



Full wwPDB EM Validation Report ⓘ

Feb 10, 2025 – 11:16 PM EST

PDB ID : 7N2C
EMDB ID : EMD-24132
Title : Elongating 70S ribosome complex in a fusidic acid-stalled intermediate state of translocation bound to EF-G(GDP) (INT2)
Authors : Rundlet, E.J.; Holm, M.; Schacherl, M.; Natchiar, K.S.; Altman, R.B.; Spahn, C.M.T.; Myasnikov, A.G.; Blanchard, S.C.
Deposited on : 2021-05-28
Resolution : 2.72 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

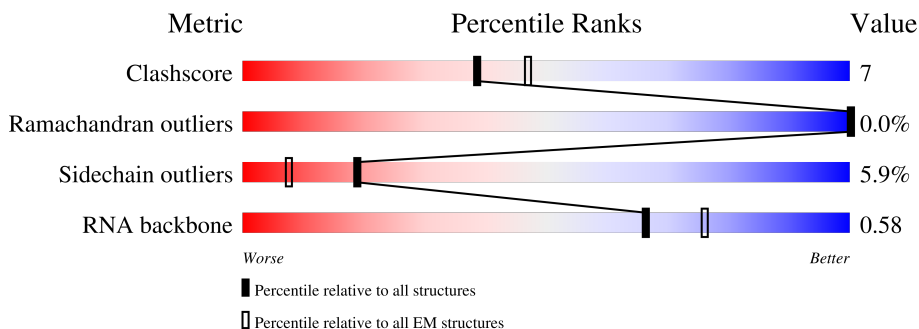
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.72 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	16	1534	
2	SB	241	
3	SC	233	
4	SD	206	
5	SE	167	
6	SF	135	
7	SG	179	





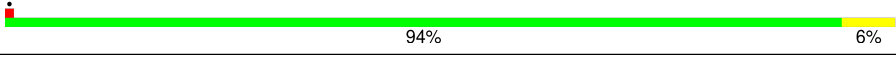










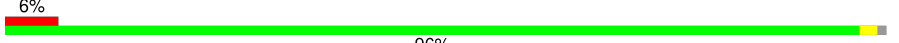
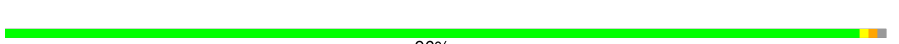






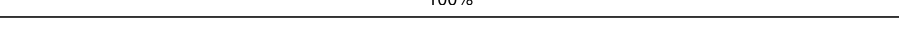
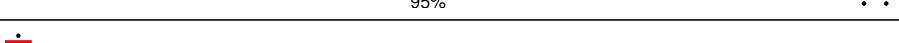
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Mol	Chain	Length	Quality of chain
8	SH	130	
9	SI	130	
10	SJ	103	
11	SK	129	
12	SL	124	
13	SM	118	
14	SN	101	
15	SO	89	
16	SP	82	
17	SQ	84	
18	SR	75	
19	SS	92	
20	ST	87	
21	SU	71	
22	mR	60	
23	23	2904	
24	5	120	
25	LA	234	
26	LB	273	
27	LC	209	
28	LD	201	
29	LE	179	
30	LF	177	
31	LG	121	
32	LI	149	

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Mol	Chain	Length	Quality of chain
33	LJ	165	
34	LK	142	
35	LM	142	
36	LN	123	
37	LO	144	
38	LP	136	
39	LQ	127	
40	LR	117	
41	LS	115	
42	LT	118	
43	LU	103	
44	LV	110	
45	LW	100	
46	LX	104	
47	LY	94	
48	La	85	
49	Lb	78	
50	Lc	63	
51	Ld	59	
52	Le	70	
53	Lf	57	
54	Lg	55	
55	Lh	46	
56	Li	65	
57	Lj	38	

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Mol	Chain	Length	Quality of chain
58	EF	704	<div><div></div><div>6%</div><div>75%</div><div>21%</div><div></div><div>• •</div></div>
59	Pp	3	<div><div></div><div>67%</div><div>33%</div><div></div><div></div></div>
60	Pt	76	<div><div></div><div>5%</div><div>72%</div><div>24%</div><div></div><div>•</div></div>
61	Dt	76	<div><div></div><div>7%</div><div>63%</div><div>33%</div><div></div><div>•</div></div>

2 Entry composition [i](#)

There are 68 unique types of molecules in this entry. The entry contains 155157 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
1	16	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SB	226	Total	C	N	O	S	0	0
			1769	1119	317	325	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SC	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SD	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SE	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SF	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SG	156	Total	C	N	O	S	0	0
			1235	773	237	221	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SH	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SI	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SJ	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SK	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SL	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SM	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SN	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SO	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SP	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SQ	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SR	67	Total	C	N	O	S	0	0
			555	351	106	97	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SS	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	ST	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SU	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 22 is a RNA chain called Chains: mR.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	mR	12	Total	C	N	O	P	0	0
			252	113	41	86	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	23	2903	Total	C	N	O	P	0	0
			62334	27815	11467	20149	2903		

- Molecule 24 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	5	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 25 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LA	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LB	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LC	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LD	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LE	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LF	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 31 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	LG	68	Total	C	N	O	0	0
			487	306	82	99		

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LI	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 33 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LJ	135	Total	C	N	O	S	0	0
			1023	648	179	192	4		

- Molecule 34 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LK	134	Total	C	N	O	S	0	0
			973	616	166	185	6		

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LM	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LN	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LO	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LP	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LQ	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	LR	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LS	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	LT	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LU	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LV	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LW	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	LX	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LY	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	La	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lb	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Lc	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Ld	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Le	67	Total	C	N	O	S	0	0
			529	328	100	95	6		

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Lf	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 54 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	Lg	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 55 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Lh	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 56 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Li	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 57 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Lj	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 58 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	EF	685	Total	C	N	O	S	0	0
			4999	3161	893	927	18		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EF	1	SER	MET	engineered mutation	UNP P0A6M8

- Molecule 59 is a protein called Polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Pp	3	Total	C	N	O	S	0	0
			28	20	4	3	1		

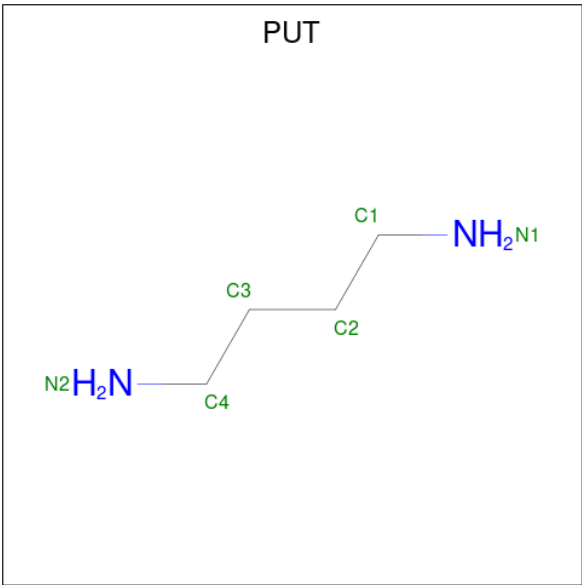
- Molecule 60 is a RNA chain called Chains: Pt.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	Pt	76	Total	C	N	O	P	S	0	0
			1636	733	284	542	76	1		

- Molecule 61 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	Dt	76	Total	C	N	O	P	S	0	0
			1641	735	294	534	76	2		

- Molecule 62 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: C₄H₁₂N₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
62	16	1	Total	C	N	0
			6	4	2	
62	16	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	

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Mol	Chain	Residues	Atoms			AltConf
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	LC	1	Total	C	N	0
			6	4	2	

