85:LYS:HE3	1.84	0.59
27:Y2:29:LYS:HE3	27:Y2:57:ILE:HG21	1.84	0.59
33:Y8:13:ARG:HG3	45:YP:61:ARG:NH2	2.16	0.59
1:QA:439:A:OP2	1:QA:493:G:N1	2.34	0.59
1:QA:582:U:OP1	15:QO:68:ARG:NH2	2.33	0.59
1:QA:945:G:N2	1:QA:1334:G:O2'	2.36	0.59
1:QA:1002:G:H1	1:QA:1038:C:H42	1.49	0.59
27:R2:66:GLU:OE2	27:R2:70:GLN:NE2	2.35	0.59
36:RB:44:G:O2'	36:RB:47:C:N4	2.36	0.59
51:RV:1:MET:HE2	51:RV:43:GLU:HB2	1.85	0.59
1:XA:587:G:N2	1:XA:754:C:OP2	2.35	0.59
35:YA:309:G:N3	35:YA:329:G:O2'	2.34	0.59
35:YA:662:G:H5''	45:YP:17:LYS:HG2	1.85	0.59
35:YA:2291:U:O2'	35:YA:2374:C:O2	2.20	0.59
35:YA:2680:C:OP2	38:YE:111:ARG:NH2	2.35	0.59
48:YS:106:ARG:NH1	48:YS:107:GLU:OE2	2.35	0.59
34:R9:22:ARG:HH12	35:RA:2741:A:H5''	1.66	0.59
35:RA:750:A:OP1	35:RA:1615:C:N4	2.35	0.59
35:RA:2207:C:O2	37:RD:151:LYS:NZ	2.35	0.59
46:RQ:12:GLN:HE21	46:RQ:72:LYS:HG3	1.68	0.59
49:RT:16:ARG:NH1	49:RT:80:SER:O	2.35	0.59
2:XB:118:LEU:HB3	2:XB:142:LEU:HD12	1.84	0.59
35:YA:2032:G:N2	38:YE:146:THR:OG1	2.33	0.59
35:YA:2680:C:H5'	38:YE:189:PRO:HA	1.85	0.59
49:YT:16:ARG:HH21	49:YT:19:LEU:HD21	1.66	0.59
24:QY:53:G:O2'	46:RQ:51:ARG:NH2	2.36	0.59
35:YA:184:C:O2'	35:YA:217:G:N3	2.34	0.59
35:YA:517:C:O2'	52:YW:18:ARG:NH2	2.36	0.59
1:QA:1259:C:H42	1:QA:1276:G:H1	1.51	0.59
35:RA:414:C:O2	35:RA:1864:U:O2'	2.21	0.59
40:RG:4:ASP:OD1	40:RG:9:ARG:NH1	2.36	0.59
35:YA:729:G:OP2	37:YD:13:ARG:NH1	2.35	0.59
52:YW:88:ARG:HB2	52:YW:92:ARG:HB3	1.84	0.59
7:QG:152:ALA:O	7:QG:155:ARG:HD2	2.03	0.59
16:QP:15:PRO:HD2	16:QP:42:ARG:HD2	1.85	0.59
1:XA:1510:U:H3	1:XA:1525:G:H1	1.50	0.59
9:XI:25:LYS:N	9:XI:60:ASP:OD1	2.36	0.59
35:YA:2701:C:H3'	35:YA:2702:U:H5''	1.84	0.59
27:R2:51:ARG:HH21	27:R2:55:ARG:HH22	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:405:U:O4	4:XD:2:GLY:N	2.36	0.59
35:YA:952:G:OP1	46:YQ:16:ARG:NH1	2.36	0.59
35:YA:1364:G:N2	35:YA:1367:A:OP2	2.29	0.59
1:QA:410:G:N2	1:QA:431:A:N7	2.51	0.58
14:QN:27:CYS:SG	14:QN:28:GLY:N	2.75	0.58
28:R3:12:PRO:O	28:R3:20:LYS:NZ	2.35	0.58
35:RA:960:A:H61	46:RQ:82:ARG:HH21	1.50	0.58
35:RA:1309:G:HO2'	35:RA:1611:C:HO2'	1.46	0.58
44:RO:17:ARG:HE	44:RO:47:ILE:HD13	1.68	0.58
1:XA:1296:C:OP1	13:XM:44:ARG:NH2	2.36	0.58
10:QJ:78:ASN:HB2	10:QJ:81:THR:HG23	1.84	0.58
27:R2:47:ASN:O	27:R2:48:HIS:ND1	2.36	0.58
35:RA:955:C:OP1	46:RQ:85:LYS:NZ	2.35	0.58
49:RT:62:THR:HG22	49:RT:75:ILE:HG12	1.85	0.58
1:XA:1241:G:OP1	7:XG:35:LYS:NZ	2.36	0.58
33:Y8:14:VAL:HG23	45:YP:61:ARG:NH2	2.18	0.58
46:YQ:20:ALA:HB3	55:YZ:79:ARG:HE	1.68	0.58
19:QS:50:ALA:HB1	19:QS:57:HIS:HB3	1.84	0.58
1:XA:407:G:H5''	4:XD:115:ARG:HB3	1.83	0.58
38:RE:116:VAL:HG23	38:RE:120:TRP:HD1	1.68	0.58
1:XA:1503:A:O2'	23:XX:12:A:N6	2.36	0.58
35:YA:2304:G:H22	35:YA:2312:U:H3	1.51	0.58
35:YA:2787:C:H1'	38:YE:62:PRO:HG3	1.86	0.58
42:YI:12:LEU:HG	42:YI:19:VAL:HG11	1.85	0.58
9:QI:33:PHE:CE1	9:QI:37:PHE:HD2	2.21	0.58
9:QI:121:ARG:NH1	9:QI:122:ALA:O	2.36	0.58
6:XF:94:GLN:OE1	18:XR:32:ARG:NH1	2.37	0.58
39:YF:101:LEU:O	39:YF:106:ARG:NH1	2.36	0.58
6:XF:36:ARG:NH2	6:XF:38:GLU:OE2	2.36	0.58
13:XM:77:ASN:OD1	29:Y4:71:ARG:NH1	2.36	0.58
3:QC:47:LEU:HB3	3:QC:52:LEU:HD23	1.85	0.58
46:RQ:81:VAL:O	46:RQ:82:ARG:NH1	2.36	0.58
35:YA:10:G:N2	35:YA:2802:G:OP1	2.35	0.58
35:YA:1454:U:O2'	35:YA:1455:G:N7	2.35	0.58
2:XB:20:GLU:HG3	2:XB:191:ASP:OD1	2.04	0.58
2:XB:185:ILE:HG22	2:XB:199:TYR:HB2	1.85	0.58
35:YA:2118:U:H3	35:YA:2147:G:HO2'	1.51	0.58
39:YF:11:VAL:HG22	39:YF:125:LEU:HB2	1.86	0.58
55:YZ:5:LEU:H	55:YZ:59:LEU:HA	1.67	0.58
43:RN:99:LEU:O	43:RN:103:VAL:HG23	2.03	0.58
35:YA:2111:C:N3	35:YA:2118:U:O2'	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:YD:16:MET:HE3	37:YD:211:ARG:HD2	1.84	0.58
1:QA:189:U:O2	17:QQ:63:ARG:NH2	2.37	0.58
1:QA:593:G:H1	1:QA:646:U:H3	1.51	0.58
1:QA:811:C:O2'	1:QA:901:A:N1	2.37	0.58
31:R6:46:HIS:HD1	35:RA:2371:G:HO2'	1.41	0.58
35:RA:223:A:O2'	35:RA:420:C:O2	2.20	0.58
45:RP:135:LEU:HB3	45:RP:139:LYS:HE2	1.84	0.58
42:YI:68:LEU:HD13	42:YI:71:ILE:HD11	1.85	0.58
1:QA:437:U:H3	1:QA:495:A:H62	1.51	0.57
13:QM:99:ARG:HB2	13:QM:101:GLN:HE22	1.69	0.57
35:RA:486:C:O2'	52:RW:60:ASN:ND2	2.35	0.57
37:RD:17:THR:HB	37:RD:205:VAL:H	1.68	0.57
38:RE:141:ILE:O	38:RE:154:LYS:NZ	2.36	0.57
1:XA:1494:G:N7	57:XA:1670:PAR:N32	2.52	0.57
35:YA:1057:A:N6	35:YA:1087:G:OP2	2.37	0.57
1:QA:1004:A:H1'	1:QA:1036:G:H22	1.70	0.57
35:RA:807:U:OP2	45:RP:41:ARG:NH1	2.37	0.57
35:RA:1791:A:H5'	37:RD:206:LEU:HD12	1.86	0.57
9:XI:42:ARG:NH1	9:XI:71:SER:OG	2.37	0.57
35:YA:1266:G:O5'	52:YW:15:ARG:NH2	2.37	0.57
27:R2:66:GLU:OE1	27:R2:69:ARG:NH1	2.37	0.57
35:RA:605:C:O2	35:RA:657:U:O2'	2.21	0.57
35:RA:1140:C:OP2	43:RN:66:LYS:NZ	2.34	0.57
35:RA:1266:G:O5'	52:RW:15:ARG:NH2	2.36	0.57
37:RD:76:PRO:HB2	37:RD:116:GLN:HE21	1.69	0.57
39:RF:101:LEU:O	39:RF:106:ARG:NH1	2.37	0.57
39:RF:200:GLU:O	39:RF:204:ASN:ND2	2.37	0.57
1:XA:352:C:O2'	1:XA:354:G:OP1	2.22	0.57
6:XF:80:ARG:NH2	6:XF:88:VAL:O	2.37	0.57
27:Y2:23:LYS:NZ	27:Y2:27:GLU:OE2	2.35	0.57
1:QA:538:G:H5''	12:QL:114:LYS:HB2	1.86	0.57
26:R1:6:GLU:O	26:R1:91:LYS:NZ	2.36	0.57
35:RA:2258:C:O2'	35:RA:2427:C:OP2	2.21	0.57
1:XA:486:U:H2'	1:XA:487:A:H8	1.68	0.57
35:YA:138:G:N2	53:YX:44:GLU:OE1	2.32	0.57
35:YA:1859:A:N6	35:YA:1883:G:O2'	2.38	0.57
39:YF:31:HIS:NE2	39:YF:35:GLU:OE2	2.37	0.57
1:QA:1074:G:OP1	5:QE:64:ARG:NH2	2.37	0.57
35:RA:900:A:H3'	35:RA:901:A:H8	1.70	0.57
35:RA:2055:C:OP1	35:RA:2056:G:H5''	2.04	0.57
2:XB:54:THR:HG22	2:XB:199:TYR:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y0:39:ARG:HH21	35:YA:2355:C:H1'	1.68	0.57
35:YA:2777:G:OP2	35:YA:2781:A:O2'	2.23	0.57
13:QM:80:ARG:O	13:QM:84:ILE:CG2	2.52	0.57
15:QO:29:VAL:HG21	15:QO:81:LEU:HD21	1.86	0.57
1:XA:532:A:H2	1:XA:1206:G:H21	1.52	0.57
35:YA:918:A:N3	36:YB:80:U:O2'	2.35	0.57
1:QA:1309:G:O2'	13:QM:77:ASN:ND2	2.37	0.57
2:QB:118:LEU:HB3	2:QB:142:LEU:HD12	1.86	0.57
33:R8:28:GLY:O	33:R8:36:LYS:NZ	2.38	0.57
55:RZ:53:ILE:HG22	55:RZ:71:VAL:HG13	1.87	0.57
3:XC:138:VAL:HG13	3:XC:149:ALA:HB3	1.87	0.57
22:XV:50:U:H3	22:XV:64:G:H1	1.53	0.57
3:QC:179:ARG:HD2	3:QC:206:GLU:HG2	1.86	0.57
38:RE:78:LEU:HG	38:RE:79:ARG:HG2	1.85	0.57
4:QD:72:GLU:OE2	4:QD:207:TYR:OH	2.23	0.57
9:QI:13:ALA:HB2	9:QI:68:GLY:HA3	1.85	0.57
24:QY:18:G:N2	24:QY:57:G:N7	2.51	0.57
35:YA:1853:A:N3	35:YA:2233:U:O2'	2.33	0.57
35:YA:2287:A:H62	35:YA:2344:U:H3	1.49	0.57
47:YR:96:ARG:HE	47:YR:117:VAL:HG12	1.70	0.57
35:RA:2396:G:H1	35:RA:2420:C:H42	1.53	0.57
35:YA:612:G:N2	35:YA:616:A:O2'	2.37	0.57
29:R4:56:VAL:HG12	29:R4:61:ARG:HG2	1.87	0.56
55:RZ:97:GLU:HB3	55:RZ:125:LEU:HD11	1.87	0.56
43:YN:12:ARG:NH1	43:YN:50:ASP:OD2	2.38	0.56
4:QD:98:GLU:OE2	4:QD:107:ARG:HG3	2.04	0.56
35:RA:2010:G:H5''	52:RW:42:ARG:HB2	1.86	0.56
10:XJ:3:LYS:N	10:XJ:74:ILE:O	2.38	0.56
24:XY:4:G:H1	24:XY:69:C:H42	1.52	0.56
48:YS:106:ARG:HA	48:YS:110:LEU:HD11	1.87	0.56
49:YT:20:PRO:HD2	49:YT:86:ILE:HG23	1.87	0.56
1:QA:376:G:H5''	16:QP:5:ARG:HB2	1.86	0.56
2:QB:74:LYS:NZ	2:QB:206:ASP:OD1	2.36	0.56
11:QK:50:TYR:HD2	11:QK:54:ARG:HB3	1.70	0.56
36:RB:104:A:OP1	55:RZ:72:ARG:NH2	2.38	0.56
43:RN:108:PRO:HG2	43:RN:113:GLY:HA2	1.87	0.56
20:XT:100:ILE:HG12	20:XT:102:GLY:H	1.68	0.56
24:XY:56:C:H5''	35:YA:896:A:H2'	1.87	0.56
38:YE:128:SER:OG	38:YE:129:HIS:N	2.38	0.56
7:QG:94:ARG:NH1	7:QG:98:SER:OG	2.38	0.56
35:RA:868:U:O2	46:RQ:8:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R1:47:GLN:OE1	35:RA:2228:G:N2	2.39	0.56
55:RZ:126:VAL:HG11	55:RZ:161:VAL:HG13	1.87	0.56
1:XA:937:A:O2'	7:XG:76:ARG:NH2	2.38	0.56
38:YE:8:LYS:HA	38:YE:26:ILE:HG22	1.88	0.56
20:QT:100:ILE:HG22	20:QT:102:GLY:H	1.69	0.56
30:Y5:53:ALA:O	47:YR:96:ARG:NH1	2.34	0.56
39:YF:12:LEU:HB3	39:YF:126:VAL:HG12	1.87	0.56
42:YI:26:ALA:HA	42:YI:30:LEU:HB2	1.87	0.56
55:YZ:72:ARG:NH1	55:YZ:97:GLU:O	2.38	0.56
17:QQ:100:LYS:O	17:QQ:101:ARG:NH2	2.38	0.56
57:XA:1670:PAR:N64	57:XA:1670:PAR:O44	2.39	0.56
35:YA:861:A:N3	36:YB:79:C:O2'	2.36	0.56
38:RE:2:LYS:HB2	38:RE:95:ILE:HD12	1.88	0.56
1:XA:811:C:O2'	1:XA:901:A:N1	2.38	0.56
1:XA:971:G:N2	1:XA:1363:A:OP2	2.39	0.56
11:XK:87:THR:HA	11:XK:91:ARG:HD2	1.86	0.56
30:Y5:7:PRO:O	35:YA:2016:U:O2'	2.22	0.56
29:R4:18:CYS:SG	29:R4:19:GLY:N	2.78	0.56
35:RA:2832:U:H4'	35:RA:2833:G:H5''	1.88	0.56
49:RT:50:ILE:HD11	49:RT:100:TYR:HA	1.88	0.56
4:XD:187:ARG:NH2	4:XD:193:ASP:OD2	2.37	0.56
9:XI:19:LEU:HB3	9:XI:59:PHE:HD2	1.71	0.56
35:YA:956:G:OP2	46:YQ:14:ARG:NH2	2.38	0.56
1:QA:689:C:OP2	11:QK:55:LYS:NZ	2.39	0.56
1:QA:1422:G:H5''	44:RO:48:PRO:HB3	1.87	0.56
3:QC:159:GLY:CA	3:QC:193:TYR:CD2	2.83	0.56
31:R6:43:CYS:SG	31:R6:44:ARG:NH1	2.78	0.56
39:RF:155:LEU:HB2	39:RF:189:THR:HG21	1.88	0.56
1:XA:1305:G:O2'	1:XA:1332:A:N6	2.39	0.56
35:YA:1754:C:H5	49:YT:96:ARG:HH21	1.52	0.56
35:YA:2127:G:H22	35:YA:2162:G:H1'	1.71	0.56
37:YD:134:ARG:HG3	37:YD:135:PHE:HD1	1.71	0.56
13:QM:23:TYR:HB3	13:QM:67:GLU:HG2	1.88	0.55
35:RA:859:G:O2'	35:RA:916:G:O6	2.23	0.55
35:RA:1019:U:H3	35:RA:1142(A):A:H62	1.53	0.55
35:RA:1490:A:O2'	37:RD:99:ASP:OD1	2.24	0.55
35:YA:1327:C:O2'	47:YR:105:ARG:NH2	2.37	0.55
1:QA:1224:G:O2'	1:QA:1322:C:OP2	2.24	0.55
1:QA:1338:G:N3	22:QV:41:C:O2'	2.39	0.55
43:RN:25:ARG:O	43:RN:29:LYS:NZ	2.39	0.55
49:RT:27:THR:HG22	49:RT:48:ILE:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:757:U:O2'	1:QA:879:C:O2	2.24	0.55
9:QI:3:GLN:OE1	9:QI:20:ARG:NH2	2.38	0.55
1:XA:708:C:OP1	11:XK:85:ARG:NH2	2.38	0.55
26:R1:87:PRO:O	26:R1:91:LYS:N	2.37	0.55
35:RA:138:G:N2	53:RX:44:GLU:OE2	2.39	0.55
40:RG:63:ILE:HG13	40:RG:64:THR:HG23	1.88	0.55
14:YN:29:ARG:HD3	14:YN:40:CYS:HB2	1.89	0.55
18:XR:48:GLY:O	18:XR:74:ARG:NH2	2.39	0.55
35:YA:942:G:O2'	35:YA:1189:A:N3	2.38	0.55
41:YH:156:ALA:O	41:YH:158:HIS:N	2.39	0.55
42:YI:79:ILE:HB	42:YI:142:VAL:HA	1.88	0.55
3:QC:131:ARG:HE	5:QE:50:GLU:HG2	1.71	0.55
35:RA:910:A:N3	35:RA:2264:C:O2'	2.38	0.55
39:YF:155:LEU:HB2	39:YF:189:THR:HG21	1.87	0.55
16:QP:66:PRO:HG2	16:QP:71:ARG:HE	1.71	0.55
47:RR:53:HIS:HA	47:RR:56:LYS:HD3	1.89	0.55
1:XA:1086:U:H3	1:XA:1099:G:H22	1.54	0.55
1:QA:253:U:OP1	17:QQ:67:LYS:NZ	2.37	0.55
1:QA:1129:C:OP1	9:QI:62:TYR:OH	2.24	0.55
1:QA:1422:G:O3'	44:RO:49:ARG:NH1	2.40	0.55
13:QM:80:ARG:HH12	19:QS:69:HIS:HE1	1.55	0.55
35:RA:942:G:O2'	35:RA:1189:A:N3	2.38	0.55
35:RA:1638:C:O2	35:RA:2698:U:O2'	2.23	0.55
35:RA:2096:U:H3	35:RA:2193:G:H1	1.55	0.55
35:RA:2406:U:OP1	35:RA:2411:A:N6	2.39	0.55
1:XA:105:G:OP2	20:XT:18:GLN:NE2	2.39	0.55
35:YA:574:C:N3	38:YE:145:LYS:NZ	2.54	0.55
35:YA:2033:A:O2'	35:YA:2035:G:OP2	2.22	0.55
40:YG:161:THR:HG22	40:YG:163:ALA:H	1.71	0.55
50:YU:90:VAL:O	50:YU:92:ARG:N	2.34	0.55
49:RT:30:VAL:HG12	49:RT:86:ILE:HG12	1.89	0.55
1:XA:1498:U:OP2	23:XX:16:A:O2'	2.25	0.55
3:XC:11:ARG:NH2	3:XC:177:THR:O	2.39	0.55
35:YA:776:G:N7	35:YA:793:A:O2'	2.40	0.55
49:YT:24:PRO:HA	49:YT:49:VAL:HG23	1.89	0.55
1:QA:376:G:H1	1:QA:387:U:H3	1.55	0.55
33:R8:48:PHE:HE2	35:RA:650:C:OP1	1.89	0.55
35:RA:297:C:OP1	54:RY:87:LYS:NZ	2.40	0.55
35:RA:307:G:H21	35:RA:330:A:H62	1.53	0.55
36:RB:48:A:OP2	48:RS:30:ARG:NH2	2.40	0.55
38:RE:6:GLY:HA3	38:RE:26:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:XD:98:GLU:HA	4:XD:103:ASN:HD22	1.70	0.55
6:XF:81:ILE:HD11	37:YD:125:ILE:HB	1.89	0.55
7:XG:151:TYR:HE1	11:XK:54:ARG:HG2	1.71	0.55
8:XH:73:ASP:OD1	8:XH:75:ARG:NH1	2.40	0.55
37:YD:71:ASP:HB2	37:YD:103:ARG:HH12	1.71	0.55
43:YN:96:GLU:HB2	43:YN:122:VAL:HG12	1.89	0.55
1:QA:642:A:N3	8:QH:113:SER:OG	2.37	0.55
24:QY:30:G:H1	24:QY:40:C:H42	1.55	0.55
33:R8:7:HIS:HD2	45:RP:50:ARG:HH11	1.55	0.55
35:RA:768:G:O2'	35:RA:1379:A:N6	2.40	0.55
42:RI:73:GLU:HG3	42:RI:136:VAL:HG23	1.89	0.55
35:YA:27:G:N2	35:YA:512:G:O2'	2.40	0.55
1:QA:1372:U:OP1	9:QI:72:GLY:N	2.41	0.54
4:QD:98:GLU:HG2	4:QD:189:PRO:HG2	1.88	0.54
1:XA:1152:A:OP1	10:XJ:70:ARG:NH2	2.36	0.54
27:Y2:14:ARG:NH1	27:Y2:66:GLU:OE1	2.40	0.54
47:YR:38:VAL:HG22	47:YR:112:ALA:HB2	1.89	0.54
1:QA:356:A:N3	1:QA:368:U:O2'	2.34	0.54
1:QA:448:A:OP2	1:QA:485:G:N2	2.35	0.54
3:QC:159:GLY:HA3	3:QC:193:TYR:CE2	2.42	0.54
44:RO:23:ARG:NH2	44:RO:28:SER:O	2.40	0.54
1:XA:152:A:H62	1:XA:169:C:H42	1.54	0.54
1:XA:278:G:OP2	17:XQ:92:ARG:NH2	2.40	0.54
4:XD:23:GLY:N	4:XD:26:CYS:SG	2.79	0.54
40:YG:29:TRP:O	40:YG:33:ARG:NH1	2.40	0.54
45:YP:64:LYS:O	45:YP:66:GLY:N	2.39	0.54
46:YQ:77:LYS:NZ	46:YQ:80:GLU:OE2	2.38	0.54
1:QA:1240:U:OP1	7:QG:119:ARG:NH2	2.40	0.54
35:RA:2119:A:N6	35:RA:2170:A:N7	2.53	0.54
35:YA:1791:A:N6	35:YA:1828:G:O2'	2.35	0.54
35:YA:2683:C:O2	44:YO:70:LYS:NZ	2.40	0.54
36:YB:5:C:O2'	36:YB:27:C:O2	2.25	0.54
49:YT:27:THR:HA	49:YT:48:ILE:HA	1.87	0.54
16:QP:13:HIS:O	16:QP:42:ARG:NH1	2.40	0.54
35:RA:1093:G:H21	35:RA:1098:A:H62	1.53	0.54
1:XA:1316:G:H4'	14:XN:18:VAL:HG11	1.90	0.54
13:XM:80:ARG:NH1	19:XS:65:ASN:O	2.40	0.54
18:XR:51:LEU:HD22	18:XR:55:ARG:HD2	1.90	0.54
33:Y8:4:MET:HE3	33:Y8:61:LEU:CD1	2.36	0.54
52:YW:69:LEU:HD13	52:YW:107:LEU:HD13	1.89	0.54
1:QA:1321:C:H5''	1:QA:1322:C:H5''	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:QJ:33:GLN:HE21	10:QJ:75:ILE:HD13	1.72	0.54
13:QM:37:THR:O	13:QM:55:ARG:NH1	2.40	0.54
35:RA:83:G:N2	35:RA:103:A:OP2	2.41	0.54
35:RA:2692:C:O2	35:RA:2847:U:O2'	2.21	0.54
36:RB:9:G:OP1	48:RS:15:ARG:NH1	2.41	0.54
28:Y3:8:LEU:HB2	28:Y3:28:LEU:HD13	1.89	0.54
35:YA:1651:G:N7	47:YR:11:ASN:ND2	2.55	0.54
35:YA:1800:C:OP2	37:YD:183:ARG:NH1	2.38	0.54
24:QY:76:A:H2'	35:RA:2585:U:H5	1.72	0.54
33:R8:4:MET:HE2	35:RA:666:G:H1'	1.90	0.54
20:XT:89:ARG:HD2	20:XT:104:LEU:HD11	1.90	0.54
33:Y8:4:MET:CE	33:Y8:61:LEU:HD13	2.37	0.54
55:YZ:74:VAL:HG22	55:YZ:86:VAL:HG23	1.87	0.54
25:R0:23:VAL:HG13	25:R0:38:VAL:HG22	1.89	0.54
35:RA:637:A:OP1	45:RP:133:SER:OG	2.22	0.54
35:RA:2857:G:N2	35:RA:2860:A:OP2	2.35	0.54
1:XA:508:C:OP1	4:XD:209:ARG:NH2	2.39	0.54
1:XA:943:U:H1'	9:XI:124:GLN:HE22	1.72	0.54
3:XC:20:SER:OG	3:XC:22:TRP:NE1	2.39	0.54
29:Y4:23:GLU:O	29:Y4:25:TYR:N	2.39	0.54
35:YA:1728:G:N1	35:YA:1730:U:OP2	2.41	0.54
35:YA:2010:G:H5''	52:YW:42:ARG:HB2	1.90	0.54
43:YN:22:THR:OG1	43:YN:23:LEU:N	2.41	0.54
2:QB:69:LEU:HB3	2:QB:162:ILE:HG22	1.90	0.54
6:QF:94:GLN:OE1	18:QR:32:ARG:NH1	2.41	0.54
26:R1:40:ARG:NH2	35:RA:2232:U:OP2	2.41	0.54
29:R4:42:PHE:O	29:R4:44:THR:N	2.41	0.54
35:RA:1815:A:OP2	37:RD:54:ARG:NH2	2.40	0.54
35:RA:2111:C:N3	35:RA:2118:U:O2'	2.40	0.54
37:YD:146:GLU:HB3	37:YD:189:CYS:HB3	1.90	0.54
41:YH:46:GLU:OE1	41:YH:51:ARG:NH1	2.41	0.54
1:QA:11:G:O2'	1:QA:506:G:N2	2.40	0.54
1:QA:573:A:N3	1:QA:883:C:O2'	2.39	0.54
7:QG:26:PHE:HD2	7:QG:43:PHE:CE2	2.26	0.54
10:QJ:38:ILE:HD11	10:QJ:71:LEU:HD23	1.89	0.54
35:RA:372:G:N2	35:RA:401:A:OP2	2.33	0.54
49:RT:52:ILE:HG12	49:RT:61:PHE:HB3	1.90	0.54
1:XA:1119:C:OP2	9:XI:9:ARG:NH2	2.41	0.54
35:YA:2065:C:O2	35:YA:2449:U:N3	2.34	0.54
38:YE:81:ILE:HG21	38:YE:84:PHE:HD2	1.73	0.54
45:YP:18:ARG:HH21	45:YP:32:THR:HG21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:444:C:H2'	1:QA:445:G:H8	1.73	0.54
1:QA:1166:G:N2	1:QA:1170:A:OP2	2.40	0.54
3:QC:88:ARG:HE	3:QC:101:LEU:HB2	1.72	0.54
29:R4:5:ILE:HB	40:RG:67:LYS:HD2	1.89	0.54
35:RA:1689:A:H62	35:RA:1698:A:H2	1.56	0.54
1:XA:439:A:OP2	1:XA:493:G:N1	2.37	0.54
2:XB:16:HIS:HD2	2:XB:210:SER:HA	1.72	0.54
3:XC:14:ILE:HG12	3:XC:15:THR:HG23	1.90	0.54
33:R8:34:TRP:O	33:R8:35:GLN:NE2	2.41	0.53
35:RA:1065:U:O2'	35:RA:1074:G:N2	2.41	0.53
40:YG:38:VAL:HG22	40:YG:93:THR:HG23	1.89	0.53
5:QE:108:ALA:HA	5:QE:111:GLU:HG2	1.89	0.53
7:QG:75:VAL:HA	7:QG:88:PRO:HA	1.89	0.53
1:XA:103:C:OP2	20:XT:17:ARG:NH2	2.39	0.53
1:XA:339:C:OP1	44:YO:13:ASN:ND2	2.41	0.53
13:XM:65:LYS:HB3	29:Y4:50:VAL:HG11	1.90	0.53
1:QA:23:C:OP2	1:QA:561:U:N3	2.40	0.53
1:QA:414:A:OP2	1:QA:428:G:N2	2.41	0.53
2:QB:115:LEU:HD12	2:QB:145:LEU:HG	1.89	0.53
31:R6:7:ILE:HG13	31:R6:8:LYS:H	1.72	0.53
35:RA:1652:A:OP1	47:RR:8:ARG:NH1	2.36	0.53
35:RA:2777:G:OP2	35:RA:2781:A:O2'	2.25	0.53
20:XT:73:HIS:HB3	20:XT:74:LYS:HD3	1.90	0.53
35:YA:307:G:H21	35:YA:330:A:H62	1.57	0.53
35:YA:1065:U:O2'	35:YA:1074:G:N2	2.41	0.53
46:YQ:66:ILE:HA	46:YQ:104:PHE:HA	1.90	0.53
2:XB:126:GLU:OE2	2:XB:130:ARG:NH1	2.41	0.53
8:XH:4:ASP:OD2	8:XH:85:ARG:NE	2.39	0.53
1:QA:582:U:OP2	1:QA:758:G:N1	2.33	0.53
1:QA:689:C:H3'	1:QA:690:G:H21	1.74	0.53
5:QE:50:GLU:HG3	5:QE:52:PRO:HD2	1.89	0.53
8:QH:110:ALA:HB3	8:QH:121:ASP:HB3	1.90	0.53
24:QY:76:A:H2	35:RA:2583:G:N2	1.96	0.53
1:XA:953:G:N7	13:XM:104:ARG:NH2	2.57	0.53
8:XH:91:ARG:NE	17:XQ:32:TYR:O	2.41	0.53
35:YA:2469:A:H2	35:YA:2481:G:H21	1.56	0.53
1:QA:544:G:OP2	4:QD:66:ARG:NH2	2.42	0.53
11:QK:33:THR:OG1	11:QK:34:ASP:N	2.41	0.53
35:RA:530:G:O2'	35:RA:532:A:N7	2.41	0.53
1:XA:953:G:H5'	1:XA:965:A:H61	1.73	0.53
10:XJ:26:ALA:O	10:XJ:84:GLN:NE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:YD:179:SER:O	37:YD:273:ARG:NH2	2.41	0.53
1:QA:769:G:H4'	1:QA:1513:A:H4'	1.91	0.53
10:QJ:45:ARG:HB2	10:QJ:65:LEU:HB3	1.91	0.53
35:RA:918:A:N3	36:RB:80:U:O2'	2.41	0.53
35:YA:486:C:O2'	52:YW:60:ASN:ND2	2.41	0.53
35:YA:1342:A:O2'	35:YA:1344:G:OP2	2.27	0.53
1:QA:571:U:O4	1:QA:864:A:N6	2.42	0.53
24:QY:75:C:O5'	24:QY:75:C:H6	1.92	0.53
40:RG:16:ARG:HH21	40:RG:28:VAL:HG22	1.74	0.53
1:XA:564:C:OP2	12:XL:15:ARG:NH2	2.37	0.53
1:XA:618:C:H5'	1:XA:619:U:H5''	1.89	0.53
35:YA:1087:G:O4'	35:YA:1103:A:N6	2.42	0.53
1:QA:662:G:H1	1:QA:743:U:H3	1.56	0.53
2:QB:78:GLN:O	2:QB:94:ASN:ND2	2.36	0.53
39:RF:134:GLY:H	39:RF:162:LEU:HD12	1.73	0.53
45:RP:59:LEU:HA	45:RP:61:ARG:HH21	1.73	0.53
1:XA:1316:G:N1	1:XA:1319:A:OP2	2.41	0.53
13:XM:3:ARG:O	13:XM:57:ARG:NH1	2.40	0.53
33:Y8:14:VAL:CG2	45:YP:61:ARG:NH2	2.72	0.53
35:YA:526:A:O2'	35:YA:2043:C:O2	2.23	0.53
37:YD:134:ARG:HG3	37:YD:135:PHE:CD1	2.44	0.53
45:YP:115:LEU:HA	45:YP:134:ALA:HB2	1.90	0.53
51:YV:60:GLU:OE1	51:YV:97:LYS:NZ	2.38	0.53
1:QA:1348:U:H4'	9:QI:120:ARG:HG3	1.92	0.53
11:QK:87:THR:HA	11:QK:91:ARG:HD2	1.91	0.53
55:RZ:57:ILE:HG23	55:RZ:69:THR:HG23	1.91	0.53
1:XA:573:A:N3	1:XA:883:C:O2'	2.41	0.53
2:XB:87:ARG:NH2	2:XB:220:ASP:OD1	2.38	0.53
48:YS:26:LEU:HB3	48:YS:87:PHE:HA	1.90	0.53
3:QC:191:THR:OG1	3:QC:194:GLY:O	2.28	0.52
35:RA:819:A:OP2	35:RA:1187:G:N2	2.29	0.52
35:RA:1139:G:O2'	35:RA:1143:A:N1	2.38	0.52
35:RA:2680:C:H5'	38:RE:189:PRO:HA	1.90	0.52
40:RG:75:LYS:HE3	40:RG:77:ILE:HD11	1.91	0.52
53:RX:11:PRO:HA	53:RX:28:PHE:HA	1.91	0.52
40:YG:47:LYS:HD3	40:YG:81:LYS:HB2	1.91	0.52
1:QA:673:G:O3'	6:QF:87:ARG:NH2	2.43	0.52
3:QC:182:ILE:HG12	3:QC:203:PHE:HA	1.92	0.52
9:QI:104:ARG:NH1	9:QI:105:ASP:O	2.43	0.52
12:QL:33:ARG:HG2	12:QL:60:LEU:HD12	1.90	0.52
26:R1:92:LYS:HE2	26:R1:96:LYS:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2787:C:H1'	38:RE:62:PRO:HG3	1.90	0.52
39:RF:113:ALA:HB2	39:RF:183:VAL:HG23	1.92	0.52
1:XA:60:A:OP1	1:XA:111:G:N2	2.42	0.52
1:XA:62:U:O2'	1:XA:379:C:O2	2.25	0.52
13:XM:58:GLU:O	13:XM:62:ASN:ND2	2.42	0.52
1:QA:1256:A:OP1	3:QC:26:LYS:NZ	2.39	0.52
37:RD:146:GLU:HB3	37:RD:189:CYS:HB3	1.90	0.52
1:XA:401:C:O2'	1:XA:621:A:N3	2.38	0.52
31:Y6:43:CYS:SG	31:Y6:44:ARG:N	2.82	0.52
35:YA:1769:G:O2'	35:YA:1958:C:OP1	2.21	0.52
35:YA:2547:U:O2	44:YO:23:ARG:NH1	2.41	0.52
52:YW:18:ARG:NH1	52:YW:76:VAL:O	2.42	0.52
1:QA:866:C:O2'	1:QA:919:A:OP1	2.27	0.52
35:RA:1394:U:H4'	35:RA:1603:A:H4'	1.92	0.52
35:RA:1791:A:N6	35:RA:1828:G:O2'	2.43	0.52
1:XA:67:C:H2'	1:XA:68:G:C8	2.45	0.52
1:XA:1150:U:O4	1:XA:1151:A:N6	2.43	0.52
1:XA:1422:G:H5''	44:YO:48:PRO:HB3	1.92	0.52
2:XB:7:VAL:HG22	2:XB:11:LEU:HD21	1.91	0.52
9:XI:121:ARG:NH1	9:XI:122:ALA:O	2.43	0.52
24:XY:9:A:O2'	24:XY:10:G:N7	2.41	0.52
35:YA:958:U:OP2	46:YQ:14:ARG:NH1	2.42	0.52
35:YA:1113:U:OP1	41:YH:2:SER:N	2.42	0.52
44:YO:68:GLU:OE2	44:YO:78:ARG:NH1	2.42	0.52
7:QG:116:ALA:HA	7:QG:119:ARG:HE	1.75	0.52
22:QV:1:C:O3'	46:RQ:87:LYS:NZ	2.42	0.52
35:RA:1999:C:O2	35:RA:2687:U:O2'	2.27	0.52
35:RA:2503:A:O2'	35:RA:2505:G:OP2	2.25	0.52
38:RE:34:VAL:HG21	38:RE:77:ILE:HD11	1.91	0.52
13:XM:14:ARG:NH2	13:XM:41:PRO:O	2.41	0.52
1:QA:279:A:OP2	17:QQ:95:TYR:OH	2.27	0.52
1:QA:1239:A:O2'	1:QA:1298:C:N4	2.43	0.52
35:RA:1651:G:OP1	47:RR:40:LYS:NZ	2.37	0.52
35:YA:2115:G:N2	35:YA:2165:G:O6	2.43	0.52
38:YE:176:ILE:HB	38:YE:181:LEU:HB2	1.92	0.52
49:YT:19:LEU:HD22	49:YT:86:ILE:HG22	1.92	0.52
50:YU:50:ARG:HG2	50:YU:53:ARG:HH22	1.74	0.52
52:YW:29:LEU:HD22	52:YW:69:LEU:HD11	1.91	0.52
1:QA:824:C:O2'	8:QH:1:MET:N	2.42	0.52
35:RA:906:G:O2'	46:RQ:67:ARG:NH2	2.39	0.52
35:RA:2308:G:H22	35:RA:2311:A:H2	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2635:C:H5''	38:RE:78:LEU:HA	1.92	0.52
1:XA:191:G:O2'	20:XT:101:GLY:O	2.27	0.52
1:XA:745:C:OP1	1:XA:851:G:O2'	2.27	0.52
7:XG:5:ARG:HE	7:XG:6:ARG:H	1.58	0.52
40:YG:59:GLU:OE1	40:YG:153:ARG:NH2	2.35	0.52
31:R6:36:LEU:HD13	31:R6:50:ARG:HE	1.75	0.52
35:RA:1138:G:O2'	43:RN:102:ALA:O	2.27	0.52
35:RA:2666:C:O2	41:RH:152:ARG:NH1	2.42	0.52
41:RH:3:ARG:NH1	41:RH:4:ILE:O	2.43	0.52
9:XI:17:VAL:HA	9:XI:63:ILE:HG22	1.91	0.52
35:YA:1252:G:N7	50:YU:36:ARG:NH1	2.57	0.52
48:YS:39:ILE:HD12	48:YS:85:VAL:HG11	1.91	0.52
1:QA:1446:A:O2'	49:RT:125:ARG:NH1	2.43	0.52
36:RB:44:G:H1'	36:RB:47:C:H42	1.74	0.52
42:RI:92:VAL:HG23	42:RI:120:ILE:HG23	1.91	0.52
46:RQ:67:ARG:NH1	46:RQ:105:GLU:OE2	2.42	0.52
1:XA:227:G:N2	16:XP:62:VAL:O	2.38	0.52
1:XA:262:A:H5''	20:XT:76:ALA:HB2	1.92	0.52
15:XO:24:SER:OG	15:XO:25:THR:N	2.42	0.52
19:XS:19:VAL:HG21	19:XS:44:MET:HB3	1.92	0.52
35:YA:1291:C:H5'	35:YA:1536:A:H5'	1.92	0.52
41:YH:153:LYS:HB3	41:YH:162:ILE:H	1.74	0.52
1:QA:1382:C:O2'	7:QG:79:ARG:NH1	2.43	0.52
13:QM:57:ARG:NH1	29:R4:34:GLU:O	2.43	0.52
35:RA:971:C:O2'	35:RA:983:A:N3	2.38	0.52
54:RY:39:VAL:HG13	54:RY:42:VAL:HB	1.91	0.52
10:XJ:38:ILE:HD12	10:XJ:39:PRO:HD2	1.92	0.52
12:XL:24:VAL:HG13	12:XL:98:TYR:HE1	1.75	0.52
35:YA:259:G:H21	35:YA:621:A:H8	1.58	0.52
35:YA:1296:G:OP1	35:YA:2709:G:O2'	2.22	0.52
35:YA:1478:G:H2'	35:YA:1479:G:H8	1.74	0.52
35:YA:1824:G:N3	37:YD:254:THR:OG1	2.42	0.52
44:YO:106:LEU:HB3	44:YO:111:PHE:HB2	1.92	0.52
1:QA:264:U:O2'	17:QQ:64:PRO:O	2.26	0.51
30:R5:36:CYS:SG	30:R5:37:LYS:N	2.83	0.51
35:RA:2343:C:O2'	35:RA:2373:G:O2'	2.27	0.51
35:YA:180:G:N2	35:YA:215:G:O6	2.43	0.51
35:YA:598:G:H5'	45:YP:11:GLY:HA3	1.92	0.51
35:YA:2597:G:H5'	37:YD:243:GLY:HA3	1.92	0.51
7:QG:20:ASP:HB3	7:QG:23:VAL:HG23	1.92	0.51
16:QP:34:GLU:OE1	16:QP:55:ARG:NH2	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:R4:54:GLY:HA3	29:R4:71:ARG:HG2	1.93	0.51
41:RH:153:LYS:HB3	41:RH:162:ILE:H	1.75	0.51
53:RX:34:ALA:O	53:RX:77:LYS:NZ	2.39	0.51
55:RZ:137:ILE:HG21	55:RZ:155:LEU:HD23	1.92	0.51
1:XA:410:G:H21	1:XA:432:A:H62	1.58	0.51
1:XA:464:G:N2	1:XA:467:G:N7	2.59	0.51
35:YA:2295:C:OP1	48:YS:10:ARG:NH1	2.43	0.51
1:QA:676:A:H1'	11:QK:115:PRO:HB3	1.92	0.51
1:QA:986:A:N3	19:QS:52:TYR:OH	2.32	0.51
1:QA:1130:A:O2'	9:QL:3:GLN:NE2	2.42	0.51
1:QA:1359:C:O2'	1:QA:1362:C:N4	2.42	0.51
7:XG:27:ILE:HA	7:XG:30:ILE:HD12	1.91	0.51
15:XO:4:THR:HG23	15:XO:7:GLU:H	1.75	0.51
35:YA:958:U:O2	36:YB:89(A):A:O2'	2.26	0.51
36:YB:8:U:O2'	48:YS:25:ARG:NH2	2.43	0.51
49:YT:62:THR:HG22	49:YT:75:ILE:HG12	1.93	0.51
3:QC:127:ARG:HH22	3:QC:192:THR:H	1.58	0.51
35:RA:523:C:O2	35:RA:553:U:O2'	2.29	0.51
1:XA:375:U:O2	16:XP:28:ARG:NH1	2.43	0.51
1:XA:1367:C:H5''	9:XI:114:TYR:HA	1.93	0.51
1:XA:1392:G:H21	1:XA:1502:A:H8	1.58	0.51
33:Y8:62:LEU:CD1	35:YA:242:G:H5''	2.41	0.51
48:YS:15:ARG:NE	48:YS:88:ASP:OD1	2.43	0.51
53:YX:57:LEU:HG	53:YX:78:LYS:HB2	1.91	0.51
1:QA:64:G:H4'	1:QA:65:U:H5'	1.93	0.51
1:QA:375:U:H5''	16:QP:69:THR:HG21	1.92	0.51
2:QB:54:THR:HG22	2:QB:199:TYR:HB3	1.91	0.51
16:QP:18:ARG:HA	16:QP:38:TYR:HA	1.93	0.51
1:XA:405:U:OP2	4:XD:3:ARG:NH2	2.38	0.51
4:XD:105:VAL:HG13	4:XD:110:PHE:HB2	1.92	0.51
35:YA:806:C:O2	35:YA:2444:G:O2'	2.25	0.51
1:QA:130:A:N3	1:QA:263:A:O2'	2.41	0.51
1:QA:559:A:H4'	1:QA:560:U:H3'	1.91	0.51
1:QA:794:A:HO2'	1:QA:1521:G:HO2'	1.57	0.51
1:QA:1123:A:H4'	10:QJ:36:GLY:HA3	1.92	0.51
1:QA:1287:A:H2	1:QA:1353:G:H1'	1.76	0.51
47:RR:70:LEU:HD12	47:RR:76:VAL:HG12	1.92	0.51
3:XC:62:ASP:HA	3:XC:97:LYS:HD3	1.93	0.51
33:Y8:14:VAL:HG13	33:Y8:22:VAL:HG13	1.92	0.51
34:Y9:36:GLN:NE2	35:YA:1124:C:O2	2.43	0.51
41:YH:52:VAL:O	41:YH:65:HIS:NE2	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:YI:114:LEU:HD13	42:YI:130:TYR:HD1	1.76	0.51
1:QA:7:G:O2'	5:QE:120:THR:O	2.29	0.51
3:QC:14:ILE:HG12	3:QC:15:THR:HG23	1.93	0.51
37:RD:141:VAL:HG13	37:RD:162:SER:HB2	1.91	0.51
19:XS:36:ARG:NH2	19:XS:72:GLY:O	2.44	0.51
27:Y2:41:ILE:HG13	27:Y2:44:LEU:HD13	1.92	0.51
35:YA:701:G:O2'	35:YA:1631:A:N1	2.44	0.51
49:YT:54:ARG:HA	49:YT:59:THR:HG23	1.93	0.51
3:QC:184:TYR:CE1	3:QC:201:TYR:HE1	2.29	0.51
11:QK:21:ILE:HB	11:QK:84:VAL:HG12	1.91	0.51
13:QM:66:LEU:HD12	13:QM:68:GLY:H	1.74	0.51
28:R3:9:VAL:HG11	28:R3:55:ARG:HD3	1.93	0.51
28:R3:29:ARG:NH1	35:RA:1183:G:O3'	2.44	0.51
35:RA:259:G:H21	35:RA:621:A:H8	1.58	0.51
35:RA:336:C:O2'	54:RY:35:TYR:OH	2.27	0.51
35:RA:1817:G:OP1	37:RD:88:ARG:NH2	2.44	0.51
35:RA:1962:C:O2'	35:RA:1964:G:OP2	2.29	0.51
41:RH:18:GLU:HB3	41:RH:25:LYS:HB3	1.93	0.51
44:RO:8:LEU:HB2	44:RO:19:ILE:HG13	1.92	0.51
6:XF:9:VAL:HB	6:XF:87:ARG:HB2	1.92	0.51
35:YA:535:C:O3'	50:YU:53:ARG:NH1	2.44	0.51
35:YA:878:A:N6	35:YA:899:A:O2'	2.38	0.51
36:YB:48:A:OP2	48:YS:30:ARG:NH2	2.44	0.51
39:YF:59:TYR:HD2	39:YF:78:ILE:HG13	1.76	0.51
18:QR:58:LEU:HB3	18:QR:62:GLU:HG3	1.93	0.51
24:QY:55:U:H3	55:RZ:183:LEU:HB3	1.76	0.51
31:R6:6:ARG:HD2	31:R6:7:ILE:H	1.75	0.51
37:RD:108:PRO:HB3	37:RD:143:HIS:CE1	2.46	0.51
10:XJ:3:LYS:NZ	10:XJ:75:ILE:O	2.41	0.51
35:YA:220:G:O2'	35:YA:233:A:N3	2.41	0.51
35:YA:242:G:O2'	35:YA:254:G:O6	2.28	0.51
35:YA:2287:A:N6	35:YA:2344:U:H3	2.08	0.51
38:YE:10:GLY:HA3	49:YT:8:LYS:HD3	1.92	0.51
52:YW:86:LEU:HD22	52:YW:96:ILE:HD11	1.92	0.51
1:QA:335:C:O2'	1:QA:1433:A:N3	2.38	0.51
13:QM:84:ILE:CD1	13:QM:86:CYS:HB2	2.39	0.51
35:RA:1681:G:HO2'	35:RA:1762:A:HO2'	1.54	0.51
39:RF:198:ALA:HA	39:RF:201:VAL:HG22	1.92	0.51
41:RH:23:ARG:HA	41:RH:36:PRO:HA	1.91	0.51
1:XA:1192:C:OP2	3:XC:4:LYS:NZ	2.34	0.51
3:XC:70:VAL:HG12	3:XC:72:LYS:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:XE:12:LEU:HB3	5:XE:31:LEU:HB3	1.93	0.51
38:YE:52:LEU:HB2	38:YE:75:VAL:HG22	1.93	0.51
1:QA:165:C:H2'	1:QA:166:G:H8	1.77	0.50
24:QY:58:A:N7	55:RZ:183:LEU:HB2	2.26	0.50
25:R0:32:ARG:H	25:R0:35:ASN:ND2	2.09	0.50
35:RA:2055:C:O2	35:RA:2572:A:N6	2.44	0.50
9:XI:10:ARG:NH1	9:XI:75:ASP:OD2	2.45	0.50
17:XQ:28:PRO:HA	17:XQ:35:VAL:HA	1.92	0.50
35:YA:793:A:N6	35:YA:2073:C:OP1	2.43	0.50
50:YU:29:SER:OG	50:YU:30:LYS:NZ	2.40	0.50
50:YU:52:ARG:HD2	50:YU:55:ARG:NH2	2.26	0.50
35:RA:579:G:O2'	35:RA:2019:A:OP1	2.27	0.50
35:RA:2291:U:O2'	35:RA:2374:C:O2	2.25	0.50
1:XA:1002:G:H2'	1:XA:1003:G:H8	1.76	0.50
2:XB:9:GLU:HG3	2:XB:48:MET:HE3	1.94	0.50
8:XH:13:ILE:HG23	8:XH:63:LEU:HD11	1.92	0.50
49:YT:39:ARG:HH22	49:YT:41:ARG:HD3	1.77	0.50
55:YZ:45:ASP:OD1	55:YZ:49:ARG:NE	2.43	0.50
14:QN:45:ARG:O	14:QN:49:HIS:ND1	2.30	0.50
19:QS:32:LYS:HA	19:QS:50:ALA:HB3	1.93	0.50
29:R4:6:HIS:CE1	40:RG:67:LYS:H	2.30	0.50
38:RE:92:THR:OG1	38:RE:93:VAL:N	2.44	0.50
47:RR:3:HIS:O	47:RR:5:LYS:N	2.45	0.50
50:RU:91:ASP:HA	50:RU:95:LEU:HD12	1.94	0.50
1:XA:578:C:O2'	1:XA:728:A:N3	2.42	0.50
14:XN:4:LYS:HA	14:XN:7:ILE:HG12	1.94	0.50
20:XT:26:ASN:HB2	20:XT:71:THR:HG23	1.93	0.50
35:YA:907:U:O2'	46:YQ:101:ARG:NH2	2.44	0.50
1:QA:651:C:N4	1:QA:753:A:OP2	2.44	0.50
38:RE:48:GLN:OE1	38:RE:64:LYS:NZ	2.44	0.50
49:RT:54:ARG:HA	49:RT:59:THR:CG2	2.33	0.50
26:Y1:5:CYS:SG	26:Y1:8:SER:OG	2.69	0.50
35:YA:363(A):A:H2'	35:YA:363(B):G:H8	1.76	0.50
35:YA:1203:G:O6	35:YA:1204:A:N6	2.44	0.50
35:YA:1980:G:O2'	35:YA:1982:C:OP2	2.29	0.50
51:YV:52:VAL:HG21	51:YV:55:ALA:HB3	1.93	0.50
1:QA:1422:G:H2'	1:QA:1423:G:H8	1.77	0.50
12:QL:70:ILE:HG13	12:QL:100:ILE:HD12	1.92	0.50
35:RA:458:G:N2	35:RA:470:A:OP2	2.36	0.50
35:RA:1327:C:HO2'	47:RR:105:ARG:HH12	1.55	0.50
35:RA:2120:G:H2'	35:RA:2121:G:H8	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:RV:24:LYS:HA	51:RV:92:THR:HG23	1.92	0.50
52:RW:86:LEU:HD22	52:RW:96:ILE:HD11	1.93	0.50
2:XB:84:GLU:HG3	2:XB:215:LEU:HB3	1.94	0.50
1:QA:1060:C:OP1	14:QN:45:ARG:NH2	2.44	0.50
31:R6:14:THR:HG1	31:R6:19:ARG:HE	1.56	0.50
35:RA:265:A:N6	35:RA:427:U:O2'	2.45	0.50
35:RA:1213:A:N3	35:RA:1238:G:O2'	2.41	0.50
35:RA:2730:C:O2'	38:RE:168:MET:O	2.23	0.50
44:RO:106:LEU:HB3	44:RO:111:PHE:HB2	1.93	0.50
1:XA:296:U:O2'	1:XA:556:C:O2	2.30	0.50
1:XA:1249:C:O2'	9:XI:73:GLN:NE2	2.45	0.50
2:XB:192:SER:OG	2:XB:193:ASP:N	2.45	0.50
37:YD:164:GLN:OE1	37:YD:176:ARG:NH2	2.37	0.50
39:YF:60:SER:OG	39:YF:61:GLY:N	2.43	0.50
1:QA:618:C:H5'	1:QA:619:U:H5''	1.94	0.50
2:QB:21:ARG:HB3	2:QB:39:ILE:HG13	1.93	0.50
19:QS:3:ARG:HH12	19:QS:11:VAL:CG1	2.25	0.50
32:R7:7:PRO:HB2	35:RA:1309:G:H4'	1.93	0.50
35:RA:1990:C:H2'	35:RA:1991:U:C6	2.47	0.50
35:RA:2130:U:O2'	35:RA:2133:G:O2'	2.26	0.50
55:RZ:47:VAL:O	55:RZ:51:ALA:N	2.39	0.50
1:XA:1452:C:H4'	1:XA:1453:G:H5'	1.93	0.50
35:YA:2688:U:OP1	35:YA:2713:A:N6	2.45	0.50
44:YO:120:GLU:OE1	49:YT:67:SER:OG	2.27	0.50
1:QA:1128:C:H1'	1:QA:1146:A:H61	1.76	0.50
35:RA:224:G:O6	35:RA:419:C:O2'	2.27	0.50
35:RA:270(E):G:H1	35:RA:270(U):C:H42	1.59	0.50
35:RA:2032:G:H21	38:RE:146:THR:HG1	1.58	0.50
52:RW:59:VAL:HG21	52:RW:66:GLU:HB2	1.94	0.50
1:XA:1077:G:N2	1:XA:1080:A:OP2	2.37	0.50
35:YA:2646:C:OP2	35:YA:2732:G:O2'	2.25	0.50
39:YF:179:GLU:HA	39:YF:205:ARG:HH22	1.74	0.50
45:YP:36:LYS:O	45:YP:40:SER:OG	2.25	0.50
50:YU:40:PHE:HB3	51:YV:75:PHE:CD2	2.47	0.50
1:QA:1336:C:H1'	1:QA:1337:G:C2	2.47	0.50
19:QS:33:THR:OG1	19:QS:34:TRP:N	2.45	0.50
25:R0:39:ARG:HH21	35:RA:2355:C:H1'	1.77	0.50
35:RA:677:A:O2'	35:RA:2070:G:O2'	2.29	0.50
49:RT:49:VAL:HG12	49:RT:63:VAL:HG22	1.92	0.50
1:XA:1318:A:H4'	19:XS:11:VAL:HG11	1.94	0.50
29:Y4:33:VAL:HG21	40:YG:109:VAL:HG13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:429:U:OP2	4:QD:36:ARG:NH2	2.43	0.49
1:QA:1366:C:O2'	10:QJ:60:ARG:NH2	2.39	0.49
20:QT:71:THR:HG22	20:QT:72:LEU:HG	1.93	0.49
35:RA:2064:C:O2'	35:RA:2251:G:N2	2.41	0.49
35:RA:2773:C:OP1	38:RE:166:THR:OG1	2.26	0.49
39:RF:135:LYS:HB3	39:RF:138:GLU:HG3	1.94	0.49
44:RO:2:ILE:HG23	44:RO:6:THR:CG2	2.42	0.49
1:QA:974:A:OP2	14:QN:29:ARG:NH2	2.35	0.49
2:QB:84:GLU:OE2	2:QB:235:SER:OG	2.30	0.49
25:R0:19:LYS:NZ	35:RA:2387:U:O2'	2.44	0.49
27:R2:32:LEU:O	27:R2:36:ARG:N	2.43	0.49
35:RA:2839:G:H5'	47:RR:46:GLY:HA2	1.94	0.49
1:XA:110:C:O2'	16:XP:25:ARG:O	2.29	0.49
1:XA:390:C:O3'	16:XP:28:ARG:NH2	2.41	0.49
3:XC:150:LYS:HG3	3:XC:167:TRP:HE1	1.77	0.49
3:XC:150:LYS:HB3	3:XC:201:TYR:HB2	1.94	0.49
33:Y8:62:LEU:HD13	35:YA:242:G:C5'	2.41	0.49
41:YH:56:SER:OG	41:YH:61:HIS:ND1	2.35	0.49
8:QH:96:GLY:H	8:QH:99:GLU:HG3	1.77	0.49
1:XA:757:U:O2'	1:XA:879:C:O2	2.30	0.49
1:XA:1028(B):C:N4	1:XA:1032(B):G:O6	2.45	0.49
33:Y8:4:MET:HE3	33:Y8:61:LEU:HD13	1.94	0.49
35:YA:1479:G:OP2	35:YA:1510:A:N6	2.38	0.49
35:YA:2502:G:H5''	35:YA:2503:A:H5''	1.93	0.49
1:QA:578:C:O2'	1:QA:728:A:N3	2.37	0.49
35:RA:820:A:N3	35:RA:943:U:O2'	2.43	0.49
35:RA:1112:G:O3'	41:RH:2:SER:N	2.45	0.49
35:RA:1669:A:N3	35:RA:1669:A:H2'	2.27	0.49
51:RV:23:GLU:OE2	51:RV:89:GLN:NE2	2.45	0.49
31:Y6:47:THR:HG22	31:Y6:48:VAL:H	1.76	0.49
35:YA:1020:A:N6	35:YA:1141:U:O2'	2.45	0.49
38:YE:118:LYS:HE2	47:YR:1:MET:HE1	1.95	0.49
44:YO:107:ARG:HG3	44:YO:115:VAL:HG11	1.94	0.49
2:QB:28:PHE:HD1	2:QB:194:PRO:HD3	1.78	0.49
25:R0:27:GLU:HG3	25:R0:68:GLU:HA	1.95	0.49
35:RA:327:G:N2	54:RY:70:SER:OG	2.46	0.49
38:RE:36:ARG:HH12	38:RE:86:PRO:HD2	1.77	0.49
44:RO:64:ARG:HB2	44:RO:83:ALA:HB3	1.94	0.49
50:RU:90:VAL:HG11	51:RV:40:LEU:HG	1.93	0.49
1:XA:676:A:H1'	11:XK:115:PRO:HB3	1.94	0.49
1:XA:1002:G:H1	1:XA:1038:C:H42	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1147:C:O2	9:QI:16:ARG:NH1	2.46	0.49
2:QB:70:PHE:O	2:QB:93:VAL:N	2.44	0.49
18:QR:34:TYR:CD1	18:QR:35:ARG:HG3	2.48	0.49
26:R1:11:ARG:HD3	26:R1:12:PRO:HD2	1.93	0.49
27:R2:22:GLU:OE2	27:R2:68:ARG:NH2	2.45	0.49
35:RA:442:G:N3	39:RF:48:THR:OG1	2.44	0.49
35:RA:1403:C:H5'	35:RA:1471:A:H1'	1.93	0.49
35:RA:1638:C:O3'	35:RA:2709:G:N2	2.46	0.49
35:RA:2115:G:N1	35:RA:2164:C:OP2	2.45	0.49
37:RD:12:SER:HB2	37:RD:208:LYS:HB3	1.93	0.49
45:RP:9:ASN:OD1	45:RP:9:ASN:N	2.44	0.49
2:XB:84:GLU:HB3	2:XB:219:VAL:HG21	1.92	0.49
8:XH:7:ALA:HB2	8:XH:85:ARG:HD3	1.95	0.49
31:Y6:25:LYS:HE2	31:Y6:27:LYS:NZ	2.28	0.49
35:YA:380:U:H2'	35:YA:381:G:H8	1.77	0.49
1:QA:1325:C:H4'	21:QU:17:THR:HG21	1.95	0.49
35:RA:2392:A:OP2	35:RA:2422:A:N6	2.46	0.49
48:RS:15:ARG:HD2	48:RS:25:ARG:HH11	1.78	0.49
1:XA:452:A:H62	1:XA:480:U:H3	1.59	0.49
9:XI:9:ARG:HG2	9:XI:14:VAL:HG22	1.94	0.49
35:YA:833:U:O2	45:YP:55:ARG:NH1	2.46	0.49
18:QR:44:LEU:HD11	18:QR:79:LEU:HD23	1.95	0.49
35:RA:238:C:O2'	35:RA:608:A:N3	2.43	0.49
35:RA:807:U:O2'	35:RA:2060:A:N1	2.40	0.49
35:RA:1190:G:H2'	35:RA:1191:G:H8	1.77	0.49
1:XA:1128:C:N3	1:XA:1144:G:N2	2.60	0.49
35:YA:243:U:OP2	35:YA:254:G:N1	2.44	0.49
35:YA:900:A:H3'	35:YA:901:A:H8	1.77	0.49
35:YA:2656:U:H3	35:YA:2665:A:H2	1.61	0.49
26:R1:42:GLN:OE1	35:RA:379:G:N2	2.39	0.49
26:R1:45:ASN:HB2	35:RA:397:G:H5''	1.94	0.49
2:XB:184:VAL:HG13	2:XB:198:ASP:H	1.78	0.49
28:Y3:15:TYR:O	28:Y3:20:LYS:NZ	2.46	0.49
35:YA:1490:A:O2'	37:YD:99:ASP:OD1	2.31	0.49
49:YT:64:ARG:HG3	49:YT:73:GLU:HG2	1.94	0.49
1:QA:953:G:N7	13:QM:104:ARG:NH2	2.56	0.49
13:QM:37:THR:OG1	13:QM:55:ARG:NH1	2.46	0.49
31:R6:27:LYS:HE2	35:RA:2284:C:H3'	1.94	0.49
35:RA:2470:G:OP1	46:RQ:56:ARG:NH2	2.46	0.49
49:RT:24:PRO:HD3	49:RT:52:ILE:HD12	1.94	0.49
54:RY:83:THR:OG1	54:RY:84:ARG:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:RZ:5:LEU:HD22	55:RZ:43:GLU:HB3	1.95	0.49
4:XD:98:GLU:HG2	4:XD:189:PRO:HG2	1.95	0.49
35:YA:1530:G:O6	35:YA:1542:G:N2	2.45	0.49
51:YV:76:LYS:HG3	51:YV:81:TYR:HD1	1.75	0.49
55:YZ:61:LEU:HB3	55:YZ:65:GLN:HB2	1.95	0.49
35:RA:2865:U:OP2	49:RT:119:LYS:NZ	2.39	0.48
42:RI:64:GLU:HG3	42:RI:67:ARG:HH21	1.78	0.48
1:XA:642:A:N3	8:XH:113:SER:OG	2.38	0.48
2:XB:164:VAL:HG12	2:XB:166:ASP:H	1.77	0.48
5:XE:75:THR:OG1	5:XE:76:ILE:N	2.46	0.48
24:XY:75:C:H2'	24:XY:76:A:C8	2.48	0.48
35:YA:868:U:O2	46:YQ:8:LYS:NZ	2.45	0.48
35:YA:994:C:O2'	35:YA:996:A:OP1	2.29	0.48
35:YA:996:A:H4'	50:YU:92:ARG:HE	1.77	0.48
1:QA:545:C:OP2	4:QD:65:ARG:NH2	2.41	0.48
11:QK:34:ASP:OD1	11:QK:38:ASN:N	2.46	0.48
35:RA:514:A:N3	35:RA:581:C:O2'	2.42	0.48
35:RA:984:A:H5''	35:RA:985:C:H5	1.77	0.48
35:RA:2295:C:H5	48:RS:13:ARG:HH12	1.59	0.48
46:RQ:24:GLY:H	46:RQ:101:ARG:HD2	1.79	0.48
35:YA:807:U:OP2	45:YP:41:ARG:NH1	2.46	0.48
35:YA:2125:G:N1	35:YA:2172:U:OP1	2.43	0.48
4:QD:23:GLY:N	4:QD:26:CYS:SG	2.72	0.48
6:QF:36:ARG:NH1	6:QF:66:GLU:OE1	2.46	0.48
7:QG:105:VAL:O	7:QG:109:ASN:ND2	2.46	0.48
35:RA:335:C:H4'	54:RY:73:ARG:HE	1.78	0.48
50:RU:92:ARG:HE	50:RU:94:ASN:HB3	1.77	0.48
35:YA:300:A:OP2	54:YY:84:ARG:NH1	2.47	0.48
35:YA:335:C:H4'	54:YY:73:ARG:HE	1.76	0.48
35:YA:1246:A:OP1	45:YP:15:ARG:NH2	2.37	0.48
1:QA:403:C:OP2	4:QD:74:GLN:NE2	2.46	0.48
1:QA:662:G:O2'	1:QA:836:G:OP1	2.32	0.48
1:QA:1392:G:H21	1:QA:1502:A:H8	1.60	0.48
2:QB:178:ARG:NH2	8:QH:71:GLY:O	2.46	0.48
13:QM:82:MET:CE	13:QM:92:HIS:HB3	2.42	0.48
27:R2:4:SER:OG	27:R2:5:GLU:N	2.34	0.48
35:RA:1666:G:O2'	44:RO:6:THR:OG1	2.28	0.48
37:RD:25:THR:O	37:RD:27:THR:N	2.46	0.48
43:RN:22:THR:OG1	43:RN:23:LEU:N	2.45	0.48
55:RZ:5:LEU:H	55:RZ:59:LEU:HA	1.79	0.48
25:Y0:18:ALA:O	25:Y0:20:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Y8:4:MET:HE1	33:Y8:61:LEU:HD11	1.93	0.48
40:YG:12:TYR:HA	40:YG:16:ARG:HD3	1.94	0.48
1:QA:129(A):G:N2	1:QA:188:U:O2'	2.46	0.48
1:QA:1213:A:N6	1:QA:1215:G:N3	2.61	0.48
35:RA:363:G:H2'	35:RA:363(A):A:H8	1.78	0.48
35:RA:476:G:N1	35:RA:479:A:OP2	2.43	0.48
35:RA:1651:G:H4'	47:RR:39:PRO:HG2	1.96	0.48
35:RA:2619:C:OP1	38:RE:152:LYS:NZ	2.34	0.48
37:RD:31:LYS:HB3	37:RD:35:LYS:HG2	1.94	0.48
1:XA:413:G:O2'	1:XA:428:G:N2	2.46	0.48
1:XA:1236:A:H4'	1:XA:1304:G:H4'	1.95	0.48
8:XH:10:LEU:HD22	8:XH:83:ILE:HD11	1.95	0.48
22:XV:58:A:O2'	22:XV:60:U:OP2	2.30	0.48
22:XV:63:G:H4'	25:Y0:11:ARG:HH22	1.79	0.48
37:YD:108:PRO:HB3	37:YD:143:HIS:CE1	2.49	0.48
1:QA:297:G:N2	1:QA:300:A:OP2	2.45	0.48
1:QA:976:G:P	14:QN:32:SER:H	2.36	0.48
4:QD:59:ARG:HA	4:QD:59:ARG:HE	1.78	0.48
35:RA:281:G:H21	35:RA:359:A:H62	1.61	0.48
35:RA:1568:G:OP2	37:RD:63:ARG:NH2	2.42	0.48
37:RD:231:HIS:CD2	37:RD:249:PRO:HG3	2.48	0.48
55:RZ:48:PHE:HA	55:RZ:51:ALA:HB3	1.95	0.48
9:XI:26:VAL:HG22	9:XI:61:ALA:HB3	1.96	0.48
1:QA:532:A:H2	1:QA:1206:G:H21	1.61	0.48
28:R3:8:LEU:HA	28:R3:54:VAL:HG12	1.96	0.48
33:R8:26:LYS:NZ	35:RA:2361:A:OP2	2.46	0.48
35:RA:1296:G:OP1	35:RA:2709:G:O2'	2.22	0.48
52:RW:29:LEU:HD22	52:RW:69:LEU:HD11	1.95	0.48
1:XA:864:A:O2'	1:XA:1078:U:O4	2.29	0.48
10:XJ:44:VAL:HG22	10:XJ:66:ARG:HG2	1.96	0.48
19:XS:68:GLY:HA2	29:Y4:68:ARG:HB2	1.95	0.48
35:YA:2470:G:H5'	46:YQ:56:ARG:HH21	1.79	0.48
55:YZ:130:PRO:HA	55:YZ:133:ILE:HD11	1.95	0.48
1:QA:1080:A:H5''	5:QE:16:THR:HG21	1.94	0.48
6:QF:9:VAL:HB	6:QF:87:ARG:HB2	1.94	0.48
35:RA:1479:G:OP2	35:RA:1510:A:N6	2.39	0.48
35:RA:2245:U:H5'	35:RA:2246:G:H5'	1.95	0.48
35:RA:2572:A:OP1	35:RA:2574:G:O2'	2.31	0.48
48:RS:26:LEU:HB3	48:RS:87:PHE:HA	1.95	0.48
19:XS:32:LYS:HA	19:XS:50:ALA:HB3	1.96	0.48
27:Y2:41:ILE:HD11	27:Y2:44:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1780:A:O2'	35:YA:1781:C:O2	2.27	0.48
35:YA:1858:G:H2'	35:YA:1883:G:H22	1.78	0.48
35:RA:2415:G:H4'	45:RP:67:MET:H	1.79	0.48
47:RR:42:LYS:HG2	47:RR:45:ARG:HH12	1.79	0.48
55:RZ:28:MET:HE1	55:RZ:61:LEU:HD11	1.95	0.48
17:XQ:15:MET:HE1	17:XQ:43:LEU:HD22	1.94	0.48
25:Y0:23:VAL:HG22	25:Y0:38:VAL:HG22	1.96	0.48
35:YA:299:A:N3	35:YA:319:C:O2'	2.43	0.48
37:YD:35:LYS:NZ	37:YD:102:LYS:O	2.47	0.48
37:YD:95:LEU:HD22	37:YD:117:VAL:HG21	1.96	0.48
1:QA:970:C:N4	9:QI:128:ARG:OXT	2.46	0.48
27:R2:31:GLU:O	27:R2:35:LEU:N	2.45	0.48
35:RA:2816:C:O2	35:RA:2883:A:O2'	2.28	0.48
44:RO:19:ILE:HG22	44:RO:43:VAL:HA	1.94	0.48
44:RO:71:ARG:HH22	44:RO:122:LEU:C	2.17	0.48
49:RT:73:GLU:OE2	49:RT:103:ARG:NE	2.41	0.48
12:XL:60:LEU:HD12	12:XL:62:SER:H	1.78	0.48
29:Y4:55:ARG:HG3	29:Y4:56:VAL:HG23	1.95	0.48
32:Y7:7:PRO:HB2	35:YA:1309:G:H4'	1.96	0.48
35:YA:414:C:H2'	35:YA:415:A:C8	2.48	0.48
35:YA:1638:C:O2	35:YA:2698:U:O2'	2.31	0.48
35:YA:1682:G:OP1	35:YA:1699:G:N1	2.45	0.48
35:YA:2258:C:O2'	35:YA:2427:C:OP2	2.32	0.48
35:YA:2446:G:N2	35:YA:2449:U:O2	2.38	0.48
38:YE:25:VAL:HG12	38:YE:183:LEU:HG	1.96	0.48
41:YH:103:LEU:HD13	41:YH:131:VAL:HG21	1.96	0.48
42:YI:1:MET:HE1	42:YI:27:ARG:HH21	1.78	0.48
1:QA:924:C:O2'	1:QA:1502:A:N6	2.47	0.47
12:QL:117:ARG:HB2	12:QL:122:THR:HB	1.96	0.47
33:R8:30:ARG:HH21	45:RP:62:LEU:HD13	1.79	0.47
42:RI:128:LEU:O	42:RI:138:ILE:N	2.40	0.47
1:XA:79:G:H2'	1:XA:80:G:H8	1.78	0.47
31:Y6:24:GLU:HG3	31:Y6:25:LYS:H	1.79	0.47
35:YA:1568:G:H5''	37:YD:61:LEU:HG	1.97	0.47
51:YV:76:LYS:HG3	51:YV:81:TYR:CE1	2.48	0.47
54:YY:14:LEU:HB2	54:YY:75:ILE:HD11	1.96	0.47
1:QA:323:U:OP1	20:QT:26:ASN:ND2	2.47	0.47
1:QA:980:C:O2'	14:QN:9:LYS:NZ	2.46	0.47
35:RA:995:C:O2	43:RN:3:THR:OG1	2.32	0.47
35:RA:1779:U:OP2	35:RA:1784:A:N6	2.39	0.47
35:RA:2012:G:OP1	52:RW:11:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:826:C:H5'	8:XH:12:ARG:HH21	1.79	0.47
1:XA:1065:U:O2	1:XA:1067:A:N6	2.43	0.47
16:XP:14:ASN:HA	16:XP:42:ARG:HH11	1.79	0.47
20:XT:74:LYS:HD3	20:XT:74:LYS:H	1.80	0.47
35:YA:223:A:O2'	35:YA:420:C:O2	2.27	0.47
35:YA:2632:A:HO2'	35:YA:2811:G:HO2'	1.52	0.47
55:YZ:125:LEU:HG	55:YZ:164:ALA:HB3	1.95	0.47
1:QA:346:G:OP1	49:RT:41:ARG:NH2	2.40	0.47
24:QY:4:G:H1	24:QY:69:C:H42	1.62	0.47
35:RA:2393:A:H5'	45:RP:62:LEU:HB3	1.96	0.47
35:RA:2495:G:H5''	46:RQ:81:VAL:HG12	1.96	0.47
35:RA:2734:A:H62	35:RA:2770:G:H21	1.61	0.47
35:RA:2791:C:OP1	35:RA:2893:G:N2	2.47	0.47
42:RI:1:MET:N	42:RI:21:VAL:O	2.40	0.47
1:XA:689:C:H3'	1:XA:690:G:H21	1.79	0.47
1:XA:1321:C:H5''	1:XA:1322:C:H5''	1.97	0.47
1:XA:1347:G:N2	1:XA:1374:A:OP2	2.38	0.47
2:XB:109:SER:O	2:XB:113:HIS:ND1	2.46	0.47
24:XY:55:U:O2'	24:XY:57:G:OP2	2.24	0.47
34:Y9:25:VAL:HB	34:Y9:34:GLN:HB2	1.96	0.47
1:QA:191:G:O2'	20:QT:101:GLY:O	2.32	0.47
1:QA:559:A:OP1	5:QE:126:ARG:NH2	2.48	0.47
1:QA:718:G:H5'	11:QK:117:ASN:HB2	1.96	0.47
4:XD:59:ARG:HA	4:XD:59:ARG:HE	1.79	0.47
24:XY:58:A:O2'	24:XY:61:C:N4	2.46	0.47
25:Y0:32:ARG:H	25:Y0:35:ASN:ND2	2.12	0.47
35:YA:1250:G:OP2	45:YP:21:ARG:NH1	2.47	0.47
35:YA:2402:C:H1'	35:YA:2403:C:H5	1.79	0.47
38:YE:75:VAL:HG23	38:YE:76:ARG:HG2	1.96	0.47
45:YP:90:ARG:NH2	45:YP:105:LEU:HD11	2.29	0.47
50:YU:91:ASP:C	50:YU:93:LYS:H	2.22	0.47
1:QA:153:C:N3	1:QA:169:C:N4	2.63	0.47
1:QA:254:G:O2'	17:QQ:16:GLN:O	2.32	0.47
1:QA:816:A:OP1	1:QA:1526:G:O2'	2.28	0.47
13:QM:84:ILE:O	13:QM:84:ILE:HG13	2.15	0.47
33:R8:16:ILE:HD12	33:R8:57:ARG:HG2	1.95	0.47
35:RA:994:C:OP2	50:RU:54:LYS:NZ	2.34	0.47
41:RH:24:VAL:N	41:RH:35:VAL:O	2.44	0.47
45:RP:4:SER:O	45:RP:7:ARG:NH1	2.48	0.47
47:RR:103:ARG:NH1	47:RR:108:GLY:O	2.47	0.47
35:YA:603:A:H5''	35:YA:655:A:H61	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1568:G:OP2	37:YD:63:ARG:NH2	2.42	0.47
35:YA:2543:G:H2'	35:YA:2544:G:C8	2.49	0.47
55:YZ:97:GLU:HG2	55:YZ:125:LEU:HD11	1.96	0.47
1:QA:1294:G:H2'	1:QA:1295:G:C8	2.50	0.47
1:QA:1321:C:OP1	13:QM:88:ARG:NH2	2.48	0.47
5:QE:145:LYS:NZ	5:QE:149:GLU:OE2	2.43	0.47
35:RA:2068:U:H3	35:RA:2430:A:H2	1.62	0.47
38:RE:9:VAL:HB	38:RE:25:VAL:HG23	1.97	0.47
1:XA:792:A:O2'	1:XA:794:A:N7	2.47	0.47
1:XA:1281:U:H5''	1:XA:1282:C:H5	1.79	0.47
7:XG:20:ASP:HB3	7:XG:23:VAL:HG12	1.95	0.47
26:Y1:78:LYS:HG2	35:YA:270(R):G:H21	1.80	0.47
33:Y8:4:MET:CE	33:Y8:61:LEU:HD12	2.35	0.47
37:YD:43:ARG:HB2	37:YD:54:ARG:HB2	1.95	0.47
39:YF:134:GLY:H	39:YF:162:LEU:HD22	1.80	0.47
50:YU:91:ASP:O	50:YU:93:LYS:N	2.46	0.47
53:YX:61:GLY:N	53:YX:75:ASP:OD1	2.39	0.47
1:QA:1286:A:N6	1:QA:1354:C:O3'	2.47	0.47
3:QC:20:SER:OG	3:QC:22:TRP:NE1	2.48	0.47
9:QI:112:LYS:HA	9:QI:119:ALA:HB2	1.97	0.47
12:QL:49:ASN:ND2	12:QL:92:ASP:OD2	2.39	0.47
24:QY:19:G:C6	35:RA:881:G:H4'	2.50	0.47
29:R4:38:LYS:HE3	40:RG:112:PRO:HG3	1.97	0.47
30:R5:3:LYS:HB3	30:R5:4:HIS:H	1.41	0.47
35:RA:1860:G:H1	35:RA:1882:C:H42	1.63	0.47
35:RA:2635:C:H5'	38:RE:77:ILE:HG23	1.97	0.47
48:RS:10:ARG:NE	48:RS:91:PRO:O	2.40	0.47
48:RS:38:GLN:HE21	48:RS:47:THR:HG21	1.80	0.47
54:RY:99:CYS:SG	54:RY:100:ALA:N	2.87	0.47
1:XA:1316:G:N2	1:XA:1318:A:H3'	2.29	0.47
26:Y1:8:SER:HB3	26:Y1:66:HIS:CE1	2.50	0.47
26:Y1:80:LEU:HG	26:Y1:81:LYS:HG3	1.97	0.47
35:YA:1130:U:O2	38:YE:149:ARG:NH2	2.42	0.47
35:YA:1826:G:H4'	37:YD:242:ARG:HH21	1.79	0.47
39:YF:157:VAL:HB	39:YF:194:MET:HB3	1.97	0.47
46:YQ:50:ALA:HB1	46:YQ:121:ALA:HB1	1.96	0.47
1:QA:1294:G:H2'	1:QA:1295:G:H8	1.79	0.47
3:QC:184:TYR:HE1	3:QC:201:TYR:HE1	1.63	0.47
29:R4:43:TYR:O	29:R4:45:GLY:N	2.47	0.47
35:RA:1217:C:OP1	50:RU:15:LYS:NZ	2.43	0.47
35:RA:2043:C:OP1	35:RA:2777:G:O2'	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2056:G:N3	35:RA:2056:G:C2'	2.77	0.47
44:RO:71:ARG:NH2	44:RO:122:LEU:O	2.48	0.47
46:RQ:29:PHE:N	46:RQ:105:GLU:OE1	2.41	0.47
1:XA:938:A:N3	1:XA:1376:U:O2'	2.44	0.47
34:Y9:22:ARG:HH12	35:YA:2741:A:H5''	1.79	0.47
35:YA:807:U:O2'	35:YA:2060:A:N1	2.41	0.47
39:YF:9:ILE:HD11	39:YF:20:LEU:HD22	1.96	0.47
39:YF:63:LYS:NZ	39:YF:75:HIS:O	2.37	0.47
6:QF:97:PHE:HB2	18:QR:32:ARG:HH21	1.80	0.47
15:QO:24:SER:HB3	15:QO:27:VAL:HG23	1.97	0.47
29:R4:25:TYR:HE2	40:RG:3:LEU:HD12	1.80	0.47
32:R7:35:ARG:NH1	35:RA:54:G:O2'	2.46	0.47
35:RA:392:C:H5''	35:RA:409:C:H5''	1.96	0.47
35:RA:535:C:O3'	50:RU:53:ARG:NH1	2.46	0.47
35:RA:2133:G:H1'	35:RA:2158:A:H61	1.79	0.47
52:RW:68:ARG:HH21	52:RW:112:GLY:HA3	1.79	0.47
1:XA:356:A:N3	1:XA:368:U:O2'	2.34	0.47
35:YA:579:G:O2'	35:YA:2019:A:OP1	2.33	0.47
35:YA:648:G:O2'	35:YA:2351:G:OP1	2.29	0.47
35:YA:1607:C:N4	35:YA:1622:G:OP2	2.33	0.47
1:QA:941:G:OP1	7:QG:32:ARG:NH1	2.48	0.47
12:QL:71:PRO:O	12:QL:102:ARG:NH1	2.47	0.47
24:QY:56:C:H5''	35:RA:897:C:H5'	1.96	0.47
35:RA:1388:G:O2'	35:RA:1525:G:O2'	2.28	0.47
35:RA:1697:G:OP2	35:RA:1698:A:O2'	2.28	0.47
36:RB:42:C:N4	40:RG:91:ARG:HH12	2.12	0.47
43:RN:133:GLN:HG2	43:RN:135:PRO:HD3	1.97	0.47
1:XA:1129:C:O2'	1:XA:1131:G:N7	2.48	0.47
8:XH:110:ALA:HB3	8:XH:121:ASP:HB3	1.97	0.47
35:YA:2126:A:N6	35:YA:2163:C:O2'	2.47	0.47
35:YA:2788:C:O2'	35:YA:2809:A:N3	2.40	0.47
44:YO:64:ARG:HH12	49:YT:70:VAL:HG21	1.80	0.47
45:YP:29:LYS:HD3	45:YP:30:THR:HG23	1.97	0.47
1:QA:1150:U:O4	1:QA:1151:A:N6	2.48	0.46
13:QM:13:LYS:HG3	13:QM:44:ARG:HD2	1.97	0.46
35:RA:674:G:H21	39:RF:74:ARG:HH12	1.62	0.46
35:RA:2377:A:H2'	35:RA:2378:A:C8	2.50	0.46
35:RA:2749:A:H5''	41:RH:4:ILE:HD11	1.97	0.46
37:RD:122:ASP:N	37:RD:122:ASP:OD1	2.42	0.46
1:XA:1463:C:OP1	49:YT:111:ARG:NH1	2.48	0.46
2:XB:101:MET:HA	2:XB:108:ILE:HG13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:2012:G:OP1	52:YW:11:ARG:NH2	2.48	0.46
39:YF:133:ASN:H	39:YF:162:LEU:HD13	1.80	0.46
3:QC:184:TYR:CE1	3:QC:201:TYR:CE1	3.03	0.46
11:QK:93:GLN:OE1	11:QK:96:ARG:NH2	2.43	0.46
13:QM:80:ARG:HH12	19:QS:69:HIS:CE1	2.34	0.46
24:QY:54:U:O4	55:RZ:183:LEU:N	2.48	0.46
35:RA:987:G:O2'	35:RA:1000:A:N3	2.43	0.46
35:RA:2008:C:H2'	35:RA:2009:G:H8	1.80	0.46
35:RA:2055:C:OP1	35:RA:2056:G:H4'	2.15	0.46
35:RA:2597:G:H5'	37:RD:243:GLY:HA3	1.97	0.46
36:RB:5:C:OP1	36:RB:61:G:O2'	2.24	0.46
38:RE:52:LEU:O	38:RE:74:PRO:HA	2.15	0.46
55:RZ:115:GLY:H	55:RZ:177:PRO:HD3	1.80	0.46
4:XD:3:ARG:HD3	4:XD:118:ARG:NE	2.30	0.46
35:YA:1077:A:H5'	35:YA:1078:U:H5''	1.96	0.46
37:YD:122:ASP:OD1	37:YD:122:ASP:N	2.48	0.46
29:R4:53:GLU:OE2	29:R4:55:ARG:NE	2.47	0.46
35:RA:1921:G:H2'	35:RA:1922:G:H8	1.80	0.46
35:RA:2219:G:OP1	37:RD:172:TYR:OH	2.27	0.46
36:RB:5:C:O2'	36:RB:27:C:O2	2.34	0.46
50:RU:102:GLU:OE2	51:RV:13:ARG:NH2	2.48	0.46
54:RY:46:LYS:HG2	54:RY:60:PHE:HD2	1.80	0.46
35:YA:195:A:H61	35:YA:198:C:H3'	1.81	0.46
35:YA:693:C:O2'	35:YA:1353:A:N3	2.43	0.46
35:YA:784:A:O4'	37:YD:227:ASN:ND2	2.48	0.46
35:YA:1858:G:O2'	35:YA:1884:A:N6	2.48	0.46
35:YA:2150:U:H2'	35:YA:2151:G:H8	1.81	0.46
1:QA:62:U:O2'	1:QA:379:C:O2	2.33	0.46
18:QR:58:LEU:HD23	18:QR:62:GLU:HG3	1.97	0.46
30:R5:19:ARG:NH1	35:RA:1264:G:OP1	2.33	0.46
35:RA:746:A:HO2'	35:RA:2611:U:HO2'	1.63	0.46
35:RA:1006:C:C2	43:RN:106:MET:HE2	2.49	0.46
44:RO:71:ARG:NH1	49:RT:74:ARG:HH12	2.14	0.46
1:XA:323:U:OP1	20:XT:26:ASN:ND2	2.46	0.46
2:XB:69:LEU:HB3	2:XB:162:ILE:HG22	1.97	0.46
2:XB:178:ARG:NH1	2:XB:196:LEU:O	2.49	0.46
35:YA:676:A:H8	35:YA:2069:G:H21	1.64	0.46
35:YA:2404:C:O3'	45:YP:77:ARG:NH2	2.48	0.46
2:QB:16:HIS:HD2	2:QB:210:SER:HA	1.81	0.46
16:QP:53:VAL:HG13	16:QP:79:VAL:HG22	1.97	0.46
32:R7:49:ARG:NH2	35:RA:128:C:O3'	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1048:A:H2	35:RA:1112:G:H21	1.63	0.46
35:RA:1454:U:O2'	35:RA:1455:G:N7	2.41	0.46
48:RS:36:TYR:HD2	48:RS:52:SER:OG	1.99	0.46
1:XA:486:U:H2'	1:XA:487:A:C8	2.49	0.46
8:XH:21:LYS:O	8:XH:65:TYR:OH	2.29	0.46
26:Y1:87:PRO:HA	26:Y1:90:ILE:HB	1.98	0.46
35:YA:1153:C:H5'	50:YU:76:TYR:HE2	1.81	0.46
1:QA:150:C:H42	1:QA:171:A:H62	1.64	0.46
10:QJ:7:LYS:HB2	10:QJ:97:GLU:HB2	1.98	0.46
11:XK:19:ALA:HA	11:XK:32:ILE:HA	1.98	0.46
35:YA:630:G:N2	35:YA:633:A:OP2	2.38	0.46
35:YA:994:C:OP1	50:YU:53:ARG:NH2	2.48	0.46
35:YA:2816:C:O2	35:YA:2883:A:O2'	2.30	0.46
37:YD:12:SER:HB2	37:YD:208:LYS:HB3	1.98	0.46
45:YP:106:LEU:HD13	45:YP:112:LEU:HD13	1.98	0.46
4:QD:8:VAL:HG11	4:QD:22:LYS:HD3	1.98	0.46
29:R4:43:TYR:O	29:R4:46:GLN:N	2.47	0.46
30:R5:4:HIS:HB3	30:R5:5:PRO:HD3	1.97	0.46
42:RI:79:ILE:HB	42:RI:142:VAL:HG12	1.97	0.46
43:RN:96:GLU:HB2	43:RN:122:VAL:HG12	1.97	0.46
55:YZ:149:SER:OG	55:YZ:150:LEU:N	2.48	0.46
2:QB:60:ASP:O	2:QB:64:ARG:NH1	2.49	0.46
16:QP:14:ASN:HA	16:QP:42:ARG:HH11	1.80	0.46
37:RD:130:ALA:HB2	37:RD:192:THR:HG22	1.97	0.46
38:RE:47:VAL:HG11	38:RE:86:PRO:HD2	1.98	0.46
41:RH:125:VAL:HG22	41:RH:131:VAL:HG23	1.97	0.46
1:XA:1291:G:H4'	9:XI:39:GLY:HA3	1.96	0.46
3:XC:131:ARG:NH1	3:XC:166:GLU:OE1	2.48	0.46
33:Y8:65:GLU:CD	33:Y8:65:GLU:N	2.72	0.46
49:YT:27:THR:HB	49:YT:48:ILE:HG13	1.96	0.46
1:QA:1412:C:H2'	1:QA:1413:A:C8	2.51	0.46
2:QB:5:ILE:HG12	2:QB:221:LEU:HB2	1.98	0.46
17:QQ:28:PRO:HA	17:QQ:35:VAL:HA	1.98	0.46
35:RA:458:G:O2'	35:RA:469:G:O6	2.23	0.46
35:RA:630:G:N2	35:RA:633:A:OP2	2.37	0.46
35:RA:1077:A:H5'	35:RA:1078:U:H5''	1.97	0.46
35:RA:2156:G:O6	35:RA:2157:G:N2	2.48	0.46
35:RA:2313:C:O4'	40:RG:40:ASN:ND2	2.49	0.46
35:RA:2795:G:H21	35:RA:2801:A:H62	1.64	0.46
1:XA:909:A:N3	1:XA:1413:A:O2'	2.42	0.46
4:XD:173:TRP:CD1	4:XD:174:LEU:HG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:685:A:OP1	35:YA:686:G:N2	2.49	0.46
35:YA:783:A:H8	35:YA:784:A:H4'	1.80	0.46
35:YA:1204:A:H1'	35:YA:1206:G:C5	2.51	0.46
36:YB:37:C:O2	48:YS:95:HIS:NE2	2.43	0.46
37:YD:35:LYS:HG2	37:YD:104:TYR:CD2	2.51	0.46
37:YD:123:ALA:HB3	37:YD:131:LEU:HG	1.98	0.46
1:QA:522:C:H41	12:QL:53:ARG:HH22	1.64	0.46
1:QA:859:A:OP2	1:QA:869:G:N2	2.41	0.46
4:QD:105:VAL:HG13	4:QD:110:PHE:HB2	1.98	0.46
11:QK:16:SER:OG	11:QK:106:LYS:NZ	2.46	0.46
13:QM:82:MET:CE	13:QM:92:HIS:CB	2.93	0.46
35:RA:587:C:OP2	45:RP:21:ARG:NH2	2.31	0.46
35:RA:2146:C:H4'	35:RA:2147:G:C8	2.51	0.46
35:RA:2851:A:O2'	47:RR:64:ARG:NH2	2.49	0.46
35:RA:2851:A:O3'	47:RR:64:ARG:NH2	2.49	0.46
37:RD:35:LYS:HD3	37:RD:104:TYR:CE1	2.50	0.46
1:XA:952:U:H2'	1:XA:953:G:H8	1.80	0.46
35:YA:2118:U:N3	35:YA:2147:G:O2'	2.45	0.46
35:YA:2659:G:N2	35:YA:2662:A:OP2	2.49	0.46
41:YH:103:LEU:HD22	41:YH:123:PHE:CD2	2.51	0.46
50:YU:92:ARG:HD3	50:YU:94:ASN:HB3	1.97	0.46
30:R5:56:LYS:HE2	30:R5:58:LEU:HD23	1.98	0.45
34:R9:30:PRO:HB3	35:RA:2527:C:H5''	1.97	0.45
35:RA:483:A:O2'	54:RY:49:VAL:O	2.27	0.45
35:RA:675:A:OP1	39:RF:63:LYS:NZ	2.41	0.45
35:RA:2564:A:OP1	35:RA:2648:C:O2'	2.32	0.45
43:RN:10:GLU:HA	43:RN:11:PRO:HD3	1.78	0.45
50:RU:66:ASN:HD21	50:RU:70:ARG:HH21	1.63	0.45
32:Y7:47:ARG:HH22	53:YX:60:ARG:CZ	2.28	0.45
36:YB:80:U:H2'	36:YB:81:G:H21	1.80	0.45
38:YE:16:ARG:HG2	38:YE:21:VAL:HG11	1.98	0.45
38:YE:52:LEU:O	38:YE:74:PRO:HA	2.16	0.45
39:YF:167:ALA:HB1	39:YF:173:VAL:HG11	1.98	0.45
1:QA:1127:G:H21	1:QA:1147:C:H41	1.63	0.45
22:QV:58:A:O2'	22:QV:60:U:OP2	2.29	0.45
35:RA:270:A:OP2	35:RA:270(Y):G:N1	2.39	0.45
35:RA:526:A:O2'	35:RA:2043:C:O2	2.29	0.45
35:RA:1652:A:N6	47:RR:11:ASN:OD1	2.42	0.45
35:RA:1859:A:N6	35:RA:1883:G:O2'	2.50	0.45
38:RE:8:LYS:O	38:RE:193:GLY:N	2.47	0.45
42:RI:3:VAL:HG12	42:RI:38:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:RP:7:ARG:HA	45:RP:8:PRO:HD2	1.87	0.45
53:RX:27:THR:HB	53:RX:80:ILE:HG12	1.97	0.45
1:XA:1095:U:P	1:XA:1108:G:H1	2.39	0.45
8:XH:49:GLU:OE2	8:XH:62:TYR:OH	2.23	0.45
11:XK:34:ASP:OD1	11:XK:38:ASN:N	2.50	0.45
19:XS:27:GLU:HG3	19:XS:29:ARG:HG2	1.98	0.45
30:Y5:12:SER:OG	35:YA:2021:C:OP1	2.32	0.45
35:YA:141:A:H8	35:YA:1408:C:H1'	1.81	0.45
35:YA:626:U:O4	45:YP:107:LYS:HE2	2.17	0.45
35:YA:870:A:OP1	46:YQ:6:ARG:NH2	2.49	0.45
35:YA:1105:U:H2'	35:YA:1106:G:H8	1.79	0.45
35:YA:2308:G:H22	35:YA:2311:A:H2	1.64	0.45
2:QB:4:GLU:HG2	2:QB:5:ILE:H	1.81	0.45
5:QE:122:GLU:O	5:QE:126:ARG:NH1	2.49	0.45
1:XA:105:G:OP1	20:XT:22:ARG:NH2	2.50	0.45
35:YA:742:G:H2'	35:YA:743:G:H8	1.81	0.45
35:YA:2580:U:H4'	38:YE:130:GLY:HA3	1.98	0.45
35:YA:2781:A:H5''	35:YA:2782:G:H5'	1.99	0.45
39:YF:113:ALA:HB2	39:YF:183:VAL:HG23	1.98	0.45
41:YH:4:ILE:HG22	41:YH:6:ARG:HG2	1.97	0.45
33:R8:59:LYS:HZ1	45:RP:50:ARG:NE	2.15	0.45
35:RA:993:G:OP1	50:RU:50:ARG:NH2	2.47	0.45
35:RA:1155:A:H5''	50:RU:55:ARG:HH11	1.81	0.45
38:RE:117:MET:HA	38:RE:122:PHE:N	2.30	0.45
27:Y2:17:SER:HB3	27:Y2:20:GLU:OE1	2.17	0.45
35:YA:1891:G:O2'	35:YA:2235:G:O2'	2.34	0.45
38:YE:9:VAL:HB	38:YE:25:VAL:HG23	1.98	0.45
1:QA:950:U:H2'	1:QA:951:G:H8	1.82	0.45
34:R9:25:VAL:HB	34:R9:34:GLN:HB2	1.99	0.45
35:RA:2073:C:HO2'	35:RA:2598:A:HO2'	1.61	0.45
51:RV:49:THR:HG23	51:RV:50:PRO:CD	2.46	0.45
55:RZ:76:LEU:HA	55:RZ:83:PRO:HA	1.97	0.45
35:YA:1210:A:H5'	35:YA:1210:A:H8	1.80	0.45
40:YG:73:ALA:HB2	40:YG:82:LEU:HD11	1.98	0.45
1:QA:545:C:O2'	1:QA:549:C:OP1	2.35	0.45
1:QA:745:C:OP1	1:QA:851:G:O2'	2.30	0.45
2:QB:219:VAL:HA	2:QB:222:ILE:HD12	1.99	0.45
35:RA:1071:G:H22	35:RA:1091:G:H8	1.65	0.45
35:RA:2392:A:H2	35:RA:2424:C:H42	1.63	0.45
36:RB:45:A:O4'	40:RG:95:ARG:NH1	2.50	0.45
46:RQ:12:GLN:HG2	46:RQ:73:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y3:10:LYS:NZ	28:Y3:15:TYR:OH	2.37	0.45
35:YA:2006:C:O2'	35:YA:2823:A:N3	2.49	0.45
37:YD:44:ASN:OD1	37:YD:44:ASN:N	2.46	0.45
42:YI:30:LEU:HB3	42:YI:36:ALA:HB3	1.97	0.45
46:YQ:39:PRO:HB3	46:YQ:99:PRO:HD3	1.99	0.45
55:YZ:47:VAL:O	55:YZ:51:ALA:N	2.42	0.45
1:QA:1159:U:O2'	1:QA:1160:G:N7	2.40	0.45
12:QL:56:ALA:O	12:QL:68:ALA:N	2.44	0.45
35:RA:39:C:O2	39:RF:46:ARG:NH2	2.50	0.45
35:RA:2850:A:OP2	35:RA:2866:U:N3	2.44	0.45
50:RU:36:ARG:HG2	50:RU:40:PHE:HE1	1.82	0.45
1:XA:1188:A:OP1	9:XI:114:TYR:OH	2.30	0.45
1:XA:1224:G:O2'	1:XA:1322:C:OP2	2.35	0.45
1:XA:1414:U:H3	1:XA:1486:G:H1	1.63	0.45
29:Y4:6:HIS:CE1	40:YG:66:GLN:HA	2.51	0.45
52:YW:73:ALA:HB3	52:YW:106:ILE:HB	1.98	0.45
1:QA:1141:C:H2'	1:QA:1142:G:H8	1.82	0.45
1:QA:1250:A:N3	1:QA:1370:G:O2'	2.44	0.45
2:QB:146:GLN:HG3	2:QB:153:ARG:HH12	1.82	0.45
33:R8:5:LYS:HG2	35:RA:242:G:C8	2.52	0.45
35:RA:30:G:O2'	35:RA:1214:A:N3	2.47	0.45
35:RA:1190:G:H2'	35:RA:1191:G:C8	2.52	0.45
37:RD:148:GLU:HB2	37:RD:151:LYS:HD2	1.99	0.45
38:RE:59:VAL:HG11	38:RE:73:GLU:HB2	1.99	0.45
1:XA:23:C:OP2	1:XA:561:U:N3	2.44	0.45
2:XB:178:ARG:HH22	8:XH:74:PRO:HB3	1.80	0.45
5:XE:110:LEU:HD13	5:XE:118:ILE:HG21	1.97	0.45
6:XF:97:PHE:HB2	18:XR:32:ARG:HE	1.82	0.45
27:Y2:18:PRO:HA	27:Y2:21:LEU:HB2	1.99	0.45
35:YA:1187:G:N2	35:YA:1188:U:O4	2.49	0.45
35:YA:1434:A:H61	35:YA:1558:A:N6	2.15	0.45
47:YR:13:HIS:NE2	47:YR:15:SER:OG	2.46	0.45
49:YT:24:PRO:HD3	49:YT:52:ILE:HD12	1.98	0.45
17:QQ:45:HIS:CD2	17:QQ:47:PRO:HG3	2.52	0.45
27:R2:65:ASN:ND2	35:RA:111:A:O3'	2.49	0.45
31:R6:6:ARG:HD2	31:R6:7:ILE:HG22	1.99	0.45
32:R7:8:ASN:HB3	32:R7:11:LYS:HB3	1.98	0.45
35:RA:627:A:H4'	35:RA:628:G:H5'	1.98	0.45
35:RA:2831:G:OP1	38:RE:58:ARG:NH1	2.50	0.45
49:RT:24:PRO:HA	49:RT:49:VAL:HG23	1.98	0.45
1:XA:157:G:H1	1:XA:164:U:H3	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:553:A:O2'	12:XL:29:GLY:O	2.32	0.45
1:XA:890:G:O2'	1:XA:906:G:O6	2.28	0.45
18:XR:45:SER:OG	18:XR:47:THR:OG1	2.29	0.45
35:YA:1652:A:N6	47:YR:11:ASN:OD1	2.46	0.45
35:YA:2315:G:OP1	40:YG:36:LYS:NZ	2.43	0.45
41:YH:41:MET:HB2	41:YH:41:MET:HE3	1.68	0.45
42:YI:130:TYR:HB3	42:YI:136:VAL:HG13	1.99	0.45
1:QA:738:C:OP1	6:QF:4:TYR:OH	2.31	0.45
1:QA:954:G:H21	1:QA:1227:A:H62	1.65	0.45
1:QA:1077:G:N2	1:QA:1080:A:OP2	2.46	0.45
4:QD:68:TYR:HE1	4:QD:103:ASN:HD21	1.57	0.45
8:QH:120:THR:OG1	8:QH:121:ASP:N	2.50	0.45
13:QM:40:ASN:HB3	13:QM:43:THR:HG23	1.99	0.45
13:QM:84:ILE:HD11	13:QM:86:CYS:CB	2.45	0.45
35:RA:2319:G:N1	35:RA:2334:G:OP2	2.45	0.45
49:RT:54:ARG:HG3	49:RT:59:THR:HG21	1.99	0.45
51:RV:49:THR:HG23	51:RV:50:PRO:HD3	1.99	0.45
1:XA:522:C:OP2	12:XL:69:TYR:OH	2.30	0.45
35:YA:2150:U:H2'	35:YA:2151:G:C8	2.52	0.45
40:YG:37:VAL:HG23	40:YG:99:MET:HE3	1.98	0.45
50:YU:83:LEU:HD12	50:YU:113:ALA:HB2	1.99	0.45
1:QA:947:G:O3'	13:QM:109:THR:OG1	2.34	0.44
25:R0:55:ARG:NH1	35:RA:2364:C:OP1	2.46	0.44
35:RA:1138:G:C2	43:RN:106:MET:HE1	2.44	0.44
38:RE:32:PRO:HB3	38:RE:90:THR:HG22	1.98	0.44
39:RF:110:LEU:HD11	39:RF:181:LEU:HB3	1.98	0.44
51:RV:28:GLU:HB2	51:RV:31:ALA:HB2	1.99	0.44
24:XY:53:G:N1	55:YZ:183:LEU:O	2.50	0.44
30:Y5:2:ALA:HA	35:YA:2015:A:H1'	1.99	0.44
35:YA:2880:C:O3'	47:YR:90:ARG:NH1	2.49	0.44
39:YF:158:THR:O	39:YF:164:ARG:NH2	2.38	0.44
2:QB:53:ARG:HH22	2:QB:199:TYR:HA	1.83	0.44
12:QL:113:ARG:HH21	12:QL:116:SER:HB2	1.82	0.44
19:QS:10:PHE:CD1	19:QS:10:PHE:O	2.70	0.44
35:RA:2723:C:OP2	38:RE:109:LYS:NZ	2.50	0.44
20:XT:74:LYS:HB3	20:XT:75:ASN:H	1.68	0.44
29:Y4:37:SER:HB3	40:YG:112:PRO:HB3	2.00	0.44
1:QA:552:U:O2'	12:QL:86:ARG:O	2.35	0.44
9:QI:19:LEU:HD22	9:QI:59:PHE:HD2	1.82	0.44
35:RA:1341:U:OP2	35:RA:1394:U:O2'	2.28	0.44
35:RA:2416:C:H5''	45:RP:64:LYS:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:RN:97:ARG:HA	43:RN:100:GLU:HB2	1.98	0.44
1:XA:247:G:OP2	17:XQ:99:SER:OG	2.36	0.44
1:XA:376:G:H5''	16:XP:5:ARG:HD2	1.99	0.44
18:XR:43:PHE:HE2	18:XR:58:LEU:HD11	1.83	0.44
31:Y6:7:ILE:HG13	31:Y6:8:LYS:H	1.81	0.44
35:YA:224:G:O6	35:YA:419:C:O2'	2.30	0.44
1:QA:362:G:N2	1:QA:365:U:OP2	2.49	0.44
44:RO:102:VAL:HG23	44:RO:121:VAL:HG23	1.98	0.44
45:RP:126:VAL:HG13	45:RP:145:PRO:HB2	1.98	0.44
51:RV:72:VAL:HG13	51:RV:85:LYS:HB2	2.00	0.44
9:XI:5:TYR:HE1	9:XI:16:ARG:HB3	1.83	0.44
35:YA:617:G:OP1	39:YF:40:GLN:NE2	2.50	0.44
44:YO:122:LEU:HD13	49:YT:72:VAL:HG11	1.99	0.44
55:YZ:76:LEU:HA	55:YZ:83:PRO:HA	2.00	0.44
1:QA:691:G:N7	11:QK:26:ASN:ND2	2.65	0.44
1:QA:950:U:H2'	1:QA:951:G:C8	2.53	0.44
1:QA:1298:C:C4	7:QG:114:ARG:HD2	2.52	0.44
3:QC:24:ALA:HB2	3:QC:32:LEU:HD12	1.99	0.44
6:QF:15:ASP:OD1	6:QF:15:ASP:N	2.48	0.44
24:QY:19:G:H3'	24:QY:20:G:H8	1.82	0.44
35:RA:33:U:O4	35:RA:446:G:O2'	2.28	0.44
35:RA:1863:G:O2'	35:RA:2411:A:O2'	2.27	0.44
35:RA:2502:G:H5''	35:RA:2503:A:H5''	1.99	0.44
55:RZ:117:LEU:HD11	55:RZ:172:ALA:HB1	1.99	0.44
1:XA:509:A:N3	1:XA:543:C:O2'	2.45	0.44
1:XA:911:U:OP2	12:XL:97:ARG:NH2	2.50	0.44
13:XM:49:THR:HB	13:XM:52:GLU:HG3	1.99	0.44
29:Y4:48:ARG:HH21	29:Y4:51:ASP:HA	1.83	0.44
35:YA:860:U:OP2	35:YA:916:G:N1	2.41	0.44
35:YA:2249:U:N3	35:YA:2253:G:OP2	2.45	0.44
37:YD:231:HIS:CD2	37:YD:249:PRO:HG3	2.53	0.44
49:YT:74:ARG:HG2	49:YT:76:PHE:CE1	2.53	0.44
1:QA:6:G:H4'	1:QA:298:A:H4'	1.99	0.44
1:QA:377:G:OP1	16:QP:3:LYS:NZ	2.38	0.44
19:QS:9:VAL:CG1	19:QS:39:THR:CB	2.94	0.44
35:RA:407:G:H2'	35:RA:408:G:H8	1.81	0.44
35:RA:1062:G:H2'	35:RA:1063:G:C8	2.52	0.44
35:RA:1942:C:OP2	35:RA:1943:U:O2'	2.32	0.44
35:RA:2880:C:O3'	47:RR:90:ARG:NH1	2.51	0.44
36:RB:111:U:H2'	36:RB:112:G:H8	1.82	0.44
37:RD:123:ALA:HB3	37:RD:131:LEU:HG	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:RG:71:THR:N	40:RG:89:GLY:O	2.48	0.44
3:XC:134:ILE:HG23	3:XC:151:VAL:HB	1.99	0.44
5:XE:11:ILE:HD12	5:XE:105:VAL:HG13	1.99	0.44
35:YA:2707:G:H5'	47:YR:68:ARG:HH21	1.83	0.44
46:YQ:36:ALA:HB2	46:YQ:103:MET:HE3	2.00	0.44
55:YZ:94:GLU:CG	55:YZ:95:PRO:CD	2.66	0.44
1:QA:165:C:H2'	1:QA:166:G:C8	2.53	0.44
1:QA:673:G:H2'	1:QA:674:G:C8	2.52	0.44
12:QL:60:LEU:HD21	12:QL:64:TYR:HB2	2.00	0.44
13:QM:91:ARG:HB2	13:QM:98:VAL:HG12	1.99	0.44
35:RA:1568:G:P	37:RD:63:ARG:HH12	2.39	0.44
39:RF:102:PRO:HB2	39:RF:105:VAL:HG23	2.00	0.44
55:RZ:19:ARG:NH1	55:RZ:84:GLU:O	2.51	0.44
1:XA:1393:U:O2'	1:XA:1501:C:O2'	2.32	0.44
8:XH:106:GLY:O	8:XH:122:ARG:NH2	2.35	0.44
20:XT:11:SER:HA	20:XT:13:LEU:HD23	1.99	0.44
35:YA:793:A:OP2	35:YA:2071:A:O2'	2.35	0.44
35:YA:1055:G:O2'	35:YA:1085:A:N1	2.43	0.44
37:YD:143:HIS:ND1	37:YD:194:GLY:O	2.49	0.44
1:QA:18:C:H5''	5:QE:127:ASN:HD21	1.83	0.44
9:QI:55:ALA:HA	9:QI:58:HIS:HD2	1.83	0.44
14:QN:24:CYS:HB3	14:QN:28:GLY:H	1.83	0.44
24:QY:25:C:H2'	24:QY:26:G:H8	1.82	0.44
35:RA:1444(A):A:O2'	35:RA:1460:A:N3	2.45	0.44
39:RF:29:ASN:HB3	39:RF:112:MET:HE1	2.00	0.44
39:RF:167:ALA:HA	39:RF:170:LEU:HD13	2.00	0.44
52:RW:69:LEU:HD13	52:RW:107:LEU:HD13	1.99	0.44
1:XA:632:A:OP1	8:XH:98:LYS:NZ	2.33	0.44
1:XA:1264:C:H2'	1:XA:1265:G:H8	1.82	0.44
16:XP:59:TRP:HA	16:XP:62:VAL:HG22	2.00	0.44
35:YA:1338:G:N7	53:YX:62:LYS:NZ	2.54	0.44
42:YI:77:LEU:HD13	42:YI:101:LEU:HD13	2.00	0.44
44:YO:104:ARG:HG3	44:YO:121:VAL:HG12	2.00	0.44
1:QA:1203:C:H5''	14:QN:3:ARG:HH21	1.83	0.44
1:QA:1309:G:N7	13:QM:99:ARG:NH2	2.66	0.44
16:QP:22:THR:HA	16:QP:33:ILE:HG12	2.00	0.44
35:RA:1992:G:OP1	35:RA:1992:G:C8	2.71	0.44
40:RG:38:VAL:HG22	40:RG:93:THR:HG22	2.00	0.44
41:RH:8:PRO:HG2	41:RH:69:ARG:CZ	2.48	0.44
44:RO:71:ARG:NH2	44:RO:122:LEU:OXT	2.39	0.44
44:RO:77:ILE:HD12	49:RT:74:ARG:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:RP:64:LYS:O	45:RP:66:GLY:N	2.51	0.44
1:XA:1318:A:H4'	19:XS:11:VAL:HG21	1.99	0.44
10:XJ:26:ALA:O	10:XJ:30:SER:OG	2.27	0.44
18:XR:74:ARG:HB3	18:XR:81:PHE:CE1	2.52	0.44
25:Y0:33:ALA:N	25:Y0:64:ASP:OD1	2.50	0.44
35:YA:219:G:N3	35:YA:234:C:O2'	2.50	0.44
44:YO:23:ARG:NH2	44:YO:28:SER:O	2.51	0.44
45:YP:126:VAL:HG23	45:YP:145:PRO:HB2	1.99	0.44
46:YQ:8:LYS:HE3	46:YQ:9:TYR:HE1	1.83	0.44
2:QB:200:ILE:HG22	2:QB:202:PRO:HD3	2.00	0.43
9:QI:33:PHE:HE2	9:QI:47:LEU:HD11	1.83	0.43
33:R8:54:GLU:O	33:R8:58:ILE:HG12	2.18	0.43
35:RA:2151:G:H2'	35:RA:2152:G:H8	1.83	0.43
37:RD:67:PHE:HB3	37:RD:153:ALA:HB3	2.00	0.43
1:XA:1286:A:H2'	1:XA:1287:A:H4'	2.00	0.43
1:XA:1404:C:H2'	1:XA:1405:G:C8	2.53	0.43
4:XD:163:GLU:HA	4:XD:166:LYS:HE3	2.00	0.43
14:XN:24:CYS:HB3	14:XN:29:ARG:H	1.83	0.43
20:XT:73:HIS:HB3	20:XT:74:LYS:H	1.45	0.43
29:Y4:67:TYR:HB2	29:Y4:68:ARG:H	1.66	0.43
33:Y8:61:LEU:HD23	33:Y8:61:LEU:HA	1.87	0.43
35:YA:392:C:H5''	35:YA:409:C:H5''	1.99	0.43
35:YA:956:G:N2	35:YA:960:A:OP2	2.51	0.43
35:YA:1063:G:H22	35:YA:1076:C:H1'	1.83	0.43
35:YA:2119:A:N1	35:YA:2170:A:N6	2.65	0.43
35:YA:2343:C:O2'	35:YA:2373:G:O2'	2.25	0.43
35:YA:2845:G:H2'	35:YA:2846:G:C8	2.53	0.43
45:YP:90:ARG:HH22	45:YP:105:LEU:HD11	1.83	0.43
48:YS:29:PHE:HB3	48:YS:36:TYR:HD2	1.83	0.43
10:QJ:76:ASN:OD1	10:QJ:76:ASN:N	2.51	0.43
15:QO:87:ILE:HG22	15:QO:88:ARG:H	1.83	0.43
22:QV:63:G:H4'	25:R0:11:ARG:HH12	1.83	0.43
35:RA:1394:U:O2	53:RX:16:LYS:NZ	2.44	0.43
38:RE:54:GLN:HG3	38:RE:55:ASN:H	1.83	0.43
2:XB:95:GLN:HB3	2:XB:96:ARG:H	1.69	0.43
8:XH:19:VAL:HG13	8:XH:21:LYS:HG3	2.00	0.43
9:XI:3:GLN:OE1	9:XI:20:ARG:NE	2.39	0.43
33:Y8:61:LEU:HD13	35:YA:593:G:H4'	1.99	0.43
35:YA:1407:C:H42	35:YA:1595:G:H1	1.66	0.43
35:YA:2298:A:H62	35:YA:2318:G:H8	1.65	0.43
1:QA:258:G:OP1	20:QT:86:ARG:NH1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:QM:49:THR:OG1	13:QM:50:GLU:N	2.51	0.43
35:RA:229:A:H4'	35:RA:230:U:H5'	2.00	0.43
35:RA:861:A:N3	36:RB:79:C:O2'	2.50	0.43
42:RI:69:LYS:HG3	42:RI:136:VAL:HB	1.99	0.43
44:RO:69:ILE:HD12	44:RO:69:ILE:N	2.32	0.43
19:XS:40:ILE:HD11	19:XS:62:ILE:HG12	2.00	0.43
32:Y7:5:TRP:O	35:YA:1612:C:O2'	2.35	0.43
37:YD:254:THR:OG1	37:YD:254:THR:O	2.35	0.43
55:YZ:137:ILE:HG23	55:YZ:156:LYS:HB3	1.99	0.43
1:QA:790:A:OP1	22:QV:38:A:O2'	2.30	0.43
1:QA:1223:C:P	19:QS:78:ARG:HH12	2.41	0.43
13:QM:84:ILE:O	19:QS:74:PHE:CE1	2.72	0.43
33:R8:59:LYS:HG2	45:RP:49:ARG:HE	1.84	0.43
35:RA:1041:C:H2'	35:RA:1042:G:H8	1.84	0.43
35:RA:2006:C:O2'	35:RA:2823:A:N3	2.50	0.43
1:XA:1408:A:N1	57:XA:1670:PAR:O61	2.50	0.43
27:Y2:70:GLN:HG3	27:Y2:71:ASN:H	1.83	0.43
33:Y8:29:LYS:HG2	33:Y8:30:ARG:H	1.83	0.43
35:YA:1005:C:O2	35:YA:1138:G:N2	2.41	0.43
35:YA:2630:G:H2'	35:YA:2631:G:C8	2.53	0.43
48:YS:27:SER:HA	48:YS:88:ASP:HB3	2.00	0.43
1:QA:1002:G:H2'	1:QA:1003:G:C8	2.53	0.43
1:QA:1125:U:O4	10:QJ:5:ARG:NE	2.51	0.43
1:QA:1229:A:OP2	13:QM:114:ARG:NH1	2.50	0.43
19:QS:18:LYS:HD2	19:QS:29:ARG:HH22	1.84	0.43
35:RA:500:G:N1	35:RA:503:A:OP2	2.50	0.43
36:RB:24:G:O6	36:RB:56:G:O2'	2.32	0.43
54:RY:99:CYS:SG	54:RY:101:LYS:N	2.91	0.43
20:XT:75:ASN:N	20:XT:75:ASN:OD1	2.49	0.43
29:Y4:67:TYR:HB2	29:Y4:68:ARG:HD3	2.00	0.43
35:YA:83:G:N2	35:YA:103:A:OP2	2.32	0.43
35:YA:764:A:N3	37:YD:213:ARG:NH1	2.66	0.43
35:YA:1290:C:O2'	35:YA:1536:A:OP2	2.28	0.43
40:YG:43:LEU:HD12	40:YG:90:LEU:HD13	1.99	0.43
41:YH:149:ARG:CZ	41:YH:154:PRO:HG2	2.48	0.43
1:QA:1502:A:H2	1:QA:1505:G:H1	1.66	0.43
10:QJ:27:ALA:HA	10:QJ:30:SER:HB3	1.99	0.43
35:RA:1278:A:H4'	47:RR:34:ILE:HD11	2.00	0.43
1:XA:261:U:OP2	20:XT:79:ARG:NH2	2.52	0.43
13:XM:86:CYS:SG	13:XM:87:TYR:N	2.91	0.43
32:Y7:47:ARG:HH12	53:YX:60:ARG:HH22	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:YD:33:LEU:HD21	37:YD:102:LYS:HD2	2.00	0.43
41:YH:103:LEU:HD23	41:YH:115:VAL:HB	2.01	0.43
44:YO:8:LEU:HD13	44:YO:82:ASN:HB3	2.00	0.43
47:YR:3:HIS:O	47:YR:5:LYS:N	2.52	0.43
52:YW:6:ILE:HG12	52:YW:104:THR:HG23	1.99	0.43
1:QA:599:C:O2'	8:QH:129:VAL:O	2.27	0.43
2:QB:187:LEU:HA	2:QB:201:ILE:HB	2.01	0.43
4:QD:88:VAL:HG13	5:QE:97:GLY:HA3	1.99	0.43
5:QE:28:PHE:CD2	5:QE:51:VAL:HG13	2.54	0.43
6:QF:42:GLU:OE2	6:QF:59:TYR:OH	2.27	0.43
10:QJ:51:ARG:NE	10:QJ:60:ARG:O	2.49	0.43
13:QM:37:THR:HG23	13:QM:39:ILE:HG12	2.00	0.43
35:RA:2122:U:H2'	35:RA:2123:G:H8	1.83	0.43
51:RV:40:LEU:HD23	51:RV:47:VAL:HA	2.00	0.43
1:XA:522:C:H41	12:XL:53:ARG:HH22	1.66	0.43
1:XA:1437:C:H2'	1:XA:1438:G:H8	1.84	0.43
2:XB:51:LEU:HD23	2:XB:201:ILE:HD12	2.01	0.43
4:XD:111:ALA:HB1	4:XD:116:GLN:HB3	2.01	0.43
35:YA:960:A:H61	46:YQ:82:ARG:NH2	2.15	0.43
35:YA:2445:G:OP1	39:YF:74:ARG:NH1	2.45	0.43
35:YA:2729:G:H1'	38:YE:187:ALA:HB2	2.00	0.43
44:YO:19:ILE:HG22	44:YO:43:VAL:HA	2.00	0.43
47:YR:59:ASP:N	47:YR:59:ASP:OD1	2.51	0.43
1:QA:1151:A:H2'	1:QA:1152:A:C8	2.54	0.43
37:RD:35:LYS:HB2	37:RD:63:ARG:HA	2.00	0.43
46:RQ:36:ALA:HB2	46:RQ:103:MET:HE2	2.01	0.43
16:XP:18:ARG:NH1	16:XP:32:TYR:OH	2.52	0.43
31:Y6:6:ARG:HG3	31:Y6:7:ILE:H	1.84	0.43
35:YA:1667:G:O2'	35:YA:1991:U:O4	2.33	0.43
35:YA:2572:A:OP1	35:YA:2574:G:O2'	2.36	0.43
35:YA:2619:C:H5''	38:YE:152:LYS:HD3	2.01	0.43
41:YH:6:ARG:HB2	41:YH:65:HIS:CG	2.54	0.43
1:QA:35:G:O2'	12:QL:118:SER:O	2.23	0.43
1:QA:628:G:H2'	1:QA:629:G:C8	2.54	0.43
15:QO:76:GLU:HA	15:QO:79:ARG:HH21	1.84	0.43
24:QY:6:U:H2'	24:QY:7:A:H8	1.83	0.43
24:QY:58:A:C6	55:RZ:183:LEU:HD13	2.54	0.43
35:RA:117:G:OP2	35:RA:119:A:O2'	2.28	0.43
1:XA:35:G:N2	12:XL:118:SER:OG	2.37	0.43
1:XA:977:A:O2'	1:XA:979:C:OP2	2.31	0.43
1:XA:1376:U:H2'	1:XA:1377:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:XH:12:ARG:HD3	8:XH:26:VAL:HG22	1.99	0.43
22:XV:15:G:H21	22:XV:21:A:H1'	1.84	0.43
35:YA:1138:G:O2'	43:YN:102:ALA:O	2.34	0.43
35:YA:1656:C:P	38:YE:136:ARG:HE	2.41	0.43
37:YD:67:PHE:HB3	37:YD:153:ALA:HB3	2.00	0.43
37:YD:245:PRO:HA	37:YD:246:PRO:HD3	1.93	0.43
39:YF:156:LEU:HD21	39:YF:163:VAL:HG12	2.01	0.43
40:YG:135:LEU:HD13	40:YG:140:ILE:HD11	2.01	0.43
43:YN:47:ALA:HB2	43:YN:112:LEU:HD11	1.99	0.43
48:YS:110:LEU:HB2	48:YS:112:PHE:CE2	2.54	0.43
55:YZ:54:HIS:HB3	55:YZ:101:PRO:HD3	2.00	0.43
1:QA:1286:A:N3	21:QU:18:TYR:OH	2.52	0.43
3:QC:184:TYR:CD1	3:QC:201:TYR:CE1	3.06	0.43
12:QL:70:ILE:HG12	12:QL:77:LEU:HD12	2.01	0.43
19:QS:31:ILE:HB	19:QS:49:ILE:HD13	2.00	0.43
24:QY:6:U:H2'	24:QY:7:A:C8	2.53	0.43
24:QY:76:A:OP2	35:RA:2602:A:C6	2.72	0.43
33:R8:13:ARG:NH1	45:RP:61:ARG:O	2.51	0.43
33:R8:61:LEU:HD13	35:RA:593:G:H4'	2.01	0.43
37:RD:71:ASP:HB2	37:RD:103:ARG:HH12	1.84	0.43
46:RQ:21:THR:HB	46:RQ:22:LYS:H	1.58	0.43
51:RV:62:LEU:HD21	51:RV:95:LEU:HB2	2.00	0.43
35:YA:30:G:O2'	35:YA:1214:A:N3	2.42	0.43
35:YA:1638:C:OP1	35:YA:2710:C:O2'	2.30	0.43
39:YF:39:TRP:NE1	39:YF:99:TYR:O	2.45	0.43
1:QA:1314:C:N4	19:QS:2:PRO:O	2.50	0.42
27:R2:9:GLN:HE22	27:R2:56:GLN:HG2	1.83	0.42
31:R6:24:GLU:OE2	35:RA:2286:A:N6	2.51	0.42
35:RA:511:U:O4	35:RA:512:G:N1	2.51	0.42
37:RD:145:VAL:HB	37:RD:155:LEU:HB2	2.00	0.42
40:RG:101:ILE:HG22	40:RG:105:LYS:HE2	2.00	0.42
42:RI:131:LYS:HA	42:RI:132:PRO:HD3	1.91	0.42
44:RO:104:ARG:NH2	49:RT:43:GLN:OE1	2.30	0.42
45:RP:122:PRO:HB3	45:RP:141:ALA:HB1	2.01	0.42
55:RZ:4:ARG:HD3	55:RZ:60:GLU:OE1	2.19	0.42
55:RZ:74:VAL:HG12	55:RZ:86:VAL:HG23	2.00	0.42
1:XA:1130:A:O5'	9:XI:20:ARG:NH2	2.52	0.42
12:XL:77:LEU:HD21	12:XL:107:ALA:HB2	2.01	0.42
26:Y1:19:GLN:HG3	35:YA:2080:G:H5'	1.99	0.42
35:YA:554:U:H2'	35:YA:556:G:C8	2.54	0.42
1:QA:184:G:H2'	1:QA:185:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:674:G:H2'	1:QA:675:A:C8	2.53	0.42
1:QA:985:C:H2'	1:QA:986:A:H8	1.84	0.42
1:QA:1095:U:P	1:QA:1108:G:H1	2.42	0.42
1:QA:1129:C:N4	1:QA:1133:G:O6	2.48	0.42
9:QI:92:TYR:HB3	9:QI:96:LEU:HD23	2.00	0.42
10:QJ:55:LYS:HB3	10:QJ:55:LYS:HE3	1.69	0.42
18:QR:34:TYR:HD1	18:QR:35:ARG:HG3	1.83	0.42
35:RA:224:G:OP2	35:RA:408:G:N2	2.48	0.42
35:RA:581:C:H2'	35:RA:582:G:C8	2.53	0.42
1:XA:1405:G:OP2	57:XA:1670:PAR:O34	2.29	0.42
2:XB:220:ASP:HA	2:XB:223:ILE:HG22	2.01	0.42
35:YA:639:U:H3	35:YA:649:G:H1	1.67	0.42
35:YA:1779:U:OP2	35:YA:1784:A:N6	2.38	0.42
37:YD:36:PRO:HA	37:YD:62:TYR:O	2.19	0.42
37:YD:122:ASP:CG	37:YD:123:ALA:H	2.26	0.42
43:YN:116:LEU:HD23	43:YN:116:LEU:HA	1.88	0.42
47:YR:79:LEU:HA	47:YR:83:ILE:HD12	2.00	0.42
49:YT:60:THR:HG22	49:YT:77:PRO:HA	2.00	0.42
55:YZ:48:PHE:O	55:YZ:52:SER:N	2.50	0.42
1:QA:738:C:OP1	6:QF:2:ARG:NH1	2.53	0.42
1:QA:1151:A:H2'	1:QA:1152:A:H8	1.84	0.42
2:QB:95:GLN:HG3	2:QB:96:ARG:H	1.84	0.42
13:QM:57:ARG:NH2	29:R4:32:TYR:OH	2.47	0.42
25:R0:69:PHE:HE2	25:R0:79:VAL:CG2	2.26	0.42
35:RA:2210:G:OP1	37:RD:68:LYS:NZ	2.50	0.42
35:RA:2745:C:O2	41:RH:139:GLN:NE2	2.48	0.42
37:RD:35:LYS:HD3	37:RD:104:TYR:CZ	2.53	0.42
37:RD:69:ARG:HH11	37:RD:105:ILE:HG12	1.84	0.42
47:RR:83:ILE:HG23	47:RR:86:ARG:HH21	1.85	0.42
1:XA:619:U:N3	4:XD:134:ASP:OD1	2.40	0.42
7:XG:16:LEU:HD11	9:XI:45:ALA:HB2	2.02	0.42
12:XL:38:THR:HG23	12:XL:39:VAL:HG23	2.00	0.42
12:XL:124:LYS:HD2	12:XL:125:PRO:HD2	2.00	0.42
35:YA:582:G:OP1	50:YU:14:HIS:ND1	2.50	0.42
35:YA:747:U:H5''	35:YA:748:G:H5'	2.00	0.42
35:YA:2293:C:OP1	48:YS:89:ARG:NH2	2.53	0.42
35:YA:2308:G:H1	35:YA:2311:A:H2	1.67	0.42
1:QA:902:G:H2'	1:QA:903:G:H8	1.85	0.42
1:QA:1010:G:H2'	1:QA:1011:G:H8	1.85	0.42
35:RA:563:G:H21	50:RU:37:GLU:CD	2.27	0.42
35:RA:1067:A:H5''	35:RA:1068:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2788:C:O2'	35:RA:2809:A:N3	2.49	0.42
36:RB:80:U:H2'	36:RB:81:G:H21	1.84	0.42
1:XA:542:G:OP1	4:XD:10:ARG:NH2	2.46	0.42
1:XA:812:C:H4'	1:XA:813:U:H5'	2.01	0.42
30:Y5:55:ARG:HD2	30:Y5:55:ARG:HA	1.76	0.42
35:YA:742:G:H2'	35:YA:743:G:C8	2.54	0.42
35:YA:1394:U:O2	53:YX:16:LYS:NZ	2.47	0.42
38:YE:134:ILE:HA	38:YE:137:HIS:CD2	2.54	0.42
40:YG:107:LEU:HD23	40:YG:111:LEU:HD12	2.01	0.42
1:QA:67:C:H2'	1:QA:68:G:C8	2.55	0.42
1:QA:272:C:H2'	1:QA:273:A:H8	1.84	0.42
1:QA:429:U:H5'	4:QD:9:CYS:HB2	2.01	0.42
1:QA:444:C:H2'	1:QA:445:G:C8	2.52	0.42
1:QA:765:G:N2	1:QA:813:U:OP2	2.40	0.42
3:QC:70:VAL:HG12	3:QC:72:LYS:H	1.83	0.42
4:QD:31:CYS:SG	4:QD:32:ALA:N	2.92	0.42
13:QM:82:MET:HE3	13:QM:92:HIS:HB3	2.01	0.42
26:R1:47:GLN:NE2	35:RA:2229:C:O2	2.53	0.42
35:RA:1262:A:OP1	52:RW:99:ARG:NH1	2.48	0.42
35:RA:1654:A:OP1	47:RR:1:MET:N	2.47	0.42
41:RH:107:VAL:HB	41:RH:153:LYS:HZ2	1.84	0.42
44:RO:76:ALA:HB3	49:RT:75:ILE:HD12	2.01	0.42
1:XA:395:C:N4	1:XA:396:G:O6	2.52	0.42
1:XA:940:C:H1'	1:XA:1374:A:H62	1.85	0.42
10:XJ:34:VAL:HG23	10:XJ:74:ILE:HG22	2.02	0.42
35:YA:255:A:O2'	35:YA:384:U:OP1	2.34	0.42
35:YA:639:U:H2'	35:YA:640:C:C6	2.55	0.42
35:YA:2405:G:H5'	45:YP:75:ILE:HD13	2.01	0.42
39:YF:127:GLU:OE1	39:YF:196:LEU:HB2	2.20	0.42
43:YN:130:HIS:HB3	43:YN:134:ARG:NH2	2.34	0.42
45:YP:98:GLU:HA	45:YP:101:VAL:HG22	2.02	0.42
46:YQ:111:GLU:OE2	46:YQ:133:ARG:NH2	2.52	0.42
48:YS:83:LYS:HG3	48:YS:109:GLY:HA3	2.02	0.42
53:YX:53:LYS:H	53:YX:82:GLN:HB3	1.83	0.42
1:QA:254:G:H2'	1:QA:255:G:H8	1.84	0.42
4:QD:31:CYS:SG	4:QD:33:MET:N	2.92	0.42
21:QU:10:ARG:HA	21:QU:13:ILE:HD12	2.01	0.42
35:RA:807:U:O2	39:RF:74:ARG:NH2	2.51	0.42
35:RA:2102:U:H3	35:RA:2187:G:H1	1.68	0.42
37:RD:3:VAL:HG23	37:RD:19:ALA:HA	2.00	0.42
53:RX:21:PHE:CE2	53:RX:92:LEU:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:XC:189:ALA:HB3	3:XC:196:LEU:HB2	2.01	0.42
8:XH:86:ILE:HG22	8:XH:93:VAL:HG21	2.01	0.42
35:YA:1045:A:O2'	35:YA:1046:A:OP2	2.34	0.42
35:YA:1105:U:H2'	35:YA:1106:G:C8	2.53	0.42
38:YE:144:ARG:HB3	38:YE:145:LYS:H	1.65	0.42
39:YF:24:LEU:HD23	39:YF:115:ALA:HA	2.00	0.42
44:YO:8:LEU:HB2	44:YO:19:ILE:HG13	2.01	0.42
50:YU:92:ARG:C	50:YU:94:ASN:H	2.27	0.42
1:QA:701:C:O2	1:QA:703:G:N1	2.53	0.42
5:QE:12:LEU:HB3	5:QE:31:LEU:HB3	2.01	0.42
12:QL:27:LEU:O	12:QL:33:ARG:NH2	2.52	0.42
17:QQ:4:LYS:HE3	17:QQ:6:LEU:HD21	2.02	0.42
26:R1:50:ARG:NH2	35:RA:2199:A:OP1	2.53	0.42
35:RA:574:C:N3	38:RE:145:LYS:NZ	2.68	0.42
35:RA:1666:G:OP1	44:RO:66:LYS:HD3	2.19	0.42
35:RA:2133:G:H2'	35:RA:2157:G:N2	2.34	0.42
35:RA:2306:C:H3'	35:RA:2307:G:H5''	2.02	0.42
40:RG:122:PRO:HB3	40:RG:180:PHE:HD2	1.84	0.42
43:RN:48:MET:HE2	43:RN:48:MET:HB2	1.88	0.42
50:RU:66:ASN:OD1	50:RU:70:ARG:NE	2.50	0.42
52:RW:88:ARG:NH1	52:RW:94:ASP:OD2	2.52	0.42
13:XM:16:ASP:HB3	13:XM:41:PRO:HB3	2.01	0.42
17:XQ:45:HIS:CD2	17:XQ:47:PRO:HG3	2.55	0.42
55:YZ:80:ARG:HH11	55:YZ:82:ARG:HH12	1.68	0.42
1:QA:464:G:N2	1:QA:467:G:N7	2.68	0.42
2:QB:24:TRP:CD1	2:QB:24:TRP:H	2.37	0.42
2:QB:93:VAL:HG11	2:QB:97:TRP:HD1	1.84	0.42
6:QF:45:LEU:HD12	6:QF:59:TYR:HD1	1.85	0.42
35:RA:307:G:N1	35:RA:310:A:OP2	2.49	0.42
35:RA:363:G:H2'	35:RA:363(A):A:C8	2.54	0.42
35:RA:1005:C:O2'	43:RN:28:THR:HG21	2.20	0.42
35:RA:1417:C:O2'	35:RA:1587:A:N3	2.48	0.42
35:RA:1567:A:H3'	37:RD:86:PRO:HG3	2.01	0.42
39:RF:167:ALA:HB1	39:RF:173:VAL:HG11	2.02	0.42
51:RV:2:PHE:HB2	51:RV:3:ALA:H	1.72	0.42
55:RZ:89:PHE:HE2	55:RZ:96:VAL:HG11	1.85	0.42
1:XA:79:G:H2'	1:XA:80:G:C8	2.54	0.42
1:XA:781:A:O2'	1:XA:1522:U:O2	2.32	0.42
1:XA:1517:G:N3	35:YA:1919:A:O2'	2.47	0.42
6:XF:5:GLU:HB3	6:XF:62:TRP:HE1	1.85	0.42
37:YD:25:THR:HG22	37:YD:82:ILE:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:YE:134:ILE:HA	38:YE:137:HIS:HD2	1.85	0.42
40:YG:126:ASP:OD2	40:YG:130:ASN:ND2	2.50	0.42
49:YT:3:ARG:HG3	49:YT:7:ILE:HG12	2.02	0.42
1:QA:1299:A:C8	1:QA:1301:U:H1'	2.54	0.42
25:R0:26:TYR:HA	25:R0:69:PHE:HE1	1.85	0.42
53:RX:53:LYS:HB2	53:RX:82:GLN:HB3	2.02	0.42
13:XM:47:ASP:OD1	13:XM:47:ASP:N	2.53	0.42
20:XT:29:LYS:O	20:XT:33:ILE:HG12	2.20	0.42
31:Y6:44:ARG:HB2	31:Y6:45:LYS:H	1.67	0.42
33:Y8:4:MET:HE2	35:YA:592:G:N3	2.35	0.42
40:YG:86:MET:HA	40:YG:87:PRO:HD2	1.97	0.42
40:YG:101:ILE:HG22	40:YG:105:LYS:HE2	2.01	0.42
1:QA:730:G:C5	1:QA:731:G:H1'	2.55	0.42
1:QA:909:A:N3	1:QA:1413:A:O2'	2.45	0.42
13:QM:14:ARG:H	13:QM:44:ARG:HA	1.84	0.42
18:QR:35:ARG:HH11	18:QR:35:ARG:HD2	1.70	0.42
35:RA:1902:C:H5'	37:RD:246:PRO:HD3	2.02	0.42
1:XA:1279:A:O2'	1:XA:1281:U:OP2	2.37	0.42
35:YA:297:C:H5''	54:YY:87:LYS:HG3	2.02	0.42
35:YA:363:G:H2'	35:YA:363(A):A:H8	1.85	0.42
35:YA:500:G:N1	35:YA:503:A:OP2	2.50	0.42
35:YA:1817:G:OP1	37:YD:88:ARG:NH2	2.53	0.42
35:YA:2233:U:H2'	35:YA:2234:G:C8	2.55	0.42
36:YB:8:U:H3	36:YB:112:G:H1	1.68	0.42
37:YD:145:VAL:HB	37:YD:155:LEU:HB2	2.01	0.42
45:YP:91:PHE:CE2	45:YP:95:VAL:HG22	2.55	0.42
1:QA:1004:A:P	1:QA:1025:U:H3	2.43	0.41
3:QC:37:GLN:NE2	14:QN:52:GLN:OE1	2.38	0.41
5:QE:33:VAL:HG13	5:QE:112:LEU:HD12	2.01	0.41
10:QJ:61:GLU:OE2	14:QN:58:LYS:HE2	2.20	0.41
27:R2:50:ILE:H	27:R2:50:ILE:HG12	1.70	0.41
35:RA:2618:G:H21	38:RE:150:VAL:HG21	1.85	0.41
38:RE:37:ARG:HB2	38:RE:46:ALA:H	1.85	0.41
50:RU:17:ILE:HG23	50:RU:39:LEU:HD12	2.02	0.41
1:XA:1238:A:H62	1:XA:1301:U:H3	1.68	0.41
2:XB:166:ASP:HB3	2:XB:169:LYS:HB3	2.02	0.41
12:XL:105:TYR:O	12:XL:107:ALA:N	2.53	0.41
35:YA:1827:C:O2'	35:YA:1970:A:N3	2.46	0.41
35:YA:2503:A:O2'	35:YA:2505:G:OP2	2.29	0.41
37:YD:31:LYS:HD3	37:YD:94:LEU:HD11	2.02	0.41
41:YH:103:LEU:CD2	41:YH:123:PHE:HE2	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:QB:102:LEU:HB3	2:QB:180:LEU:HD12	2.02	0.41
13:QM:32:GLU:O	13:QM:36:LYS:HG2	2.20	0.41
31:R6:30:THR:HG23	31:R6:31:PRO:HD3	2.02	0.41
35:RA:1043:C:N3	35:RA:1112:G:N2	2.47	0.41
35:RA:1062:G:H2'	35:RA:1063:G:H8	1.85	0.41
35:RA:2777:G:H5''	35:RA:2778:A:H3'	2.01	0.41
35:RA:2847:U:OP1	49:RT:98:LYS:NZ	2.34	0.41
41:RH:126:PRO:HG2	41:RH:130:ARG:HE	1.85	0.41
46:RQ:56:ARG:HA	46:RQ:56:ARG:HD2	1.89	0.41
50:RU:92:ARG:HD2	51:RV:11:GLN:HB2	2.02	0.41
52:RW:45:TYR:CZ	52:RW:49:LYS:HD2	2.54	0.41
1:XA:7:G:O2'	5:XE:120:THR:O	2.38	0.41
1:XA:824:C:H2'	1:XA:825:G:H8	1.82	0.41
29:Y4:18:CYS:SG	29:Y4:19:GLY:N	2.93	0.41
33:Y8:54:GLU:O	33:Y8:58:ILE:HG12	2.19	0.41
35:YA:363(A):A:H2'	35:YA:363(B):G:C8	2.53	0.41
35:YA:2468:G:O2'	35:YA:2481:G:N2	2.54	0.41
1:QA:769:G:OP2	1:QA:803:G:O2'	2.36	0.41
1:QA:1355:G:H2'	1:QA:1356:G:H8	1.85	0.41
10:QJ:25:GLU:CD	10:QJ:28:ARG:HH21	2.27	0.41
24:QY:20:G:OP2	24:QY:60:C:N4	2.54	0.41
25:R0:26:TYR:HA	25:R0:69:PHE:CE1	2.56	0.41
32:R7:49:ARG:HH12	35:RA:1600:C:H4'	1.85	0.41
35:RA:1342:A:OP1	53:RX:36:LYS:NZ	2.35	0.41
44:RO:78:ARG:HH12	49:RT:75:ILE:HD11	1.85	0.41
54:RY:46:LYS:HG2	54:RY:60:PHE:CD2	2.56	0.41
55:RZ:75:ASN:HB2	55:RZ:85:HIS:HB3	2.02	0.41
55:RZ:91:LEU:HD23	55:RZ:130:PRO:HG3	2.02	0.41
1:XA:445:G:H2'	1:XA:446:G:C8	2.55	0.41
3:XC:23:TYR:HE1	10:XJ:67:THR:HG23	1.84	0.41
19:XS:63:THR:HG22	19:XS:66:MET:HE3	2.02	0.41
35:YA:1266:G:O2'	35:YA:2012:G:O6	2.32	0.41
52:YW:45:TYR:CZ	52:YW:49:LYS:HD2	2.55	0.41
53:YX:26:TYR:HD2	53:YX:92:LEU:HD22	1.85	0.41
1:QA:581:G:OP1	15:QO:65:ARG:NH1	2.53	0.41
1:QA:855:G:OP2	1:QA:871:U:N3	2.44	0.41
1:QA:1172:C:H2'	1:QA:1173:G:H8	1.85	0.41
4:QD:57:ARG:HB3	4:QD:206:PHE:HB2	2.02	0.41
4:QD:116:GLN:HE21	4:QD:157:LEU:HD11	1.85	0.41
10:QJ:79:ARG:HD3	10:QJ:79:ARG:HA	1.91	0.41
19:QS:63:THR:OG1	19:QS:64:GLU:OE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1254:A:H5''	35:RA:1255:U:H5''	2.02	0.41
35:RA:1649:G:O2'	47:RR:107:ASP:OD2	2.23	0.41
35:RA:1710:C:O2'	35:RA:2858:C:N3	2.53	0.41
38:RE:30:PRO:HA	38:RE:92:THR:HA	2.02	0.41
39:RF:11:VAL:HG22	39:RF:125:LEU:HB2	2.02	0.41
41:RH:85:LYS:HB3	41:RH:86:GLU:H	1.64	0.41
47:RR:57:ARG:HE	47:RR:62:ALA:HB2	1.85	0.41
54:RY:10:GLY:H	54:RY:27:VAL:HG23	1.85	0.41
1:XA:152:A:H62	1:XA:169:C:N4	2.16	0.41
1:XA:243:A:H4'	1:XA:244:U:H3'	2.01	0.41
1:XA:411:A:C4	1:XA:413:G:H1'	2.55	0.41
1:XA:562:C:H1'	12:XL:15:ARG:HD2	2.02	0.41
1:XA:711:G:H2'	1:XA:712:A:C8	2.55	0.41
1:XA:1130:A:N6	1:XA:1131:G:O6	2.53	0.41
26:Y1:97:LEU:HD13	35:YA:270(T):G:H5''	2.02	0.41
35:YA:729:G:H5'	35:YA:730:C:H5''	2.01	0.41
35:YA:1056:G:H4'	35:YA:1086:A:H8	1.85	0.41
2:QB:115:LEU:HD22	2:QB:153:ARG:HD3	2.02	0.41
9:QL:33:PHE:CD1	9:QL:37:PHE:HD2	2.37	0.41
12:QL:85:ILE:HG23	12:QL:98:TYR:HB3	2.02	0.41
13:QM:84:ILE:CG1	13:QM:86:CYS:HB2	2.50	0.41
19:QS:63:THR:OG1	19:QS:64:GLU:N	2.52	0.41
21:QU:6:ARG:HE	21:QU:15:ARG:NH1	2.18	0.41
25:R0:38:VAL:HG21	25:R0:45:PHE:CD2	2.55	0.41
35:RA:195:A:H61	35:RA:198:C:H3'	1.85	0.41
35:RA:2579:C:O2'	38:RE:131:ALA:O	2.34	0.41
35:RA:2630:G:H2'	35:RA:2631:G:H8	1.86	0.41
35:RA:2849:U:O4	49:RT:23:ARG:NH2	2.38	0.41
40:RG:12:TYR:HA	40:RG:16:ARG:HD3	2.03	0.41
45:RP:121:LYS:O	45:RP:123:LEU:N	2.54	0.41
53:RX:12:VAL:HG12	53:RX:29:TRP:CD2	2.56	0.41
1:XA:861:G:HO2'	1:XA:874:G:HO2'	1.63	0.41
1:XA:861:G:O2'	1:XA:874:G:O2'	2.38	0.41
33:Y8:16:ILE:HD12	33:Y8:63:PRO:HB2	2.02	0.41
35:YA:566:U:P	51:YV:80:GLN:HE21	2.43	0.41
35:YA:1657:C:H4'	38:YE:133:LYS:HB3	2.03	0.41
39:YF:185:ASP:HA	39:YF:188:ARG:HD3	2.03	0.41
3:QC:29:TYR:OH	14:QN:54:PRO:O	2.37	0.41
4:QD:57:ARG:HH12	5:QE:107:ARG:NH1	2.19	0.41
4:QD:140:VAL:HG11	4:QD:146:ILE:HD11	2.03	0.41
13:QM:106:ASN:OD1	13:QM:106:ASN:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R2:41:ILE:HD11	27:R2:44:LEU:HD22	2.03	0.41
35:RA:629:G:N3	35:RA:639:U:O2'	2.52	0.41
41:RH:103:LEU:HD22	41:RH:123:PHE:HD2	1.85	0.41
45:RP:99:LEU:HA	45:RP:102:ARG:NE	2.35	0.41
46:RQ:24:GLY:HA2	46:RQ:67:ARG:HH22	1.86	0.41
1:XA:437:U:H2'	1:XA:438:G:O4'	2.21	0.41
1:XA:1055:A:O2'	3:XC:161:GLU:O	2.36	0.41
1:XA:1345:U:OP1	9:XI:120:ARG:NH1	2.53	0.41
3:XC:141:VAL:O	3:XC:144:SER:OG	2.29	0.41
35:YA:1992:G:N2	35:YA:1996:C:O2'	2.53	0.41
35:YA:2705:A:O2'	35:YA:2852:G:OP1	2.34	0.41
37:YD:241:PRO:O	37:YD:242:ARG:HG2	2.20	0.41
54:YY:90:LEU:HB3	54:YY:91:GLU:H	1.71	0.41
1:QA:243:A:H4'	1:QA:244:U:H3'	2.03	0.41
1:QA:1512:U:H3	1:QA:1523:G:H1	1.69	0.41
10:QJ:13:HIS:HB3	10:QJ:68:HIS:CD2	2.55	0.41
11:QK:80:VAL:HG13	11:QK:103:LEU:HD12	2.02	0.41
35:RA:494:G:H4'	52:RW:6:ILE:HB	2.03	0.41
35:RA:919:G:N2	35:RA:2269:A:OP2	2.54	0.41
35:RA:1441:G:H2'	35:RA:1442:G:H8	1.84	0.41
35:RA:1588:C:H2'	35:RA:1589:C:H6	1.85	0.41
35:RA:2345:G:O2'	35:RA:2381:C:O2	2.33	0.41
38:RE:21:VAL:HA	38:RE:22:PRO:HD3	1.93	0.41
40:RG:52:ILE:HG23	40:RG:55:LYS:HB3	2.03	0.41
45:RP:99:LEU:HA	45:RP:102:ARG:HE	1.85	0.41
1:XA:1022:G:H2'	1:XA:1023:G:C8	2.56	0.41
9:XI:46:ALA:HA	9:XI:78:LYS:HB2	2.02	0.41
12:XL:49:ASN:HD22	12:XL:92:ASP:CG	2.29	0.41
24:XY:19:G:H4'	24:XY:57:G:H22	1.85	0.41
25:Y0:68:GLU:HG3	25:Y0:80:HIS:HB2	2.01	0.41
33:Y8:62:LEU:N	33:Y8:63:PRO:CD	2.83	0.41
55:YZ:59:LEU:HD11	55:YZ:88:PHE:HD2	1.86	0.41
1:QA:1355:G:H2'	1:QA:1356:G:C8	2.56	0.41
9:QI:77:ILE:O	9:QI:81:ILE:HG12	2.20	0.41
16:QP:5:ARG:NH2	16:QP:27:LYS:O	2.53	0.41
29:R4:7:PRO:HG2	40:RG:65:GLY:HA2	2.03	0.41
30:R5:25:LEU:HD11	52:RW:41:LYS:HE3	2.03	0.41
31:R6:46:HIS:ND1	35:RA:2371:G:O2'	2.35	0.41
35:RA:259:G:H2'	35:RA:260:G:H8	1.86	0.41
35:RA:593:G:H2'	35:RA:594:U:C6	2.55	0.41
35:RA:672:C:H5	45:RP:42:SER:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1467:C:C5	35:RA:1546:C:H2'	2.56	0.41
35:RA:1991:U:H6	35:RA:1991:U:C5'	2.32	0.41
35:RA:2630:G:H2'	35:RA:2631:G:C8	2.55	0.41
51:RV:2:PHE:CD1	51:RV:13:ARG:NH2	2.89	0.41
1:XA:973:G:H3'	1:XA:974:A:H5''	2.03	0.41
26:Y1:7:ILE:HD12	26:Y1:62:VAL:HG21	2.02	0.41
35:YA:458:G:O2'	35:YA:469:G:O6	2.28	0.41
35:YA:2076:U:OP2	35:YA:2238:G:N2	2.37	0.41
35:YA:2661:G:H2'	35:YA:2662:A:C8	2.56	0.41
35:YA:2702:U:H5	47:YR:73:VAL:HG21	1.86	0.41
37:YD:232:PRO:HB3	37:YD:244:ARG:NH1	2.36	0.41
40:YG:10:LYS:NZ	40:YG:175:LEU:O	2.54	0.41
1:QA:34:C:H2'	1:QA:35:G:H8	1.85	0.41
3:QC:6:HIS:HB3	14:QN:49:HIS:CD2	2.55	0.41
5:QE:144:THR:N	5:QE:147:ASP:OD1	2.48	0.41
9:QI:24:GLY:N	9:QI:60:ASP:OD1	2.44	0.41
10:QJ:47:PHE:CE1	10:QJ:63:PHE:HB2	2.56	0.41
16:QP:20:VAL:HG23	16:QP:35:LYS:HA	2.03	0.41
17:QQ:83:ASP:N	17:QQ:83:ASP:OD1	2.53	0.41
21:QU:6:ARG:HE	21:QU:15:ARG:HH11	1.69	0.41
27:R2:52:ASP:O	27:R2:56:GLN:HG3	2.20	0.41
29:R4:68:ARG:HB3	29:R4:69:LYS:H	1.56	0.41
32:R7:5:TRP:NE1	32:R7:7:PRO:HG3	2.36	0.41
33:R8:34:TRP:CD1	33:R8:35:GLN:HG2	2.56	0.41
35:RA:907:U:O2'	46:RQ:101:ARG:NH2	2.40	0.41
35:RA:1142(A):A:H4'	43:RN:25:ARG:HH22	1.86	0.41
35:RA:1817:G:OP1	37:RD:62:TYR:OH	2.27	0.41
35:RA:2036:C:H2'	35:RA:2037:G:H8	1.86	0.41
35:RA:2055:C:H1'	38:RE:145:LYS:HE3	2.03	0.41
35:RA:2375:G:N2	35:RA:2378:A:OP2	2.49	0.41
35:RA:2656:U:H3	35:RA:2665:A:H2	1.69	0.41
1:XA:884:U:H4'	1:XA:885:G:H5''	2.02	0.41
1:XA:920:U:O2'	1:XA:1081:G:O2'	2.32	0.41
1:XA:1022:G:H2'	1:XA:1023:G:H8	1.86	0.41
1:XA:1192:C:O2	5:XE:25:ARG:NH2	2.34	0.41
10:XJ:57:LYS:CD	10:XJ:60:ARG:HH21	2.23	0.41
11:XK:25:TYR:HD1	11:XK:88:GLY:HA2	1.85	0.41
11:XK:127:LYS:HE3	23:XX:10:G:H5'	2.03	0.41
13:XM:108:ARG:HD2	13:XM:114:ARG:HG3	2.03	0.41
28:Y3:26:LEU:O	28:Y3:35:ARG:NE	2.53	0.41
31:Y6:39:TYR:HB3	31:Y6:40:CYS:H	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1341:U:OP2	35:YA:1394:U:O2'	2.32	0.41
35:YA:1568:G:P	37:YD:63:ARG:HH22	2.42	0.41
35:YA:1662:C:O2'	35:YA:2687:U:OP1	2.34	0.41
35:YA:2100:G:H1	35:YA:2189:U:H3	1.68	0.41
35:YA:2331:G:O2'	35:YA:2336:A:N1	2.51	0.41
35:YA:2564:A:OP1	35:YA:2648:C:O2'	2.32	0.41
36:YB:111:U:H2'	36:YB:112:G:H8	1.85	0.41
38:YE:12:THR:OG1	38:YE:13:ARG:N	2.53	0.41
39:YF:198:ALA:HA	39:YF:201:VAL:HG12	2.02	0.41
41:YH:126:PRO:HB3	41:YH:131:VAL:HA	2.02	0.41
44:YO:64:ARG:HB2	44:YO:83:ALA:HB3	2.03	0.41
1:QA:67:C:O2'	1:QA:171:A:N3	2.46	0.41
1:QA:346:G:H1'	1:QA:347:G:H5'	2.03	0.41
1:QA:553:A:O2'	12:QL:29:GLY:O	2.34	0.41
26:R1:91:LYS:HB3	26:R1:92:LYS:H	1.58	0.41
33:R8:29:LYS:O	33:R8:33:ASN:ND2	2.38	0.41
35:RA:745:G:HO2'	35:RA:748:G:HO2'	1.65	0.41
35:RA:1012:U:OP1	50:RU:75:ASN:ND2	2.51	0.41
35:RA:2470:G:H5'	46:RQ:56:ARG:HH21	1.86	0.41
39:RF:24:LEU:HB3	39:RF:115:ALA:HB2	2.02	0.41
39:RF:157:VAL:HB	39:RF:194:MET:HG2	2.03	0.41
42:RI:14:ASP:OD1	42:RI:14:ASP:N	2.54	0.41
44:RO:85:VAL:HG11	44:RO:114:ILE:HD12	2.02	0.41
55:RZ:10:ARG:HE	55:RZ:36:LYS:HB3	1.85	0.41
1:XA:25:C:H2'	1:XA:26:A:C8	2.56	0.41
27:Y2:50:ILE:HD12	35:YA:61:G:H5'	2.01	0.41
29:Y4:37:SER:HB2	29:Y4:42:PHE:HB3	2.02	0.41
30:Y5:38:ALA:HB3	30:Y5:40:LYS:NZ	2.31	0.41
33:Y8:29:LYS:HE3	33:Y8:44:LYS:HB2	2.02	0.41
34:Y9:2:LYS:HB2	34:Y9:34:GLN:HG2	2.02	0.41
34:Y9:14:CYS:HA	34:Y9:27:CYS:HB2	2.02	0.41
47:YR:56:LYS:NZ	47:YR:90:ARG:O	2.54	0.41
1:QA:501:C:H2'	1:QA:502:G:H8	1.86	0.40
3:QC:159:GLY:HA2	3:QC:193:TYR:HD2	1.74	0.40
4:QD:165:MET:SD	4:QD:168:ARG:NH1	2.94	0.40
8:QH:49:GLU:HG3	8:QH:51:VAL:HG13	2.03	0.40
18:QR:74:ARG:HB3	18:QR:81:PHE:CE1	2.55	0.40
35:RA:571:A:N6	35:RA:2499:C:O3'	2.54	0.40
35:RA:2212:A:H1'	35:RA:2215:G:C4	2.56	0.40
38:RE:101:ARG:NH1	38:RE:171:GLU:HB2	2.36	0.40
39:RF:29:ASN:ND2	39:RF:32:LEU:HD23	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:RG:97:ASP:HA	40:RG:100:TRP:HD1	1.86	0.40
50:RU:40:PHE:HB3	51:RV:75:PHE:CD2	2.55	0.40
1:XA:277:C:OP1	17:XQ:68:ARG:NH1	2.54	0.40
1:XA:662:G:H2'	1:XA:663:A:C8	2.56	0.40
29:Y4:23:GLU:C	29:Y4:25:TYR:H	2.29	0.40
33:Y8:26:LYS:HD3	33:Y8:47:LYS:HB3	2.03	0.40
35:YA:1190:G:H5'	45:YP:32:THR:HA	2.03	0.40
35:YA:1266:G:O6	52:YW:13:SER:OG	2.30	0.40
35:YA:1565:C:H5''	37:YD:18:VAL:HG21	2.03	0.40
36:YB:44:G:H1'	36:YB:47:C:N4	2.36	0.40
47:YR:86:ARG:HH21	47:YR:118:GLU:HB2	1.85	0.40
5:QE:110:LEU:HD13	5:QE:118:ILE:HG21	2.03	0.40
24:QY:3:G:H22	24:QY:70:U:H3	1.68	0.40
35:RA:1094:U:O2'	35:RA:1096:A:OP1	2.34	0.40
41:RH:41:MET:HG2	41:RH:55:PRO:HD2	2.03	0.40
49:RT:19:LEU:HA	49:RT:20:PRO:HD3	1.97	0.40
50:RU:90:VAL:HG12	50:RU:91:ASP:H	1.86	0.40
1:XA:1302:U:H1'	13:XM:17:VAL:HG11	2.02	0.40
19:XS:64:GLU:O	29:Y4:60:GLN:NE2	2.54	0.40
35:YA:486:C:HO2'	52:YW:60:ASN:ND2	2.19	0.40
35:YA:2749:A:OP2	35:YA:2750:A:O2'	2.33	0.40
42:YI:4:ILE:HG12	42:YI:18:VAL:HG22	2.02	0.40
46:YQ:75:THR:HG21	46:YQ:85:LYS:HE3	2.03	0.40
46:YQ:81:VAL:O	46:YQ:82:ARG:NH1	2.45	0.40
47:YR:58:GLY:HA2	47:YR:80:PHE:HE2	1.86	0.40
1:QA:1111:A:H61	3:QC:177:THR:HG22	1.85	0.40
1:QA:1342:C:H2'	1:QA:1343:G:C8	2.56	0.40
3:QC:153:VAL:HG22	3:QC:198:VAL:HG22	2.02	0.40
12:QL:11:VAL:HG11	17:QQ:36:ILE:HG21	2.03	0.40
18:QR:86:VAL:HG12	18:QR:87:ARG:HG2	2.03	0.40
20:QT:37:SER:O	20:QT:41:ILE:HG12	2.22	0.40
30:R5:51:TYR:HB3	30:R5:52:TYR:H	1.48	0.40
35:RA:620:G:H4'	35:RA:621:A:H5''	2.04	0.40
35:RA:1193:G:OP1	45:RP:14:LYS:NZ	2.51	0.40
35:RA:1657:C:OP1	38:RE:136:ARG:N	2.54	0.40
35:RA:2577:A:H5''	35:RA:2578:G:H5'	2.03	0.40
41:RH:41:MET:HB2	41:RH:41:MET:HE3	1.79	0.40
49:RT:73:GLU:OE1	49:RT:103:ARG:NH2	2.52	0.40
1:XA:170:U:H2'	1:XA:171:A:H8	1.86	0.40
1:XA:979:C:O2	14:YN:19:ARG:NE	2.55	0.40
2:XB:31:TYR:HD2	2:XB:202:PRO:HB3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:XC:71:ALA:HA	3:XC:106:VAL:HG22	2.03	0.40
8:XH:39:LEU:HB3	8:XH:45:ILE:HG12	2.03	0.40
24:XY:19:G:C6	35:YA:881:G:H4'	2.57	0.40
25:Y0:46:LYS:HB2	25:Y0:78:TYR:CD1	2.56	0.40
35:YA:33:U:O4	35:YA:446:G:O2'	2.31	0.40
35:YA:530:G:C5	35:YA:2022:U:H5''	2.55	0.40
35:YA:2576:G:O2'	35:YA:2579:C:OP2	2.39	0.40
35:YA:2847:U:OP1	49:YT:98:LYS:NZ	2.40	0.40
43:YN:16:ILE:HG21	43:YN:26:LEU:HD11	2.02	0.40
46:YQ:21:THR:HB	46:YQ:22:LYS:H	1.51	0.40
55:YZ:155:LEU:HD21	55:YZ:163:LEU:HD22	2.03	0.40
1:QA:392:G:H5'	16:QP:12:LYS:HG3	2.04	0.40
1:QA:427:U:OP2	1:QA:428:G:O2'	2.36	0.40
1:QA:877:C:O2'	8:QH:3:THR:OG1	2.33	0.40
1:QA:985:C:H2'	1:QA:986:A:C8	2.56	0.40
1:QA:1292:U:H5'	9:QL:38:GLN:HE22	1.86	0.40
1:QA:1318:A:OP1	19:QS:3:ARG:NH2	2.54	0.40
24:QY:55:U:H5	24:QY:57:G:H8	1.69	0.40
30:R5:51:TYR:HB2	30:R5:56:LYS:HG2	2.03	0.40
33:R8:46:ARG:NH1	35:RA:630:G:OP1	2.55	0.40
35:RA:818:G:N1	35:RA:1188:U:OP2	2.42	0.40
35:RA:845:G:O2'	35:RA:847:U:O4	2.40	0.40
35:RA:1024:G:H5''	35:RA:1025:G:H5''	2.03	0.40
45:RP:115:LEU:HA	45:RP:134:ALA:HB2	2.02	0.40
1:XA:19:C:H5''	5:XE:86:ALA:HB3	2.02	0.40
1:XA:130:A:H5'	17:XQ:63:ARG:NH2	2.37	0.40
1:XA:1292:U:H2'	1:XA:1293:G:C8	2.57	0.40
17:XQ:66:SER:OG	17:XQ:67:LYS:N	2.55	0.40
32:Y7:19:ARG:HD3	35:YA:125:G:H5''	2.03	0.40
35:YA:49:A:N7	35:YA:120:U:H5	2.20	0.40
35:YA:483:A:O2'	54:YY:49:VAL:O	2.27	0.40
35:YA:729:G:P	37:YD:13:ARG:HD3	2.61	0.40
37:YD:159:ALA:HB1	37:YD:198:ASN:HB3	2.03	0.40
42:YI:6:LEU:HD13	42:YI:36:ALA:HA	2.02	0.40
1:QA:627:G:H2'	1:QA:628:G:C8	2.57	0.40
1:QA:767:A:O2'	1:QA:1524:C:O2	2.38	0.40
3:QC:134:ILE:HG23	3:QC:151:VAL:HB	2.04	0.40
4:QD:53:ASP:HB3	4:QD:57:ARG:HH12	1.86	0.40
11:QK:43:SER:HB3	11:QK:68:ALA:HB2	2.03	0.40
23:QX:20:C:H2'	23:QX:21:A:C8	2.57	0.40
35:RA:227:A:H5''	45:RP:76:LYS:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:446:G:OP1	50:RU:3:ARG:NH1	2.54	0.40
35:RA:1636:C:H2'	35:RA:1637:A:C8	2.56	0.40
38:RE:201:THR:HG22	38:RE:203:LYS:H	1.87	0.40
39:RF:150:GLY:HA2	39:RF:172:TRP:CD2	2.57	0.40
45:RP:88:LEU:HD12	45:RP:95:VAL:HG11	2.04	0.40
1:XA:170:U:H2'	1:XA:171:A:C8	2.56	0.40
1:XA:468:A:H5''	16:XP:80:PHE:HB3	2.03	0.40
1:XA:626:U:H4'	16:XP:38:TYR:CE2	2.55	0.40
3:XC:8:ILE:HD12	3:XC:16:ARG:NE	2.36	0.40
4:XD:191:ARG:NH2	4:XD:200:GLU:OE1	2.53	0.40
13:XM:16:ASP:N	13:XM:16:ASP:OD1	2.54	0.40
32:Y7:12:ARG:NH2	32:Y7:44:PRO:HB3	2.37	0.40
33:Y8:63:PRO:CD	33:Y8:63:PRO:O	2.70	0.40
39:YF:82:ILE:HG13	39:YF:83:PHE:HD1	1.86	0.40
39:YF:178:PRO:HB3	39:YF:198:ALA:HB2	2.04	0.40
41:YH:54:ARG:NH2	41:YH:57:ASP:OD1	2.55	0.40
44:YO:120:GLU:HB2	49:YT:68:TYR:HE2	1.86	0.40
45:YP:46:LYS:HE3	45:YP:46:LYS:HB3	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	206 (88%)	27 (12%)	2 (1%)	14	44
2	XB	235/256 (92%)	207 (88%)	28 (12%)	0	100	100
3	QC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
3	XC	203/239 (85%)	186 (92%)	17 (8%)	0	100	100
4	QD	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	24	57
4	XD	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	24	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	QE	149/162 (92%)	138 (93%)	11 (7%)	0	100	100
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	18	49
6	QF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
6	XF	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	145 (95%)	7 (5%)	1 (1%)	18	49
8	QH	136/138 (99%)	121 (89%)	15 (11%)	0	100	100
8	XH	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
9	QI	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
9	XI	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	16	47
10	QJ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
10	XJ	97/105 (92%)	84 (87%)	13 (13%)	0	100	100
11	QK	117/129 (91%)	109 (93%)	8 (7%)	0	100	100
11	XK	117/129 (91%)	108 (92%)	9 (8%)	0	100	100
12	QL	123/131 (94%)	107 (87%)	15 (12%)	1 (1%)	16	47
12	XL	123/131 (94%)	108 (88%)	10 (8%)	5 (4%)	2	13
13	QM	119/126 (94%)	99 (83%)	19 (16%)	1 (1%)	16	47
13	XM	119/126 (94%)	102 (86%)	17 (14%)	0	100	100
14	QN	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	7	30
14	XN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	7	30
15	QO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
15	XO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	QP	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
16	XP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	QQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
17	XQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
18	QR	68/88 (77%)	67 (98%)	1 (2%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	82/93 (88%)	69 (84%)	13 (16%)	0	100	100
19	XS	82/93 (88%)	71 (87%)	8 (10%)	3 (4%)	2	15
20	QT	97/106 (92%)	83 (86%)	14 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	XT	97/106 (92%)	86 (89%)	8 (8%)	3 (3%)	3	18
21	QU	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
21	XU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
25	R0	80/85 (94%)	75 (94%)	5 (6%)	0	100	100
25	Y0	80/85 (94%)	76 (95%)	4 (5%)	0	100	100
26	R1	95/98 (97%)	80 (84%)	12 (13%)	3 (3%)	3	18
26	Y1	95/98 (97%)	85 (90%)	8 (8%)	2 (2%)	5	25
27	R2	67/72 (93%)	59 (88%)	7 (10%)	1 (2%)	8	32
27	Y2	67/72 (93%)	60 (90%)	7 (10%)	0	100	100
28	R3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	R4	69/71 (97%)	44 (64%)	18 (26%)	7 (10%)	0	3
29	Y4	69/71 (97%)	41 (59%)	26 (38%)	2 (3%)	3	19
30	R5	57/60 (95%)	48 (84%)	9 (16%)	0	100	100
30	Y5	57/60 (95%)	48 (84%)	9 (16%)	0	100	100
31	R6	47/54 (87%)	31 (66%)	13 (28%)	3 (6%)	1	6
31	Y6	47/54 (87%)	32 (68%)	12 (26%)	3 (6%)	1	6
32	R7	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
32	Y7	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
33	R8	62/65 (95%)	50 (81%)	10 (16%)	2 (3%)	3	18
33	Y8	62/65 (95%)	51 (82%)	10 (16%)	1 (2%)	7	30
34	R9	35/37 (95%)	35 (100%)	0	0	100	100
34	Y9	35/37 (95%)	35 (100%)	0	0	100	100
37	RD	270/276 (98%)	244 (90%)	21 (8%)	5 (2%)	6	27
37	YD	270/276 (98%)	243 (90%)	26 (10%)	1 (0%)	30	61
38	RE	203/206 (98%)	165 (81%)	35 (17%)	3 (2%)	8	32
38	YE	203/206 (98%)	168 (83%)	30 (15%)	5 (2%)	4	21
39	RF	200/210 (95%)	184 (92%)	13 (6%)	3 (2%)	8	32
39	YF	200/210 (95%)	185 (92%)	13 (6%)	2 (1%)	12	41
40	RG	179/182 (98%)	158 (88%)	21 (12%)	0	100	100
40	YG	179/182 (98%)	156 (87%)	22 (12%)	1 (1%)	21	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	RH	168/180 (93%)	134 (80%)	30 (18%)	4 (2%)	4	22
41	YH	168/180 (93%)	140 (83%)	26 (16%)	2 (1%)	10	37
42	RI	144/148 (97%)	115 (80%)	21 (15%)	8 (6%)	1	8
42	YI	144/148 (97%)	116 (81%)	22 (15%)	6 (4%)	2	13
43	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	18	49
43	YN	136/140 (97%)	117 (86%)	18 (13%)	1 (1%)	18	49
44	RO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
44	YO	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16	47
45	RP	148/150 (99%)	117 (79%)	27 (18%)	4 (3%)	4	20
45	YP	148/150 (99%)	118 (80%)	28 (19%)	2 (1%)	9	34
46	RQ	139/141 (99%)	111 (80%)	27 (19%)	1 (1%)	18	49
46	YQ	139/141 (99%)	116 (84%)	19 (14%)	4 (3%)	3	19
47	RR	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	7	30
47	YR	116/118 (98%)	108 (93%)	6 (5%)	2 (2%)	7	30
48	RS	109/112 (97%)	91 (84%)	15 (14%)	3 (3%)	4	20
48	YS	109/112 (97%)	92 (84%)	16 (15%)	1 (1%)	14	44
49	RT	135/146 (92%)	121 (90%)	14 (10%)	0	100	100
49	YT	135/146 (92%)	117 (87%)	17 (13%)	1 (1%)	18	49
50	RU	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	14	44
50	YU	115/118 (98%)	107 (93%)	5 (4%)	3 (3%)	4	21
51	RV	99/101 (98%)	85 (86%)	12 (12%)	2 (2%)	6	25
51	YV	99/101 (98%)	82 (83%)	16 (16%)	1 (1%)	12	41
52	RW	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
52	YW	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
53	RX	90/96 (94%)	81 (90%)	9 (10%)	0	100	100
53	YX	90/96 (94%)	82 (91%)	7 (8%)	1 (1%)	11	39
54	RY	100/110 (91%)	91 (91%)	9 (9%)	0	100	100
54	YY	100/110 (91%)	94 (94%)	6 (6%)	0	100	100
55	RZ	181/206 (88%)	152 (84%)	24 (13%)	5 (3%)	4	20
55	YZ	181/206 (88%)	158 (87%)	19 (10%)	4 (2%)	5	24
All	All	11470/12126 (95%)	10176 (89%)	1168 (10%)	126 (1%)	11	39