- Molecule 63 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

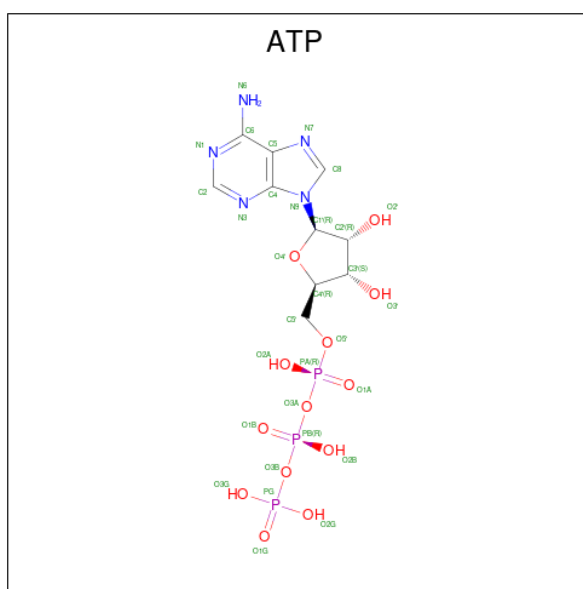
Mol	Chain	Residues	Atoms		AltConf
63	16	40	Total	Mg	0
			40	40	
63	SN	2	Total	Mg	0
			2	2	
63	23	144	Total	Mg	0
			144	144	
63	5	4	Total	Mg	0
			4	4	
63	LB	1	Total	Mg	0
			1	1	
63	LC	1	Total	Mg	0
			1	1	
63	LD	1	Total	Mg	0
			1	1	
63	LQ	1	Total	Mg	0
			1	1	
63	LW	1	Total	Mg	0
			1	1	
63	Lf	1	Total	Mg	0
			1	1	
63	EF	1	Total	Mg	0
			1	1	

- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of

Interest" by depositor).

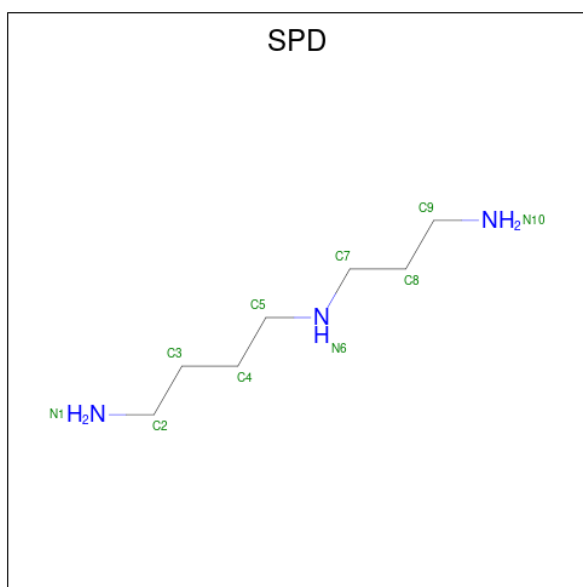
Mol	Chain	Residues	Atoms		AltConf
64	SB	1	Total	Zn	0
			1	1	
64	Le	1	Total	Zn	0
			1	1	
64	Lj	1	Total	Zn	0
			1	1	

- Molecule 65 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



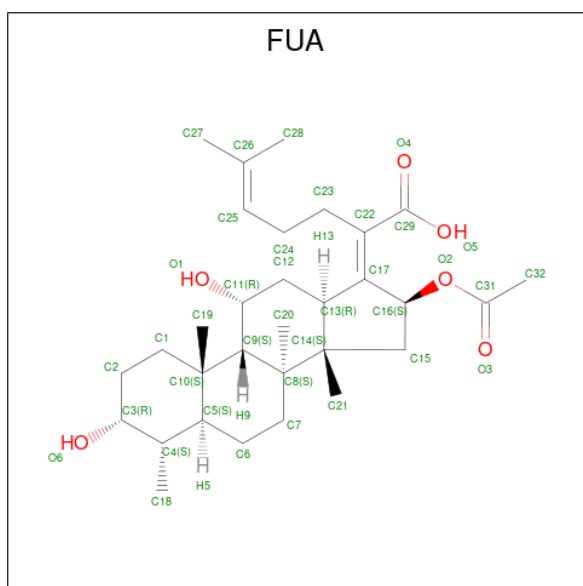
Mol	Chain	Residues	Atoms					AltConf
65	23	1	Total	C	N	O	P	0
			31	10	5	13	3	
65	23	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 66 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



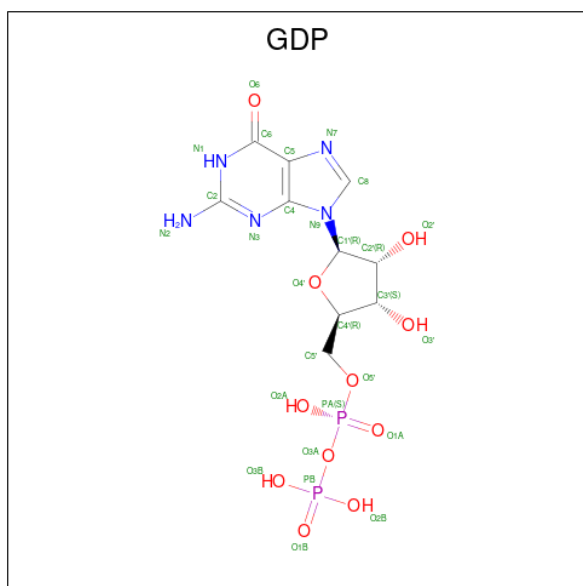
Mol	Chain	Residues	Atoms			AltConf
66	23	1	Total	C	N	0
			10	7	3	
66	23	1	Total	C	N	0
			10	7	3	
66	23	1	Total	C	N	0
			10	7	3	

- Molecule 67 is FUSIDIC ACID (three-letter code: FUA) (formula: $C_{31}H_{48}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
67	EF	1	Total	C	O	0
			37	31	6	