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	QD	5	ILE
26	R1	92	LYS
29	R4	24	THR
29	R4	43	TYR
31	R6	8	LYS
33	R8	62	LEU
37	RD	33	LEU
41	RH	168	PRO
42	RI	15	VAL
45	RP	108	LYS
47	RR	4	LEU
48	RS	88	ASP
48	RS	89	ARG
50	RU	92	ARG
55	RZ	53	ILE
4	XD	5	ILE
12	XL	105	TYR
12	XL	106	ASP
20	XT	74	LYS
26	Y1	92	LYS
29	Y4	24	THR
38	YE	72	VAL
41	YH	157	TYR
41	YH	168	PRO
42	YI	12	LEU
45	YP	108	LYS
47	YR	4	LEU
50	YU	91	ASP
50	YU	92	ARG
55	YZ	53	ILE
55	YZ	94	GLU
2	QB	208	ILE
14	QN	17	LYS
37	RD	243	GLY
38	RE	83	ASP
42	RI	12	LEU
42	RI	13	GLY
45	RP	15	ARG
47	RR	3	HIS
51	RV	45	THR
51	RV	100	ARG
12	XL	104	VAL

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Mol	Chain	Res	Type
12	XL	116	SER
14	XN	17	LYS
19	XS	27	GLU
20	XT	73	HIS
20	XT	75	ASN
31	Y6	8	LYS
38	YE	132	HIS
39	YF	129	PHE
39	YF	134	GLY
42	YI	15	VAL
43	YN	22	THR
47	YR	3	HIS
48	YS	110	LEU
53	YX	68	ARG
2	QB	238	LEU
13	QM	12	ASN
27	R2	70	GLN
29	R4	23	GLU
31	R6	45	LYS
33	R8	63	PRO
37	RD	32	SER
39	RF	129	PHE
41	RH	40	GLU
42	RI	86	THR
45	RP	6	LEU
19	XS	3	ARG
26	Y1	91	LYS
33	Y8	30	ARG
38	YE	83	ASP
38	YE	129	HIS
42	YI	14	ASP
45	YP	65	ARG
46	YQ	22	LYS
46	YQ	25	ASP
26	R1	91	LYS
29	R4	41	PRO
39	RF	67	GLN
39	RF	130	ALA
41	RH	155	SER
42	RI	134	PRO
48	RS	87	PHE
55	RZ	52	SER