- Molecule 68 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

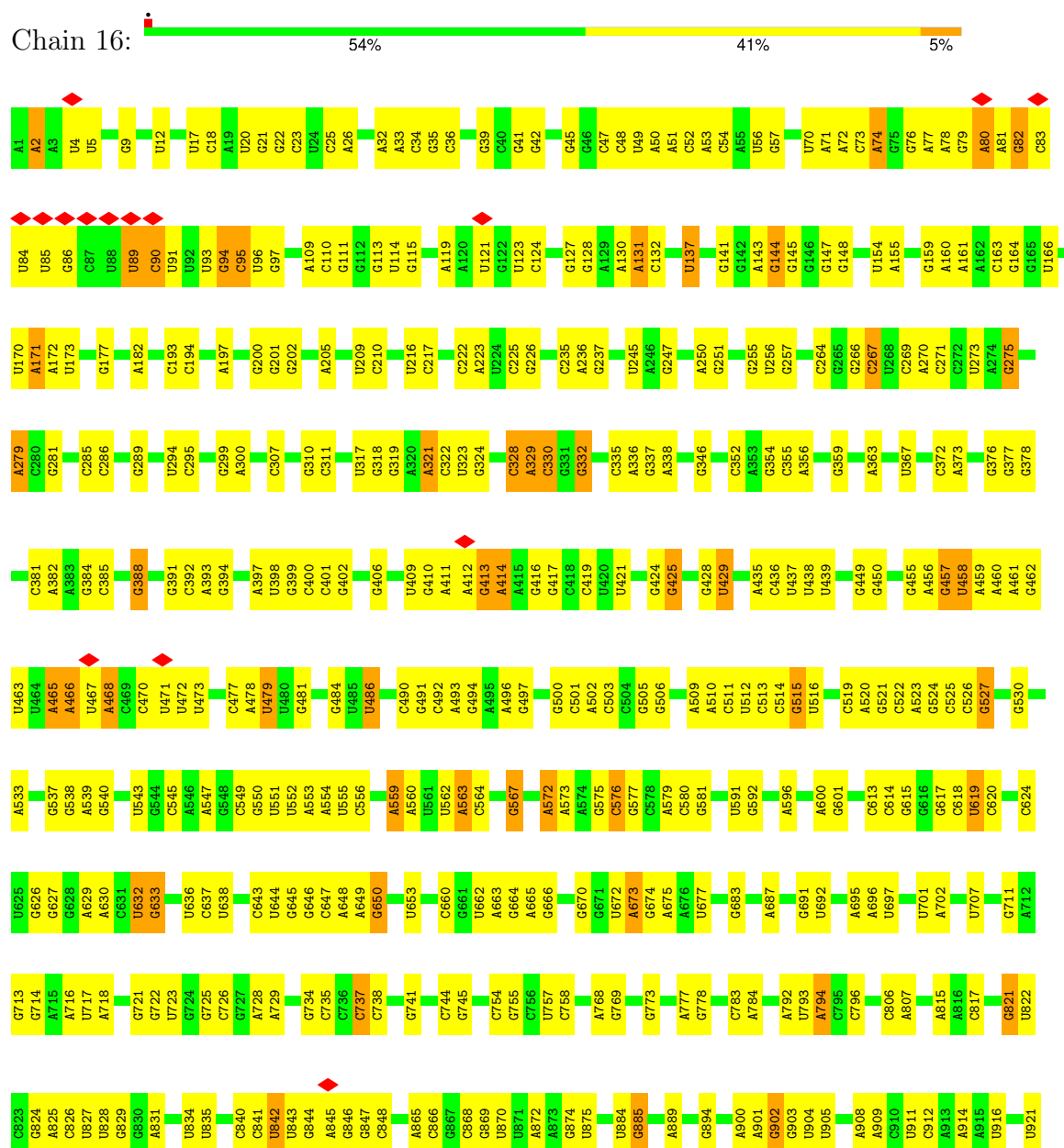


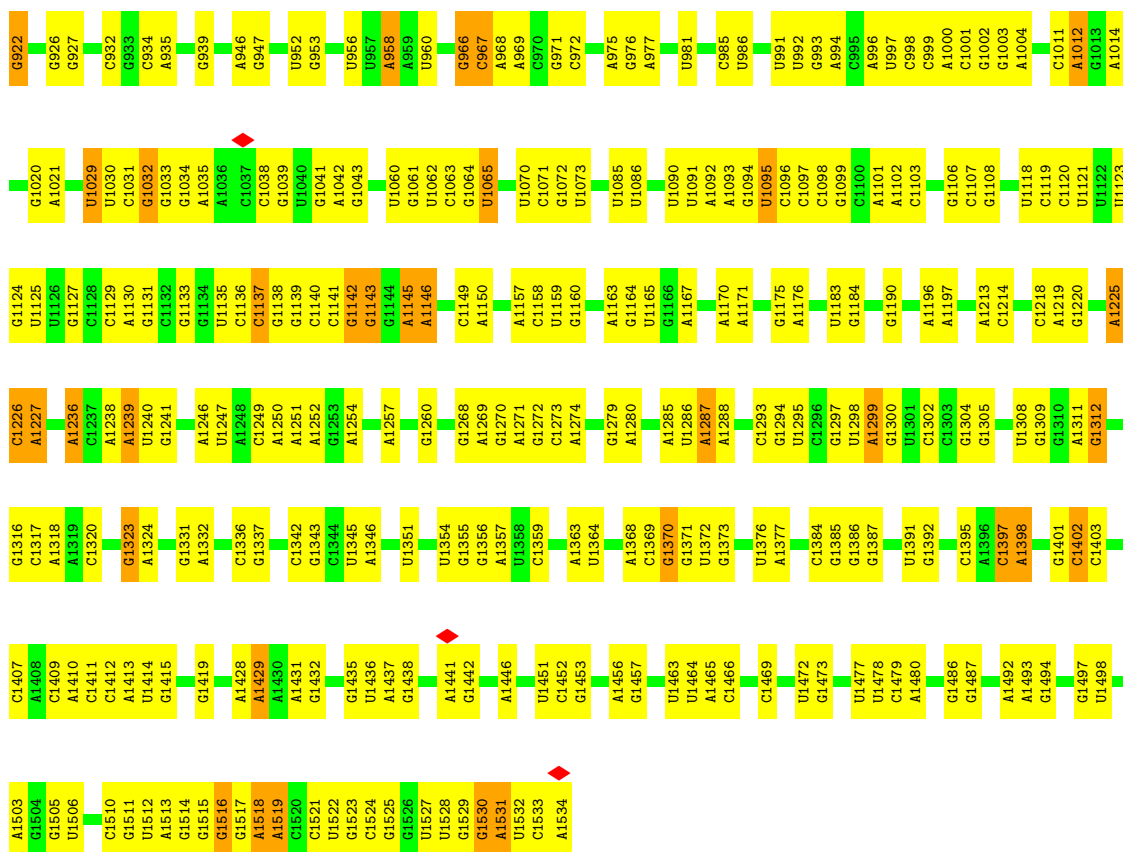
Mol	Chain	Residues	Atoms					AltConf
68	EF	1	Total 28	C 10	N 5	O 11	P 2	0

3 Residue-property plots

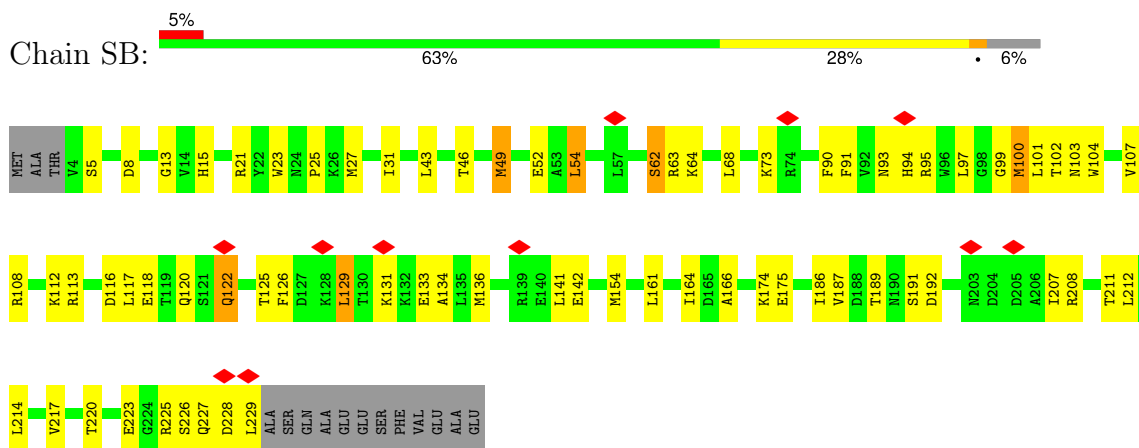
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S rRNA

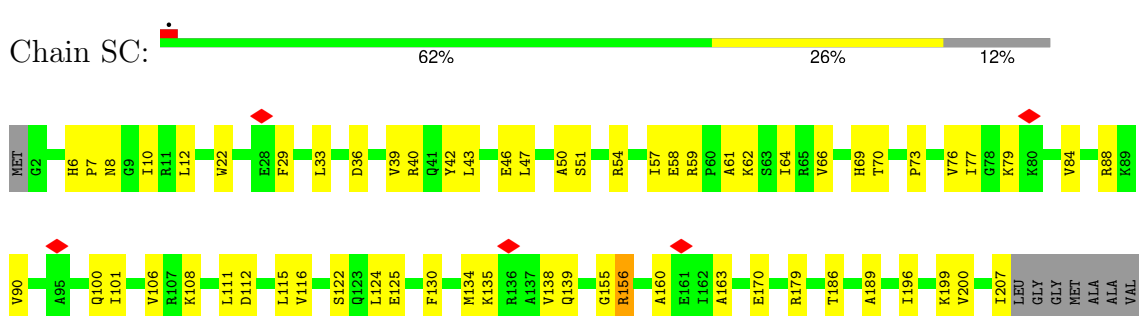




- Molecule 2: 30S ribosomal protein S2



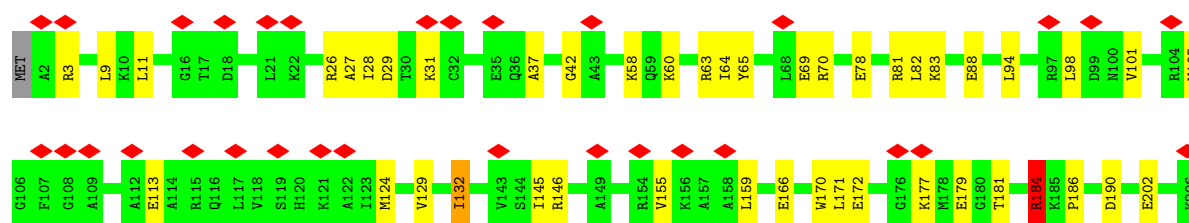
- Molecule 3: 30S ribosomal protein S3



GLU
GLN
PRO
GLU
LYS
PRO
ALA
GLN
PRO
LYS
LYS
GLN
GLN
ARG
LYS
GLY
ARG
LYS

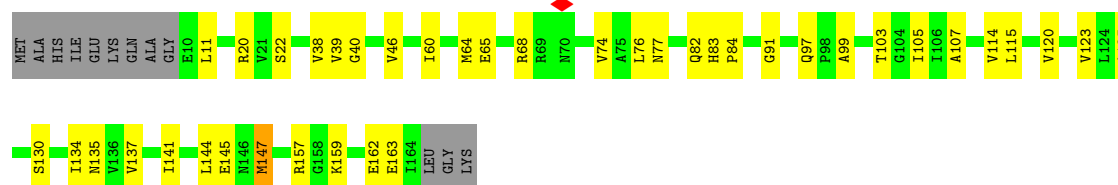
• Molecule 4: 30S ribosomal protein S4

Chain SD:



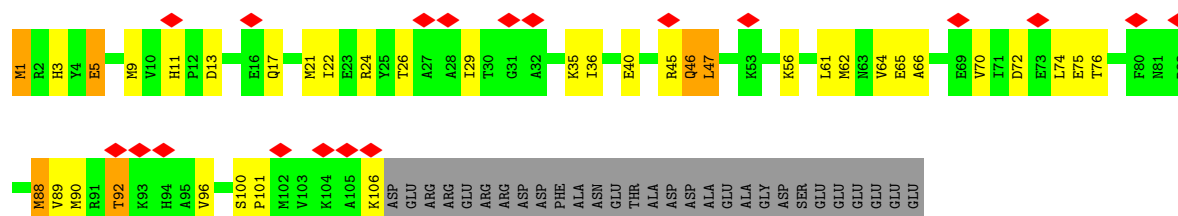
• Molecule 5: 30S ribosomal protein S5

Chain SE:



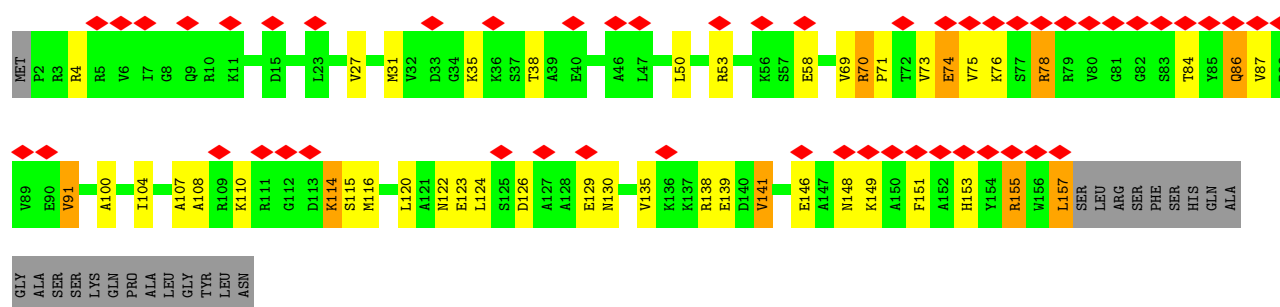
• Molecule 6: 30S ribosomal protein S6

Chain SF:



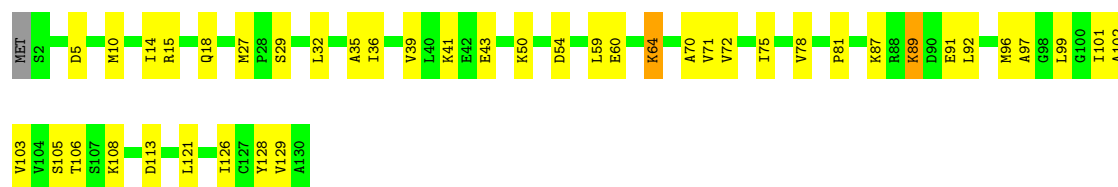
• Molecule 7: 30S ribosomal protein S7

Chain SG:



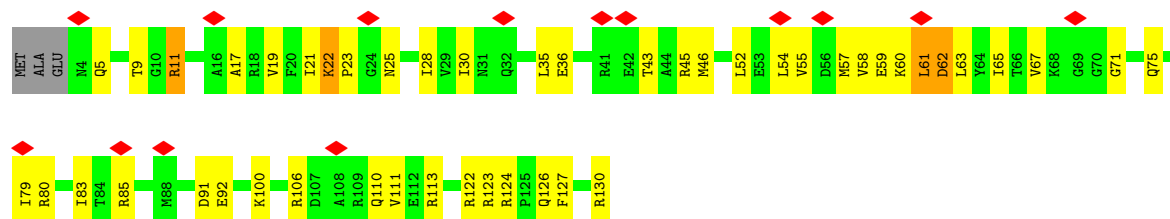
• Molecule 8: 30S ribosomal protein S8

Chain SH:  67% 31% ..



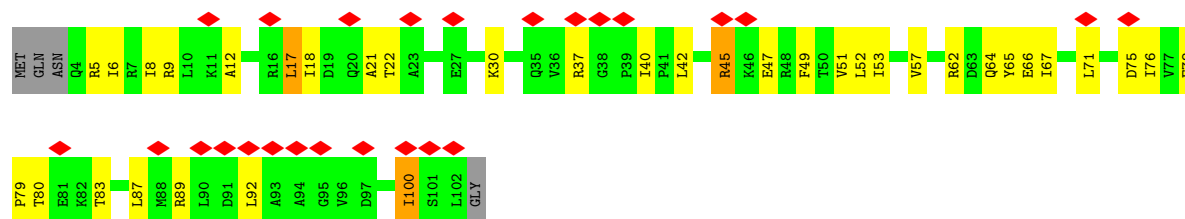
• Molecule 9: 30S ribosomal protein S9

Chain SI:  11% 62% 33% ..



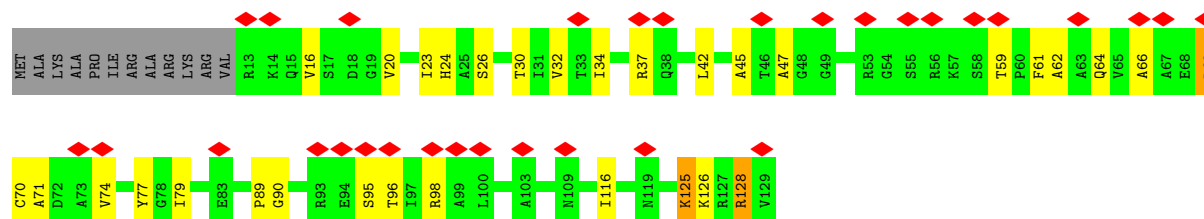
• Molecule 10: 30S ribosomal protein S10

Chain SJ:  24% 61% 32% ..




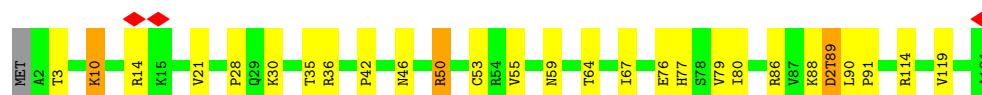
• Molecule 11: 30S ribosomal protein S11

Chain SK:  24% 66% 22% 9% ..

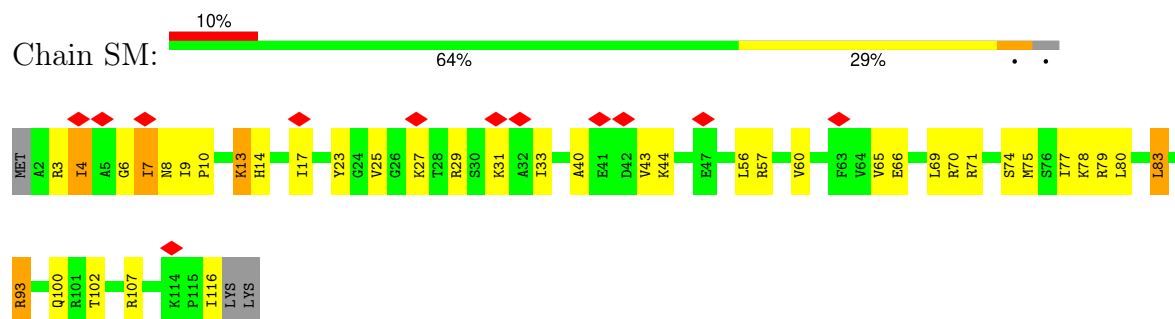


• Molecule 12: 30S ribosomal protein S12

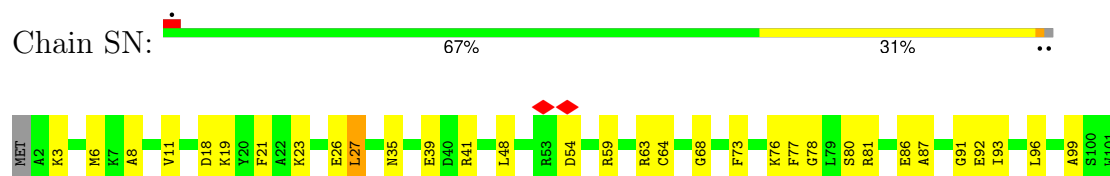
Chain SL:  77% 19% ..