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Mol	Chain	Res	Type
55	RZ	61	LEU
12	XL	115	LYS
31	Y6	7	ILE
40	YG	81	LYS
46	YQ	78	PRO
49	YT	108	ARG
50	YU	90	VAL
29	R4	40	HIS
29	R4	42	PHE
29	R4	44	THR
43	RN	96	GLU
46	RQ	22	LYS
7	XG	8	GLU
19	XS	10	PHE
31	Y6	45	LYS
42	YI	10	GLU
42	YI	16	GLY
51	YV	50	PRO
12	QL	27	LEU
26	R1	54	ALA
38	RE	92	THR
38	RE	93	VAL
45	RP	7	ARG
5	XE	74	GLY
38	YE	131	ALA
44	YO	49	ARG
46	YQ	105	GLU
55	YZ	52	SER
37	RD	123	ALA
55	RZ	180	VAL
37	YD	123	ALA
41	RH	169	VAL
42	RI	16	GLY
42	RI	132	PRO
42	YI	13	GLY
31	R6	7	ILE
42	RI	118	LYS
9	XI	90	PRO
29	Y4	40	HIS
37	RD	36	PRO
55	RZ	111	VAL
55	YZ	61	LEU

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	205/220 (93%)	205 (100%)	0	100	100
2	XB	205/220 (93%)	205 (100%)	0	100	100
3	QC	159/188 (85%)	159 (100%)	0	100	100
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	173/181 (96%)	173 (100%)	0	100	100
4	XD	173/181 (96%)	173 (100%)	0	100	100
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	116 (100%)	0	100	100
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	119/119 (100%)	119 (100%)	0	100	100
8	XH	119/119 (100%)	119 (100%)	0	100	100
9	QI	98/99 (99%)	98 (100%)	0	100	100
9	XI	98/99 (99%)	98 (100%)	0	100	100
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	89/92 (97%)	89 (100%)	0	100	100
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	90/99 (91%)	90 (100%)	0	100	100
12	QL	104/108 (96%)	104 (100%)	0	100	100
12	XL	104/108 (96%)	104 (100%)	0	100	100
13	QM	97/101 (96%)	96 (99%)	1 (1%)	68	79
13	XM	97/101 (96%)	97 (100%)	0	100	100
14	QN	49/50 (98%)	49 (100%)	0	100	100
14	XN	49/50 (98%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	95 (100%)	0	100	100
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	73/80 (91%)	71 (97%)	2 (3%)	39	67
19	XS	73/80 (91%)	73 (100%)	0	100	100
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
25	R0	65/67 (97%)	65 (100%)	0	100	100
25	Y0	65/67 (97%)	65 (100%)	0	100	100
26	R1	82/83 (99%)	82 (100%)	0	100	100
26	Y1	82/83 (99%)	82 (100%)	0	100	100
27	R2	64/67 (96%)	64 (100%)	0	100	100
27	Y2	64/67 (96%)	64 (100%)	0	100	100
28	R3	51/52 (98%)	51 (100%)	0	100	100
28	Y3	51/52 (98%)	51 (100%)	0	100	100
29	R4	63/63 (100%)	63 (100%)	0	100	100
29	Y4	63/63 (100%)	63 (100%)	0	100	100
30	R5	51/52 (98%)	51 (100%)	0	100	100
30	Y5	51/52 (98%)	51 (100%)	0	100	100
31	R6	48/52 (92%)	48 (100%)	0	100	100
31	Y6	48/52 (92%)	48 (100%)	0	100	100
32	R7	42/42 (100%)	42 (100%)	0	100	100
32	Y7	42/42 (100%)	42 (100%)	0	100	100
33	R8	54/55 (98%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	Y8	54/55 (98%)	52 (96%)	2 (4%)	30	61
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	214/218 (98%)	214 (100%)	0	100	100
38	RE	165/166 (99%)	165 (100%)	0	100	100
38	YE	165/166 (99%)	165 (100%)	0	100	100
39	RF	161/166 (97%)	161 (100%)	0	100	100
39	YF	161/166 (97%)	161 (100%)	0	100	100
40	RG	155/156 (99%)	155 (100%)	0	100	100
40	YG	155/156 (99%)	155 (100%)	0	100	100
41	RH	142/148 (96%)	142 (100%)	0	100	100
41	YH	142/148 (96%)	142 (100%)	0	100	100
42	RI	122/124 (98%)	122 (100%)	0	100	100
42	YI	122/124 (98%)	122 (100%)	0	100	100
43	RN	117/119 (98%)	116 (99%)	1 (1%)	70	80
43	YN	117/119 (98%)	117 (100%)	0	100	100
44	RO	100/100 (100%)	99 (99%)	1 (1%)	68	79
44	YO	100/100 (100%)	100 (100%)	0	100	100
45	RP	116/116 (100%)	116 (100%)	0	100	100
45	YP	116/116 (100%)	116 (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	87/88 (99%)	87 (100%)	0	100	100
49	RT	120/127 (94%)	120 (100%)	0	100	100
49	YT	120/127 (94%)	120 (100%)	0	100	100
50	RU	93/94 (99%)	93 (100%)	0	100	100
50	YU	93/94 (99%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	RV	82/82 (100%)	82 (100%)	0	100	100
51	YV	82/82 (100%)	82 (100%)	0	100	100
52	RW	92/92 (100%)	92 (100%)	0	100	100
52	YW	92/92 (100%)	92 (100%)	0	100	100
53	RX	74/78 (95%)	74 (100%)	0	100	100
53	YX	74/78 (95%)	74 (100%)	0	100	100
54	RY	85/91 (93%)	85 (100%)	0	100	100
54	YY	85/91 (93%)	85 (100%)	0	100	100
55	RZ	162/179 (90%)	162 (100%)	0	100	100
55	YZ	162/179 (90%)	162 (100%)	0	100	100
All	All	9688/10064 (96%)	9681 (100%)	7 (0%)	88	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	QM	83	ASP
19	QS	9	VAL
19	QS	11	VAL
43	RN	106	MET
44	RO	6	THR
33	Y8	62	LEU
33	Y8	65	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
2	QB	16	HIS
2	QB	40	HIS
2	QB	95	GLN
2	QB	224	GLN
3	QC	28	GLN
3	QC	162	GLN
5	QE	38	GLN
6	QF	7	ASN
7	QG	11	GLN
7	QG	84	ASN
7	QG	109	ASN

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Mol	Chain	Res	Type
9	QI	29	ASN
9	QI	58	HIS
10	QJ	33	GLN
10	QJ	68	HIS
11	QK	99	GLN
12	QL	80	HIS
13	QM	77	ASN
13	QM	92	HIS
15	QO	50	HIS
16	QP	16	HIS
19	QS	47	HIS
19	QS	56	GLN
19	QS	69	HIS
20	QT	16	HIS
27	R2	9	GLN
28	R3	52	HIS
29	R4	6	HIS
29	R4	60	GLN
37	RD	116	GLN
38	RE	54	GLN
39	RF	40	GLN
39	RF	203	GLN
39	RF	204	ASN
44	RO	5	GLN
46	RQ	12	GLN
47	RR	24	GLN
47	RR	50	HIS
48	RS	38	GLN
49	RT	58	ASN
49	RT	90	GLN
50	RU	44	ASN
51	RV	80	GLN
52	RW	60	ASN
53	RX	41	ASN
55	RZ	121	HIS
2	XB	16	HIS
2	XB	40	HIS
2	XB	140	HIS
2	XB	212	GLN
3	XC	37	GLN
3	XC	123	GLN
4	XD	45	GLN

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Mol	Chain	Res	Type
4	XD	161	ASN
4	XD	201	GLN
7	XG	86	GLN
7	XG	109	ASN
8	XH	78	GLN
8	XH	82	HIS
9	XI	31	GLN
9	XI	73	GLN
9	XI	124	GLN
10	XJ	78	ASN
10	XJ	84	GLN
12	XL	80	HIS
13	XM	62	ASN
13	XM	101	GLN
15	XO	50	HIS
15	XO	62	GLN
19	XS	23	ASN
19	XS	47	HIS
25	Y0	12	ASN
27	Y2	38	GLN
27	Y2	65	ASN
28	Y3	46	ASN
29	Y4	47	GLN
34	Y9	20	HIS
37	YD	201	HIS
37	YD	227	ASN
38	YE	132	HIS
38	YE	137	HIS
38	YE	143	ASN
39	YF	40	GLN
39	YF	203	GLN
40	YG	41	GLN
42	YI	104	GLN
42	YI	105	HIS
43	YN	101	HIS
49	YT	38	ASN
52	YW	60	ASN
52	YW	61	ASN
55	YZ	34	ASN
55	YZ	55	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	271 (18%)	29 (1%)
1	XA	1498/1522 (98%)	282 (18%)	27 (1%)
22	QV	76/77 (98%)	15 (19%)	0
22	XV	76/77 (98%)	14 (18%)	0
23	QX	17/19 (89%)	8 (47%)	1 (5%)
23	XX	17/19 (89%)	8 (47%)	1 (5%)
24	QY	74/76 (97%)	28 (37%)	0
24	XY	74/76 (97%)	25 (33%)	0
35	RA	2879/2915 (98%)	591 (20%)	47 (1%)
35	YA	2880/2915 (98%)	589 (20%)	44 (1%)
36	RB	119/122 (97%)	21 (17%)	1 (0%)
36	YB	119/122 (97%)	18 (15%)	0
All	All	9327/9462 (98%)	1870 (20%)	150 (1%)

All (1870) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	31	G
1	QA	32	A
1	QA	39	G
1	QA	48	C
1	QA	50	A
1	QA	51	A
1	QA	54	C
1	QA	64	G
1	QA	65	U
1	QA	66	G
1	QA	78	G
1	QA	79	G
1	QA	90	C
1	QA	91	C
1	QA	95	G
1	QA	101	A
1	QA	108	G
1	QA	116	A
1	QA	121	C
1	QA	129(A)	G
1	QA	144	G
1	QA	146	G
1	QA	163	C
1	QA	169	C
1	QA	173	U

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Mol	Chain	Res	Type
1	QA	174	C
1	QA	182	U
1	QA	187	C
1	QA	191(A)	G
1	QA	195	A
1	QA	197	A
1	QA	209	U
1	QA	210	U
1	QA	216	G
1	QA	244	U
1	QA	245	C
1	QA	247	G
1	QA	251	G
1	QA	267	C
1	QA	270	A
1	QA	281	G
1	QA	289	G
1	QA	306	G
1	QA	321	A
1	QA	328	C
1	QA	329	A
1	QA	332	G
1	QA	344	A
1	QA	346	G
1	QA	347	G
1	QA	348	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	384	G
1	QA	388	G
1	QA	389	A
1	QA	390	C
1	QA	397	A
1	QA	398	C
1	QA	406	G
1	QA	411	A
1	QA	412	A
1	QA	413	G