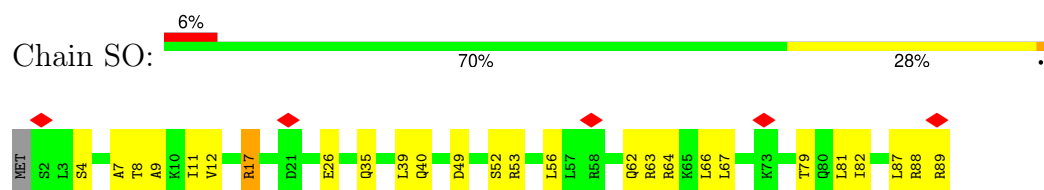
- Molecule 13: 30S ribosomal protein S13



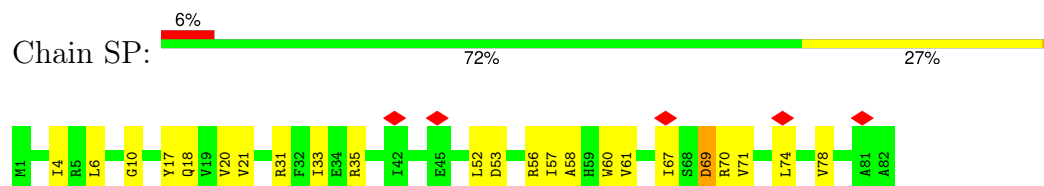
- Molecule 14: 30S ribosomal protein S14



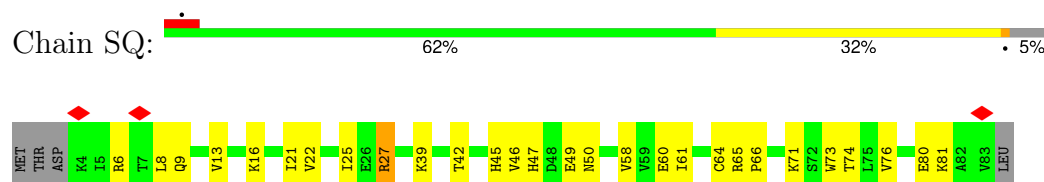
- Molecule 15: 30S ribosomal protein S15



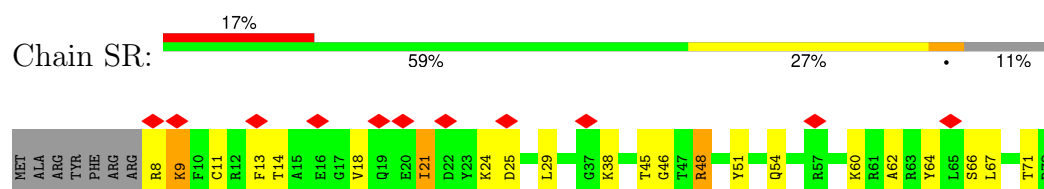
- Molecule 16: 30S ribosomal protein S16



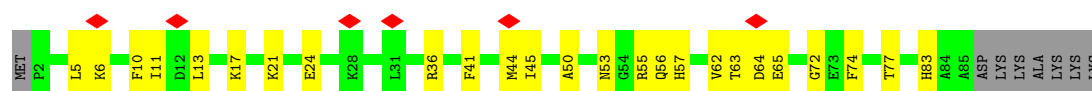
- Molecule 17: 30S ribosomal protein S17



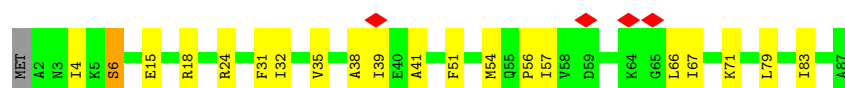
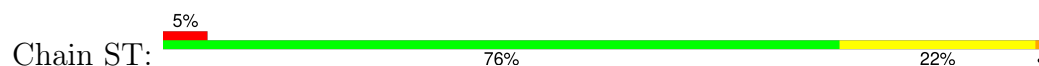
- Molecule 18: 30S ribosomal protein S18



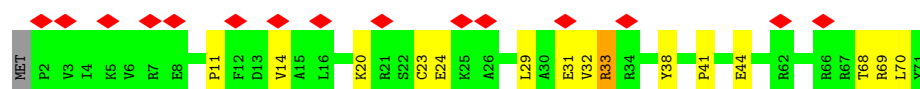
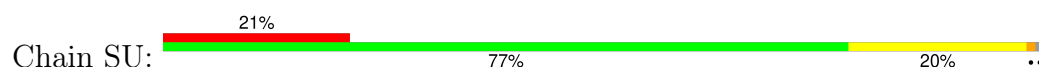
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



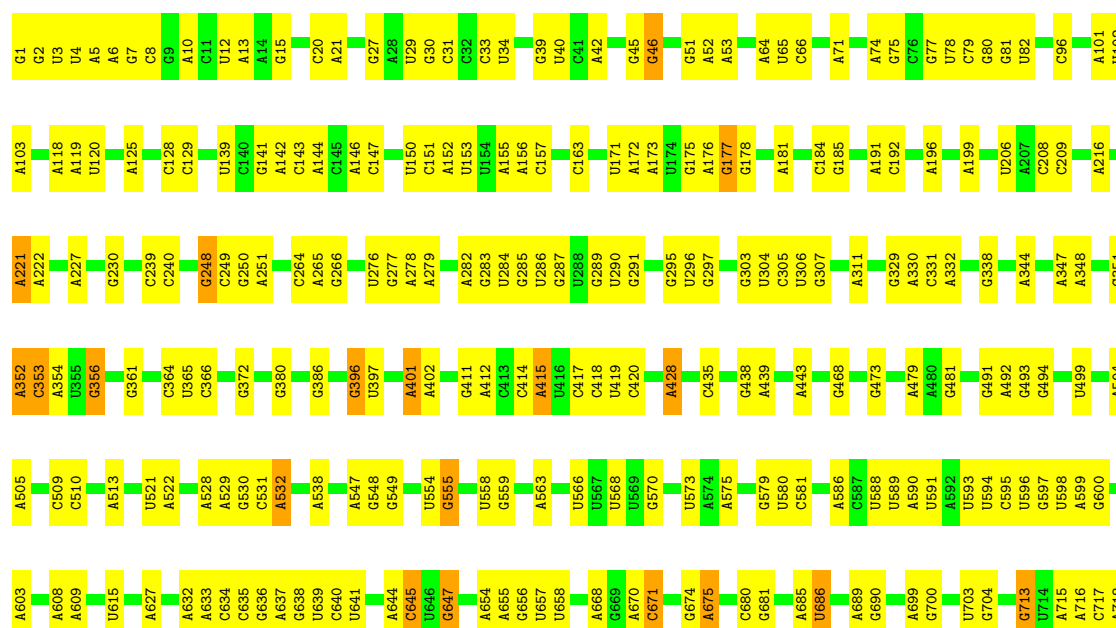
- Molecule 21: 30S ribosomal protein S21



- Molecule 22: Chains: mR



- Molecule 23: 23S rRNA

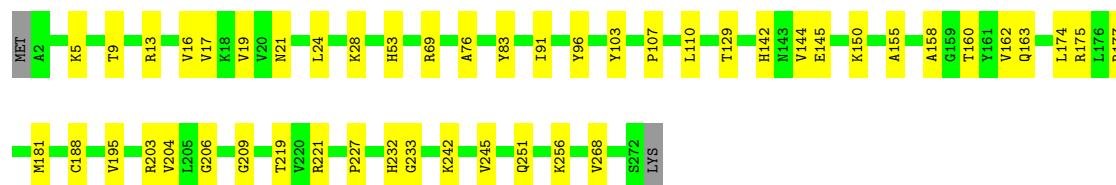


G2046	C1947	A1854	C1764	G1649	C1532	C1428	G1299	C1196	G1107	U1023	U906	A905	G827	A721
C2047	G1954	G1857	G1770	A1665	A1533	G1428	G1300	C1197	G1110	U1023	U906	A905	U828	A721
G2048	U1955	A1858	G1771	G1666	U1534	G1429	A1301	U1198	G1111	G830	A829	C908	U828	C723
C2050	C1957	G1862	A1772	G1667	C1536	G1432	A1307	C1200	G1112	G1026	A908	C908	G830	U724
A2051	C1958	G1866	A1773	A1672	G1537	G1433	A1307	G1212	G1115	A1027	A910	A910	A833	G729
C2055	C1962	A1866	C1774	G1673	U1537	A1433	U1313	U1219	G1116	A1028	A911	C912	G834	A730
G2056	U1963	G1867	U1782	G1674	G1540	A1434	C1314	U1219	C1117	A1029	A911	C912	G843	C740
A2060	G1964	C1868	U1783	C1675	C1541	G1435	C1315	U1223	C1118	U1033	A917	U917	A845	U741
C2061	C1965	G1869	A1783	A1676	U1542	G1436	C1316	G1223	G1125	G1034	G926	G926	A846	A742
A2062	G1965	C1870	A1784	A1677	G1543	U1438	G1317	U1224	G1132	U1035	A927	A927	A847	A743
C2063	A1966	A1871	A1785	A1678	U1548	A1439	U1318	G1225	U1133	G1038	A928	A928	A848	G745
C2064	C1967	A1872	A1786	A1679	A1549	U1440	U1318	A1226	U1132	A1039	U746	U746	A849	U850
C2065	G1873	G1873	A1876	A1680	A1548	G1441	A1322	G1227	C1134	C1045	C851	C851	C851	U747
C2066	A1876	C1881	C1795	G1681	G1560	U1442	C1323	U1231	C1135	G1045	C851	C851	C851	U747
G2069	G1972	U1882	G1797	U1683	U1563	C1444	A1327	G1232	G1136	A1046	A941	A941	U852	U754
A2070	G1983	A1885	C1800	G1685	C1564	C1447	A1328	G1233	G1137	G1047	C946	C946	G856	U755
C2071	A1987	A1885	A1801	C1704	C1565	G1448	A1327	G1235	G1139	A1050	A947	A947	G857	A756
C2072	G1988	A1802	A1689	A1705	A1566	G1448	G1339	G1236	C1152	G1051	C948	C948	G858	G757
C2073	C1989	A1889	A1690	G1706	A1566	G1448	G1339	G1236	C1152	G1051	C948	C948	G858	G757
U2074	C1990	A1889	A1690	G1707	A1569	G1452	A1365	A1237	U1141	A1054	C949	C949	G859	G760
U2075	G1991	G1896	A1693	C1708	A1570	A1453	A1365	G1238	A1142	G1055	U955	U955	A861	G761
C2078	U1992	A1896	A1808	G1709	A1571	G1459	G1368	A1247	G1149	G1056	U955	U955	A861	U762
U2079	U1993	A1900	A1810	A1705	A1572	G1459	C1357	G1248	C1150	A1059	A959	A959	A863	G763
C2080	C1994	A1901	G1811	G1706	U1578	A1470	G1358	U1249	C1151	G1059	A960	A960	G864	A764
U2081	G1997	G1906	U1812	G1707	U1578	A1470	A1365	G1251	C1153	U1060	C961	C961	G869	G775
A2082	C2008	G1907	G1813	C1708	A1583	G1478	A1365	G1252	G1154	A1067	U963	U963	G869	G776
U2086	A2009	G1910	C1816	U1709	U1584	G1482	G1368	A1253	C1155	G1068	C964	C964	U871	A782
G2087	U2011	U1911	A1819	G1715	A1584	G1482	A1378	U1254	A1155	A1069	C965	C965	U872	A783
G2093	G2012	A1913	A1912	G1715	A1586	G1483	A1378	U1255	C1156	A1070	C966	C966	U872	A784
C2096	A2013	C1914	C1822	U1720	A1587	U1484	U1379	G1256	G1161	C1076	C967	C967	G875	G784
U2098	A2014	A1916	A1821	G1721	A1590	U1485	A1383	G1266	G1162	A1077	C968	C968	A877	G785
U2099	A2015	U1917	C1827	G1727	A1591	U1486	A1384	U1267	G1163	U1078	C969	C969	A877	C786
C2100	G2021	A1918	G1828	C1727	A1597	U1486	A1384	G1271	C1164	C1079	G879	G879	A878	C787
A2101	U2022	A1919	A1829	U1730	A1598	U1486	A1387	U1272	A1165	A1080	G880	G880	A789	G788
G2102	C2023	C1920	G1731	G1730	C1604	A1495	A1387	U1273	A1169	U1083	G881	G881	A789	G796
U2106	G2024	G1921	C1832	U1736	C1605	A1496	A1395	U1278	G1170	A1084	G882	G882	C796	G797
G2107	C2025	A1927	G1835	G1738	A1608	U1496	A1395	C1278	C1171	A1085	U884	U884	G801	G801
G2107	U2026	G1928	C1838	A1739	A1610	U1504	U1405	U1282	U1175	A1088	C885	C885	G805	G805
G2110	A2030	G1929	G1842	G1740	A1616	C1507	U1406	A1286	U1176	A1090	C888	C888	U811	U811
U2111	C2031	U1931	C1843	C1741	C1617	A1508	U1406	A1287	G1177	G1091	C889	C889	C812	C812
G2112	A2032	G1932	C1844	U1742	A1618	A1509	G1410	G1288	C1178	U1094	C890	C890	C813	C813
U2113	C2033	G1933	C1844	U1743	A1618	G1510	U1411	G1288	U1179	U1094	C891	C891	C814	C814
A2114	A2036	A1936	G1845	A1744	U1636	G1511	U1412	G1292	U1180	A1009	A892	A892	C817	C817
G2115	C2037	A1937	G1846	A1745	A1637	C1512	A1413	C1293	U1181	U1010	C893	C893	G818	G818
G2116	A2037	A1937	G1847	A1746	A1637	U1513	A1413	U1294	U1182	G1011	C894	C894	A819	A819
A2117	A1938	A1848	A1847	U1747	G1645	G1514	G1416	U1296	U1183	U1012	C895	C895	G819	G819
U2118	U2039	U1939	G1849	C1748	U1646	G1514	G1416	G1296	U1184	C1102	U896	U896	G822	G822
A2119	C2043	U1946	A1853	G1756	U1647	A1515	A1419	C1297	G1187	U1105	C897	C897	C823	C823
					U1648	G1524	A1420	C1298	G1195	G1106	C903	C903		