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Mol	Chain	Res	Type
1	QA	421	U
1	QA	422	C
1	QA	423	G
1	QA	429	U
1	QA	440	A
1	QA	452	A
1	QA	466	C
1	QA	467	G
1	QA	484	G
1	QA	485	G
1	QA	486	U
1	QA	496	A
1	QA	497	U
1	QA	505	G
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	527	G
1	QA	531	U
1	QA	532	A
1	QA	533	A
1	QA	547	A
1	QA	559	A
1	QA	564	C
1	QA	572	A
1	QA	573	A
1	QA	576	G
1	QA	577	G
1	QA	579	G
1	QA	607	A
1	QA	618	C
1	QA	620	C
1	QA	630	G
1	QA	631	G
1	QA	652	U
1	QA	653	A
1	QA	665	A
1	QA	671	G
1	QA	688	G

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Mol	Chain	Res	Type
1	QA	693	G
1	QA	701	C
1	QA	702	A
1	QA	703	G
1	QA	704	A
1	QA	723	U
1	QA	724	G
1	QA	731	G
1	QA	748	C
1	QA	753	A
1	QA	754	C
1	QA	755	G
1	QA	773	G
1	QA	777	A
1	QA	792	A
1	QA	793	U
1	QA	794	A
1	QA	813	U
1	QA	815	A
1	QA	817	C
1	QA	819	A
1	QA	820	U
1	QA	821	G
1	QA	828	A
1	QA	841	U
1	QA	843	U
1	QA	848	C
1	QA	859	A
1	QA	872	A
1	QA	889	A
1	QA	902	G
1	QA	914	A
1	QA	927	G
1	QA	934	C
1	QA	935	A
1	QA	948	C
1	QA	960	U
1	QA	966	G
1	QA	968	A
1	QA	969	A
1	QA	971	G
1	QA	972	C

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Mol	Chain	Res	Type
1	QA	974	A
1	QA	976	G
1	QA	977	A
1	QA	981	U
1	QA	982	U
1	QA	991	U
1	QA	992	U
1	QA	993	G
1	QA	994	A
1	QA	1004	A
1	QA	1006	C
1	QA	1009	G
1	QA	1020	U
1	QA	1024	G
1	QA	1025	U
1	QA	1028	C
1	QA	1029	G
1	QA	1030	C
1	QA	1032(A)	G
1	QA	1040	U
1	QA	1054	C
1	QA	1065	U
1	QA	1066	C
1	QA	1081	G
1	QA	1094	G
1	QA	1095	U
1	QA	1101	A
1	QA	1124	G
1	QA	1125	U
1	QA	1126	U
1	QA	1130	A
1	QA	1131	G
1	QA	1132	C
1	QA	1136	U
1	QA	1137	C
1	QA	1138	G
1	QA	1139	G
1	QA	1146	A
1	QA	1157	A
1	QA	1158	C
1	QA	1159	U
1	QA	1163	C

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Mol	Chain	Res	Type
1	QA	1171	G
1	QA	1178	G
1	QA	1181	G
1	QA	1183	A
1	QA	1187	G
1	QA	1190	G
1	QA	1196	U
1	QA	1197	G
1	QA	1201	A
1	QA	1202	G
1	QA	1211	U
1	QA	1212	U
1	QA	1213	A
1	QA	1225	A
1	QA	1227	A
1	QA	1238	A
1	QA	1240	U
1	QA	1241	G
1	QA	1256	A
1	QA	1257	U
1	QA	1258	G
1	QA	1260	C
1	QA	1270	C
1	QA	1280	A
1	QA	1281	U
1	QA	1282	C
1	QA	1285	A
1	QA	1286	A
1	QA	1287	A
1	QA	1290	G
1	QA	1297	C
1	QA	1298	C
1	QA	1299	A
1	QA	1300	G
1	QA	1301	U
1	QA	1302	U
1	QA	1305	G
1	QA	1321	C
1	QA	1322	C
1	QA	1323	G
1	QA	1326	C
1	QA	1331	G

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Mol	Chain	Res	Type
1	QA	1335	C
1	QA	1336	C
1	QA	1337	G
1	QA	1345	U
1	QA	1346	A
1	QA	1347	G
1	QA	1348	U
1	QA	1353	G
1	QA	1358	U
1	QA	1362(A)	C
1	QA	1370	G
1	QA	1379	G
1	QA	1400	C
1	QA	1419	G
1	QA	1442	G
1	QA	1443	G
1	QA	1446	A
1	QA	1447	G
1	QA	1452	C
1	QA	1453	G
1	QA	1469	G
1	QA	1492	A
1	QA	1497	G
1	QA	1498	U
1	QA	1499	A
1	QA	1502	A
1	QA	1503	A
1	QA	1504	G
1	QA	1506	U
1	QA	1517	G
1	QA	1519	A
1	QA	1520	G
1	QA	1525	G
1	QA	1529	G
1	QA	1530	G
22	QV	7	G
22	QV	8	U
22	QV	9	G
22	QV	16	C
22	QV	17	C
22	QV	17(A)	U
22	QV	18	G

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Mol	Chain	Res	Type
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
22	QV	76	A
23	QX	7	G
23	QX	10	G
23	QX	11	U
23	QX	12	A
23	QX	13	A
23	QX	14	A
23	QX	19	G
23	QX	23	A
24	QY	8	U
24	QY	12	U
24	QY	13	C
24	QY	15	G
24	QY	16	C
24	QY	17	U
24	QY	18	G
24	QY	19	G
24	QY	20	G
24	QY	21	A
24	QY	23	A
24	QY	30	G
24	QY	34	G
24	QY	43	G
24	QY	46	G
24	QY	47	U
24	QY	48	C
24	QY	50	G
24	QY	55	U
24	QY	57	G
24	QY	58	A
24	QY	59	U
24	QY	61	C
24	QY	68	G
24	QY	71	C
24	QY	74	C

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Mol	Chain	Res	Type
24	QY	75	C
24	QY	76	A
35	RA	14	A
35	RA	15	G
35	RA	34	C
35	RA	35	G
35	RA	46	C
35	RA	51	G
35	RA	55	G
35	RA	61	G
35	RA	64	A
35	RA	71	A
35	RA	74	A
35	RA	75	G
35	RA	83	G
35	RA	90	U
35	RA	101	G
35	RA	102	G
35	RA	103	A
35	RA	118	A
35	RA	119	A
35	RA	120	U
35	RA	131	G
35	RA	138	G
35	RA	161	U
35	RA	177	G
35	RA	181	A
35	RA	196	A
35	RA	199	A
35	RA	201	C
35	RA	215	G
35	RA	216	A
35	RA	221	A
35	RA	222	A
35	RA	223	A
35	RA	228	A
35	RA	229	A
35	RA	230	U
35	RA	232	G
35	RA	233	A
35	RA	243	U
35	RA	248	G

Continued on next page...

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Mol	Chain	Res	Type
35	RA	249	C
35	RA	252	G
35	RA	265	A
35	RA	266	G
35	RA	269	U
35	RA	270(L)	U
35	RA	270(M)	U
35	RA	270(P)	C
35	RA	271(C)	U
35	RA	271	G
35	RA	273(F)	C
35	RA	275	G
35	RA	276	A
35	RA	277	C
35	RA	285	C
35	RA	299	A
35	RA	309	G
35	RA	311	A
35	RA	323	G
35	RA	324	A
35	RA	327	G
35	RA	329	G
35	RA	330	A
35	RA	346	A
35	RA	352	G
35	RA	364	C
35	RA	371	A
35	RA	372	G
35	RA	373	U
35	RA	386	G
35	RA	395	U
35	RA	405	U
35	RA	411	G
35	RA	412	A
35	RA	428	A
35	RA	444	C
35	RA	448	U
35	RA	451	C
35	RA	454	A
35	RA	455	C
35	RA	457	A
35	RA	470	A

Continued on next page...

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Mol	Chain	Res	Type
35	RA	481	G
35	RA	503	A
35	RA	504	U
35	RA	505	A
35	RA	508	G
35	RA	509	C
35	RA	512	G
35	RA	513	A
35	RA	529	A
35	RA	531	C
35	RA	532	A
35	RA	533	G
35	RA	537	C
35	RA	539	G
35	RA	540	G
35	RA	546	C
35	RA	547	A
35	RA	554	U
35	RA	556	G
35	RA	563	G
35	RA	573	G
35	RA	574	C
35	RA	575	A
35	RA	583	G
35	RA	588	U
35	RA	603	A
35	RA	607	U
35	RA	614	U
35	RA	615	G
35	RA	616	A
35	RA	617	G
35	RA	621	A
35	RA	622	G
35	RA	627	A
35	RA	634	C
35	RA	637	A
35	RA	638	G
35	RA	645	C
35	RA	646	A
35	RA	651	G
35	RA	654	A
35	RA	654(A)	G

Continued on next page...

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Mol	Chain	Res	Type
35	RA	654(T)	C
35	RA	669	G
35	RA	670	A
35	RA	686	G
35	RA	702	G
35	RA	717	G
35	RA	722	A
35	RA	730	C
35	RA	747	U
35	RA	752	A
35	RA	753	C
35	RA	765	G
35	RA	771	G
35	RA	776	G
35	RA	782	A
35	RA	783	A
35	RA	784	A
35	RA	785	G
35	RA	788	A
35	RA	790	C
35	RA	793	A
35	RA	800	A
35	RA	805	G
35	RA	812	C
35	RA	819	A
35	RA	827	U
35	RA	828	U
35	RA	847	U
35	RA	856	C
35	RA	857	C
35	RA	859	G
35	RA	869	G
35	RA	880	G
35	RA	881	G
35	RA	884	C
35	RA	885	C
35	RA	886	C
35	RA	888	C
35	RA	889	C
35	RA	893	C
35	RA	896	A
35	RA	897	C

Continued on next page...

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Mol	Chain	Res	Type
35	RA	898	C
35	RA	900	A
35	RA	901	A
35	RA	904	C
35	RA	907	U
35	RA	910	A
35	RA	917	A
35	RA	932	G
35	RA	938	G
35	RA	941	A
35	RA	945	A
35	RA	946	G
35	RA	953	A
35	RA	959	A
35	RA	961	C
35	RA	973	A
35	RA	974	G
35	RA	974(A)	C
35	RA	980	A
35	RA	983	A
35	RA	989	G
35	RA	996	A
35	RA	1003	G
35	RA	1005	C
35	RA	1012	U
35	RA	1013	C
35	RA	1015	G
35	RA	1022	G
35	RA	1023	U
35	RA	1024	G
35	RA	1025	G
35	RA	1026	U
35	RA	1027	A
35	RA	1033	U
35	RA	1044	G
35	RA	1045	A
35	RA	1046	A
35	RA	1049	C
35	RA	1050	A
35	RA	1053	C
35	RA	1055	G
35	RA	1057	A

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Mol	Chain	Res	Type
35	RA	1059	G
35	RA	1060	U
35	RA	1061	U
35	RA	1062	G
35	RA	1065	U
35	RA	1066	U
35	RA	1067	A
35	RA	1068	G
35	RA	1071	G
35	RA	1073	A
35	RA	1076	C
35	RA	1077	A
35	RA	1078	U
35	RA	1079	C
35	RA	1080	C
35	RA	1082	U
35	RA	1083	U
35	RA	1084	A
35	RA	1085	A
35	RA	1086	A
35	RA	1087	G
35	RA	1088	A
35	RA	1090	U
35	RA	1091	G
35	RA	1093	G
35	RA	1095	A
35	RA	1096	A
35	RA	1104	C
35	RA	1105	U
35	RA	1110	G
35	RA	1111	A
35	RA	1112	G
35	RA	1113	U
35	RA	1122	G
35	RA	1131	G
35	RA	1135	C
35	RA	1136	G
35	RA	1139	G
35	RA	1140	C
35	RA	1142(A)	A
35	RA	1168	G
35	RA	1170	G

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Mol	Chain	Res	Type
35	RA	1173	G
35	RA	1174	A
35	RA	1175	U
35	RA	1176	G
35	RA	1179	C
35	RA	1195	G
35	RA	1204	A
35	RA	1205	U
35	RA	1206	G
35	RA	1210	A
35	RA	1211	U
35	RA	1220	A
35	RA	1236	G
35	RA	1238	G
35	RA	1240	U
35	RA	1244	G
35	RA	1252	G
35	RA	1253	A
35	RA	1256	G
35	RA	1271	G
35	RA	1272	A
35	RA	1273	U
35	RA	1284	A
35	RA	1300	U
35	RA	1301	A
35	RA	1312	U
35	RA	1313	U
35	RA	1314	C
35	RA	1319	G
35	RA	1329	U
35	RA	1341	U
35	RA	1349	A
35	RA	1352	U
35	RA	1365	A
35	RA	1368	G
35	RA	1370	C
35	RA	1378	A
35	RA	1379	A
35	RA	1380	G
35	RA	1384	A
35	RA	1385	G
35	RA	1395	A

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Mol	Chain	Res	Type
35	RA	1403	C
35	RA	1404	C
35	RA	1407	C
35	RA	1411	C
35	RA	1416	G
35	RA	1419	A
35	RA	1420	U
35	RA	1421	G
35	RA	1428	C
35	RA	1444(A)	A
35	RA	1445	C
35	RA	1449	A
35	RA	1449(A)	G
35	RA	1455	G
35	RA	1458	C
35	RA	1460	A
35	RA	1461	G
35	RA	1467	C
35	RA	1471	A
35	RA	1482	U
35	RA	1483	G
35	RA	1485	G
35	RA	1490	A
35	RA	1493	C
35	RA	1495	A
35	RA	1497	U
35	RA	1507	A
35	RA	1508	A
35	RA	1510	A
35	RA	1511	A
35	RA	1513	C
35	RA	1514	U
35	RA	1525	G
35	RA	1533	C
35	RA	1535	U
35	RA	1536	A
35	RA	1537	C
35	RA	1538	G
35	RA	1543	A
35	RA	1544	C
35	RA	1545	A
35	RA	1554	A

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Mol	Chain	Res	Type
35	RA	1558	A
35	RA	1559	G
35	RA	1566	A
35	RA	1569	A
35	RA	1578	U
35	RA	1586	A
35	RA	1598	C
35	RA	1608	A
35	RA	1609	A
35	RA	1616	A
35	RA	1617	C
35	RA	1618	A
35	RA	1630(A)	C
35	RA	1640	C
35	RA	1648	C
35	RA	1654	A
35	RA	1667	G
35	RA	1668	A
35	RA	1674	G
35	RA	1675	C
35	RA	1688	U
35	RA	1695	G
35	RA	1703	G
35	RA	1725	G
35	RA	1728	G
35	RA	1729	A
35	RA	1730	U
35	RA	1731	G
35	RA	1734	C
35	RA	1742	C
35	RA	1743	G
35	RA	1756	G
35	RA	1763	G
35	RA	1764	G
35	RA	1773	A
35	RA	1780	A
35	RA	1782	C
35	RA	1787	A
35	RA	1791	A
35	RA	1799	G
35	RA	1800	C
35	RA	1811	G

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Mol	Chain	Res	Type
35	RA	1816	G
35	RA	1820	U
35	RA	1828	G
35	RA	1829	A
35	RA	1835	G
35	RA	1847	A
35	RA	1848	A
35	RA	1858	G
35	RA	1860	G
35	RA	1869	G
35	RA	1872	A
35	RA	1878	G
35	RA	1882	C
35	RA	1885	A
35	RA	1888	G
35	RA	1889	A
35	RA	1900	A
35	RA	1906	G
35	RA	1913	A
35	RA	1929	G
35	RA	1931	U
35	RA	1936	A
35	RA	1938	A
35	RA	1939	U
35	RA	1955	U
35	RA	1963	U
35	RA	1964	G
35	RA	1967	C
35	RA	1969	A
35	RA	1970	A
35	RA	1971	A
35	RA	1972	A
35	RA	1982	C
35	RA	1991	U
35	RA	1992	G
35	RA	1993	U
35	RA	2020	A
35	RA	2023	G
35	RA	2031	A
35	RA	2032	G
35	RA	2033	A
35	RA	2039	C

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Mol	Chain	Res	Type
35	RA	2043	C
35	RA	2052	G
35	RA	2055	C
35	RA	2056	G
35	RA	2059	A
35	RA	2060	A
35	RA	2061	G
35	RA	2062	A
35	RA	2069	G
35	RA	2107	C
35	RA	2111	C
35	RA	2113	U
35	RA	2114	A
35	RA	2115	G
35	RA	2116	G
35	RA	2117	A
35	RA	2119	A
35	RA	2126	A
35	RA	2127	G
35	RA	2128	C
35	RA	2131	G
35	RA	2132	U
35	RA	2133	G
35	RA	2135	A
35	RA	2136	C
35	RA	2145	C
35	RA	2146	C
35	RA	2147	G
35	RA	2148	G
35	RA	2158	A
35	RA	2166	G
35	RA	2168	G
35	RA	2169	A
35	RA	2171	A
35	RA	2173	A
35	RA	2176	A
35	RA	2190	G
35	RA	2198	A
35	RA	2199	A
35	RA	2210	G
35	RA	2211	G
35	RA	2212	A

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Mol	Chain	Res	Type
35	RA	2213	U
35	RA	2215	G
35	RA	2225	A
35	RA	2238	G
35	RA	2239	G
35	RA	2243	U
35	RA	2249	U
35	RA	2266	A
35	RA	2275	C
35	RA	2283	C
35	RA	2284	C
35	RA	2287	A
35	RA	2288	A
35	RA	2307	G
35	RA	2308	G
35	RA	2311	A
35	RA	2319	G
35	RA	2320	A
35	RA	2321	G
35	RA	2325	G
35	RA	2334	G
35	RA	2335	A
35	RA	2345	G
35	RA	2346	A
35	RA	2347	C
35	RA	2350	C
35	RA	2354	G
35	RA	2358	G
35	RA	2372	G
35	RA	2383	G
35	RA	2385	C
35	RA	2392	A
35	RA	2402	C
35	RA	2405	G
35	RA	2406	U
35	RA	2410	G
35	RA	2420	C
35	RA	2421	G
35	RA	2423	U
35	RA	2424	C
35	RA	2425	A
35	RA	2429	G

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Mol	Chain	Res	Type
35	RA	2430	A
35	RA	2435	A
35	RA	2439	A
35	RA	2440	C
35	RA	2441	C
35	RA	2445	G
35	RA	2448	A
35	RA	2469	A
35	RA	2470	G
35	RA	2475	C
35	RA	2482	G
35	RA	2484	G
35	RA	2494	G
35	RA	2498	C
35	RA	2502	G
35	RA	2505	G
35	RA	2518	A
35	RA	2519	U
35	RA	2529	G
35	RA	2542	A
35	RA	2543	G
35	RA	2554	U
35	RA	2562	U
35	RA	2564	A
35	RA	2567	G
35	RA	2569	G
35	RA	2573	C
35	RA	2576	G
35	RA	2578	G
35	RA	2582	G
35	RA	2586	C
35	RA	2602	A
35	RA	2609	U
35	RA	2611	U
35	RA	2612	C
35	RA	2615	U
35	RA	2621	A
35	RA	2623	G
35	RA	2629	A
35	RA	2642	G
35	RA	2646	C
35	RA	2654	A

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Mol	Chain	Res	Type
35	RA	2655	G
35	RA	2665	A
35	RA	2673	G
35	RA	2689	U
35	RA	2690	C
35	RA	2700	C
35	RA	2702	U
35	RA	2707	G
35	RA	2712	U
35	RA	2712(A)	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	2734	A
35	RA	2739	U
35	RA	2744	G
35	RA	2748	A
35	RA	2757	A
35	RA	2761	G
35	RA	2765	A
35	RA	2766	G
35	RA	2777	G
35	RA	2778	A
35	RA	2779	U
35	RA	2780	G
35	RA	2790	A
35	RA	2791	C
35	RA	2797	U
35	RA	2807	G
35	RA	2818	G
35	RA	2820	A
35	RA	2821	A
35	RA	2823	A
35	RA	2825	C
35	RA	2833	G
35	RA	2834	G
35	RA	2835	A
35	RA	2866	U
35	RA	2872	G

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Mol	Chain	Res	Type
35	RA	2879	C
35	RA	2880	C
35	RA	2882	A
35	RA	2892	A
35	RA	2894	G
36	RB	7	G
36	RB	8	U
36	RB	9	G
36	RB	12	C
36	RB	13	A
36	RB	15	A
36	RB	16	G
36	RB	22	U
36	RB	25	A
36	RB	26	A
36	RB	30	C
36	RB	41	U
36	RB	42	C
36	RB	44	G
36	RB	45	A
36	RB	56	G
36	RB	67	G
36	RB	73	A
36	RB	81	G
36	RB	105	G
36	RB	109	G
1	XA	6	G
1	XA	32	A
1	XA	39	G
1	XA	47	C
1	XA	48	C
1	XA	51	A
1	XA	61	G
1	XA	65	U
1	XA	66	G
1	XA	78	G
1	XA	79	G
1	XA	81	G
1	XA	89	U
1	XA	90	C
1	XA	91	C
1	XA	92	G

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Mol	Chain	Res	Type
1	XA	95	G
1	XA	101	A
1	XA	108	G
1	XA	115	G
1	XA	116	A
1	XA	121	C
1	XA	130	A
1	XA	144	G
1	XA	147	G
1	XA	163	C
1	XA	169	C
1	XA	172	A
1	XA	173	U
1	XA	174	C
1	XA	187	C
1	XA	188	U
1	XA	190	G
1	XA	191(A)	G
1	XA	195	A
1	XA	197	A
1	XA	201	C
1	XA	209	U
1	XA	216	G
1	XA	220	G
1	XA	244	U
1	XA	245	C
1	XA	247	G
1	XA	251	G
1	XA	267	C
1	XA	270	A
1	XA	281	G
1	XA	289	G
1	XA	321	A
1	XA	328	C
1	XA	329	A
1	XA	332	G
1	XA	345	C
1	XA	346	G
1	XA	347	G
1	XA	348	G
1	XA	351	G
1	XA	352	C

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Mol	Chain	Res	Type
1	XA	353	A
1	XA	354	G
1	XA	356	A
1	XA	367	U
1	XA	372	C
1	XA	382	A
1	XA	384	G
1	XA	388	G
1	XA	390	C
1	XA	397	A
1	XA	398	C
1	XA	406	G
1	XA	411	A
1	XA	412	A
1	XA	413	G
1	XA	414	A
1	XA	422	C
1	XA	423	G
1	XA	424	G
1	XA	429	U
1	XA	435	C
1	XA	440	A
1	XA	452	A
1	XA	465	A
1	XA	466	C
1	XA	467	G
1	XA	483	C
1	XA	485	G
1	XA	486	U
1	XA	496	A
1	XA	497	U
1	XA	509	A
1	XA	510	A
1	XA	511	C
1	XA	518	C
1	XA	521	G
1	XA	527	G
1	XA	531	U
1	XA	532	A
1	XA	533	A
1	XA	546	G
1	XA	547	A

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Mol	Chain	Res	Type
1	XA	548	G
1	XA	559	A
1	XA	561	U
1	XA	564	C
1	XA	565	U
1	XA	568	G
1	XA	572	A
1	XA	573	A
1	XA	576	G
1	XA	577	G
1	XA	596	C
1	XA	614	A
1	XA	618	C
1	XA	630	G
1	XA	631	G
1	XA	652	U
1	XA	653	A
1	XA	661	G
1	XA	665	A
1	XA	688	G
1	XA	702	A
1	XA	703	G
1	XA	704	A
1	XA	721	G
1	XA	724	G
1	XA	731	G
1	XA	748	C
1	XA	749	C
1	XA	754	C
1	XA	755	G
1	XA	774	G
1	XA	777	A
1	XA	792	A
1	XA	793	U
1	XA	794	A
1	XA	799	G
1	XA	812	C
1	XA	813	U
1	XA	816	A
1	XA	817	C
1	XA	821	G
1	XA	828	A

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Mol	Chain	Res	Type
1	XA	841	U
1	XA	842	C
1	XA	843	U
1	XA	848	C
1	XA	859	A
1	XA	872	A
1	XA	888	G
1	XA	902	G
1	XA	914	A
1	XA	926	G
1	XA	927	G
1	XA	934	C
1	XA	948	C
1	XA	958	A
1	XA	960	U
1	XA	967	C
1	XA	968	A
1	XA	969	A
1	XA	972	C
1	XA	974	A
1	XA	975	A
1	XA	976	G
1	XA	977	A
1	XA	981	U
1	XA	991	U
1	XA	992	U
1	XA	993	G
1	XA	1004	A
1	XA	1005	A
1	XA	1006	C
1	XA	1009	G
1	XA	1017	G
1	XA	1021	G
1	XA	1024	G
1	XA	1025	U
1	XA	1028	C
1	XA	1029	G
1	XA	1032(A)	G
1	XA	1036	G
1	XA	1042	G
1	XA	1054	C
1	XA	1055	A

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Mol	Chain	Res	Type
1	XA	1066	C
1	XA	1081	G
1	XA	1094	G
1	XA	1095	U
1	XA	1101	A
1	XA	1124	G
1	XA	1125	U
1	XA	1126	U
1	XA	1130	A
1	XA	1131	G
1	XA	1136	U
1	XA	1137	C
1	XA	1138	G
1	XA	1139	G
1	XA	1146	A
1	XA	1152	A
1	XA	1154	G
1	XA	1157	A
1	XA	1158	C
1	XA	1159	U
1	XA	1160	G
1	XA	1162	C
1	XA	1171	G
1	XA	1176	A
1	XA	1177	G
1	XA	1181	G
1	XA	1182	G
1	XA	1183	A
1	XA	1184	G
1	XA	1187	G
1	XA	1190	G
1	XA	1196	U
1	XA	1197	G
1	XA	1211	U
1	XA	1212	U
1	XA	1238	A
1	XA	1240	U
1	XA	1241	G
1	XA	1256	A
1	XA	1257	U
1	XA	1258	G
1	XA	1260	C

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Mol	Chain	Res	Type
1	XA	1270	C
1	XA	1273	G
1	XA	1280	A
1	XA	1281	U
1	XA	1282	C
1	XA	1286	A
1	XA	1287	A
1	XA	1298	C
1	XA	1300	G
1	XA	1301	U
1	XA	1302	U
1	XA	1303	C
1	XA	1305	G
1	XA	1318	A
1	XA	1320	C
1	XA	1321	C
1	XA	1322	C
1	XA	1323	G
1	XA	1331	G
1	XA	1335	C
1	XA	1336	C
1	XA	1346	A
1	XA	1347	G
1	XA	1353	G
1	XA	1362(A)	C
1	XA	1363	A
1	XA	1364	U
1	XA	1367	C
1	XA	1368	G
1	XA	1370	G
1	XA	1379	G
1	XA	1397	C
1	XA	1398	A
1	XA	1419	G
1	XA	1442	G
1	XA	1443	G
1	XA	1446	A
1	XA	1452	C
1	XA	1453	G
1	XA	1454	G
1	XA	1469	G
1	XA	1487	G

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Mol	Chain	Res	Type
1	XA	1492	A
1	XA	1497	G
1	XA	1498	U
1	XA	1499	A
1	XA	1502	A
1	XA	1503	A
1	XA	1504	G
1	XA	1506	U
1	XA	1517	G
1	XA	1519	A
1	XA	1520	G
1	XA	1529	G
1	XA	1530	G
1	XA	1531	A
22	XV	3	C
22	XV	16	C
22	XV	17	C
22	XV	17(A)	U
22	XV	18	G
22	XV	19	G
22	XV	20	U
22	XV	21	A
22	XV	22	G
22	XV	34	C
22	XV	47	U
22	XV	48	C
22	XV	59	A
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	18	G
23	XX	19	G
23	XX	23	A
24	XY	4	G
24	XY	8	U
24	XY	9	A
24	XY	12	U
24	XY	16	C
24	XY	17	U

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Mol	Chain	Res	Type
24	XY	18	G
24	XY	19	G
24	XY	20	G
24	XY	21	A
24	XY	22	G
24	XY	23	A
24	XY	43	G
24	XY	46	G
24	XY	47	U
24	XY	50	G
24	XY	55	U
24	XY	56	C
24	XY	57	G
24	XY	58	A
24	XY	59	U
24	XY	61	C
24	XY	71	C
24	XY	73	A
24	XY	74	C
35	YA	9	U
35	YA	15	G
35	YA	34	C
35	YA	35	G
35	YA	46	C
35	YA	50	U
35	YA	51	G
35	YA	55	G
35	YA	61	G
35	YA	63	U
35	YA	74	A
35	YA	75	G
35	YA	91	A
35	YA	96	G
35	YA	101	G
35	YA	102	G
35	YA	103	A
35	YA	118	A
35	YA	119	A
35	YA	120	U
35	YA	125	G
35	YA	131	G
35	YA	149	A

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Mol	Chain	Res	Type
35	YA	161	U
35	YA	162	U
35	YA	181	A
35	YA	188	G
35	YA	196	A
35	YA	199	A
35	YA	204	A
35	YA	215	G
35	YA	216	A
35	YA	221	A
35	YA	222	A
35	YA	223	A
35	YA	229	A
35	YA	230	U
35	YA	232	G
35	YA	242	G
35	YA	243	U
35	YA	248	G
35	YA	249	C
35	YA	252	G
35	YA	264	C
35	YA	265	A
35	YA	266	G
35	YA	269	U
35	YA	270(L)	U
35	YA	270(M)	U
35	YA	270(N)	G
35	YA	270(P)	C
35	YA	271(A)	C
35	YA	271(B)	G
35	YA	271(C)	U
35	YA	271	G
35	YA	274	G
35	YA	275	G
35	YA	276	A
35	YA	278	A
35	YA	279	C
35	YA	299	A
35	YA	311	A
35	YA	323	G
35	YA	324	A
35	YA	329	G

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Mol	Chain	Res	Type
35	YA	330	A
35	YA	332	A
35	YA	342	G
35	YA	352	G
35	YA	363	G
35	YA	363(F)	A
35	YA	364	C
35	YA	371	A
35	YA	372	G
35	YA	386	G
35	YA	387	U
35	YA	396	G
35	YA	405	U
35	YA	406	G
35	YA	411	G
35	YA	412	A
35	YA	421	U
35	YA	428	A
35	YA	443	A
35	YA	444	C
35	YA	448	U
35	YA	455	C
35	YA	457	A
35	YA	467	G
35	YA	470	A
35	YA	480	A
35	YA	481	G
35	YA	504	U
35	YA	505	A
35	YA	509	C
35	YA	518	G
35	YA	528	A
35	YA	530	G
35	YA	531	C
35	YA	532	A
35	YA	533	G
35	YA	537	C
35	YA	539	G
35	YA	540	G
35	YA	546	C
35	YA	547	A
35	YA	554	U

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Mol	Chain	Res	Type
35	YA	563	G
35	YA	573	G
35	YA	575	A
35	YA	588	U
35	YA	603	A
35	YA	607	U
35	YA	614	U
35	YA	615	G
35	YA	616	A
35	YA	617	G
35	YA	618	G
35	YA	622	G
35	YA	627	A
35	YA	634	C
35	YA	637	A
35	YA	638	G
35	YA	645	C
35	YA	646	A
35	YA	651	G
35	YA	654	A
35	YA	654(A)	G
35	YA	686	G
35	YA	695	G
35	YA	702	G
35	YA	717	G
35	YA	722	A
35	YA	730	C
35	YA	734	A
35	YA	747	U
35	YA	752	A
35	YA	753	C
35	YA	764	A
35	YA	765	G
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	790	C
35	YA	792	G

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Mol	Chain	Res	Type
35	YA	800	A
35	YA	805	G
35	YA	812	C
35	YA	819	A
35	YA	827	U
35	YA	828	U
35	YA	829	A
35	YA	846	C
35	YA	847	U
35	YA	856	C
35	YA	857	C
35	YA	859	G
35	YA	860	U
35	YA	866	A
35	YA	880	G
35	YA	881	G
35	YA	882	G
35	YA	884	C
35	YA	885	C
35	YA	886	C
35	YA	888	C
35	YA	889	C
35	YA	890	A
35	YA	896	A
35	YA	897	C
35	YA	900	A
35	YA	901	A
35	YA	907	U
35	YA	910	A
35	YA	917	A
35	YA	918	A
35	YA	932	G
35	YA	941	A
35	YA	945	A
35	YA	946	G
35	YA	953	A
35	YA	959	A
35	YA	961	C
35	YA	973	A
35	YA	974	G
35	YA	974(A)	C
35	YA	983	A

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Mol	Chain	Res	Type
35	YA	989	G
35	YA	996	A
35	YA	1003	G
35	YA	1005	C
35	YA	1011	G
35	YA	1012	U
35	YA	1013	C
35	YA	1015	G
35	YA	1022	G
35	YA	1023	U
35	YA	1024	G
35	YA	1025	G
35	YA	1026	U
35	YA	1027	A
35	YA	1033	U
35	YA	1045	A
35	YA	1046	A
35	YA	1047	G
35	YA	1050	A
35	YA	1054	A
35	YA	1057	A
35	YA	1059	G
35	YA	1060	U
35	YA	1061	U
35	YA	1062	G
35	YA	1065	U
35	YA	1066	U
35	YA	1067	A
35	YA	1068	G
35	YA	1069	A
35	YA	1071	G
35	YA	1076	C
35	YA	1077	A
35	YA	1078	U
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	1089	G

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Mol	Chain	Res	Type
35	YA	1093	G
35	YA	1095	A
35	YA	1096	A
35	YA	1097	U
35	YA	1103	A
35	YA	1104	C
35	YA	1110	G
35	YA	1111	A
35	YA	1112	G
35	YA	1122	G
35	YA	1126	A
35	YA	1129	A
35	YA	1130	U
35	YA	1131	G
35	YA	1135	C
35	YA	1136	G
35	YA	1139	G
35	YA	1142	U
35	YA	1142(A)	A
35	YA	1173	G
35	YA	1174	A
35	YA	1175	U
35	YA	1176	G
35	YA	1179	C
35	YA	1195	G
35	YA	1204	A
35	YA	1205	U
35	YA	1210	A
35	YA	1211	U
35	YA	1218	C
35	YA	1220	A
35	YA	1238	G
35	YA	1240	U
35	YA	1250	G
35	YA	1252	G
35	YA	1253	A
35	YA	1256	G
35	YA	1265	A
35	YA	1271	G
35	YA	1272	A
35	YA	1300	U
35	YA	1301	A

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Mol	Chain	Res	Type
35	YA	1306	C
35	YA	1309	G
35	YA	1329	U
35	YA	1341	U
35	YA	1349	A
35	YA	1352	U
35	YA	1365	A
35	YA	1368	G
35	YA	1370	C
35	YA	1379	A
35	YA	1384	A
35	YA	1385	G
35	YA	1386	C
35	YA	1391	U
35	YA	1395	A
35	YA	1407	C
35	YA	1411	C
35	YA	1416	G
35	YA	1419	A
35	YA	1420	U
35	YA	1421	G
35	YA	1427	A
35	YA	1428	C
35	YA	1444(A)	A
35	YA	1449	A
35	YA	1449(A)	G
35	YA	1455	G
35	YA	1458	C
35	YA	1460	A
35	YA	1461	G
35	YA	1467	C
35	YA	1471	A
35	YA	1483	G
35	YA	1485	G
35	YA	1493	C
35	YA	1497	U
35	YA	1507	A
35	YA	1508	A
35	YA	1510	A
35	YA	1511	A
35	YA	1514	U
35	YA	1523	U

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Mol	Chain	Res	Type
35	YA	1534	G
35	YA	1535	U
35	YA	1536	A
35	YA	1537	C
35	YA	1538	G
35	YA	1540	G
35	YA	1543	A
35	YA	1544	C
35	YA	1545	A
35	YA	1558	A
35	YA	1559	G
35	YA	1566	A
35	YA	1569	A
35	YA	1578	U
35	YA	1579	A
35	YA	1581	G
35	YA	1585	C
35	YA	1586	A
35	YA	1598	C
35	YA	1607	C
35	YA	1608	A
35	YA	1609	A
35	YA	1617	C
35	YA	1618	A
35	YA	1640	C
35	YA	1648	C
35	YA	1653	G
35	YA	1654	A
35	YA	1668	A
35	YA	1674	G
35	YA	1675	C
35	YA	1693	U
35	YA	1695	G
35	YA	1699	G
35	YA	1700	A
35	YA	1725	G
35	YA	1728	G
35	YA	1729	A
35	YA	1730	U
35	YA	1731	G
35	YA	1733	G
35	YA	1742	C

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Mol	Chain	Res	Type
35	YA	1743	G
35	YA	1754	C
35	YA	1756	G
35	YA	1762	A
35	YA	1763	G
35	YA	1764	G
35	YA	1773	A
35	YA	1780	A
35	YA	1791	A
35	YA	1799	G
35	YA	1800	C
35	YA	1801	G
35	YA	1808	U
35	YA	1811	G
35	YA	1816	G
35	YA	1820	U
35	YA	1828	G
35	YA	1829	A
35	YA	1835	G
35	YA	1847	A
35	YA	1858	G
35	YA	1869	G
35	YA	1872	A
35	YA	1878	G
35	YA	1881	C
35	YA	1882	C
35	YA	1888	G
35	YA	1889	A
35	YA	1896	G
35	YA	1900	A
35	YA	1906	G
35	YA	1919	A
35	YA	1929	G
35	YA	1937	A
35	YA	1938	A
35	YA	1939	U
35	YA	1940	U
35	YA	1955	U
35	YA	1956	U
35	YA	1963	U
35	YA	1964	G
35	YA	1965	C

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Mol	Chain	Res	Type
35	YA	1966	A
35	YA	1967	C
35	YA	1969	A
35	YA	1970	A
35	YA	1971	A
35	YA	1972	A
35	YA	1982	C
35	YA	1991	U
35	YA	1992	G
35	YA	1993	U
35	YA	2020	A
35	YA	2021	C
35	YA	2023	G
35	YA	2031	A
35	YA	2032	G
35	YA	2033	A
35	YA	2039	C
35	YA	2043	C
35	YA	2054	A
35	YA	2055	C
35	YA	2056	G
35	YA	2059	A
35	YA	2060	A
35	YA	2061	G
35	YA	2062	A
35	YA	2069	G
35	YA	2090	G
35	YA	2093	G
35	YA	2099	U
35	YA	2111	C
35	YA	2113	U
35	YA	2114	A
35	YA	2115	G
35	YA	2116	G
35	YA	2119	A
35	YA	2120	G
35	YA	2126	A
35	YA	2127	G
35	YA	2128	C
35	YA	2131	G
35	YA	2132	U
35	YA	2133	G

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Mol	Chain	Res	Type
35	YA	2146	C
35	YA	2147	G
35	YA	2148	G
35	YA	2158	A
35	YA	2165	G
35	YA	2166	G
35	YA	2167	U
35	YA	2168	G
35	YA	2169	A
35	YA	2171	A
35	YA	2173	A
35	YA	2176	A
35	YA	2178	C
35	YA	2190	G
35	YA	2192	G
35	YA	2198	A
35	YA	2210	G
35	YA	2211	G
35	YA	2212	A
35	YA	2213	U
35	YA	2215	G
35	YA	2225	A
35	YA	2234	G
35	YA	2238	G
35	YA	2239	G
35	YA	2243	U
35	YA	2246	G
35	YA	2249	U
35	YA	2269	A
35	YA	2275	C
35	YA	2283	C
35	YA	2287	A
35	YA	2288	A
35	YA	2289	G
35	YA	2307	G
35	YA	2308	G
35	YA	2310	A
35	YA	2311	A
35	YA	2318	G
35	YA	2319	G
35	YA	2320	A
35	YA	2325	G

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Mol	Chain	Res	Type
35	YA	2334	G
35	YA	2336	A
35	YA	2342	C
35	YA	2346	A
35	YA	2347	C
35	YA	2350	C
35	YA	2354	G
35	YA	2377	A
35	YA	2383	G
35	YA	2385	C
35	YA	2403	C
35	YA	2406	U
35	YA	2410	G
35	YA	2423	U
35	YA	2425	A
35	YA	2429	G
35	YA	2430	A
35	YA	2435	A
35	YA	2439	A
35	YA	2440	C
35	YA	2441	C
35	YA	2445	G
35	YA	2448	A
35	YA	2465	C
35	YA	2469	A
35	YA	2470	G
35	YA	2474	C
35	YA	2475	C
35	YA	2478	A
35	YA	2480	C
35	YA	2491	U
35	YA	2494	G
35	YA	2498	C
35	YA	2502	G
35	YA	2505	G
35	YA	2518	A
35	YA	2525	G
35	YA	2529	G
35	YA	2542	A
35	YA	2543	G
35	YA	2554	U
35	YA	2562	U

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Mol	Chain	Res	Type
35	YA	2564	A
35	YA	2567	G
35	YA	2573	C
35	YA	2578	G
35	YA	2586	C
35	YA	2602	A
35	YA	2609	U
35	YA	2611	U
35	YA	2612	C
35	YA	2615	U
35	YA	2629	A
35	YA	2646	C
35	YA	2653	U
35	YA	2654	A
35	YA	2665	A
35	YA	2673	G
35	YA	2679	A
35	YA	2681	C
35	YA	2682	U
35	YA	2689	U
35	YA	2690	C
35	YA	2691	C
35	YA	2702	U
35	YA	2707	G
35	YA	2712	U
35	YA	2712(A)	A
35	YA	2713	A
35	YA	2714	G
35	YA	2718	G
35	YA	2726	U
35	YA	2732	G
35	YA	2733	A
35	YA	2744	G
35	YA	2761	G
35	YA	2765	A
35	YA	2766	G
35	YA	2776	A
35	YA	2777	G
35	YA	2778	A
35	YA	2779	U
35	YA	2780	G
35	YA	2790	A

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Mol	Chain	Res	Type
35	YA	2791	C
35	YA	2797	U
35	YA	2798	C
35	YA	2807	G
35	YA	2808	U
35	YA	2818	G
35	YA	2820	A
35	YA	2821	A
35	YA	2823	A
35	YA	2833	G
35	YA	2834	G
35	YA	2835	A
35	YA	2849	U
35	YA	2866	U
35	YA	2872	G
35	YA	2879	C
35	YA	2880	C
35	YA	2891	G
35	YA	2892	A
35	YA	2894	G
36	YB	7	G
36	YB	8	U
36	YB	9	G
36	YB	12	C
36	YB	13	A
36	YB	15	A
36	YB	19	G
36	YB	22	U
36	YB	40	U
36	YB	42	C
36	YB	45	A
36	YB	52	A
36	YB	53	A
36	YB	56	G
36	YB	73	A
36	YB	81	G
36	YB	82	G
36	YB	109	G

All (150) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	QA	115	G
1	QA	181	G
1	QA	243	A
1	QA	244	U
1	QA	250	A
1	QA	266	G
1	QA	328	C
1	QA	410	G
1	QA	412	A
1	QA	484	G
1	QA	485	G
1	QA	509	A
1	QA	687	A
1	QA	703	G
1	QA	753	A
1	QA	792	A
1	QA	812	C
1	QA	913	A
1	QA	992	U
1	QA	1027	C
1	QA	1065	U
1	QA	1285	A
1	QA	1297	C
1	QA	1336	C
1	QA	1346	A
1	QA	1347	G
1	QA	1446	A
1	QA	1498	U
1	QA	1528	U
23	QX	18	G
35	RA	74	A
35	RA	99	U
35	RA	102	G
35	RA	221	A
35	RA	222	A
35	RA	227	A
35	RA	229	A
35	RA	242	G
35	RA	271(B)	G
35	RA	271(C)	U
35	RA	345	A

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Mol	Chain	Res	Type
35	RA	372	G
35	RA	404	C
35	RA	503	A
35	RA	508	G
35	RA	512	G
35	RA	587	C
35	RA	637	A
35	RA	752	A
35	RA	846	C
35	RA	856	C
35	RA	1022	G
35	RA	1026	U
35	RA	1045	A
35	RA	1078	U
35	RA	1085	A
35	RA	1178	C
35	RA	1210	A
35	RA	1312	U
35	RA	1427	A
35	RA	1558	A
35	RA	1653	G
35	RA	1694	C
35	RA	1799	G
35	RA	1819	A
35	RA	1930	G
35	RA	1992	G
35	RA	2060	A
35	RA	2126	A
35	RA	2405	G
35	RA	2439	A
35	RA	2566	A
35	RA	2610	C
35	RA	2689	U
35	RA	2712	U
35	RA	2776	A
35	RA	2832	U
36	RB	66	A
1	XA	60	A
1	XA	78	G
1	XA	89	U
1	XA	115	G
1	XA	243	A

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Mol	Chain	Res	Type
1	XA	244	U
1	XA	250	A
1	XA	266	G
1	XA	328	C
1	XA	345	C
1	XA	410	G
1	XA	412	A
1	XA	484	G
1	XA	485	G
1	XA	509	A
1	XA	560	U
1	XA	687	A
1	XA	703	G
1	XA	753	A
1	XA	793	U
1	XA	812	C
1	XA	913	A
1	XA	992	U
1	XA	1027	C
1	XA	1285	A
1	XA	1297	C
1	XA	1498	U
23	XX	18	G
35	YA	99	U
35	YA	102	G
35	YA	221	A
35	YA	222	A
35	YA	229	A
35	YA	242	G
35	YA	271(B)	G
35	YA	278	A
35	YA	404	C
35	YA	503	A
35	YA	587	C
35	YA	637	A
35	YA	653	A
35	YA	752	A
35	YA	827	U
35	YA	846	C
35	YA	856	C
35	YA	859	G
35	YA	1022	G

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Mol	Chain	Res	Type
35	YA	1026	U
35	YA	1045	A
35	YA	1085	A
35	YA	1178	C
35	YA	1204	A
35	YA	1210	A
35	YA	1427	A
35	YA	1558	A
35	YA	1653	G
35	YA	1694	C
35	YA	1698	A
35	YA	1799	G
35	YA	1819	A
35	YA	1955	U
35	YA	1992	G
35	YA	2126	A
35	YA	2406	U
35	YA	2439	A
35	YA	2566	A
35	YA	2610	C
35	YA	2681	C
35	YA	2689	U
35	YA	2712	U
35	YA	2776	A
35	YA	2832	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 855 ligands modelled in this entry, 851 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	501	4	0,12,12	-	-	-		
58	SF4	QD	501	-	0,12,12	-	-	-		
57	PAR	XA	1670	-	44,45,45	0.86	1 (2%)	63,67,67	1.27	6 (9%)
57	PAR	QA	1663	-	44,45,45	0.81	0	63,67,67	1.26	7 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	XD	501	4	-	-	0/6/5/5
58	SF4	QD	501	-	-	-	0/6/5/5
57	PAR	XA	1670	-	-	4/18/94/94	0/4/4/4
57	PAR	QA	1663	-	-	3/18/94/94	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	XA	1670	PAR	C24-N24	-2.02	1.44	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	QA	1663	PAR	C13-O52-C52	-3.35	110.03	117.98
57	XA	1670	PAR	C13-O52-C52	-3.01	110.85	117.98
57	XA	1670	PAR	O11-C42-C32	-2.97	102.08	109.18
57	QA	1663	PAR	O62-C62-C12	-2.58	105.08	109.90
57	QA	1663	PAR	O33-C33-C23	-2.57	103.05	111.32
57	XA	1670	PAR	O62-C62-C12	-2.42	105.38	109.90
57	XA	1670	PAR	O33-C33-C23	-2.39	103.62	111.32
57	QA	1663	PAR	O11-C42-C32	-2.18	103.98	109.18
57	QA	1663	PAR	C11-C21-N21	-2.18	106.28	110.20
57	XA	1670	PAR	O11-C11-C21	-2.13	104.59	108.08
57	QA	1663	PAR	C64-C54-C44	-2.13	107.82	112.80
57	XA	1670	PAR	C31-C41-C51	-2.12	106.39	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	QA	1663	PAR	C11-O51-C51	2.03	117.69	113.72

There are no chirality outliers.