- Molecule 26: 50S ribosomal protein L2

Chain LB: 82% 18%



- Molecule 27: 50S ribosomal protein L3

Chain LC: 89% 11%



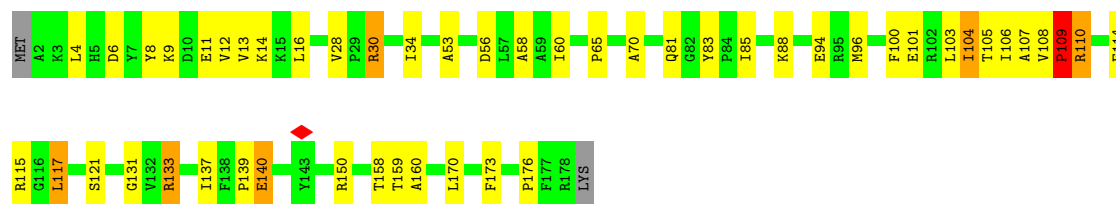
- Molecule 28: 50S ribosomal protein L4

Chain LD: 90% 10%



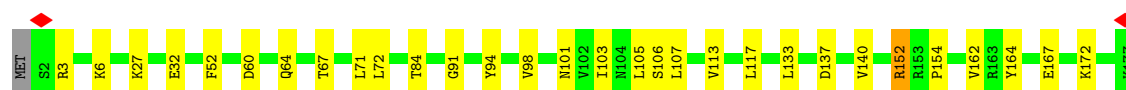
- Molecule 29: 50S ribosomal protein L5

Chain LE: 71% 24%



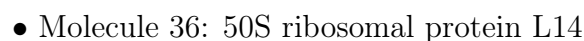
- Molecule 30: 50S ribosomal protein L6


Chain LF: 82% 16%

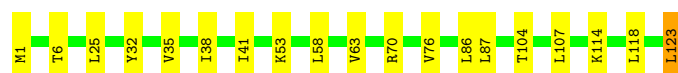


- Molecule 31: 50S ribosomal protein L7/L12

Chain LG: 35% 21% 44%



Chain LN:  85% 15%



- Molecule 37: 50S ribosomal protein L15

Chain LO:  94% 6%




- Molecule 38: 50S ribosomal protein L16

Chain LP:  85% 15%




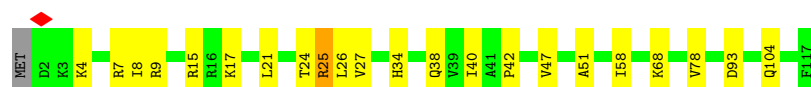
- Molecule 39: 50S ribosomal protein L17

Chain LQ:  84% 10% 6%




- Molecule 40: 50S ribosomal protein L18

Chain LR:  80% 18% ..




- Molecule 41: 50S ribosomal protein L19

Chain LS:  78% 21% .




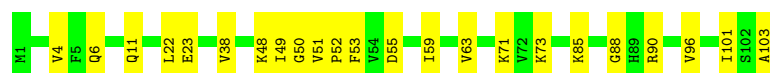
- Molecule 42: 50S ribosomal protein L20

Chain LT:  85% 14% ..




- Molecule 43: 50S ribosomal protein L21

Chain LU:  78% 22%



- Molecule 44: 50S ribosomal protein L22

Chain LV:  81% 18%



- Molecule 45: 50S ribosomal protein L23

Chain LW:  73% 20% 7%




- Molecule 46: 50S ribosomal protein L24

Chain LX:  90% 8%



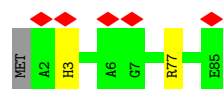
- Molecule 47: 50S ribosomal protein L25

Chain LY:  84% 14%



- Molecule 48: 50S ribosomal protein L27

Chain La:  6% 96%

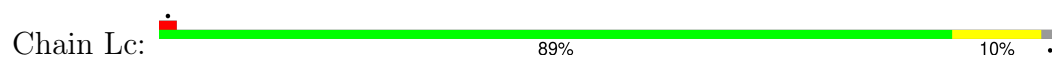


- Molecule 49: 50S ribosomal protein L28

Chain Lb:  96%



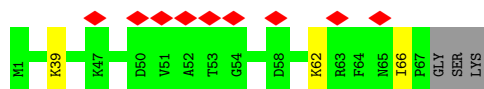
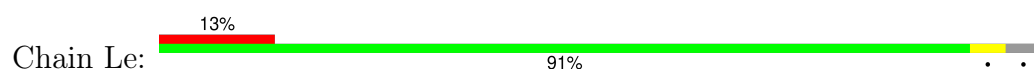
- Molecule 50: 50S ribosomal protein L29



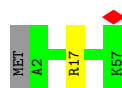
- Molecule 51: 50S ribosomal protein L30



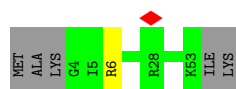
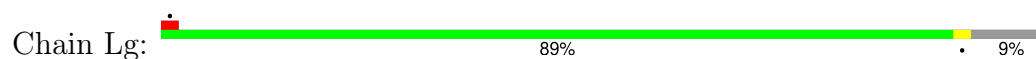
- Molecule 52: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L32



- Molecule 54: 50S ribosomal protein L33



- Molecule 55: 50S ribosomal protein L34

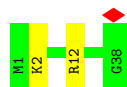


There are no outlier residues recorded for this chain.

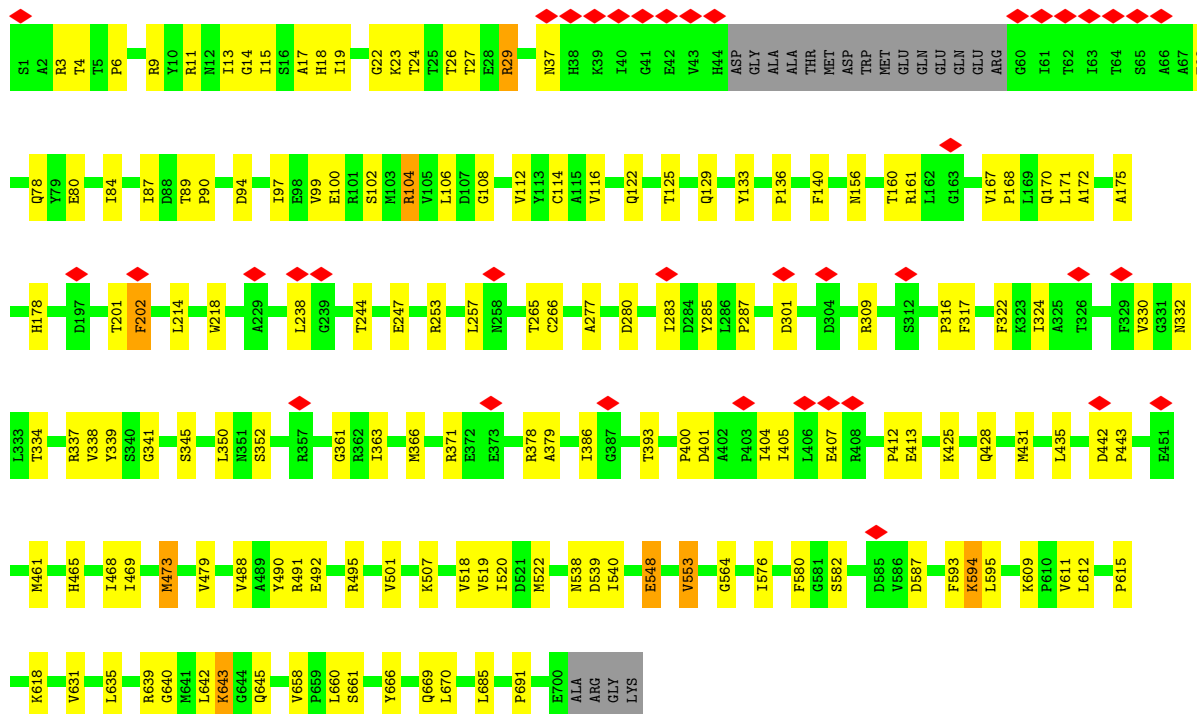
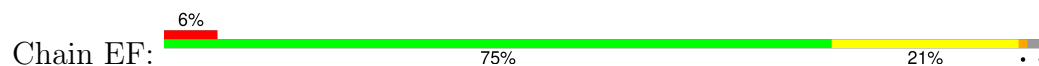
- Molecule 56: 50S ribosomal protein L35



- Molecule 57: 50S ribosomal protein L36



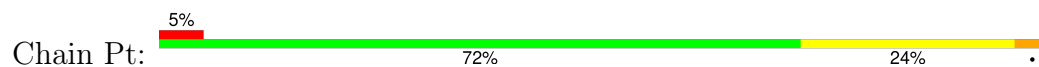
• Molecule 58: Elongation factor G



• Molecule 59: Polypeptide

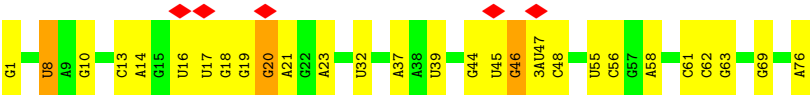


• Molecule 60: Chains: Pt



• Molecule 61: tRNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113540	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	87	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.126	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (\AA)	610.55994, 610.55994, 610.55994	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 5MU, 5MC, 1MG, MA6, UR3, FUA, GDP, 3AU, MIA, G7M, 6MZ, PUT, 2MG, 2MA, 4SU, ATP, ZN, H2U, SPD, OMG, D2T, OMC, 4OC, U8U, PSU, OMU, 3TD, T6A, 4D4