All (7) torsion outliers are listed below:

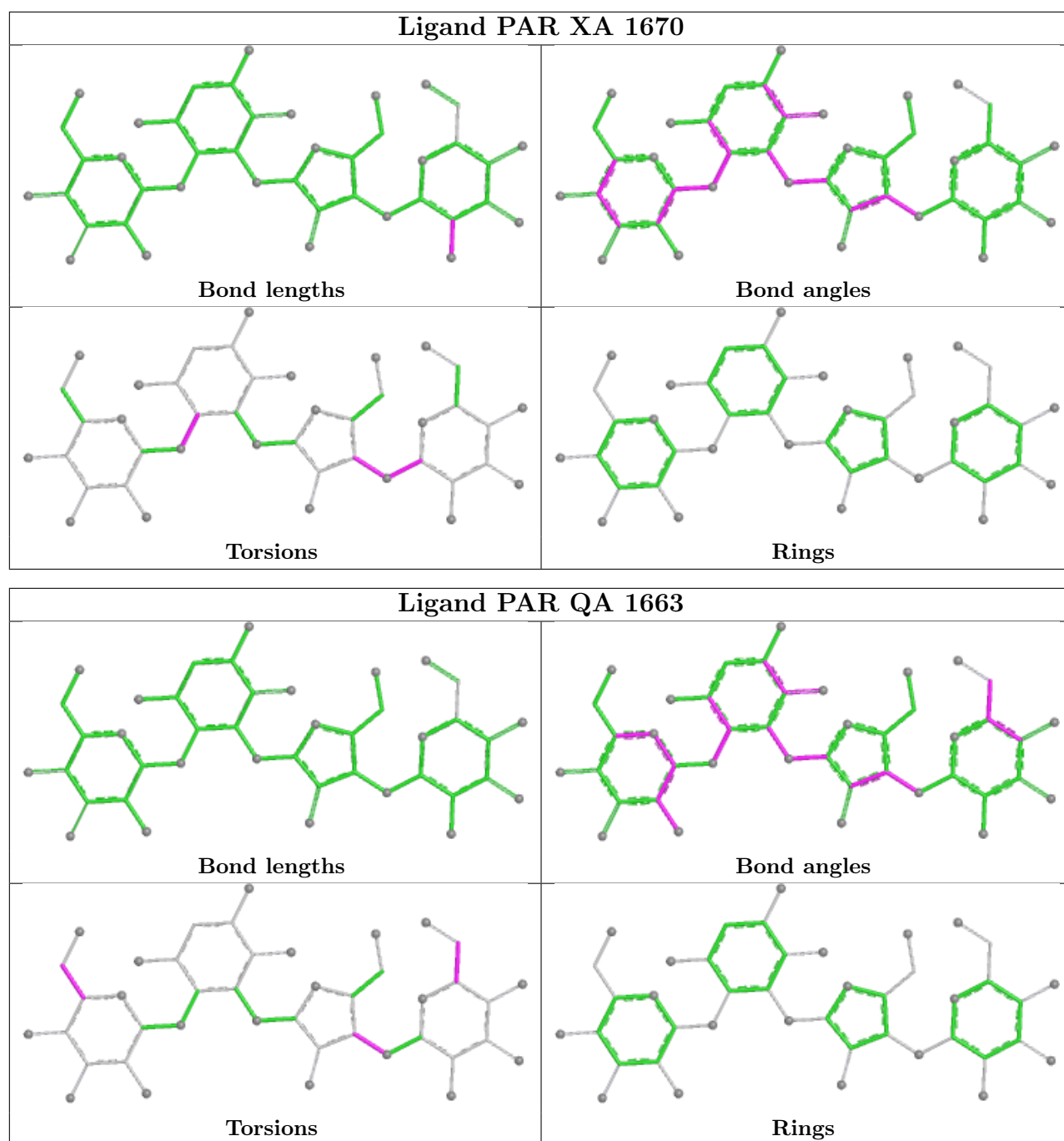
Mol	Chain	Res	Type	Atoms
57	QA	1663	PAR	O54-C54-C64-N64
57	XA	1670	PAR	O54-C14-O33-C33
57	QA	1663	PAR	O51-C51-C61-O61
57	QA	1663	PAR	C23-C33-O33-C14
57	XA	1670	PAR	C43-C33-O33-C14
57	XA	1670	PAR	C23-C33-O33-C14
57	XA	1670	PAR	C52-C42-O11-C11

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	XA	1670	PAR	4	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	1500/1522 (98%)	0.19	31 (2%) 63 42	53, 93, 175, 270	0
1	XA	1500/1522 (98%)	0.08	20 (1%) 75 56	48, 82, 158, 266	0
2	QB	237/256 (92%)	0.78	20 (8%) 17 9	86, 128, 167, 198	0
2	XB	237/256 (92%)	0.57	11 (4%) 37 20	72, 111, 154, 176	0
3	QC	205/239 (85%)	0.72	18 (8%) 15 9	90, 129, 158, 170	0
3	XC	205/239 (85%)	0.49	13 (6%) 26 14	68, 101, 144, 170	0
4	QD	208/209 (99%)	0.52	11 (5%) 32 17	62, 89, 113, 137	0
4	XD	208/209 (99%)	0.76	21 (10%) 12 6	64, 94, 123, 150	0
5	QE	151/162 (93%)	0.53	9 (5%) 27 15	78, 105, 133, 152	0
5	XE	151/162 (93%)	0.26	6 (3%) 42 23	55, 82, 115, 150	0
6	QF	101/101 (100%)	0.30	2 (1%) 65 44	55, 85, 114, 173	0
6	XF	101/101 (100%)	0.26	2 (1%) 65 44	64, 90, 115, 138	0
7	QG	155/156 (99%)	0.79	11 (7%) 22 12	92, 115, 160, 177	0
7	XG	155/156 (99%)	0.48	6 (3%) 43 24	72, 98, 135, 156	0
8	QH	138/138 (100%)	0.85	14 (10%) 12 6	72, 102, 128, 145	0
8	XH	138/138 (100%)	0.58	6 (4%) 40 22	58, 88, 117, 138	0
9	QI	127/128 (99%)	1.42	30 (23%) 2 1	101, 129, 153, 172	0
9	XI	127/128 (99%)	1.05	19 (14%) 5 3	64, 111, 147, 159	0
10	QJ	99/105 (94%)	1.52	29 (29%) 1 1	111, 138, 174, 179	0
10	XJ	99/105 (94%)	1.12	12 (12%) 8 5	66, 119, 157, 170	0
11	QK	119/129 (92%)	0.81	8 (6%) 24 13	62, 97, 132, 163	0
11	XK	119/129 (92%)	0.75	8 (6%) 24 13	59, 85, 126, 147	0
12	QL	125/131 (95%)	1.15	20 (16%) 5 2	62, 90, 129, 179	0
12	XL	125/131 (95%)	0.79	17 (13%) 7 4	49, 70, 116, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	QM	121/126 (96%)	1.16	22 (18%)	3	1	88, 126, 155, 176	0
13	XM	121/126 (96%)	1.22	18 (14%)	5	3	72, 104, 143, 188	0
14	QN	60/61 (98%)	1.74	19 (31%)	1	1	98, 129, 156, 196	0
14	XN	60/61 (98%)	1.29	14 (23%)	2	1	66, 90, 123, 139	0
15	QO	88/89 (98%)	0.66	4 (4%)	38	20	62, 90, 125, 137	0
15	XO	88/89 (98%)	0.56	4 (4%)	38	20	56, 77, 114, 123	0
16	QP	84/88 (95%)	0.75	6 (7%)	22	12	63, 86, 115, 144	0
16	XP	84/88 (95%)	0.76	4 (4%)	35	19	70, 90, 127, 147	0
17	QQ	100/105 (95%)	0.76	8 (8%)	18	10	66, 91, 123, 149	0
17	XQ	100/105 (95%)	0.67	9 (9%)	15	8	63, 88, 116, 133	0
18	QR	70/88 (79%)	0.41	1 (1%)	73	53	63, 90, 126, 161	0
18	XR	70/88 (79%)	0.43	2 (2%)	53	32	60, 93, 118, 160	0
19	QS	84/93 (90%)	1.38	19 (22%)	2	1	101, 139, 176, 223	0
19	XS	84/93 (90%)	0.79	12 (14%)	6	3	77, 107, 139, 154	0
20	QT	99/106 (93%)	1.20	19 (19%)	3	1	63, 93, 138, 181	0
20	XT	99/106 (93%)	1.38	27 (27%)	1	1	70, 97, 127, 161	0
21	QU	25/27 (92%)	1.89	10 (40%)	1	0	95, 116, 129, 131	0
21	XU	25/27 (92%)	1.49	6 (24%)	2	1	75, 99, 123, 131	0
22	QV	77/77 (100%)	0.48	3 (3%)	43	24	71, 114, 165, 197	0
22	XV	77/77 (100%)	0.37	4 (5%)	33	17	57, 94, 129, 182	0
23	QX	18/19 (94%)	1.55	6 (33%)	1	0	77, 133, 218, 227	0
23	XX	18/19 (94%)	1.71	8 (44%)	0	0	63, 135, 222, 242	0
24	QY	75/76 (98%)	1.52	21 (28%)	1	1	79, 187, 255, 279	0
24	XY	75/76 (98%)	1.06	14 (18%)	3	1	70, 166, 221, 268	0
25	R0	82/85 (96%)	0.93	9 (10%)	10	5	60, 84, 110, 154	0
25	Y0	82/85 (96%)	0.66	5 (6%)	27	15	42, 60, 91, 131	0
26	R1	97/98 (98%)	0.96	10 (10%)	12	6	49, 69, 132, 183	0
26	Y1	97/98 (98%)	0.69	14 (14%)	6	3	34, 58, 127, 176	0
27	R2	69/72 (95%)	0.79	5 (7%)	21	11	59, 90, 130, 181	0
27	Y2	69/72 (95%)	0.71	6 (8%)	16	9	47, 66, 114, 172	0
28	R3	59/60 (98%)	0.71	2 (3%)	48	28	62, 84, 113, 156	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	Y3	59/60 (98%)	0.30	0	100	100	39, 59, 105, 133	0
29	R4	71/71 (100%)	1.31	13 (18%)	3	1	104, 148, 198, 223	0
29	Y4	71/71 (100%)	1.41	15 (21%)	2	1	80, 130, 196, 204	0
30	R5	59/60 (98%)	1.03	10 (16%)	4	2	47, 68, 154, 192	0
30	Y5	59/60 (98%)	1.08	13 (22%)	2	1	32, 60, 158, 166	0
31	R6	49/54 (90%)	2.53	29 (59%)	0	0	54, 98, 149, 190	0
31	Y6	49/54 (90%)	2.08	21 (42%)	0	0	46, 76, 135, 187	0
32	R7	49/49 (100%)	0.70	4 (8%)	17	10	45, 61, 101, 150	0
32	Y7	49/49 (100%)	0.53	4 (8%)	17	10	32, 43, 95, 165	0
33	R8	64/65 (98%)	1.26	16 (25%)	2	1	50, 73, 120, 176	0
33	Y8	64/65 (98%)	1.42	16 (25%)	2	1	41, 57, 93, 204	0
34	R9	37/37 (100%)	0.79	2 (5%)	31	17	68, 89, 125, 166	0
34	Y9	37/37 (100%)	0.28	0	100	100	44, 58, 84, 87	0
35	RA	2882/2915 (98%)	0.05	94 (3%)	49	29	43, 71, 193, 277	0
35	YA	2883/2915 (98%)	-0.11	43 (1%)	72	52	35, 54, 162, 262	0
36	RB	120/122 (98%)	0.22	1 (0%)	82	65	85, 107, 133, 149	0
36	YB	120/122 (98%)	-0.02	2 (1%)	69	48	61, 74, 95, 129	0
37	RD	272/276 (98%)	0.69	24 (8%)	15	9	41, 62, 101, 150	0
37	YD	272/276 (98%)	0.43	18 (6%)	24	13	31, 53, 83, 154	0
38	RE	205/206 (99%)	0.78	22 (10%)	11	6	45, 75, 130, 185	0
38	YE	205/206 (99%)	0.64	21 (10%)	12	6	28, 59, 118, 150	0
39	RF	202/210 (96%)	0.49	4 (1%)	65	44	46, 80, 128, 155	0
39	YF	202/210 (96%)	0.39	8 (3%)	42	23	36, 58, 122, 170	0
40	RG	181/182 (99%)	0.78	14 (7%)	19	10	76, 118, 152, 165	0
40	YG	181/182 (99%)	0.53	6 (3%)	49	29	65, 87, 128, 186	0
41	RH	170/180 (94%)	1.26	35 (20%)	2	1	88, 128, 160, 194	0
41	YH	170/180 (94%)	0.80	22 (12%)	7	4	48, 74, 113, 176	0
42	RI	146/148 (98%)	0.69	8 (5%)	30	16	63, 103, 140, 152	0
42	YI	146/148 (98%)	0.71	9 (6%)	26	14	56, 100, 139, 178	0
43	RN	138/140 (98%)	0.65	10 (7%)	21	11	52, 82, 113, 159	0
43	YN	138/140 (98%)	0.49	5 (3%)	46	26	36, 57, 104, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RO	122/122 (100%)	0.39	2 (1%) 70 49	45, 71, 97, 116	0
44	YO	122/122 (100%)	0.20	1 (0%) 82 65	34, 57, 82, 100	0
45	RP	150/150 (100%)	1.38	37 (24%) 2 1	53, 93, 141, 205	0
45	YP	150/150 (100%)	0.98	22 (14%) 6 3	29, 70, 117, 168	0
46	RQ	141/141 (100%)	1.31	30 (21%) 2 1	55, 89, 135, 178	0
46	YQ	141/141 (100%)	0.94	19 (13%) 7 4	40, 63, 116, 144	0
47	RR	118/118 (100%)	0.59	5 (4%) 40 22	48, 66, 90, 130	0
47	YR	118/118 (100%)	0.56	5 (4%) 40 22	37, 55, 82, 115	0
48	RS	111/112 (99%)	0.93	16 (14%) 6 3	73, 103, 141, 187	0
48	YS	111/112 (99%)	0.59	9 (8%) 18 10	53, 76, 127, 186	0
49	RT	137/146 (93%)	0.70	13 (9%) 14 7	54, 77, 137, 165	0
49	YT	137/146 (93%)	0.65	12 (8%) 15 9	45, 68, 129, 164	0
50	RU	117/118 (99%)	0.72	9 (7%) 19 10	49, 79, 122, 169	0
50	YU	117/118 (99%)	0.40	4 (3%) 48 28	24, 53, 91, 157	0
51	RV	101/101 (100%)	0.50	7 (6%) 23 12	53, 89, 135, 184	0
51	YV	101/101 (100%)	0.41	7 (6%) 23 12	32, 65, 113, 158	0
52	RW	113/113 (100%)	0.46	6 (5%) 32 17	45, 64, 96, 171	0
52	YW	113/113 (100%)	0.19	2 (1%) 67 47	33, 49, 88, 158	0
53	RX	92/96 (95%)	0.68	8 (8%) 16 9	53, 74, 99, 105	0
53	YX	92/96 (95%)	0.31	4 (4%) 40 22	39, 55, 86, 133	0
54	RY	102/110 (92%)	1.12	14 (13%) 6 4	71, 97, 134, 158	0
54	YY	102/110 (92%)	0.49	2 (1%) 65 44	44, 70, 106, 139	0
55	RZ	183/206 (88%)	1.23	34 (18%) 3 1	93, 135, 195, 224	0
55	YZ	183/206 (88%)	1.07	30 (16%) 4 2	56, 104, 184, 226	0
All	All	21011/21588 (97%)	0.46	1442 (6%) 23 12	24, 81, 157, 279	0

All (1442) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	QK	129	SER	12.8
11	QK	128	ALA	12.1
11	XK	129	SER	12.1
45	RP	13	ASN	10.6
13	XM	101	GLN	8.5

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Mol	Chain	Res	Type	RSRZ
19	QS	11	VAL	8.4
32	R7	48	LYS	8.1
48	YS	2	ALA	7.9
46	YQ	90	VAL	7.9
12	QL	27	LEU	7.8
55	RZ	179	ASP	7.8
9	QI	105	ASP	7.6
38	RE	79	ARG	7.6
30	R5	2	ALA	7.5
37	YD	34	VAL	7.5
11	QK	127	LYS	7.3
14	XN	2	ALA	7.3
12	QL	28	LYS	6.8
29	R4	67	TYR	6.8
25	Y0	2	ALA	6.7
24	XY	17	U	6.6
19	QS	10	PHE	6.5
9	QI	64	THR	6.5
41	RH	152	ARG	6.5
26	R1	95	LEU	6.4
45	RP	24	GLY	6.4
33	Y8	64	TYR	6.3
20	XT	9	ASN	6.3
31	R6	23	THR	6.2
31	R6	20	ASN	6.2
55	YZ	113	ALA	6.2
46	RQ	87	LYS	6.2
37	RD	38	LYS	6.1
55	RZ	176	PRO	6.1
13	XM	100	GLY	6.1
46	YQ	87	LYS	6.1
10	XJ	59	SER	6.0
30	Y5	2	ALA	5.9
32	Y7	48	LYS	5.9
49	RT	58	ASN	5.8
20	XT	14	LYS	5.8
31	R6	42	TRP	5.8
11	XK	128	ALA	5.7
35	RA	1092	C	5.7
55	RZ	175	VAL	5.6
20	XT	18	GLN	5.6
37	RD	30	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
26	Y1	85	LEU	5.6
41	RH	171	LEU	5.6
13	QM	100	GLY	5.5
22	QV	1	C	5.5
45	YP	13	ASN	5.5
41	RH	169	VAL	5.5
46	RQ	90	VAL	5.5
37	RD	36	PRO	5.4
1	QA	693	G	5.4
45	RP	70	GLN	5.4
46	YQ	91	GLU	5.4
27	Y2	15	LYS	5.4
33	Y8	53	PRO	5.4
20	XT	74	LYS	5.4
50	RU	97	ASP	5.3
12	QL	26	ALA	5.3
38	YE	79	ARG	5.3
37	YD	26	LYS	5.3
41	RH	154	PRO	5.3
31	R6	12	GLU	5.3
24	XY	54	U	5.3
29	R4	70	GLY	5.2
33	R8	53	PRO	5.2
17	QQ	24	GLU	5.2
41	RH	150	ALA	5.2
14	QN	13	THR	5.2
41	YH	155	SER	5.2
9	QI	30	GLY	5.2
13	XM	99	ARG	5.2
29	Y4	69	LYS	5.2
55	YZ	175	VAL	5.2
35	RA	1026	U	5.2
50	RU	90	VAL	5.1
20	XT	11	SER	5.1
20	QT	74	LYS	5.1
55	YZ	177	PRO	5.1
4	XD	23	GLY	5.0
54	RY	62	GLU	5.0
13	XM	102	ARG	5.0
10	QJ	59	SER	5.0
12	XL	28	LYS	5.0
21	XU	26	LYS	5.0

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Mol	Chain	Res	Type	RSRZ
26	Y1	89	GLU	5.0
54	RY	12	THR	5.0
29	Y4	67	TYR	4.9
2	QB	165	VAL	4.9
9	XI	110	GLU	4.9
25	Y0	3	HIS	4.9
35	RA	1094	U	4.9
46	YQ	80	GLU	4.9
8	XH	1	MET	4.9
41	YH	168	PRO	4.8
55	RZ	116	VAL	4.8
12	XL	129	ALA	4.8
20	QT	73	HIS	4.8
37	RD	35	LYS	4.8
45	RP	25	SER	4.8
12	QL	32	PHE	4.8
38	RE	187	ALA	4.8
35	RA	1093	G	4.8
41	YH	152	ARG	4.8
31	Y6	5	VAL	4.7
10	QJ	42	THR	4.7
22	XV	1	C	4.7
35	RA	1059	G	4.7
37	RD	32	SER	4.7
46	RQ	26	TYR	4.6
26	R1	92	LYS	4.6
3	XC	15	THR	4.6
37	RD	44	ASN	4.6
20	XT	10	LEU	4.6
31	Y6	43	CYS	4.6
13	QM	121	LYS	4.6
13	QM	88	ARG	4.6
23	XX	13	A	4.5
30	R5	50	GLY	4.5
41	YH	154	PRO	4.5
45	YP	71	VAL	4.5
48	RS	2	ALA	4.5
23	QX	14	A	4.5
20	XT	12	ALA	4.4
13	QM	102	ARG	4.4
27	R2	66	GLU	4.4
30	Y5	60	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
14	QN	38	GLY	4.4
55	YZ	176	PRO	4.4
3	QC	158	GLY	4.4
31	Y6	42	TRP	4.4
37	RD	33	LEU	4.4
45	YP	61	ARG	4.4
23	XX	12	A	4.4
8	QH	99	GLU	4.4
30	Y5	57	VAL	4.4
55	YZ	108	PRO	4.4
14	XN	8	GLU	4.3
35	RA	2169	A	4.3
26	Y1	92	LYS	4.3
45	YP	24	GLY	4.3
35	YA	1536	A	4.3
41	RH	156	ALA	4.3
41	YH	156	ALA	4.3
10	XJ	64	GLU	4.3
3	XC	167	TRP	4.3
31	Y6	27	LYS	4.3
21	QU	10	ARG	4.3
55	YZ	178	GLU	4.3
41	RH	167	GLU	4.3
14	QN	39	LEU	4.2
17	XQ	101	ARG	4.2
31	Y6	23	THR	4.2
9	QI	75	ASP	4.2
10	QJ	68	HIS	4.2
37	RD	29	PRO	4.2
45	RP	26	GLY	4.2
47	YR	106	GLY	4.2
55	YZ	174	VAL	4.2
37	YD	33	LEU	4.2
43	YN	138	LEU	4.2
14	XN	14	PRO	4.2
53	RX	3	THR	4.2
17	QQ	101	ARG	4.2
40	YG	26	GLN	4.2
24	QY	2	G	4.2
25	R0	2	ALA	4.2
13	QM	122	LYS	4.2
25	Y0	5	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
41	RH	166	GLY	4.2
33	R8	64	TYR	4.2
31	Y6	12	GLU	4.1
45	RP	18	ARG	4.1
1	QA	1054	C	4.1
33	R8	65	GLU	4.1
32	Y7	49	ARG	4.1
40	RG	2	PRO	4.1
10	QJ	46	ARG	4.1
30	R5	3	LYS	4.1
39	YF	132	VAL	4.1
48	RS	110	LEU	4.1
41	YH	153	LYS	4.1
7	QG	8	GLU	4.1
38	RE	20	ALA	4.1
45	RP	61	ARG	4.1
10	QJ	62	HIS	4.1
11	XK	117	ASN	4.0
33	R8	50	LEU	4.0
46	YQ	21	THR	4.0
33	Y8	51	ALA	4.0
33	Y8	63	PRO	4.0
29	Y4	70	GLY	4.0
31	R6	5	VAL	4.0
1	XA	1397	C	4.0
14	QN	14	PRO	4.0
30	Y5	58	LEU	4.0
7	QG	81	GLY	4.0
13	XM	122	LYS	4.0
19	QS	12	ASP	4.0
38	YE	204	ALA	4.0
21	QU	26	LYS	4.0
30	Y5	49	CYS	4.0
37	RD	34	VAL	4.0
54	RY	24	VAL	4.0
55	RZ	180	VAL	4.0
46	YQ	92	GLY	4.0
24	QY	53	G	4.0
32	Y7	47	ARG	4.0
35	RA	1058	G	4.0
31	R6	7	ILE	4.0
31	R6	17	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
31	R6	27	LYS	3.9
55	RZ	163	LEU	3.9
5	QE	24	ARG	3.9
34	R9	37	GLY	3.9
9	QI	46	ALA	3.9
37	RD	259	THR	3.9
50	YU	91	ASP	3.9
24	QY	76	A	3.9
12	XL	20	LYS	3.9
13	XM	121	LYS	3.9
26	Y1	97	LEU	3.9
45	RP	62	LEU	3.9
32	R7	49	ARG	3.9
55	RZ	107	THR	3.9
19	XS	68	GLY	3.9
55	RZ	114	GLY	3.9
30	Y5	51	TYR	3.8
31	R6	22	ALA	3.8
41	YH	170	ARG	3.8
13	XM	120	LYS	3.8
31	R6	21	TYR	3.8
55	RZ	171	ILE	3.8
38	YE	66	HIS	3.8
45	RP	19	VAL	3.8
55	YZ	116	VAL	3.8
3	QC	177	THR	3.8
55	RZ	177	PRO	3.8
20	QT	10	LEU	3.8
1	QA	1397	C	3.8
38	YE	77	ILE	3.8
38	YE	146	THR	3.8
41	RH	107	VAL	3.8
49	YT	124	ASP	3.8
46	RQ	88	GLY	3.8
46	RQ	20	ALA	3.7
31	Y6	20	ASN	3.7
29	Y4	66	SER	3.7
29	Y4	68	ARG	3.7
4	XD	4	TYR	3.7
41	YH	3	ARG	3.7
42	YI	84	GLY	3.7
31	R6	39	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
24	QY	50	G	3.7
20	XT	79	ARG	3.7
23	XX	15	A	3.7
38	RE	78	LEU	3.7
35	RA	1100	C	3.7
45	RP	36	LYS	3.7
11	QK	117	ASN	3.7
13	QM	6	GLY	3.7
20	XT	70	SER	3.7
14	QN	12	ARG	3.7
38	YE	78	LEU	3.7
41	RH	153	LYS	3.7
27	R2	72	ALA	3.6
46	YQ	138	ASP	3.6
33	Y8	30	ARG	3.6
9	QI	124	GLN	3.6
24	QY	71	C	3.6
9	QI	110	GLU	3.6
46	RQ	80	GLU	3.6
45	YP	67	MET	3.6
23	QX	15	A	3.6
12	QL	18	VAL	3.6
24	XY	62	C	3.6
41	YH	169	VAL	3.6
48	RS	14	VAL	3.6
27	Y2	11	GLU	3.6
29	Y4	63	TYR	3.6
33	Y8	61	LEU	3.6
55	RZ	120	ILE	3.6
29	R4	68	ARG	3.6
31	R6	18	ARG	3.6
45	RP	16	ARG	3.6
6	XF	53	ALA	3.6
23	XX	14	A	3.6
9	XI	105	ASP	3.6
19	XS	11	VAL	3.6
6	XF	54	LYS	3.6
19	QS	85	LYS	3.6
31	Y6	8	LYS	3.6
55	YZ	117	LEU	3.6
41	RH	151	ILE	3.6
20	QT	70	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	QA	108	G	3.5
35	RA	1103	A	3.5
45	YP	70	GLN	3.5
11	XK	127	LYS	3.5
21	XU	25	LYS	3.5
24	QY	54	U	3.5
46	RQ	104	PHE	3.5
10	XJ	33	GLN	3.5
4	XD	166	LYS	3.5
33	R8	51	ALA	3.5
38	YE	187	ALA	3.5
35	RA	1096	A	3.5
45	YP	62	LEU	3.5
35	YA	2803	C	3.5
45	RP	39	LYS	3.5
50	RU	91	ASP	3.5
46	RQ	115	MET	3.5
47	YR	1	MET	3.5
37	RD	237	GLU	3.5
46	RQ	6	ARG	3.5
25	R0	10	THR	3.5
29	R4	69	LYS	3.5
31	R6	8	LYS	3.5
49	YT	106	SER	3.5
55	RZ	174	VAL	3.5
26	Y1	98	LEU	3.5
27	R2	52	ASP	3.5
1	QA	82	U	3.5
35	RA	1060	U	3.5
12	XL	21	LYS	3.5
27	Y2	72	ALA	3.5
55	YZ	109	ALA	3.5
23	XX	11	U	3.5
30	R5	51	TYR	3.4
20	QT	69	GLY	3.4
21	QU	16	GLY	3.4
13	XM	2	ALA	3.4
14	QN	61	TRP	3.4
54	RY	55	TYR	3.4
23	QX	10	G	3.4
50	YU	118	GLY	3.4
29	Y4	60	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
35	RA	1098	A	3.4
41	YH	125	VAL	3.4
21	QU	15	ARG	3.4
45	YP	22	GLY	3.4
46	RQ	21	THR	3.4
29	Y4	5	ILE	3.4
3	QC	2	GLY	3.4
9	XI	7	THR	3.4
19	QS	69	HIS	3.4
22	XV	47	U	3.4
50	YU	95	LEU	3.4
24	XY	18	G	3.4
33	R8	48	PHE	3.3
9	XI	12	GLU	3.3
46	RQ	140	ALA	3.3
37	RD	40	THR	3.3
45	YP	15	ARG	3.3
19	QS	70	LYS	3.3
35	RA	1095	A	3.3
31	Y6	22	ALA	3.3
46	YQ	1	MET	3.3
29	R4	5	ILE	3.3
51	YV	36	PRO	3.3
45	RP	30	THR	3.3
46	YQ	81	VAL	3.3
14	QN	15	LYS	3.3
55	YZ	97	GLU	3.3
35	RA	2121	G	3.3
12	QL	29	GLY	3.3
12	QL	120	TYR	3.3
30	Y5	46	CYS	3.3
55	RZ	144	LEU	3.3
41	RH	86	GLU	3.3
45	RP	117	GLU	3.3
42	RI	132	PRO	3.3
41	RH	106	THR	3.3
19	XS	85	LYS	3.3
25	R0	4	LYS	3.3
23	QX	13	A	3.3
33	Y8	40	GLU	3.3
35	YA	2179	C	3.3
26	R1	79	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
31	R6	6	ARG	3.2
37	RD	262	ARG	3.2
38	RE	74	PRO	3.2
38	RE	159	HIS	3.2
49	YT	1	MET	3.2
31	Y6	15	GLU	3.2
42	RI	10	GLU	3.2
31	Y6	41	PRO	3.2
30	R5	49	CYS	3.2
3	QC	167	TRP	3.2
9	QI	119	ALA	3.2
5	QE	25	ARG	3.2
14	QN	8	GLU	3.2
21	QU	6	ARG	3.2
31	Y6	29	ASN	3.2
48	YS	108	GLY	3.2
46	RQ	22	LYS	3.2
31	R6	41	PRO	3.2
1	QA	1451	A	3.2
46	RQ	81	VAL	3.2
37	RD	27	THR	3.2
37	YD	25	THR	3.2
49	YT	112	ARG	3.2
46	RQ	24	GLY	3.2
33	Y8	59	LYS	3.2
8	QH	112	LEU	3.2
46	YQ	104	PHE	3.2
24	QY	49	A	3.2
38	RE	204	ALA	3.2
35	RA	1099	G	3.2
39	YF	131	GLY	3.2
35	YA	2804	C	3.2
10	QJ	40	LEU	3.2
55	RZ	108	PRO	3.2
4	QD	73	ARG	3.2
31	R6	44	ARG	3.2
38	RE	77	ILE	3.2
1	QA	1196	U	3.1
19	XS	76	PRO	3.1
1	XA	422	C	3.1
35	RA	11	G	3.1
35	RA	1089	G	3.1

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Mol	Chain	Res	Type	RSRZ
35	YA	2123	G	3.1
21	XU	15	ARG	3.1
2	XB	195	ASP	3.1
3	XC	2	GLY	3.1
8	QH	73	ASP	3.1
12	QL	72	GLY	3.1
14	XN	44	LEU	3.1
55	YZ	114	GLY	3.1
55	YZ	144	LEU	3.1
31	R6	24	GLU	3.1
30	Y5	52	TYR	3.1
45	RP	67	MET	3.1
1	XA	1054	C	3.1
13	XM	8	GLU	3.1
41	YH	86	GLU	3.1
46	RQ	96	VAL	3.1
14	XN	3	ARG	3.1
4	QD	154	ASN	3.1
38	RE	65	GLY	3.1
54	RY	10	GLY	3.1
10	QJ	58	ASP	3.1
10	XJ	45	ARG	3.1
16	QP	68	ASP	3.1
33	R8	54	GLU	3.1
35	RA	1102	C	3.1
42	YI	117	GLU	3.1
35	YA	2112	G	3.1
31	Y6	26	ASN	3.1
46	YQ	140	ALA	3.1
9	XI	102	LEU	3.1
20	QT	102	GLY	3.1
13	QM	91	ARG	3.1
55	YZ	179	ASP	3.1
48	RS	7	TYR	3.1
7	QG	38	LEU	3.0
13	QM	66	LEU	3.0
41	YH	171	LEU	3.0
25	R0	3	HIS	3.0
33	R8	31	HIS	3.0
9	QI	111	ARG	3.0
17	QQ	91	ARG	3.0
29	R4	71	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
37	RD	238	GLY	3.0
7	QG	113	GLU	3.0
48	RS	27	SER	3.0
23	XX	23	A	3.0
35	YA	2119	A	3.0
7	QG	37	ASN	3.0
29	R4	40	HIS	3.0
38	YE	76	ARG	3.0
45	YP	65	ARG	3.0
14	XN	13	THR	3.0
21	QU	8	THR	3.0
33	Y8	34	TRP	3.0
1	XA	1302	U	3.0
38	YE	128	SER	3.0
35	RA	1091	G	3.0
6	QF	83	ASP	3.0
48	RS	17	ARG	3.0
37	RD	26	LYS	3.0
43	RN	84	LYS	3.0
45	RP	14	LYS	3.0
46	RQ	18	LYS	3.0
46	YQ	24	GLY	3.0
55	YZ	118	GLN	3.0
35	YA	229	A	3.0
10	QJ	67	THR	3.0
25	R0	45	PHE	3.0
31	R6	30	THR	3.0
1	QA	88	C	3.0
8	XH	2	LEU	3.0
35	YA	9	U	3.0
10	XJ	55	LYS	3.0
25	R0	76	GLY	3.0
37	RD	243	GLY	3.0
46	YQ	88	GLY	3.0
2	QB	15	VAL	3.0
19	XS	9	VAL	3.0
32	R7	46	VAL	3.0
35	RA	2168	G	3.0
31	R6	26	ASN	3.0
19	QS	39	THR	3.0
37	RD	10	THR	3.0
1	QA	1531	A	3.0

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Mol	Chain	Res	Type	RSRZ
17	XQ	98	LEU	3.0
33	Y8	62	LEU	3.0
49	YT	6	LEU	3.0
2	QB	188	ALA	3.0
49	RT	106	SER	3.0
49	YT	12	SER	3.0
55	YZ	52	SER	3.0
35	RA	2179	C	3.0
55	RZ	115	GLY	3.0
1	XA	723	U	3.0
33	R8	35	GLN	3.0
37	YD	44	ASN	3.0
21	QU	14	TRP	2.9
35	YA	2793	G	2.9
41	RH	155	SER	2.9
45	RP	71	VAL	2.9
45	YP	19	VAL	2.9
13	XM	4	ILE	2.9
32	R7	47	ARG	2.9
55	RZ	59	LEU	2.9
12	QL	31	PRO	2.9
40	RG	137	GLU	2.9
40	YG	35	GLU	2.9
46	RQ	63	LYS	2.9
2	XB	72	GLY	2.9
14	QN	36	PHE	2.9
3	XC	14	ILE	2.9
5	QE	10	MET	2.9
40	RG	86	MET	2.9
26	R1	98	LEU	2.9
54	RY	43	ASN	2.9
35	RA	1076	C	2.9
43	YN	68	GLU	2.9
53	RX	79	ALA	2.9
35	RA	1420	U	2.9
9	XI	19	LEU	2.9
15	QO	59	MET	2.9
40	RG	96	ARG	2.9
48	YS	3	ARG	2.9
54	RY	57	GLN	2.9
40	RG	97	ASP	2.9
1	QA	60	A	2.9

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Mol	Chain	Res	Type	RSRZ
1	XA	1451	A	2.9
31	R6	16	CYS	2.9
35	RA	275	G	2.9
35	RA	1087	G	2.9
35	RA	1847	A	2.9
15	QO	60	VAL	2.9
33	R8	45	GLY	2.9
35	RA	2138	C	2.9
35	RA	2803	C	2.9
35	YA	2896	C	2.9
4	XD	76	ARG	2.9
45	RP	108	LYS	2.9
51	YV	45	THR	2.9
33	Y8	54	GLU	2.9
32	Y7	46	VAL	2.9
40	RG	28	VAL	2.9
21	QU	18	TYR	2.9
45	RP	22	GLY	2.9
48	RS	20	ARG	2.9
1	QA	1001	G	2.9
1	QA	1053	G	2.9
9	XI	78	LYS	2.9
42	RI	1	MET	2.9
1	QA	723	U	2.8
35	RA	34	C	2.8
52	RW	94	ASP	2.8
31	Y6	24	GLU	2.8
37	YD	30	GLU	2.8
46	RQ	91	GLU	2.8
55	RZ	178	GLU	2.8
50	YU	90	VAL	2.8
55	YZ	180	VAL	2.8
45	RP	65	ARG	2.8
14	XN	15	LYS	2.8
31	R6	34	LEU	2.8
55	RZ	121	HIS	2.8
9	XI	94	ALA	2.8
23	XX	10	G	2.8
35	RA	2166	G	2.8
35	YA	12	U	2.8
35	YA	2121	G	2.8
3	QC	15	THR	2.8

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Mol	Chain	Res	Type	RSRZ
4	XD	80	GLU	2.8
35	RA	2896	C	2.8
9	QI	29	ASN	2.8
13	XM	85	GLY	2.8
41	YH	5	GLY	2.8
42	RI	116	LEU	2.8
55	YZ	115	GLY	2.8
2	QB	114	ARG	2.8
19	QS	9	VAL	2.8
16	XP	29	ASP	2.8
10	QJ	54	PHE	2.8
11	XK	98	LEU	2.8
16	QP	19	ILE	2.8
45	RP	20	GLY	2.8
54	RY	5	MET	2.8
1	QA	328	C	2.8
1	QA	1129	C	2.8
1	XA	1018	C	2.8
31	Y6	16	CYS	2.8
27	Y2	70	GLN	2.8
4	XD	3	ARG	2.8
9	QI	66	ARG	2.8
17	XQ	35	VAL	2.8
45	RP	101	VAL	2.8
31	R6	10	LEU	2.8
33	Y8	50	LEU	2.8
46	RQ	139	GLU	2.8
53	YX	67	GLY	2.8
3	XC	193	TYR	2.8
7	XG	85	TYR	2.8
35	RA	276	A	2.8
35	RA	1069	A	2.8
35	RA	2167	U	2.8
9	QI	73	GLN	2.8
24	XY	61	C	2.8
55	RZ	113	ALA	2.8
37	YD	38	LYS	2.8
35	YA	2805	G	2.8
26	R1	2	SER	2.8
3	QC	160	ALA	2.7
29	Y4	39	CYS	2.7
45	RP	6	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
9	QI	7	THR	2.7
9	XI	30	GLY	2.7
13	XM	64	TRP	2.7
24	QY	22	G	2.7
17	XQ	91	ARG	2.7
13	XM	12	ASN	2.7
37	RD	39	LYS	2.7
48	YS	7	TYR	2.7
10	QJ	32	ALA	2.7
8	QH	97	VAL	2.7
2	XB	155	LEU	2.7
12	QL	5	PRO	2.7
4	QD	23	GLY	2.7
35	RA	1084	A	2.7
45	YP	58	THR	2.7
47	RR	93	GLY	2.7
20	QT	8	ARG	2.7
7	QG	152	ALA	2.7
23	XX	9	G	2.7
33	Y8	35	GLN	2.7
35	YA	615	G	2.7
10	QJ	47	PHE	2.7
12	XL	89	ARG	2.7
14	QN	23	ARG	2.7
11	QK	11	LYS	2.7
12	QL	47	LYS	2.7
30	R5	26	THR	2.7
43	YN	22	THR	2.7
24	QY	73	A	2.7
26	Y1	95	LEU	2.7
46	YQ	89	ASN	2.7
13	QM	101	GLN	2.7
16	QP	8	ARG	2.7
10	QJ	64	GLU	2.7
37	RD	139	GLY	2.7
19	QS	38	SER	2.7
9	QI	43	ALA	2.7
20	QT	12	ALA	2.7
4	QD	4	TYR	2.7
11	XK	47	VAL	2.7
13	XM	90	LEU	2.7
20	QT	104	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
33	R8	62	LEU	2.7
9	QI	117	HIS	2.7
29	Y4	40	HIS	2.7
39	YF	133	ASN	2.7
3	QC	5	ILE	2.6
3	QC	162	GLN	2.6
30	Y5	5	PRO	2.6
41	YH	9	ILE	2.6
45	RP	68	GLN	2.6
12	QL	21	LYS	2.6
51	RV	76	LYS	2.6
19	QS	68	GLY	2.6
1	QA	1195	C	2.6
5	QE	50	GLU	2.6
33	R8	56	GLU	2.6
38	YE	153	GLY	2.6
46	RQ	105	GLU	2.6
55	RZ	119	GLU	2.6
51	YV	49	THR	2.6
8	QH	28	ALA	2.6
10	QJ	85	LEU	2.6
19	QS	41	VAL	2.6
26	Y1	94	LEU	2.6
45	RP	42	SER	2.6
51	YV	35	LEU	2.6
55	YZ	172	ALA	2.6
12	QL	69	TYR	2.6
17	QQ	32	TYR	2.6
20	XT	73	HIS	2.6
1	XA	1453	G	2.6
35	RA	2112	G	2.6
35	RA	2802	G	2.6
35	RA	2833	G	2.6
35	YA	2795	G	2.6
52	RW	22	ASP	2.6
54	RY	44	ILE	2.6
20	QT	9	ASN	2.6
45	RP	7	ARG	2.6
35	RA	2118	U	2.6
49	RT	2	ASN	2.6
1	XA	532	A	2.6
6	QF	95	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
14	QN	46	GLU	2.6
35	RA	2799	A	2.6
9	QI	27	THR	2.6
18	XR	78	LEU	2.6
20	QT	28	ALA	2.6
55	YZ	183	LEU	2.6
35	RA	2140	C	2.6
9	QI	62	TYR	2.6
5	QE	13	ILE	2.6
8	QH	84	ARG	2.6
10	XJ	60	ARG	2.6
49	RT	29	ARG	2.6
54	RY	6	HIS	2.6
2	QB	26	PRO	2.6
9	QI	33	PHE	2.6
41	RH	10	PRO	2.6
5	XE	22	GLY	2.6
21	XU	2	GLY	2.6
41	YH	14	GLY	2.6
5	XE	81	GLU	2.6
17	QQ	58	GLU	2.6
35	RA	2779	U	2.6
35	RA	2807	G	2.6
13	QM	99	ARG	2.6
35	RA	1085	A	2.6
19	XS	38	SER	2.6
31	Y6	21	TYR	2.6
33	Y8	48	PHE	2.6
46	RQ	1	MET	2.6
35	YA	2178	C	2.6
55	RZ	118	GLN	2.6
7	QG	82	GLY	2.6
45	RP	109	GLY	2.6
28	R3	34	GLU	2.6
54	RY	29	GLU	2.6
3	QC	168	ALA	2.6
35	RA	614	U	2.6
45	RP	15	ARG	2.6
48	YS	5	THR	2.6
50	RU	52	ARG	2.6
25	Y0	53	MET	2.6
35	RA	101	G	2.6

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Mol	Chain	Res	Type	RSRZ
46	RQ	137	TYR	2.6
49	RT	14	TYR	2.6
35	RA	1077	A	2.6
12	XL	29	GLY	2.6
19	XS	84	GLY	2.6
49	RT	104	ASN	2.6
4	XD	135	LEU	2.6
1	QA	308	C	2.6
10	XJ	34	VAL	2.6
35	RA	974(A)	C	2.6
35	RA	1052	C	2.6
12	XL	19	ARG	2.6
12	XL	26	ALA	2.6
38	RE	72	VAL	2.6
38	YE	72	VAL	2.6
13	QM	79	LYS	2.6
41	RH	165	ALA	2.6
48	RS	3	ARG	2.6
10	QJ	23	ILE	2.5
10	QJ	75	ILE	2.5
7	XG	62	PHE	2.5
35	RA	1078	U	2.5
45	YP	23	PRO	2.5
12	XL	27	LEU	2.5
31	Y6	34	LEU	2.5
55	RZ	157	LEU	2.5
7	XG	37	ASN	2.5
9	XI	41	VAL	2.5
21	XU	6	ARG	2.5
33	Y8	49	VAL	2.5
35	RA	1106	G	2.5
1	QA	572	A	2.5
22	XV	38	A	2.5
38	RE	70	ALA	2.5
39	YF	127	GLU	2.5
29	Y4	22	ILE	2.5
46	RQ	66	ILE	2.5
40	RG	155	MET	2.5
35	RA	1053	C	2.5
35	YA	277	C	2.5
51	RV	75	PHE	2.5
9	QI	115	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
29	R4	64	GLY	2.5
35	YA	2118	U	2.5
35	YA	2122	U	2.5
41	YH	7	LEU	2.5
45	YP	105	LEU	2.5
2	XB	197	VAL	2.5
13	QM	7	VAL	2.5
46	RQ	102	VAL	2.5
4	XD	134	ASP	2.5
14	XN	5	ALA	2.5
20	XT	75	ASN	2.5
38	YE	68	ALA	2.5
43	RN	100	GLU	2.5
55	RZ	172	ALA	2.5
10	QJ	4	ILE	2.5
20	XT	55	ILE	2.5
14	QN	22	THR	2.5
40	YG	80	PHE	2.5
24	XY	2	G	2.5
35	RA	1063	G	2.5
35	YA	2792	G	2.5
24	QY	61	C	2.5
41	RH	170	ARG	2.5
16	QP	62	VAL	2.5
38	RE	75	VAL	2.5
26	Y1	93	GLU	2.5
55	RZ	146	ILE	2.5
55	YZ	77	ASP	2.5
9	XI	64	THR	2.5
37	YD	27	THR	2.5
38	YE	159	HIS	2.5
51	RV	36	PRO	2.5
20	QT	20	LEU	2.5
20	QT	101	GLY	2.5
30	Y5	54	GLY	2.5
52	RW	26	GLY	2.5
38	YE	59	VAL	2.5
23	QX	9	G	2.5
30	R5	53	ALA	2.5
55	YZ	152	ALA	2.5
2	XB	214	ILE	2.5
10	XJ	75	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
41	RH	162	ILE	2.5
1	QA	1320	C	2.5
8	QH	4	ASP	2.5
24	QY	17	U	2.5
35	YA	1535	U	2.5
2	QB	137	ARG	2.5
4	XD	73	ARG	2.5
9	XI	107	ARG	2.5
20	XT	15	ARG	2.5
45	YP	148	LEU	2.5
12	XL	64	TYR	2.5
45	RP	38	GLN	2.5
12	QL	68	ALA	2.4
20	XT	76	ALA	2.4
4	XD	152	SER	2.4
10	XJ	4	ILE	2.4
1	XA	1286	A	2.4
5	XE	83	GLU	2.4
23	QX	22	A	2.4
31	R6	35	GLU	2.4
35	RA	227	A	2.4
35	RA	1057	A	2.4
43	RN	68	GLU	2.4
49	RT	1	MET	2.4
19	XS	10	PHE	2.4
37	YD	35	LYS	2.4
42	YI	121	LYS	2.4
43	RN	115	ARG	2.4
44	RO	81	ASP	2.4
52	YW	92	ARG	2.4
10	XJ	90	LEU	2.4
38	RE	56	PRO	2.4
24	QY	47	U	2.4
24	QY	55	U	2.4
35	RA	12	U	2.4
35	RA	1097	U	2.4
40	YG	25	TYR	2.4
4	XD	2	GLY	2.4
9	QI	44	VAL	2.4
29	Y4	64	GLY	2.4
3	QC	189	ALA	2.4
26	Y1	54	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
41	YH	151	ILE	2.4
17	QQ	97	SER	2.4
19	QS	4	SER	2.4
9	XI	118	LYS	2.4
14	QN	37	PHE	2.4
30	Y5	33	CYS	2.4
37	YD	32	SER	2.4
43	YN	134	ARG	2.4
48	RS	30	ARG	2.4
17	QQ	43	LEU	2.4
31	R6	11	LEU	2.4
49	YT	104	ASN	2.4
9	QI	123	PRO	2.4
55	YZ	167	PRO	2.4
2	QB	136	VAL	2.4
17	QQ	33	GLY	2.4
41	RH	164	TYR	2.4
42	YI	144	VAL	2.4
50	RU	7	GLY	2.4
55	YZ	111	VAL	2.4
1	QA	631	G	2.4
1	QA	1202	G	2.4
4	XD	204	ILE	2.4
10	QJ	74	ILE	2.4
19	QS	40	ILE	2.4
20	QT	100	ILE	2.4
24	QY	72	C	2.4
24	XY	15	G	2.4
35	RA	2165	G	2.4
35	YA	2120	G	2.4
26	Y1	96	LYS	2.4
8	QH	31	PHE	2.4
9	QI	104	ARG	2.4
38	YE	163	GLU	2.4
41	RH	3	ARG	2.4
48	RS	33	LYS	2.4
54	RY	26	LYS	2.4
18	XR	46	GLU	2.4
12	XL	118	SER	2.4
41	YH	2	SER	2.4
13	QM	70	LEU	2.4
19	QS	5	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
16	XP	68	ASP	2.4
41	RH	113	VAL	2.4
43	RN	46	VAL	2.4
43	RN	62	VAL	2.4
45	RP	35	HIS	2.4
45	YP	27	HIS	2.4
48	YS	109	GLY	2.4
8	XH	110	ALA	2.4
9	QI	106	ALA	2.4
14	QN	30	ALA	2.4
1	QA	1286	A	2.4
13	QM	78	ILE	2.4
37	RD	240	ALA	2.4
55	RZ	152	ALA	2.4
35	YA	2799	A	2.4
3	QC	4	LYS	2.4
31	Y6	18	ARG	2.4
8	XH	132	GLU	2.4
20	XT	99	LEU	2.4
26	R1	97	LEU	2.4
31	R6	15	GLU	2.4
35	RA	2145	C	2.4
40	RG	35	GLU	2.4
41	YH	124	GLU	2.4
31	R6	43	CYS	2.4
35	RA	2319	G	2.4
35	RA	2805	G	2.4
21	XU	14	TRP	2.4
7	XG	80	VAL	2.4
10	QJ	100	THR	2.4
13	QM	60	VAL	2.4
37	RD	56	GLY	2.4
53	RX	6	ASP	2.4
12	QL	129	ALA	2.4
13	QM	33	ALA	2.4
38	YE	70	ALA	2.4
48	RS	102	ALA	2.4
50	RU	17	ILE	2.4
14	QN	19	ARG	2.4
4	XD	96	LEU	2.4
38	YE	63	LEU	2.4
36	YB	52	A	2.4

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Mol	Chain	Res	Type	RSRZ
12	XL	62	SER	2.4
1	XA	1126	U	2.4
9	QI	28	VAL	2.4
51	RV	50	PRO	2.4
35	RA	2804	C	2.3
7	XG	81	GLY	2.3
33	Y8	55	ALA	2.3
43	RN	114	ARG	2.3
55	RZ	109	ALA	2.3
55	RZ	87	ASP	2.3
1	QA	1182	G	2.3
35	YA	2116	G	2.3
3	QC	87	LEU	2.3
3	XC	188	LEU	2.3
13	XM	96	LEU	2.3
41	RH	109	PHE	2.3
45	YP	59	LEU	2.3
47	YR	113	LEU	2.3
48	RS	32	LEU	2.3
49	RT	114	LEU	2.3
46	YQ	139	GLU	2.3
49	RT	11	GLU	2.3
54	YY	91	GLU	2.3
10	QJ	72	VAL	2.3
2	XB	192	SER	2.3
29	R4	7	PRO	2.3
33	R8	34	TRP	2.3
51	RV	73	SER	2.3
9	XI	11	LYS	2.3
13	QM	27	LYS	2.3
17	XQ	37	LYS	2.3
4	QD	3	ARG	2.3
20	XT	8	ARG	2.3
27	Y2	69	ARG	2.3
41	YH	132	ARG	2.3
55	RZ	12	GLY	2.3
12	QL	128	ALA	2.3
31	R6	13	CYS	2.3
39	RF	21	ALA	2.3
55	YZ	120	ILE	2.3
19	QS	80	TYR	2.3
24	XY	59	U	2.3

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Mol	Chain	Res	Type	RSRZ
24	XY	70	U	2.3
53	RX	5	TYR	2.3
20	QT	72	LEU	2.3
33	R8	61	LEU	2.3
49	YT	11	GLU	2.3
13	XM	17	VAL	2.3
35	RA	2159	G	2.3
35	YA	1110	G	2.3
41	RH	114	VAL	2.3
54	RY	45	VAL	2.3
26	R1	96	LYS	2.3
4	XD	159	ARG	2.3
8	XH	101	PRO	2.3
46	RQ	59	ARG	2.3
47	YR	45	ARG	2.3
12	XL	128	ALA	2.3
16	QP	61	SER	2.3
38	RE	130	GLY	2.3
39	YF	207	GLY	2.3
55	RZ	110	GLY	2.3
49	YT	94	ALA	2.3
55	RZ	173	ALA	2.3
10	QJ	56	HIS	2.3
43	RN	1	MET	2.3
12	QL	64	TYR	2.3
46	RQ	9	TYR	2.3
10	QJ	69	ASN	2.3
25	R0	7	LEU	2.3
35	RA	265	A	2.3
35	RA	1070	A	2.3
35	RA	2117	A	2.3
35	RA	2135	A	2.3
35	YA	276	A	2.3
35	YA	1096	A	2.3
1	QA	1212	U	2.3
17	XQ	93	GLN	2.3
35	RA	1535	U	2.3
35	YA	614	U	2.3
38	YE	73	GLU	2.3
42	RI	117	GLU	2.3
43	YN	88	GLU	2.3
4	XD	112	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
12	XL	47	LYS	2.3
34	R9	15	LYS	2.3
35	RA	1064	C	2.3
42	YI	132	PRO	2.3
20	QT	96	GLY	2.3
54	YY	59	GLY	2.3
11	QK	89	ALA	2.3
2	XB	168	THR	2.3
27	R2	4	SER	2.3
46	RQ	79	LEU	2.3
48	YS	110	LEU	2.3
1	QA	1124	G	2.3
1	XA	630	G	2.3
9	XI	18	PHE	2.3
35	RA	2894	G	2.3
35	YA	1176	G	2.3
37	YD	46	GLN	2.3
2	XB	27	LYS	2.3
1	QA	996	A	2.3
9	QI	109	VAL	2.3
11	QK	126	ARG	2.3
35	YA	1177	A	2.3
37	YD	14	ARG	2.3
46	YQ	10	ARG	2.3
1	QA	429	U	2.3
1	XA	1125	U	2.3
24	XY	55	U	2.3
19	QS	76	PRO	2.3
37	RD	64	ILE	2.3
38	YE	74	PRO	2.3
41	RH	89	ILE	2.3
24	XY	16	C	2.3
31	Y6	30	THR	2.3
45	RP	32	THR	2.3
38	RE	51	PHE	2.3
5	XE	20	GLN	2.3
45	YP	68	GLN	2.3
47	RR	5	LYS	2.3
3	QC	149	ALA	2.2
3	XC	159	GLY	2.2
13	QM	30	ALA	2.2
41	RH	108	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
45	RP	34	GLY	2.2
1	QA	994	A	2.2
19	QS	71	LEU	2.2
20	XT	13	LEU	2.2
35	RA	1101	U	2.2
35	RA	1510	A	2.2
35	YA	2629	A	2.2
37	YD	15	PHE	2.2
37	YD	262	ARG	2.2
38	RE	76	ARG	2.2
47	RR	8	ARG	2.2
19	XS	65	ASN	2.2
39	RF	6	VAL	2.2
51	RV	37	VAL	2.2
18	QR	62	GLU	2.2
29	Y4	65	ASP	2.2
31	Y6	35	GLU	2.2
45	YP	74	GLU	2.2
49	RT	110	ILE	2.2
13	XM	10	PRO	2.2
16	XP	30	GLY	2.2
26	Y1	79	GLY	2.2
29	R4	1	MET	2.2
41	RH	168	PRO	2.2
46	YQ	79	LEU	2.2
46	YQ	83	MET	2.2
49	RT	6	LEU	2.2
51	YV	38	LEU	2.2
52	YW	91	GLY	2.2
2	QB	97	TRP	2.2
29	R4	27	THR	2.2
35	RA	2318	G	2.2
38	RE	92	THR	2.2
42	YI	129	THR	2.2
51	YV	44	LYS	2.2
52	RW	111	HIS	2.2
35	RA	1065	U	2.2
20	XT	19	SER	2.2
20	XT	61	SER	2.2
2	XB	15	VAL	2.2
41	RH	115	VAL	2.2
2	QB	86	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	QB	200	ILE	2.2
3	XC	161	GLU	2.2
8	QH	136	GLU	2.2
10	QJ	98	ILE	2.2
12	XL	7	ILE	2.2
16	QP	34	GLU	2.2
1	XA	1129	C	2.2
35	RA	1104	C	2.2
35	YA	2794	C	2.2
10	QJ	27	ALA	2.2
13	QM	10	PRO	2.2
20	QT	99	LEU	2.2
20	XT	56	MET	2.2
45	RP	47	ASP	2.2
30	Y5	50	GLY	2.2
10	QJ	55	LYS	2.2
17	XQ	100	LYS	2.2
4	XD	110	PHE	2.2
7	QG	4	ARG	2.2
20	XT	23	ARG	2.2
45	YP	16	ARG	2.2
41	YH	157	TYR	2.2
9	XI	81	ILE	2.2
14	QN	42	ILE	2.2
48	RS	18	ILE	2.2
1	XA	81	G	2.2
4	QD	163	GLU	2.2
15	QO	26	GLU	2.2
2	QB	101	MET	2.2
2	QB	155	LEU	2.2
9	QI	96	LEU	2.2
24	QY	58	A	2.2
35	RA	1071	G	2.2
40	RG	139	LEU	2.2
42	RI	5	LEU	2.2
48	RS	56	LEU	2.2
2	QB	14	GLY	2.2
2	XB	14	GLY	2.2
5	QE	22	GLY	2.2
20	XT	69	GLY	2.2
37	RD	2	ALA	2.2
41	YH	150	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
45	YP	69	GLY	2.2
50	RU	48	ALA	2.2
51	YV	48	GLY	2.2
33	R8	52	LYS	2.2
13	QM	108	ARG	2.2
51	RV	82	ARG	2.2
36	YB	84	C	2.2
17	XQ	29	HIS	2.2
49	RT	40	THR	2.2
2	QB	7	VAL	2.2
43	RN	9	VAL	2.2
47	RR	73	VAL	2.2
21	QU	13	ILE	2.2
40	RG	62	LEU	2.2
42	YI	12	LEU	2.2
4	QD	150	GLU	2.2
44	RO	1	MET	2.2
38	RE	205	ALA	2.2
15	XO	19	PRO	2.2
24	QY	59	U	2.2
4	XD	168	ARG	2.2
2	QB	189	ASP	2.2
14	QN	27	CYS	2.2
53	YX	65	ARG	2.2
53	YX	68	ARG	2.2
3	XC	10	PHE	2.2
45	RP	87	ASP	2.2
1	QA	1324	A	2.2
35	RA	229	A	2.2
35	RA	1073	A	2.2
1	XA	963	G	2.2
24	XY	3	G	2.2
35	RA	2116	G	2.2
29	Y4	6	HIS	2.2
25	R0	43	THR	2.1
54	RY	42	VAL	2.1
9	QI	114	TYR	2.1
41	RH	83	TYR	2.1
1	QA	1030	C	2.1
22	QV	16	C	2.1
25	R0	36	ILE	2.1
41	RH	9	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
4	XD	137	SER	2.1
10	QJ	35	SER	2.1
40	YG	69	ALA	2.1
41	RH	2	SER	2.1
52	RW	1	MET	2.1
5	QE	111	GLU	2.1
14	QN	2	ALA	2.1
10	QJ	39	PRO	2.1
30	R5	54	GLY	2.1
31	R6	28	ARG	2.1
47	RR	46	GLY	2.1
13	XM	106	ASN	2.1
1	XA	210	U	2.1
11	XK	36	ASP	2.1
35	RA	2808	U	2.1
36	RB	1	U	2.1
10	XJ	101	VAL	2.1
2	QB	107	THR	2.1
4	XD	89	THR	2.1
53	RX	45	THR	2.1
55	YZ	107	THR	2.1
8	QH	13	ILE	2.1
35	RA	2892	A	2.1
21	QU	25	LYS	2.1
55	RZ	5	LEU	2.1
10	QJ	26	ALA	2.1
12	QL	86	ARG	2.1
15	QO	88	ARG	2.1
17	XQ	68	ARG	2.1
46	RQ	134	ARG	2.1
4	QD	179	GLU	2.1
4	XD	60	GLU	2.1
39	YF	138	GLU	2.1
35	YA	2798	C	2.1
41	RH	8	PRO	2.1
53	RX	38	GLU	2.1
3	QC	3	ASN	2.1
14	XN	16	PHE	2.1
49	YT	2	ASN	2.1
53	RX	41	ASN	2.1
10	XJ	73	ASP	2.1
39	YF	173	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	XC	192	THR	2.1
5	XE	139	LEU	2.1
8	XH	83	ILE	2.1
12	QL	91	LYS	2.1
14	XN	50	LYS	2.1
19	XS	5	LEU	2.1
20	XT	72	LEU	2.1
30	R5	29	THR	2.1
40	RG	7	LEU	2.1
42	RI	78	THR	2.1
45	RP	96	THR	2.1
3	XC	164	ARG	2.1
10	QJ	60	ARG	2.1
5	QE	20	GLN	2.1
38	RE	54	GLN	2.1
39	YF	167	ALA	2.1
49	RT	5	ALA	2.1
3	QC	161	GLU	2.1
8	QH	130	GLY	2.1
20	XT	98	PRO	2.1
24	QY	14	A	2.1
35	RA	1379	A	2.1
35	RA	1536	A	2.1
35	RA	2790	A	2.1
37	YD	238	GLY	2.1
4	QD	79	PHE	2.1
35	RA	2402	C	2.1
2	QB	140	HIS	2.1
9	XI	75	ASP	2.1
19	XS	12	ASP	2.1
30	R5	4	HIS	2.1
55	RZ	40	ASP	2.1
55	YZ	45	ASP	2.1
3	QC	191	THR	2.1
14	XN	29	ARG	2.1
15	XO	68	ARG	2.1
20	XT	25	ARG	2.1
46	RQ	82	ARG	2.1
55	YZ	80	ARG	2.1
4	QD	181	MET	2.1
8	QH	1	MET	2.1
3	XC	180	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
42	RI	115	ALA	2.1
24	QY	12	U	2.1
26	R1	47	GLN	2.1
35	YA	271(C)	U	2.1
8	QH	128	GLY	2.1
19	QS	82	GLY	2.1
39	RF	207	GLY	2.1
4	QD	98	GLU	2.1
7	XG	43	PHE	2.1
26	Y1	27	GLU	2.1
26	Y1	83	GLU	2.1
27	Y2	66	GLU	2.1
30	Y5	59	GLU	2.1
38	YE	56	PRO	2.1
44	YO	108	GLU	2.1
7	QG	80	VAL	2.1
10	QJ	34	VAL	2.1
29	Y4	21	VAL	2.1
41	RH	11	VAL	2.1
12	XL	17	LYS	2.1
24	XY	73	A	2.1
35	YA	2062	A	2.1
35	YA	2801	A	2.1
40	RG	74	LYS	2.1
40	RG	84	LYS	2.1
13	QM	4	ILE	2.1
14	XN	47	LEU	2.1
14	XN	61	TRP	2.1
16	XP	28	ARG	2.1
31	Y6	37	ARG	2.1
38	RE	195	LEU	2.1
52	RW	90	ARG	2.1
46	RQ	83	MET	2.1
55	YZ	170	THR	2.1
22	QV	70	G	2.1
26	R1	24	ALA	2.1
35	RA	277	C	2.1
35	RA	2137	C	2.1
35	YA	2138	C	2.1
35	RA	1176	G	2.1
35	RA	2792	G	2.1
35	YA	2151	G	2.1

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Mol	Chain	Res	Type	RSRZ
5	XE	85	GLY	2.1
19	QS	84	GLY	2.1
39	RF	131	GLY	2.1
2	QB	57	PHE	2.1
2	XB	202	PRO	2.1
29	R4	49	PHE	2.1
29	R4	59	PHE	2.1
40	YG	54	GLU	2.1
42	YI	135	GLU	2.1
48	YS	12	PHE	2.1
12	XL	18	VAL	2.0
14	XN	18	VAL	2.0
20	XT	65	LYS	2.0
24	QY	66	U	2.0
35	YA	1026	U	2.0
43	RN	89	LYS	2.0
45	YP	36	LYS	2.0
9	XI	126	SER	2.0
4	XD	65	ARG	2.0
9	QI	128	ARG	2.0
15	XO	3	ILE	2.0
37	YD	273	ARG	2.0
41	RH	64	LEU	2.0
13	QM	64	TRP	2.0
38	RE	168	MET	2.0
46	YQ	7	MET	2.0
2	QB	205	ASP	2.0
3	XC	169	ALA	2.0
7	QG	24	THR	2.0
9	QI	32	ASP	2.0
11	XK	89	ALA	2.0
20	QT	67	ALA	2.0
26	Y1	77	ALA	2.0
35	RA	2801	A	2.0
35	YA	887	A	2.0
35	YA	2173	A	2.0
42	YI	146	ALA	2.0
53	YX	3	THR	2.0
2	QB	17	PHE	2.0
5	QE	85	GLY	2.0
8	QH	101	PRO	2.0
14	QN	16	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
48	RS	104	GLY	2.0
50	RU	118	GLY	2.0
55	YZ	110	GLY	2.0
33	R8	63	PRO	2.0
35	RA	1109	C	2.0
37	YD	39	LYS	2.0
41	RH	85	LYS	2.0
45	RP	17	LYS	2.0
48	RS	11	LYS	2.0
48	YS	111	GLU	2.0
1	XA	63	C	2.0
9	QI	14	VAL	2.0
22	XV	17	C	2.0
55	RZ	111	VAL	2.0
20	XT	83	ARG	2.0
24	QY	18	G	2.0
26	R1	11	ARG	2.0
31	R6	36	LEU	2.0
11	QK	53	SER	2.0
19	XS	4	SER	2.0
1	QA	1240	U	2.0
1	XA	189	U	2.0
35	RA	161	U	2.0
35	YA	1060	U	2.0
41	RH	111	HIS	2.0
45	RP	27	HIS	2.0
3	QC	165	THR	2.0
12	QL	30	ALA	2.0
50	RU	46	ALA	2.0
37	YD	20	ASP	2.0
47	YR	49	ASP	2.0
9	XI	100	GLY	2.0
25	Y0	60	PHE	2.0
49	YT	25	GLY	2.0
15	XO	62	GLN	2.0
20	QT	54	LYS	2.0
38	RE	69	LYS	2.0
49	YT	8	LYS	2.0
27	R2	31	GLU	2.0
35	RA	6	A	2.0
35	RA	1460	A	2.0
7	QG	10	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
53	RX	65	ARG	2.0
55	RZ	141	VAL	2.0
28	R3	8	LEU	2.0
38	YE	195	LEU	2.0
40	RG	34	LEU	2.0
3	QC	202	ILE	2.0
1	XA	345	C	2.0
24	QY	74	C	2.0
24	XY	72	C	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
56	MG	RA	3218	1/1	0.08	1.15	161,161,161,161	0
56	MG	YA	3172	1/1	0.09	0.41	115,115,115,115	0
56	MG	RA	3148	1/1	0.11	0.52	156,156,156,156	0
56	MG	YA	3346	1/1	0.13	0.54	112,112,112,112	0
56	MG	XA	1692	1/1	0.16	0.53	126,126,126,126	0
56	MG	YA	3340	1/1	0.19	0.64	117,117,117,117	0
56	MG	QA	1625	1/1	0.22	0.47	105,105,105,105	0
56	MG	QA	1653	1/1	0.22	0.25	144,144,144,144	0
56	MG	QX	102	1/1	0.23	0.55	137,137,137,137	0
56	MG	XA	1661	1/1	0.24	0.34	139,139,139,139	0
56	MG	RA	3170	1/1	0.24	0.58	159,159,159,159	0
56	MG	QA	1659	1/1	0.24	0.24	154,154,154,154	0
56	MG	RA	3236	1/1	0.24	0.89	182,182,182,182	0
56	MG	RA	3259	1/1	0.24	0.33	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3012	1/1	0.25	0.47	120,120,120,120	0
56	MG	RA	3178	1/1	0.25	0.85	102,102,102,102	0
56	MG	RA	3217	1/1	0.26	0.49	74,74,74,74	0
56	MG	YA	3290	1/1	0.26	0.30	73,73,73,73	0
56	MG	RA	3112	1/1	0.29	0.65	131,131,131,131	0
56	MG	XA	1659	1/1	0.29	0.27	112,112,112,112	0
56	MG	YA	3233	1/1	0.32	0.44	90,90,90,90	0
56	MG	YA	3106	1/1	0.32	0.94	126,126,126,126	0
56	MG	RA	3120	1/1	0.33	0.55	106,106,106,106	0
56	MG	RA	3140	1/1	0.33	0.29	89,89,89,89	0
56	MG	RA	3164	1/1	0.34	0.83	121,121,121,121	0
56	MG	QA	1643	1/1	0.34	0.72	140,140,140,140	0
56	MG	XA	1647	1/1	0.34	0.31	129,129,129,129	0
56	MG	RA	3173	1/1	0.34	0.47	109,109,109,109	0
56	MG	RA	3159	1/1	0.35	0.72	104,104,104,104	0
56	MG	YA	3118	1/1	0.37	0.29	52,52,52,52	0
56	MG	XA	1629	1/1	0.37	0.31	82,82,82,82	0
56	MG	QA	1658	1/1	0.37	0.44	108,108,108,108	0
56	MG	RA	3219	1/1	0.38	0.38	126,126,126,126	0
56	MG	RA	3166	1/1	0.38	0.50	126,126,126,126	0
56	MG	RA	3180	1/1	0.38	0.45	80,80,80,80	0
56	MG	QA	1601	1/1	0.38	0.79	134,134,134,134	0
56	MG	RA	3139	1/1	0.38	0.58	133,133,133,133	0
56	MG	YA	3163	1/1	0.39	0.55	137,137,137,137	0
56	MG	RA	3063	1/1	0.40	0.24	111,111,111,111	0
56	MG	YA	3218	1/1	0.41	0.39	99,99,99,99	0
56	MG	XA	1636	1/1	0.42	0.23	75,75,75,75	0
56	MG	XA	1655	1/1	0.42	0.85	127,127,127,127	0
56	MG	QA	1619	1/1	0.43	0.24	79,79,79,79	0
56	MG	XA	1648	1/1	0.44	0.46	101,101,101,101	0
56	MG	RA	3122	1/1	0.44	0.56	124,124,124,124	0
56	MG	YA	3164	1/1	0.44	0.22	57,57,57,57	0
56	MG	XA	1662	1/1	0.45	0.56	105,105,105,105	0
56	MG	RA	3151	1/1	0.45	0.50	95,95,95,95	0
56	MG	XX	101	1/1	0.45	0.45	104,104,104,104	0
56	MG	RA	3206	1/1	0.45	0.47	170,170,170,170	0
56	MG	YA	3202	1/1	0.45	0.55	104,104,104,104	0
56	MG	YA	3220	1/1	0.46	0.49	86,86,86,86	0
56	MG	RA	3130	1/1	0.46	0.26	68,68,68,68	0
56	MG	RA	3215	1/1	0.46	0.48	99,99,99,99	0
56	MG	QA	1656	1/1	0.46	0.23	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3195	1/1	0.46	0.35	117,117,117,117	0
56	MG	YA	3246	1/1	0.47	0.65	82,82,82,82	0
56	MG	RA	3013	1/1	0.47	0.64	127,127,127,127	0
56	MG	YA	3155	1/1	0.48	0.54	104,104,104,104	0
56	MG	XA	1619	1/1	0.48	0.45	89,89,89,89	0
56	MG	XA	1654	1/1	0.48	0.72	108,108,108,108	0
56	MG	QA	1618	1/1	0.49	0.62	97,97,97,97	0
56	MG	RA	3102	1/1	0.49	0.23	66,66,66,66	0
56	MG	YA	3168	1/1	0.49	0.49	102,102,102,102	0
56	MG	RA	3126	1/1	0.50	0.47	77,77,77,77	0
56	MG	RA	3249	1/1	0.51	0.91	117,117,117,117	0
56	MG	RA	3057	1/1	0.51	0.57	68,68,68,68	0
56	MG	XA	1607	1/1	0.51	0.40	93,93,93,93	0
56	MG	RA	3118	1/1	0.51	0.48	153,153,153,153	0
56	MG	QA	1620	1/1	0.51	0.22	113,113,113,113	0
56	MG	YA	3342	1/1	0.51	0.27	97,97,97,97	0
56	MG	RA	3051	1/1	0.51	0.52	88,88,88,88	0
56	MG	QA	1655	1/1	0.52	0.33	125,125,125,125	0
56	MG	XA	1667	1/1	0.52	0.44	107,107,107,107	0
56	MG	R9	101	1/1	0.53	0.67	140,140,140,140	0
56	MG	XA	1608	1/1	0.54	0.15	147,147,147,147	0
56	MG	RA	3202	1/1	0.54	0.44	196,196,196,196	0
56	MG	XA	1657	1/1	0.54	0.27	96,96,96,96	0
56	MG	YA	3288	1/1	0.54	0.50	106,106,106,106	0
56	MG	YA	3321	1/1	0.55	0.54	90,90,90,90	0
56	MG	QA	1637	1/1	0.55	0.29	74,74,74,74	0
56	MG	RA	3192	1/1	0.55	0.39	101,101,101,101	0
56	MG	YA	3206	1/1	0.55	0.61	103,103,103,103	0
56	MG	YQ	203	1/1	0.55	0.49	104,104,104,104	0
56	MG	RA	3245	1/1	0.56	0.36	79,79,79,79	0
56	MG	RA	3207	1/1	0.56	0.30	77,77,77,77	0
56	MG	XA	1614	1/1	0.56	0.43	114,114,114,114	0
56	MG	XA	1658	1/1	0.56	0.26	88,88,88,88	0
56	MG	QA	1644	1/1	0.56	0.14	142,142,142,142	0
56	MG	XA	1602	1/1	0.57	0.30	85,85,85,85	0
56	MG	RA	3003	1/1	0.57	0.57	172,172,172,172	0
56	MG	RA	3220	1/1	0.57	0.20	102,102,102,102	0
56	MG	YP	201	1/1	0.58	0.55	102,102,102,102	0
56	MG	QA	1612	1/1	0.58	0.62	85,85,85,85	0
56	MG	RA	3221	1/1	0.59	0.27	90,90,90,90	0
56	MG	YA	3286	1/1	0.59	0.41	83,83,83,83	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	0.59	0.35	103,103,103,103	0
56	MG	RA	3191	1/1	0.59	0.19	102,102,102,102	0
56	MG	QA	1617	1/1	0.59	0.36	62,62,62,62	0
56	MG	XA	1689	1/1	0.60	0.23	65,65,65,65	0
56	MG	YA	3238	1/1	0.60	0.18	67,67,67,67	0
56	MG	YB	201	1/1	0.60	0.48	97,97,97,97	0
56	MG	XA	1690	1/1	0.60	0.20	49,49,49,49	0
56	MG	RA	3153	1/1	0.60	0.28	116,116,116,116	0
56	MG	QA	1657	1/1	0.61	0.28	102,102,102,102	0
56	MG	RA	3210	1/1	0.61	0.36	103,103,103,103	0
56	MG	RA	3263	1/1	0.61	0.34	75,75,75,75	0
56	MG	RA	3201	1/1	0.61	0.37	92,92,92,92	0
56	MG	QA	1647	1/1	0.61	0.28	90,90,90,90	0
56	MG	RA	3143	1/1	0.61	0.35	102,102,102,102	0
56	MG	RA	3045	1/1	0.62	0.38	105,105,105,105	0
56	MG	QA	1642	1/1	0.62	0.20	96,96,96,96	0
56	MG	QA	1626	1/1	0.62	0.13	71,71,71,71	0
56	MG	QA	1632	1/1	0.62	0.76	113,113,113,113	0
56	MG	XA	1620	1/1	0.62	0.22	83,83,83,83	0
56	MG	RA	3223	1/1	0.63	0.58	120,120,120,120	0
56	MG	RA	3133	1/1	0.63	0.35	113,113,113,113	0
56	MG	RA	3113	1/1	0.63	0.34	72,72,72,72	0
56	MG	QA	1672	1/1	0.63	0.36	82,82,82,82	0
56	MG	QA	1614	1/1	0.63	0.35	67,67,67,67	0
56	MG	YA	3234	1/1	0.63	0.35	129,129,129,129	0
56	MG	RA	3073	1/1	0.64	0.52	92,92,92,92	0
56	MG	YA	3326	1/1	0.64	0.33	78,78,78,78	0
56	MG	RA	3121	1/1	0.64	0.35	89,89,89,89	0
56	MG	YA	3241	1/1	0.64	0.34	128,128,128,128	0
56	MG	RA	3155	1/1	0.64	0.19	69,69,69,69	0
56	MG	XA	1611	1/1	0.64	0.30	73,73,73,73	0
56	MG	YA	3222	1/1	0.64	0.28	64,64,64,64	0
56	MG	RA	3264	1/1	0.64	0.18	66,66,66,66	0
56	MG	XA	1663	1/1	0.65	0.27	109,109,109,109	0
56	MG	YA	3333	1/1	0.65	0.45	74,74,74,74	0
56	MG	XA	1646	1/1	0.65	0.41	122,122,122,122	0
56	MG	RA	3181	1/1	0.65	0.32	78,78,78,78	0
56	MG	XA	1634	1/1	0.66	0.21	72,72,72,72	0
56	MG	RA	3044	1/1	0.66	0.36	78,78,78,78	0
56	MG	YA	3205	1/1	0.66	0.40	66,66,66,66	0
56	MG	QA	1638	1/1	0.66	0.41	97,97,97,97	0
56	MG	YA	3217	1/1	0.66	0.29	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3252	1/1	0.66	0.20	37,37,37,37	0
56	MG	RA	3277	1/1	0.66	0.44	71,71,71,71	0
56	MG	YB	203	1/1	0.66	0.23	77,77,77,77	0
56	MG	RA	3279	1/1	0.66	0.86	105,105,105,105	0
56	MG	XA	1632	1/1	0.66	0.49	92,92,92,92	0
56	MG	RA	3150	1/1	0.67	0.19	86,86,86,86	0
56	MG	XA	1633	1/1	0.67	0.36	95,95,95,95	0
56	MG	RA	3271	1/1	0.67	0.29	86,86,86,86	0
56	MG	XA	1691	1/1	0.67	0.57	98,98,98,98	0
56	MG	XA	1650	1/1	0.67	0.11	106,106,106,106	0
56	MG	RA	3011	1/1	0.67	0.54	108,108,108,108	0
56	MG	YA	3187	1/1	0.67	0.12	57,57,57,57	0
56	MG	XA	1644	1/1	0.67	0.22	62,62,62,62	0
56	MG	YA	3323	1/1	0.67	0.48	77,77,77,77	0
56	MG	RP	203	1/1	0.68	0.30	79,79,79,79	0
56	MG	RA	3001	1/1	0.68	0.23	64,64,64,64	0
56	MG	RA	3209	1/1	0.68	0.36	130,130,130,130	0
56	MG	RA	3142	1/1	0.68	0.42	176,176,176,176	0
56	MG	YA	3300	1/1	0.68	0.35	78,78,78,78	0
56	MG	YA	3239	1/1	0.68	0.44	133,133,133,133	0
56	MG	RA	3212	1/1	0.68	0.28	71,71,71,71	0
56	MG	YA	3193	1/1	0.68	0.67	108,108,108,108	0
56	MG	XM	201	1/1	0.69	0.16	111,111,111,111	0
56	MG	RA	3067	1/1	0.69	0.51	55,55,55,55	0
56	MG	RA	3135	1/1	0.69	0.27	52,52,52,52	0
56	MG	RA	3161	1/1	0.69	0.33	85,85,85,85	0
56	MG	YA	3182	1/1	0.69	0.49	91,91,91,91	0
56	MG	XA	1668	1/1	0.69	0.60	92,92,92,92	0
56	MG	RA	3199	1/1	0.70	0.58	93,93,93,93	0
56	MG	RA	3035	1/1	0.70	0.61	78,78,78,78	0
56	MG	YA	3337	1/1	0.70	0.58	88,88,88,88	0
56	MG	RA	3177	1/1	0.70	0.30	95,95,95,95	0
56	MG	QA	1607	1/1	0.70	0.18	76,76,76,76	0
56	MG	YA	3103	1/1	0.70	0.17	61,61,61,61	0
56	MG	RB	203	1/1	0.70	0.34	64,64,64,64	0
56	MG	RA	3262	1/1	0.70	0.45	86,86,86,86	0
56	MG	YA	3154	1/1	0.70	0.42	81,81,81,81	0
56	MG	YP	203	1/1	0.70	0.32	47,47,47,47	0
56	MG	QA	1648	1/1	0.70	0.37	97,97,97,97	0
56	MG	YA	3198	1/1	0.71	0.31	67,67,67,67	0
56	MG	YA	3162	1/1	0.71	0.42	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3294	1/1	0.71	0.55	98,98,98,98	0
56	MG	YA	3298	1/1	0.71	0.23	89,89,89,89	0
56	MG	YA	3191	1/1	0.71	0.43	80,80,80,80	0
56	MG	RA	3247	1/1	0.71	0.21	66,66,66,66	0
56	MG	QA	1661	1/1	0.72	0.10	137,137,137,137	0
56	MG	RA	3196	1/1	0.72	0.29	90,90,90,90	0
56	MG	QA	1621	1/1	0.72	0.38	118,118,118,118	0
56	MG	YA	3061	1/1	0.72	0.25	44,44,44,44	0
56	MG	QA	1645	1/1	0.72	0.34	74,74,74,74	0
56	MG	YA	3165	1/1	0.72	0.21	77,77,77,77	0
56	MG	YA	3308	1/1	0.72	0.29	83,83,83,83	0
56	MG	QA	1649	1/1	0.72	0.38	79,79,79,79	0
56	MG	RA	3123	1/1	0.72	0.40	72,72,72,72	0
56	MG	YA	3122	1/1	0.72	0.27	57,57,57,57	0
56	MG	XA	1642	1/1	0.73	0.20	81,81,81,81	0
56	MG	RA	3146	1/1	0.73	0.51	92,92,92,92	0
56	MG	YA	3329	1/1	0.73	0.23	66,66,66,66	0
56	MG	RA	3273	1/1	0.73	0.34	55,55,55,55	0
56	MG	RA	3152	1/1	0.73	0.21	48,48,48,48	0
56	MG	RA	3127	1/1	0.73	0.17	39,39,39,39	0
56	MG	XA	1664	1/1	0.73	0.36	87,87,87,87	0
56	MG	RA	3246	1/1	0.73	0.28	108,108,108,108	0
56	MG	YA	3114	1/1	0.73	0.23	43,43,43,43	0
56	MG	YA	3225	1/1	0.73	0.17	36,36,36,36	0
56	MG	QA	1602	1/1	0.73	0.26	43,43,43,43	0
56	MG	XA	1637	1/1	0.73	0.15	63,63,63,63	0
56	MG	XA	1638	1/1	0.73	0.17	66,66,66,66	0
56	MG	YA	3131	1/1	0.74	0.17	50,50,50,50	0
56	MG	RA	3275	1/1	0.74	0.36	92,92,92,92	0
56	MG	RA	3214	1/1	0.74	0.23	74,74,74,74	0
56	MG	RA	3266	1/1	0.74	0.49	80,80,80,80	0
56	MG	YQ	202	1/1	0.74	0.32	80,80,80,80	0
56	MG	XA	1680	1/1	0.74	0.36	56,56,56,56	0
56	MG	YA	3111	1/1	0.75	0.43	102,102,102,102	0
56	MG	YA	3262	1/1	0.75	0.24	70,70,70,70	0
56	MG	YA	3181	1/1	0.75	0.49	65,65,65,65	0
56	MG	RA	3083	1/1	0.75	0.25	64,64,64,64	0
56	MG	RA	3225	1/1	0.75	0.26	68,68,68,68	0
56	MG	XA	1613	1/1	0.75	0.13	52,52,52,52	0
56	MG	RA	3278	1/1	0.75	0.34	75,75,75,75	0
56	MG	RA	3233	1/1	0.75	0.48	91,91,91,91	0
56	MG	QA	1631	1/1	0.76	0.12	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3167	1/1	0.76	0.20	35,35,35,35	0
56	MG	RA	3256	1/1	0.76	0.51	74,74,74,74	0
56	MG	RD	301	1/1	0.76	0.28	57,57,57,57	0
56	MG	QA	1670	1/1	0.76	0.32	77,77,77,77	0
56	MG	RA	3186	1/1	0.76	0.13	57,57,57,57	0
56	MG	RA	3080	1/1	0.76	0.24	49,49,49,49	0
56	MG	RA	3231	1/1	0.76	0.14	50,50,50,50	0
56	MG	XA	1684	1/1	0.77	0.30	61,61,61,61	0
56	MG	YA	3035	1/1	0.77	0.45	61,61,61,61	0
56	MG	YA	3199	1/1	0.77	0.20	53,53,53,53	0
56	MG	YA	3240	1/1	0.77	0.30	95,95,95,95	0
56	MG	RA	3244	1/1	0.77	0.44	56,56,56,56	0
56	MG	YA	3203	1/1	0.77	0.28	88,88,88,88	0
56	MG	RA	3252	1/1	0.77	0.47	75,75,75,75	0
56	MG	QA	1628	1/1	0.77	0.72	96,96,96,96	0
56	MG	YA	3211	1/1	0.77	0.20	62,62,62,62	0
56	MG	YA	3179	1/1	0.77	0.26	71,71,71,71	0
56	MG	YA	3156	1/1	0.77	0.38	75,75,75,75	0
56	MG	YA	3158	1/1	0.77	0.19	43,43,43,43	0
56	MG	QA	1623	1/1	0.77	0.40	92,92,92,92	0
56	MG	YA	3190	1/1	0.77	0.21	64,64,64,64	0
56	MG	RA	3046	1/1	0.77	0.31	47,47,47,47	0
56	MG	YA	3197	1/1	0.78	0.72	82,82,82,82	0
56	MG	YA	3313	1/1	0.78	0.53	87,87,87,87	0
56	MG	RA	3099	1/1	0.78	0.40	42,42,42,42	0
56	MG	QA	1654	1/1	0.78	0.31	77,77,77,77	0
56	MG	RA	3042	1/1	0.78	0.30	46,46,46,46	0
56	MG	RB	202	1/1	0.78	0.14	75,75,75,75	0
56	MG	XA	1671	1/1	0.78	0.52	62,62,62,62	0
56	MG	YA	3144	1/1	0.78	0.10	35,35,35,35	0
56	MG	XA	1678	1/1	0.78	0.28	55,55,55,55	0
56	MG	YA	3039	1/1	0.78	0.30	44,44,44,44	0
56	MG	RA	3203	1/1	0.78	0.62	101,101,101,101	0
56	MG	YA	3189	1/1	0.78	0.28	67,67,67,67	0
56	MG	YA	3291	1/1	0.78	0.34	90,90,90,90	0
56	MG	YA	3076	1/1	0.78	0.39	54,54,54,54	0
56	MG	RA	3162	1/1	0.78	0.19	58,58,58,58	0
56	MG	RA	3183	1/1	0.78	0.22	49,49,49,49	0
56	MG	YA	3301	1/1	0.78	0.13	28,28,28,28	0
56	MG	QA	1608	1/1	0.79	0.17	79,79,79,79	0
56	MG	QA	1646	1/1	0.79	0.23	97,97,97,97	0
56	MG	YA	3338	1/1	0.79	0.74	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3149	1/1	0.79	0.48	89,89,89,89	0
56	MG	XA	1666	1/1	0.79	0.13	145,145,145,145	0
56	MG	RA	3250	1/1	0.79	0.50	63,63,63,63	0
56	MG	YA	3145	1/1	0.79	0.23	49,49,49,49	0
56	MG	YA	3151	1/1	0.79	0.15	38,38,38,38	0
56	MG	XA	1625	1/1	0.79	0.10	45,45,45,45	0
56	MG	XA	1669	1/1	0.79	0.11	43,43,43,43	0
56	MG	YA	3228	1/1	0.79	0.23	60,60,60,60	0
56	MG	R0	101	1/1	0.79	0.26	57,57,57,57	0
56	MG	YA	3285	1/1	0.80	0.23	57,57,57,57	0
56	MG	RA	3222	1/1	0.80	0.21	86,86,86,86	0
56	MG	YA	3088	1/1	0.80	0.39	45,45,45,45	0
56	MG	RA	3235	1/1	0.80	0.35	51,51,51,51	0
56	MG	QA	1630	1/1	0.80	0.12	92,92,92,92	0
56	MG	YA	3293	1/1	0.80	0.38	73,73,73,73	0
56	MG	XA	1660	1/1	0.80	0.44	72,72,72,72	0
56	MG	RA	3224	1/1	0.80	0.20	63,63,63,63	0
56	MG	QA	1660	1/1	0.80	0.09	87,87,87,87	0
56	MG	QA	1639	1/1	0.80	0.26	81,81,81,81	0
56	MG	YA	3125	1/1	0.80	0.39	51,51,51,51	0
56	MG	XA	1631	1/1	0.80	0.24	71,71,71,71	0
56	MG	XA	1687	1/1	0.80	0.50	85,85,85,85	0
56	MG	YA	3282	1/1	0.80	0.20	40,40,40,40	0
56	MG	QA	1650	1/1	0.81	0.22	68,68,68,68	0
56	MG	RA	3276	1/1	0.81	0.35	84,84,84,84	0
56	MG	RA	3132	1/1	0.81	0.31	65,65,65,65	0
56	MG	RA	3055	1/1	0.81	0.12	33,33,33,33	0
56	MG	RA	3092	1/1	0.81	0.16	57,57,57,57	0
56	MG	XA	1618	1/1	0.81	0.32	43,43,43,43	0
56	MG	YA	3046	1/1	0.81	0.24	24,24,24,24	0
56	MG	YA	3344	1/1	0.81	0.12	44,44,44,44	0
56	MG	YA	3169	1/1	0.81	0.21	58,58,58,58	0
56	MG	QF	201	1/1	0.81	0.18	87,87,87,87	0
56	MG	QA	1651	1/1	0.81	0.17	88,88,88,88	0
56	MG	RA	3125	1/1	0.81	0.21	71,71,71,71	0
56	MG	QA	1603	1/1	0.81	0.54	93,93,93,93	0
56	MG	QA	1641	1/1	0.81	0.29	72,72,72,72	0
56	MG	YA	3188	1/1	0.81	0.15	72,72,72,72	0
56	MG	YA	3157	1/1	0.82	0.10	16,16,16,16	0
56	MG	YA	3091	1/1	0.82	0.32	64,64,64,64	0
56	MG	YA	3316	1/1	0.82	0.26	47,47,47,47	0
56	MG	RA	3010	1/1	0.82	0.27	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3198	1/1	0.82	0.10	64,64,64,64	0
56	MG	RA	3138	1/1	0.82	0.37	47,47,47,47	0
56	MG	RA	3184	1/1	0.82	0.41	140,140,140,140	0
56	MG	Y6	102	1/1	0.82	0.10	9,9,9,9	0
56	MG	Y9	101	1/1	0.82	0.40	82,82,82,82	0
56	MG	YA	3033	1/1	0.82	0.24	43,43,43,43	0
56	MG	YA	3127	1/1	0.82	0.10	34,34,34,34	0
56	MG	YA	3215	1/1	0.82	0.13	36,36,36,36	0
56	MG	RA	3009	1/1	0.82	0.26	36,36,36,36	0
56	MG	XA	1681	1/1	0.82	0.32	58,58,58,58	0
56	MG	RA	3016	1/1	0.82	0.53	82,82,82,82	0
56	MG	YA	3060	1/1	0.82	0.21	39,39,39,39	0
56	MG	RA	3248	1/1	0.82	0.24	71,71,71,71	0
56	MG	YA	3226	1/1	0.82	0.10	26,26,26,26	0
56	MG	RA	3114	1/1	0.82	0.16	48,48,48,48	0
56	MG	RA	3101	1/1	0.82	0.11	32,32,32,32	0
56	MG	YA	3025	1/1	0.83	0.34	26,26,26,26	0
56	MG	RA	3238	1/1	0.83	0.28	46,46,46,46	0
56	MG	XA	1649	1/1	0.83	0.30	81,81,81,81	0
56	MG	YA	3330	1/1	0.83	0.20	84,84,84,84	0
56	MG	YA	3096	1/1	0.83	0.23	39,39,39,39	0
56	MG	YA	3140	1/1	0.83	0.27	49,49,49,49	0
56	MG	YA	3141	1/1	0.83	0.26	38,38,38,38	0
56	MG	YA	3102	1/1	0.83	0.29	48,48,48,48	0
56	MG	XA	1685	1/1	0.83	0.43	58,58,58,58	0
56	MG	YA	3147	1/1	0.83	0.30	58,58,58,58	0
56	MG	YA	3171	1/1	0.83	0.21	73,73,73,73	0
56	MG	YA	3148	1/1	0.83	0.14	36,36,36,36	0
56	MG	YA	3306	1/1	0.83	0.40	90,90,90,90	0
56	MG	YA	3045	1/1	0.83	0.17	31,31,31,31	0
56	MG	RA	3111	1/1	0.83	0.41	69,69,69,69	0
56	MG	RA	3060	1/1	0.83	0.10	26,26,26,26	0
56	MG	RA	3104	1/1	0.83	0.20	57,57,57,57	0
56	MG	YX	101	1/1	0.83	0.23	101,101,101,101	0
56	MG	YA	3263	1/1	0.84	0.68	70,70,70,70	0
56	MG	QA	1636	1/1	0.84	0.21	52,52,52,52	0
56	MG	XV	101	1/1	0.84	0.20	77,77,77,77	0
56	MG	RP	202	1/1	0.84	0.36	95,95,95,95	0
56	MG	YA	3166	1/1	0.84	0.12	27,27,27,27	0
56	MG	RA	3097	1/1	0.84	0.51	87,87,87,87	0
56	MG	YA	3071	1/1	0.84	0.18	27,27,27,27	0
56	MG	RA	3269	1/1	0.84	0.40	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3170	1/1	0.84	0.19	79,79,79,79	0
56	MG	YA	3297	1/1	0.84	0.16	56,56,56,56	0
56	MG	QA	1652	1/1	0.84	0.13	142,142,142,142	0
56	MG	RA	3048	1/1	0.84	0.33	38,38,38,38	0
56	MG	YA	3129	1/1	0.84	0.26	45,45,45,45	0
56	MG	YA	3302	1/1	0.84	0.41	85,85,85,85	0
56	MG	RA	3160	1/1	0.84	0.27	74,74,74,74	0
56	MG	YA	3132	1/1	0.84	0.15	40,40,40,40	0
56	MG	YA	3183	1/1	0.84	0.12	48,48,48,48	0
56	MG	XA	1639	1/1	0.84	0.62	79,79,79,79	0
56	MG	YA	3317	1/1	0.84	0.20	50,50,50,50	0
56	MG	YA	3261	1/1	0.85	0.60	71,71,71,71	0
56	MG	RA	3119	1/1	0.85	0.20	98,98,98,98	0
56	MG	RA	3211	1/1	0.85	0.09	60,60,60,60	0
56	MG	XA	1673	1/1	0.85	0.39	62,62,62,62	0
56	MG	RA	3145	1/1	0.85	0.23	43,43,43,43	0
56	MG	YA	3055	1/1	0.85	0.48	91,91,91,91	0
56	MG	R5	101	1/1	0.85	0.14	31,31,31,31	0
56	MG	RA	3077	1/1	0.85	0.27	41,41,41,41	0
56	MG	YA	3150	1/1	0.85	0.27	78,78,78,78	0
56	MG	XA	1621	1/1	0.85	0.29	41,41,41,41	0
56	MG	QA	1662	1/1	0.85	0.23	63,63,63,63	0
56	MG	YA	3085	1/1	0.85	0.11	23,23,23,23	0
56	MG	YA	3128	1/1	0.85	0.31	39,39,39,39	0
56	MG	RB	201	1/1	0.85	0.14	72,72,72,72	0
56	MG	YA	3242	1/1	0.85	0.27	63,63,63,63	0
56	MG	YA	3243	1/1	0.85	0.34	53,53,53,53	0
56	MG	RA	3189	1/1	0.85	0.32	69,69,69,69	0
56	MG	YA	3159	1/1	0.85	0.21	30,30,30,30	0
56	MG	YA	3259	1/1	0.85	0.33	46,46,46,46	0
56	MG	YA	3260	1/1	0.85	0.38	56,56,56,56	0
56	MG	RA	3176	1/1	0.86	0.12	51,51,51,51	0
56	MG	QA	1634	1/1	0.86	0.18	59,59,59,59	0
56	MG	YA	3196	1/1	0.86	0.29	99,99,99,99	0
56	MG	RE	301	1/1	0.86	0.24	34,34,34,34	0
56	MG	RA	3193	1/1	0.86	0.16	121,121,121,121	0
56	MG	XA	1652	1/1	0.86	0.15	46,46,46,46	0
56	MG	YA	3248	1/1	0.86	0.20	36,36,36,36	0
56	MG	RA	3134	1/1	0.86	0.31	66,66,66,66	0
56	MG	RA	3062	1/1	0.86	0.23	29,29,29,29	0
56	MG	RA	3197	1/1	0.86	0.17	75,75,75,75	0
56	MG	QA	1615	1/1	0.86	0.12	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	XA	1683	1/1	0.86	0.50	66,66,66,66	0
56	MG	YA	3213	1/1	0.86	0.33	57,57,57,57	0
56	MG	YA	3271	1/1	0.86	0.16	60,60,60,60	0
56	MG	YA	3273	1/1	0.86	0.17	37,37,37,37	0
56	MG	YA	3175	1/1	0.86	0.08	35,35,35,35	0
56	MG	YA	3176	1/1	0.86	0.29	61,61,61,61	0
56	MG	YA	3178	1/1	0.86	0.28	44,44,44,44	0
56	MG	YA	3153	1/1	0.86	0.09	27,27,27,27	0
56	MG	YA	3347	1/1	0.86	0.40	74,74,74,74	0
56	MG	RA	3251	1/1	0.86	0.47	78,78,78,78	0
56	MG	RA	3154	1/1	0.86	0.20	57,57,57,57	0
56	MG	RA	3065	1/1	0.86	0.29	25,25,25,25	0
56	MG	QA	1668	1/1	0.86	0.53	90,90,90,90	0
56	MG	YQ	201	1/1	0.86	0.33	105,105,105,105	0
56	MG	RA	3261	1/1	0.86	0.16	38,38,38,38	0
56	MG	RA	3174	1/1	0.86	0.08	52,52,52,52	0
56	MG	YA	3130	1/1	0.86	0.40	69,69,69,69	0
56	MG	RA	3074	1/1	0.87	0.20	53,53,53,53	0
56	MG	YA	3001	1/1	0.87	0.40	128,128,128,128	0
56	MG	YA	3146	1/1	0.87	0.17	48,48,48,48	0
56	MG	XA	1643	1/1	0.87	0.24	63,63,63,63	0
56	MG	YA	3257	1/1	0.87	0.23	32,32,32,32	0
56	MG	YA	3319	1/1	0.87	0.10	41,41,41,41	0
56	MG	XA	1630	1/1	0.87	0.33	68,68,68,68	0
56	MG	RA	3274	1/1	0.87	0.25	59,59,59,59	0
56	MG	QA	1610	1/1	0.87	0.17	24,24,24,24	0
56	MG	RA	3089	1/1	0.87	0.41	60,60,60,60	0
56	MG	RA	3090	1/1	0.87	0.26	51,51,51,51	0
56	MG	YA	3265	1/1	0.87	0.66	72,72,72,72	0
56	MG	YA	3334	1/1	0.87	0.74	98,98,98,98	0
56	MG	YA	3180	1/1	0.87	0.39	70,70,70,70	0
56	MG	YA	3047	1/1	0.87	0.16	19,19,19,19	0
56	MG	XA	1635	1/1	0.87	0.36	62,62,62,62	0
56	MG	XA	1651	1/1	0.87	0.28	68,68,68,68	0
56	MG	RA	3136	1/1	0.87	0.15	71,71,71,71	0
56	MG	RU	201	1/1	0.87	0.24	104,104,104,104	0
56	MG	YA	3229	1/1	0.87	0.10	38,38,38,38	0
56	MG	YA	3161	1/1	0.87	0.17	46,46,46,46	0
56	MG	RA	3165	1/1	0.87	0.20	73,73,73,73	0
56	MG	YA	3235	1/1	0.87	0.31	66,66,66,66	0
56	MG	YP	202	1/1	0.87	0.12	76,76,76,76	0
56	MG	XA	1656	1/1	0.87	0.35	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3135	1/1	0.87	0.16	42,42,42,42	0
56	MG	YA	3136	1/1	0.87	0.10	34,34,34,34	0
56	MG	Y6	101	1/1	0.87	0.09	25,25,25,25	0
56	MG	RA	3156	1/1	0.87	0.13	46,46,46,46	0
56	MG	YA	3117	1/1	0.88	0.56	68,68,68,68	0
56	MG	RA	3006	1/1	0.88	0.42	65,65,65,65	0
56	MG	YA	3212	1/1	0.88	0.16	43,43,43,43	0
56	MG	RA	3226	1/1	0.88	0.28	80,80,80,80	0
56	MG	RA	3179	1/1	0.88	0.09	15,15,15,15	0
56	MG	YA	3216	1/1	0.88	0.12	51,51,51,51	0
56	MG	YA	3324	1/1	0.88	0.18	29,29,29,29	0
56	MG	YA	3048	1/1	0.88	0.24	26,26,26,26	0
56	MG	RA	3124	1/1	0.88	0.33	61,61,61,61	0
56	MG	YA	3219	1/1	0.88	0.18	41,41,41,41	0
56	MG	RA	3015	1/1	0.88	0.16	40,40,40,40	0
56	MG	RA	3100	1/1	0.88	0.33	52,52,52,52	0
56	MG	XA	1626	1/1	0.88	0.29	71,71,71,71	0
56	MG	RA	3041	1/1	0.88	0.15	26,26,26,26	0
56	MG	RA	3258	1/1	0.88	0.31	61,61,61,61	0
56	MG	XA	1682	1/1	0.88	0.21	48,48,48,48	0
56	MG	YA	3232	1/1	0.88	0.15	65,65,65,65	0
56	MG	YA	3090	1/1	0.88	0.21	33,33,33,33	0
56	MG	RA	3239	1/1	0.88	0.44	73,73,73,73	0
56	MG	YA	3012	1/1	0.88	0.28	36,36,36,36	0
56	MG	YA	3237	1/1	0.88	0.18	58,58,58,58	0
56	MG	YB	204	1/1	0.88	0.39	58,58,58,58	0
56	MG	RA	3185	1/1	0.88	0.11	59,59,59,59	0
56	MG	YA	3029	1/1	0.88	0.15	28,28,28,28	0
56	MG	RA	3094	1/1	0.88	0.36	60,60,60,60	0
56	MG	RA	3147	1/1	0.88	0.20	67,67,67,67	0
56	MG	XA	1688	1/1	0.88	0.45	80,80,80,80	0
56	MG	YA	3173	1/1	0.88	0.38	72,72,72,72	0
56	MG	YA	3245	1/1	0.88	0.36	47,47,47,47	0
56	MG	YA	3315	1/1	0.89	0.09	30,30,30,30	0
56	MG	QA	1640	1/1	0.89	0.15	52,52,52,52	0
56	MG	RA	3232	1/1	0.89	0.45	81,81,81,81	0
56	MG	RA	3253	1/1	0.89	0.19	37,37,37,37	0
56	MG	YA	3041	1/1	0.89	0.11	9,9,9,9	0
56	MG	YA	3044	1/1	0.89	0.31	34,34,34,34	0
56	MG	QA	1629	1/1	0.89	0.15	52,52,52,52	0
56	MG	RA	3216	1/1	0.89	0.14	47,47,47,47	0
56	MG	YA	3269	1/1	0.89	0.14	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3200	1/1	0.89	0.08	22,22,22,22	0
56	MG	YA	3331	1/1	0.89	0.21	53,53,53,53	0
56	MG	RA	3260	1/1	0.89	0.30	57,57,57,57	0
56	MG	YA	3230	1/1	0.89	0.27	60,60,60,60	0
56	MG	YA	3284	1/1	0.89	0.13	16,16,16,16	0
56	MG	RA	3076	1/1	0.89	0.14	52,52,52,52	0
56	MG	RA	3023	1/1	0.89	0.27	37,37,37,37	0
56	MG	RA	3079	1/1	0.89	0.22	33,33,33,33	0
56	MG	YA	3065	1/1	0.89	0.12	45,45,45,45	0
56	MG	RA	3024	1/1	0.89	0.18	36,36,36,36	0
56	MG	YA	3075	1/1	0.89	0.08	33,33,33,33	0
56	MG	RA	3082	1/1	0.89	0.16	39,39,39,39	0
56	MG	YA	3079	1/1	0.89	0.21	26,26,26,26	0
56	MG	YA	3081	1/1	0.89	0.21	26,26,26,26	0
56	MG	YE	301	1/1	0.89	0.17	17,17,17,17	0
56	MG	YA	3299	1/1	0.89	0.20	36,36,36,36	0
56	MG	XA	1675	1/1	0.89	0.27	36,36,36,36	0
56	MG	RA	3267	1/1	0.89	0.28	29,29,29,29	0
56	MG	RA	3028	1/1	0.89	0.17	47,47,47,47	0
56	MG	RA	3034	1/1	0.89	0.27	48,48,48,48	0
56	MG	RA	3163	1/1	0.89	0.17	53,53,53,53	0
56	MG	QA	1633	1/1	0.89	0.19	84,84,84,84	0
56	MG	RA	3237	1/1	0.90	0.28	50,50,50,50	0
56	MG	RA	3110	1/1	0.90	0.09	47,47,47,47	0
56	MG	RA	3020	1/1	0.90	0.20	52,52,52,52	0
56	MG	QA	1613	1/1	0.90	0.16	47,47,47,47	0
56	MG	QA	1669	1/1	0.90	0.15	49,49,49,49	0
56	MG	YA	3126	1/1	0.90	0.09	31,31,31,31	0
56	MG	RA	3182	1/1	0.90	0.15	58,58,58,58	0
56	MG	QA	1616	1/1	0.90	0.30	70,70,70,70	0
56	MG	YA	3320	1/1	0.90	0.37	67,67,67,67	0
56	MG	YA	3255	1/1	0.90	0.32	23,23,23,23	0
56	MG	YA	3207	1/1	0.90	0.06	25,25,25,25	0
56	MG	RA	3032	1/1	0.90	0.24	34,34,34,34	0
56	MG	RA	3168	1/1	0.90	0.18	45,45,45,45	0
56	MG	YA	3328	1/1	0.90	0.10	40,40,40,40	0
56	MG	QA	1604	1/1	0.90	0.22	32,32,32,32	0
56	MG	RA	3187	1/1	0.90	0.25	60,60,60,60	0
56	MG	RA	3188	1/1	0.90	0.22	92,92,92,92	0
56	MG	YA	3264	1/1	0.90	0.27	48,48,48,48	0
56	MG	RA	3172	1/1	0.90	0.10	37,37,37,37	0
56	MG	YA	3336	1/1	0.90	0.20	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3254	1/1	0.90	0.28	63,63,63,63	0
56	MG	QA	1674	1/1	0.90	0.08	140,140,140,140	0
56	MG	YA	3143	1/1	0.90	0.09	27,27,27,27	0
56	MG	YA	3341	1/1	0.90	0.19	48,48,48,48	0
56	MG	RA	3158	1/1	0.90	0.38	76,76,76,76	0
56	MG	YA	3283	1/1	0.90	0.15	28,28,28,28	0
56	MG	XA	1674	1/1	0.90	0.12	52,52,52,52	0
56	MG	YA	3087	1/1	0.90	0.26	32,32,32,32	0
56	MG	YA	3010	1/1	0.90	0.28	36,36,36,36	0
56	MG	RA	3088	1/1	0.90	0.14	39,39,39,39	0
56	MG	YA	3013	1/1	0.90	0.16	9,9,9,9	0
56	MG	YB	206	1/1	0.90	0.13	56,56,56,56	0
56	MG	YA	3185	1/1	0.90	0.07	34,34,34,34	0
56	MG	XA	1627	1/1	0.90	0.17	48,48,48,48	0
56	MG	XA	1679	1/1	0.90	0.08	50,50,50,50	0
56	MG	YA	3031	1/1	0.90	0.26	36,36,36,36	0
56	MG	YA	3236	1/1	0.90	0.26	54,54,54,54	0
56	MG	RA	3053	1/1	0.90	0.29	39,39,39,39	0
56	MG	RB	204	1/1	0.90	0.34	57,57,57,57	0
56	MG	YA	3113	1/1	0.90	0.13	41,41,41,41	0
57	PAR	XA	1670	42/42	0.90	0.13	59,64,86,122	0
56	MG	RA	3131	1/1	0.91	0.25	56,56,56,56	0
56	MG	QV	101	1/1	0.91	0.18	47,47,47,47	0
56	MG	Y0	101	1/1	0.91	0.18	33,33,33,33	0
56	MG	RA	3029	1/1	0.91	0.17	12,12,12,12	0
56	MG	YA	3089	1/1	0.91	0.16	18,18,18,18	0
56	MG	RA	3171	1/1	0.91	0.15	35,35,35,35	0
56	MG	Y8	101	1/1	0.91	0.17	31,31,31,31	0
56	MG	RF	301	1/1	0.91	0.08	59,59,59,59	0
56	MG	YA	3098	1/1	0.91	0.18	30,30,30,30	0
56	MG	YA	3303	1/1	0.91	0.14	43,43,43,43	0
56	MG	RP	201	1/1	0.91	0.49	207,207,207,207	0
56	MG	YA	3307	1/1	0.91	0.25	147,147,147,147	0
56	MG	YA	3007	1/1	0.91	0.21	26,26,26,26	0
56	MG	YA	3310	1/1	0.91	0.11	31,31,31,31	0
56	MG	RA	3190	1/1	0.91	0.07	42,42,42,42	0
56	MG	YA	3107	1/1	0.91	0.17	38,38,38,38	0
56	MG	YA	3231	1/1	0.91	0.11	49,49,49,49	0
56	MG	RA	3072	1/1	0.91	0.30	53,53,53,53	0
56	MG	RA	3093	1/1	0.91	0.14	23,23,23,23	0
56	MG	XA	1601	1/1	0.91	0.19	24,24,24,24	0
56	MG	QA	1624	1/1	0.91	0.33	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	YA	3030	1/1	0.91	0.16	16,16,16,16	0
56	MG	YA	3120	1/1	0.91	0.31	78,78,78,78	0
56	MG	YA	3325	1/1	0.91	0.07	31,31,31,31	0
56	MG	XA	1606	1/1	0.91	0.41	57,57,57,57	0
56	MG	XA	1677	1/1	0.91	0.15	49,49,49,49	0
56	MG	RA	3194	1/1	0.91	0.12	75,75,75,75	0
56	MG	RA	3268	1/1	0.91	0.09	9,9,9,9	0
56	MG	XA	1610	1/1	0.91	0.15	37,37,37,37	0
56	MG	YA	3043	1/1	0.91	0.27	38,38,38,38	0
56	MG	QA	1671	1/1	0.91	0.13	54,54,54,54	0
56	MG	YA	3186	1/1	0.91	0.18	45,45,45,45	0
56	MG	RA	3054	1/1	0.91	0.30	29,29,29,29	0
56	MG	QA	1605	1/1	0.91	0.53	62,62,62,62	0
56	MG	RA	3141	1/1	0.91	0.20	37,37,37,37	0
56	MG	RA	3022	1/1	0.91	0.17	40,40,40,40	0
56	MG	YA	3050	1/1	0.91	0.21	21,21,21,21	0
56	MG	YA	3192	1/1	0.91	0.09	45,45,45,45	0
56	MG	YA	3052	1/1	0.91	0.26	37,37,37,37	0
56	MG	YA	3195	1/1	0.91	0.23	70,70,70,70	0
56	MG	RA	3058	1/1	0.91	0.17	32,32,32,32	0
56	MG	RA	3103	1/1	0.91	0.19	35,35,35,35	0
56	MG	QA	1606	1/1	0.91	0.10	49,49,49,49	0
56	MG	YB	205	1/1	0.91	0.47	77,77,77,77	0
56	MG	QA	1609	1/1	0.91	0.13	57,57,57,57	0
56	MG	YA	3200	1/1	0.91	0.06	41,41,41,41	0
56	MG	YA	3069	1/1	0.91	0.30	42,42,42,42	0
56	MG	YA	3070	1/1	0.91	0.11	16,16,16,16	0
56	MG	YA	3204	1/1	0.91	0.09	30,30,30,30	0
56	MG	RA	3025	1/1	0.91	0.30	29,29,29,29	0
56	MG	YA	3072	1/1	0.91	0.10	41,41,41,41	0
56	MG	XA	1628	1/1	0.91	0.07	38,38,38,38	0
56	MG	XF	201	1/1	0.91	0.21	65,65,65,65	0
56	MG	RA	3257	1/1	0.91	0.22	46,46,46,46	0
56	MG	YA	3063	1/1	0.92	0.18	23,23,23,23	0
56	MG	XA	1676	1/1	0.92	0.20	60,60,60,60	0
56	MG	YA	3109	1/1	0.92	0.26	29,29,29,29	0
56	MG	RA	3265	1/1	0.92	0.25	38,38,38,38	0
56	MG	RA	3228	1/1	0.92	0.23	45,45,45,45	0
56	MG	YA	3177	1/1	0.92	0.22	53,53,53,53	0
56	MG	YA	3296	1/1	0.92	0.61	84,84,84,84	0
56	MG	YA	3335	1/1	0.92	0.29	53,53,53,53	0
56	MG	R8	101	1/1	0.92	0.11	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3116	1/1	0.92	0.12	24,24,24,24	0
56	MG	RA	3087	1/1	0.92	0.21	28,28,28,28	0
56	MG	YA	3339	1/1	0.92	0.13	40,40,40,40	0
56	MG	YA	3073	1/1	0.92	0.27	58,58,58,58	0
56	MG	YA	3036	1/1	0.92	0.24	25,25,25,25	0
56	MG	RA	3116	1/1	0.92	0.12	24,24,24,24	0
56	MG	XA	1665	1/1	0.92	0.24	57,57,57,57	0
56	MG	YA	3305	1/1	0.92	0.22	47,47,47,47	0
56	MG	QA	1665	1/1	0.92	0.19	58,58,58,58	0
56	MG	RA	3204	1/1	0.92	0.19	72,72,72,72	0
56	MG	YB	202	1/1	0.92	0.17	34,34,34,34	0
56	MG	RA	3007	1/1	0.92	0.32	71,71,71,71	0
56	MG	YA	3160	1/1	0.92	0.15	43,43,43,43	0
56	MG	YA	3311	1/1	0.92	0.17	37,37,37,37	0
56	MG	XA	1686	1/1	0.92	0.14	61,61,61,61	0
56	MG	XA	1640	1/1	0.92	0.26	45,45,45,45	0
56	MG	XA	1641	1/1	0.92	0.16	36,36,36,36	0
56	MG	QA	1611	1/1	0.92	0.19	35,35,35,35	0
56	MG	RA	3040	1/1	0.92	0.11	19,19,19,19	0
56	MG	YA	3019	1/1	0.92	0.21	18,18,18,18	0
56	MG	YA	3138	1/1	0.92	0.08	30,30,30,30	0
56	MG	YA	3139	1/1	0.92	0.20	34,34,34,34	0
56	MG	RA	3242	1/1	0.92	0.10	28,28,28,28	0
57	PAR	QA	1663	42/42	0.92	0.11	59,59,76,103	0
56	MG	YA	3026	1/1	0.92	0.15	26,26,26,26	0
56	MG	YA	3201	1/1	0.93	0.09	71,71,71,71	0
56	MG	YA	3123	1/1	0.93	0.07	16,16,16,16	0
56	MG	XA	1623	1/1	0.93	0.06	32,32,32,32	0
56	MG	XA	1624	1/1	0.93	0.20	34,34,34,34	0
56	MG	YA	3318	1/1	0.93	0.27	49,49,49,49	0
56	MG	RA	3084	1/1	0.93	0.06	15,15,15,15	0
56	MG	RA	3213	1/1	0.93	0.15	33,33,33,33	0
56	MG	YA	3016	1/1	0.93	0.28	28,28,28,28	0
56	MG	YA	3209	1/1	0.93	0.25	52,52,52,52	0
56	MG	XA	1653	1/1	0.93	0.27	70,70,70,70	0
56	MG	RA	3085	1/1	0.93	0.07	14,14,14,14	0
56	MG	RA	3070	1/1	0.93	0.14	32,32,32,32	0
56	MG	YA	3327	1/1	0.93	0.42	59,59,59,59	0
56	MG	YA	3214	1/1	0.93	0.17	47,47,47,47	0
56	MG	YA	3268	1/1	0.93	0.13	23,23,23,23	0
56	MG	YA	3133	1/1	0.93	0.15	46,46,46,46	0
56	MG	RA	3021	1/1	0.93	0.10	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	RA	3107	1/1	0.93	0.06	35,35,35,35	0
56	MG	YA	3276	1/1	0.93	0.08	22,22,22,22	0
56	MG	YA	3278	1/1	0.93	0.12	18,18,18,18	0
56	MG	YA	3279	1/1	0.93	0.29	164,164,164,164	0
56	MG	RA	3109	1/1	0.93	0.10	43,43,43,43	0
56	MG	YA	3032	1/1	0.93	0.17	9,9,9,9	0
56	MG	RR	201	1/1	0.93	0.17	41,41,41,41	0
56	MG	RA	3031	1/1	0.93	0.17	22,22,22,22	0
56	MG	RA	3129	1/1	0.93	0.12	59,59,59,59	0
56	MG	YA	3037	1/1	0.93	0.20	39,39,39,39	0
56	MG	YA	3343	1/1	0.93	0.29	57,57,57,57	0
56	MG	YA	3227	1/1	0.93	0.07	36,36,36,36	0
56	MG	YA	3038	1/1	0.93	0.19	22,22,22,22	0
56	MG	RA	3002	1/1	0.93	0.27	118,118,118,118	0
56	MG	QA	1666	1/1	0.93	0.20	29,29,29,29	0
56	MG	RA	3061	1/1	0.93	0.09	9,9,9,9	0
56	MG	RA	3169	1/1	0.93	0.22	35,35,35,35	0
56	MG	QA	1667	1/1	0.93	0.18	33,33,33,33	0
56	MG	YA	3152	1/1	0.93	0.22	63,63,63,63	0
56	MG	RA	3095	1/1	0.93	0.14	22,22,22,22	0
56	MG	RA	3227	1/1	0.93	0.14	90,90,90,90	0
56	MG	RA	3208	1/1	0.93	0.36	69,69,69,69	0
56	MG	XA	1617	1/1	0.93	0.19	46,46,46,46	0
56	MG	YA	3051	1/1	0.93	0.25	36,36,36,36	0
56	MG	RA	3229	1/1	0.93	0.11	17,17,17,17	0
56	MG	RA	3036	1/1	0.93	0.28	44,44,44,44	0
56	MG	YA	3057	1/1	0.93	0.10	9,9,9,9	0
56	MG	RA	3018	1/1	0.93	0.13	24,24,24,24	0
56	MG	QX	101	1/1	0.93	0.28	76,76,76,76	0
56	MG	YA	3312	1/1	0.93	0.23	44,44,44,44	0
56	MG	YA	3015	1/1	0.94	0.20	31,31,31,31	0
56	MG	YA	3184	1/1	0.94	0.09	36,36,36,36	0
56	MG	YA	3101	1/1	0.94	0.10	10,10,10,10	0
56	MG	YA	3067	1/1	0.94	0.20	23,23,23,23	0
56	MG	YA	3289	1/1	0.94	0.23	39,39,39,39	0
56	MG	RA	3205	1/1	0.94	0.23	53,53,53,53	0
56	MG	YA	3018	1/1	0.94	0.14	21,21,21,21	0
56	MG	YA	3332	1/1	0.94	0.10	42,42,42,42	0
56	MG	YA	3247	1/1	0.94	0.18	30,30,30,30	0
56	MG	XA	1615	1/1	0.94	0.29	36,36,36,36	0
56	MG	YA	3249	1/1	0.94	0.12	46,46,46,46	0
56	MG	YA	3251	1/1	0.94	0.26	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	RA	3078	1/1	0.94	0.17	47,47,47,47	0
56	MG	YA	3110	1/1	0.94	0.11	29,29,29,29	0
56	MG	YA	3256	1/1	0.94	0.50	48,48,48,48	0
56	MG	RA	3069	1/1	0.94	0.15	37,37,37,37	0
56	MG	RA	3086	1/1	0.94	0.19	21,21,21,21	0
56	MG	RA	3234	1/1	0.94	0.46	65,65,65,65	0
56	MG	YA	3304	1/1	0.94	0.23	37,37,37,37	0
56	MG	RE	303	1/1	0.94	0.12	29,29,29,29	0
56	MG	YA	3002	1/1	0.94	0.17	20,20,20,20	0
56	MG	YA	3084	1/1	0.94	0.10	9,9,9,9	0
56	MG	YA	3004	1/1	0.94	0.09	9,9,9,9	0
56	MG	YA	3309	1/1	0.94	0.23	43,43,43,43	0
56	MG	YA	3121	1/1	0.94	0.07	11,11,11,11	0
56	MG	YA	3034	1/1	0.94	0.27	14,14,14,14	0
56	MG	QA	1627	1/1	0.94	0.05	34,34,34,34	0
56	MG	YA	3270	1/1	0.94	0.13	22,22,22,22	0
56	MG	YA	3124	1/1	0.94	0.24	50,50,50,50	0
56	MG	RA	3071	1/1	0.94	0.20	37,37,37,37	0
56	MG	YA	3275	1/1	0.94	0.32	49,49,49,49	0
56	MG	RA	3167	1/1	0.94	0.20	62,62,62,62	0
56	MG	YA	3277	1/1	0.94	0.26	31,31,31,31	0
56	MG	YA	3062	1/1	0.94	0.18	28,28,28,28	0
56	MG	YA	3092	1/1	0.94	0.07	23,23,23,23	0
56	MG	YR	201	1/1	0.94	0.11	28,28,28,28	0
56	MG	YA	3322	1/1	0.94	0.14	35,35,35,35	0
56	MG	YA	3208	1/1	0.94	0.13	48,48,48,48	0
56	MG	RA	3068	1/1	0.94	0.17	40,40,40,40	0
56	MG	YA	3287	1/1	0.95	0.04	9,9,9,9	0
56	MG	RA	3030	1/1	0.95	0.16	30,30,30,30	0
56	MG	RA	3014	1/1	0.95	0.44	63,63,63,63	0
56	MG	RE	302	1/1	0.95	0.18	37,37,37,37	0
56	MG	RA	3056	1/1	0.95	0.08	32,32,32,32	0
56	MG	YA	3149	1/1	0.95	0.14	36,36,36,36	0
56	MG	YA	3017	1/1	0.95	0.08	16,16,16,16	0
56	MG	RA	3091	1/1	0.95	0.15	27,27,27,27	0
56	MG	YA	3253	1/1	0.95	0.12	9,9,9,9	0
56	MG	YA	3119	1/1	0.95	0.24	33,33,33,33	0
56	MG	YA	3078	1/1	0.95	0.22	31,31,31,31	0
56	MG	Y2	101	1/1	0.95	0.16	57,57,57,57	0
56	MG	YA	3020	1/1	0.95	0.14	12,12,12,12	0
56	MG	YA	3221	1/1	0.95	0.13	33,33,33,33	0
56	MG	YA	3021	1/1	0.95	0.14	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3023	1/1	0.95	0.15	26,26,26,26	0
56	MG	Y5	101	1/1	0.95	0.09	36,36,36,36	0
56	MG	RA	3115	1/1	0.95	0.07	21,21,21,21	0
56	MG	RA	3241	1/1	0.95	0.07	33,33,33,33	0
56	MG	YA	3056	1/1	0.95	0.07	10,10,10,10	0
56	MG	RA	3108	1/1	0.95	0.13	47,47,47,47	0
56	MG	XA	1616	1/1	0.95	0.22	34,34,34,34	0
56	MG	YA	3093	1/1	0.95	0.10	13,13,13,13	0
56	MG	YA	3272	1/1	0.95	0.15	26,26,26,26	0
56	MG	RA	3117	1/1	0.95	0.05	20,20,20,20	0
56	MG	YA	3274	1/1	0.95	0.06	24,24,24,24	0
56	MG	XA	1645	1/1	0.95	0.11	37,37,37,37	0
56	MG	RA	3081	1/1	0.95	0.25	34,34,34,34	0
56	MG	YA	3064	1/1	0.95	0.17	26,26,26,26	0
56	MG	YA	3137	1/1	0.95	0.09	31,31,31,31	0
56	MG	RA	3128	1/1	0.95	0.09	38,38,38,38	0
56	MG	YA	3280	1/1	0.95	0.19	31,31,31,31	0
56	MG	YA	3104	1/1	0.95	0.17	18,18,18,18	0
56	MG	YA	3066	1/1	0.95	0.07	26,26,26,26	0
56	MG	YA	3008	1/1	0.95	0.14	11,11,11,11	0
56	MG	YA	3068	1/1	0.95	0.07	22,22,22,22	0
56	MG	QA	1673	1/1	0.95	0.32	62,62,62,62	0
56	MG	XA	1603	1/1	0.96	0.25	41,41,41,41	0
56	MG	RA	3255	1/1	0.96	0.10	48,48,48,48	0
56	MG	YA	3244	1/1	0.96	0.17	56,56,56,56	0
56	MG	RA	3005	1/1	0.96	0.31	60,60,60,60	0
56	MG	YA	3077	1/1	0.96	0.18	12,12,12,12	0
56	MG	YA	3054	1/1	0.96	0.09	9,9,9,9	0
56	MG	YA	3009	1/1	0.96	0.11	21,21,21,21	0
56	MG	YA	3080	1/1	0.96	0.11	17,17,17,17	0
56	MG	RA	3064	1/1	0.96	0.29	17,17,17,17	0
56	MG	YA	3083	1/1	0.96	0.14	19,19,19,19	0
56	MG	QA	1664	1/1	0.96	0.12	43,43,43,43	0
56	MG	RA	3272	1/1	0.96	0.06	48,48,48,48	0
56	MG	YA	3086	1/1	0.96	0.17	30,30,30,30	0
56	MG	RA	3105	1/1	0.96	0.12	22,22,22,22	0
56	MG	RA	3106	1/1	0.96	0.11	22,22,22,22	0
56	MG	YA	3174	1/1	0.96	0.11	16,16,16,16	0
56	MG	RA	3026	1/1	0.96	0.14	42,42,42,42	0
56	MG	YA	3292	1/1	0.96	0.21	40,40,40,40	0
56	MG	RA	3033	1/1	0.96	0.14	28,28,28,28	0
56	MG	YE	303	1/1	0.96	0.08	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YN	201	1/1	0.96	0.15	32,32,32,32	0
56	MG	RA	3004	1/1	0.96	0.11	34,34,34,34	0
56	MG	RA	3157	1/1	0.96	0.17	38,38,38,38	0
56	MG	RA	3019	1/1	0.96	0.12	29,29,29,29	0
56	MG	YA	3266	1/1	0.96	0.12	26,26,26,26	0
56	MG	RA	3280	1/1	0.96	0.07	35,35,35,35	0
56	MG	YA	3024	1/1	0.96	0.12	14,14,14,14	0
56	MG	YA	3100	1/1	0.96	0.13	9,9,9,9	0
56	MG	RA	3281	1/1	0.96	0.29	146,146,146,146	0
56	MG	RA	3230	1/1	0.96	0.17	9,9,9,9	0
56	MG	YA	3049	1/1	0.96	0.14	15,15,15,15	0
59	ZN	QN	101	1/1	0.96	0.10	182,182,182,182	0
56	MG	YA	3005	1/1	0.97	0.07	9,9,9,9	0
56	MG	YA	3006	1/1	0.97	0.08	14,14,14,14	0
56	MG	RA	3008	1/1	0.97	0.21	31,31,31,31	0
56	MG	YA	3250	1/1	0.97	0.26	28,28,28,28	0
56	MG	XA	1672	1/1	0.97	0.21	39,39,39,39	0
56	MG	RA	3096	1/1	0.97	0.19	23,23,23,23	0
56	MG	XA	1604	1/1	0.97	0.29	31,31,31,31	0
56	MG	YA	3254	1/1	0.97	0.14	17,17,17,17	0
56	MG	XA	1622	1/1	0.97	0.06	34,34,34,34	0
56	MG	YA	3295	1/1	0.97	0.23	31,31,31,31	0
56	MG	YA	3097	1/1	0.97	0.12	34,34,34,34	0
56	MG	RA	3047	1/1	0.97	0.11	24,24,24,24	0
56	MG	YA	3258	1/1	0.97	0.10	20,20,20,20	0
56	MG	YA	3099	1/1	0.97	0.13	11,11,11,11	0
56	MG	YA	3223	1/1	0.97	0.04	9,9,9,9	0
56	MG	YA	3224	1/1	0.97	0.07	9,9,9,9	0
56	MG	YA	3014	1/1	0.97	0.20	9,9,9,9	0
56	MG	YA	3042	1/1	0.97	0.13	9,9,9,9	0
56	MG	YA	3345	1/1	0.97	0.29	47,47,47,47	0
56	MG	RA	3098	1/1	0.97	0.07	16,16,16,16	0
56	MG	YA	3194	1/1	0.97	0.13	39,39,39,39	0
56	MG	YA	3134	1/1	0.97	0.10	10,10,10,10	0
56	MG	YA	3267	1/1	0.97	0.11	9,9,9,9	0
56	MG	RA	3017	1/1	0.97	0.11	17,17,17,17	0
56	MG	XA	1609	1/1	0.97	0.21	30,30,30,30	0
56	MG	Y1	101	1/1	0.97	0.09	49,49,49,49	0
56	MG	RA	3049	1/1	0.97	0.06	9,9,9,9	0
56	MG	YA	3108	1/1	0.97	0.06	9,9,9,9	0
56	MG	YE	302	1/1	0.97	0.10	9,9,9,9	0
56	MG	RA	3075	1/1	0.97	0.10	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	XA	1612	1/1	0.97	0.08	20,20,20,20	0
56	MG	YA	3142	1/1	0.97	0.09	18,18,18,18	0
56	MG	RA	3027	1/1	0.97	0.12	21,21,21,21	0
56	MG	RA	3175	1/1	0.97	0.08	26,26,26,26	0
56	MG	RA	3243	1/1	0.97	0.04	31,31,31,31	0
56	MG	QA	1622	1/1	0.97	0.11	41,41,41,41	0
56	MG	YA	3028	1/1	0.97	0.05	9,9,9,9	0
56	MG	YA	3281	1/1	0.97	0.17	27,27,27,27	0
56	MG	RA	3039	1/1	0.97	0.05	9,9,9,9	0
56	MG	YA	3210	1/1	0.97	0.06	51,51,51,51	0
56	MG	YA	3003	1/1	0.97	0.10	9,9,9,9	0
58	SF4	QD	501	8/8	0.97	0.07	67,82,98,141	0
56	MG	RA	3270	1/1	0.97	0.10	25,25,25,25	0
59	ZN	Y9	102	1/1	0.97	0.04	59,59,59,59	0
56	MG	YA	3314	1/1	0.98	0.26	51,51,51,51	0
56	MG	RA	3052	1/1	0.98	0.04	15,15,15,15	0
56	MG	RA	3059	1/1	0.98	0.04	22,22,22,22	0
56	MG	RA	3137	1/1	0.98	0.15	13,13,13,13	0
56	MG	YA	3082	1/1	0.98	0.12	12,12,12,12	0
56	MG	YA	3040	1/1	0.98	0.06	9,9,9,9	0
56	MG	YA	3053	1/1	0.98	0.05	9,9,9,9	0
56	MG	RA	3038	1/1	0.98	0.08	15,15,15,15	0
56	MG	RA	3240	1/1	0.98	0.10	23,23,23,23	0
56	MG	RE	304	1/1	0.98	0.20	37,37,37,37	0
56	MG	YA	3105	1/1	0.98	0.04	9,9,9,9	0
56	MG	RA	3144	1/1	0.98	0.18	16,16,16,16	0
56	MG	YA	3058	1/1	0.98	0.35	38,38,38,38	0
56	MG	QM	201	1/1	0.98	0.04	61,61,61,61	0
56	MG	YA	3022	1/1	0.98	0.11	9,9,9,9	0
56	MG	XV	102	1/1	0.98	0.11	24,24,24,24	0
56	MG	XA	1605	1/1	0.98	0.29	39,39,39,39	0
58	SF4	XD	501	8/8	0.98	0.06	59,74,81,83	0
56	MG	YA	3094	1/1	0.98	0.08	9,9,9,9	0
59	ZN	R9	102	1/1	0.98	0.04	97,97,97,97	0
59	ZN	XN	101	1/1	0.98	0.07	97,97,97,97	0
56	MG	YA	3095	1/1	0.98	0.07	11,11,11,11	0
56	MG	YA	3059	1/1	0.99	0.05	9,9,9,9	0
56	MG	YA	3115	1/1	0.99	0.07	9,9,9,9	0
56	MG	YA	3074	1/1	0.99	0.16	16,16,16,16	0
56	MG	RA	3043	1/1	0.99	0.06	11,11,11,11	0
56	MG	RA	3050	1/1	0.99	0.04	14,14,14,14	0
56	MG	RA	3066	1/1	0.99	0.04	9,9,9,9	0

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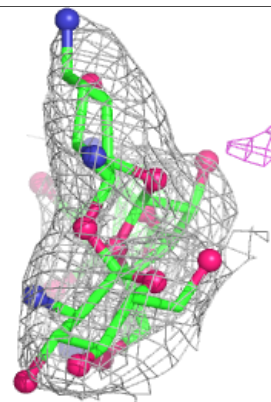
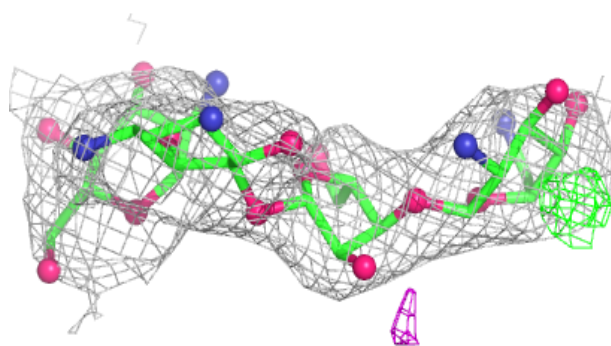
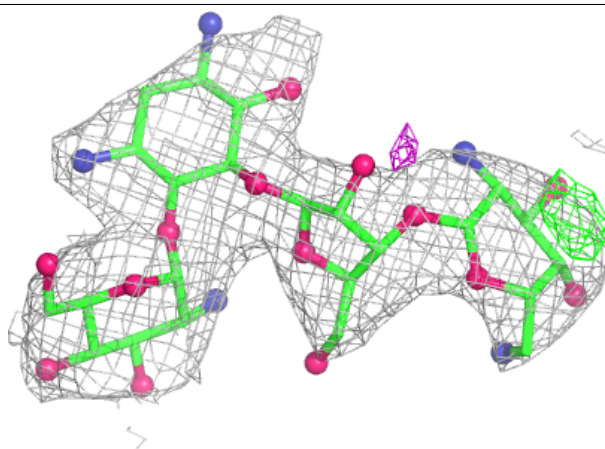
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	YA	3011	1/1	0.99	0.05	9,9,9,9	0
56	MG	YA	3027	1/1	0.99	0.23	9,9,9,9	0
56	MG	YA	3112	1/1	0.99	0.03	11,11,11,11	0
56	MG	RA	3037	1/1	0.99	0.04	9,9,9,9	0

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.

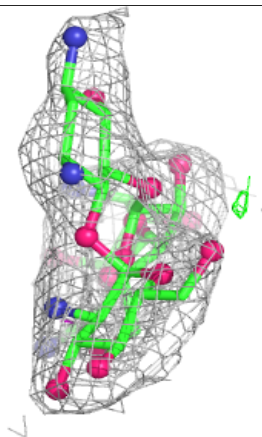
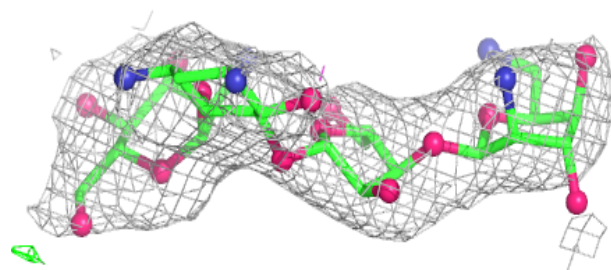
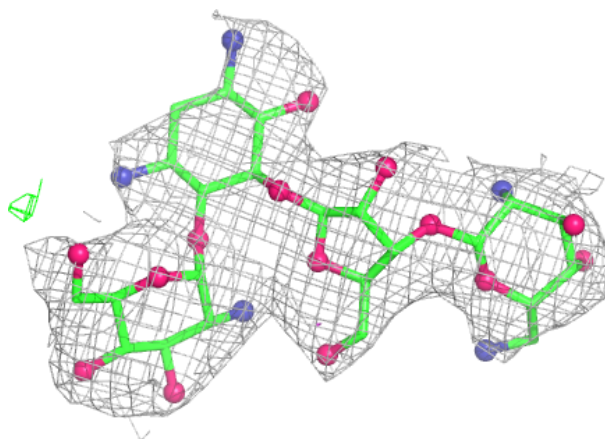
Electron density around PAR XA 1670:

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 QA 1663:

$2mF_o-DF_c$ (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.