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	16	0.32	0/36619	0.73	4/57122 (0.0%)
2	SB	0.45	0/1800	0.59	0/2425
3	SC	0.32	0/1651	0.55	0/2225
4	SD	0.34	0/1665	0.56	0/2227
5	SE	0.39	0/1157	0.57	0/1557
6	SF	0.47	0/881	0.63	0/1189
7	SG	0.56	0/1253	0.66	0/1681
8	SH	0.35	0/989	0.59	0/1326
9	SI	0.43	0/1034	0.65	0/1375
10	SJ	0.53	0/805	0.74	1/1089 (0.1%)
11	SK	0.32	0/893	0.59	0/1205
12	SL	0.46	0/960	0.62	0/1286
13	SM	0.54	0/900	1.02	3/1204 (0.2%)
14	SN	0.51	0/817	0.61	0/1088
15	SO	0.33	0/722	0.53	0/964
16	SP	0.37	0/659	0.63	0/884
17	SQ	0.36	0/657	0.59	0/881
18	SR	0.47	0/564	0.67	0/756
19	SS	0.37	0/685	0.58	0/922
20	ST	0.35	0/676	0.54	0/895
21	SU	0.33	0/597	0.59	0/792
22	mR	0.24	0/280	0.64	0/433
23	23	0.41	0/69239	0.76	8/108014 (0.0%)
24	5	0.44	1/2873 (0.0%)	0.75	0/4478
25	LA	0.38	0/1033	0.61	0/1387
26	LB	0.34	0/2121	0.59	0/2852
27	LC	0.32	0/1586	0.55	0/2134
28	LD	0.29	0/1571	0.52	0/2113
29	LE	0.42	0/1434	0.67	2/1926 (0.1%)
30	LF	0.31	0/1343	0.53	0/1816
31	LG	0.33	0/488	0.62	0/652

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LI	0.30	0/1122	0.51	0/1515
33	LJ	0.47	0/1037	0.63	0/1400
34	LK	0.52	0/987	0.64	0/1334
35	LM	0.31	0/1152	0.51	0/1551
36	LN	0.35	0/956	0.59	0/1279
37	LO	0.34	0/1062	0.59	0/1413
38	LP	0.33	0/1081	0.58	0/1443
39	LQ	0.31	0/973	0.61	0/1301
40	LR	0.33	0/902	0.58	0/1209
41	LS	0.34	0/929	0.58	0/1242
42	LT	0.35	0/960	0.53	0/1278
43	LU	0.35	0/829	0.61	0/1107
44	LV	0.34	0/864	0.57	0/1156
45	LW	0.30	0/744	0.53	0/994
46	LX	0.31	0/787	0.53	0/1051
47	LY	0.33	0/766	0.55	0/1025
48	La	0.33	0/642	0.53	0/848
49	Lb	0.33	0/635	0.57	0/848
50	Lc	0.33	0/502	0.59	1/667 (0.1%)
51	Ld	0.31	0/453	0.56	0/605
52	Le	0.37	0/539	0.62	0/721
53	Lf	0.36	0/450	0.59	0/599
54	Lg	0.28	0/416	0.49	0/554
55	Lh	0.32	0/380	0.68	0/498
56	Li	0.31	0/513	0.57	0/676
57	Lj	0.32	0/303	0.55	0/397
58	EF	0.45	0/5097	0.61	0/6933
59	Pp	0.41	0/28	0.97	0/34
60	Pt	0.41	1/1600 (0.1%)	0.73	0/2486
61	Dt	0.45	2/1654 (0.1%)	0.73	1/2572 (0.0%)
All	All	0.39	4/166315 (0.0%)	0.71	20/247634 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	SD	0	1
6	SF	0	1
7	SG	0	1
9	SI	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	SJ	0	1
15	SO	0	2
21	SU	0	1
27	LC	0	1
29	LE	0	1
40	LR	0	1
46	LX	0	1
47	LY	0	2
48	La	0	1
49	Lb	0	1
51	Ld	0	1
53	Lf	0	1
All	All	0	18

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	Pt	1	G	OP3-P	-10.66	1.48	1.61
61	Dt	1	G	OP3-P	-10.65	1.48	1.61
24	5	1	U	OP3-P	-10.55	1.48	1.61
61	Dt	20	G	O3'-P	6.27	1.68	1.61

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	SM	93	ARG	CG-CD-NE	18.53	150.71	111.80
13	SM	93	ARG	CB-CG-CD	16.38	154.19	111.60
29	LE	109	PRO	CA-N-CD	-10.29	97.10	111.50
10	SJ	37	ARG	N-CA-C	-8.11	89.09	111.00
13	SM	93	ARG	CD-NE-CZ	7.94	134.72	123.60
61	Dt	20	G	P-O3'-C3'	7.84	129.10	119.70
1	16	419	C	N3-C2-O2	-6.54	117.32	121.90
23	23	2874	C	C2-N1-C1'	6.51	125.96	118.80
1	16	754	C	C2-N1-C1'	6.35	125.79	118.80
1	16	998	C	N3-C2-O2	-6.15	117.59	121.90
23	23	1313	U	C2-N1-C1'	6.04	124.95	117.70
23	23	1314	C	C2-N1-C1'	5.68	125.05	118.80
23	23	1187	G	P-O3'-C3'	5.63	126.46	119.70
23	23	1267	U	C2-N1-C1'	5.57	124.38	117.70
23	23	1485	U	C2-N1-C1'	5.36	124.13	117.70
29	LE	110	ARG	CB-CA-C	5.29	120.98	110.40
23	23	1267	U	N1-C2-O2	5.22	126.45	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	2874	C	C6-N1-C1'	-5.17	114.60	120.80
1	16	425	G	C5-C6-O6	5.15	131.69	128.60
50	Lc	57	LEU	CA-CB-CG	5.03	126.88	115.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	LC	124	ARG	Sidechain
29	LE	133	ARG	Sidechain
40	LR	9	ARG	Sidechain
46	LX	82	ARG	Sidechain
47	LY	19	ARG	Sidechain
47	LY	93	ARG	Sidechain
48	La	77	ARG	Sidechain
49	Lb	11	ARG	Sidechain
51	Ld	30	ARG	Sidechain
53	Lf	17	ARG	Sidechain
4	SD	184	ARG	Sidechain
6	SF	45	ARG	Sidechain
7	SG	141	VAL	Mainchain
9	SI	113	ARG	Sidechain
10	SJ	89	ARG	Sidechain
15	SO	53	ARG	Sidechain
15	SO	89	ARG	Sidechain
21	SU	33	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	16	32929	0	16589	404	0
2	SB	1769	0	1795	35	0
3	SC	1624	0	1696	37	0
4	SD	1643	0	1707	24	0
5	SE	1144	0	1185	20	0
6	SF	862	0	864	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	SG	1235	0	1286	25	0
8	SH	979	0	1031	25	0
9	SI	1022	0	1070	21	0
10	SJ	795	0	836	21	0
11	SK	877	0	887	20	0
12	SL	957	0	1017	15	0
13	SM	891	0	952	23	0
14	SN	805	0	844	19	0
15	SO	714	0	734	12	0
16	SP	649	0	666	20	0
17	SQ	648	0	691	17	0
18	SR	555	0	578	13	0
19	SS	668	0	693	18	0
20	ST	670	0	719	11	0
21	SU	589	0	629	7	0
22	mR	252	0	128	0	0
23	23	62334	0	31374	584	0
24	5	2570	0	1301	10	0
25	LA	1026	0	1092	26	0
26	LB	2082	0	2154	30	0
27	LC	1565	0	1616	13	0
28	LD	1552	0	1618	15	0
29	LE	1410	0	1444	37	0
30	LF	1323	0	1371	16	0
31	LG	487	0	515	16	0
32	LI	1111	0	1148	18	0
33	LJ	1023	0	1050	15	0
34	LK	973	0	1017	25	0
35	LM	1129	0	1162	13	0
36	LN	947	0	1023	12	0
37	LO	1053	0	1129	7	0
38	LP	1075	0	1155	9	0
39	LQ	960	0	1000	8	0
40	LR	892	0	923	11	0
41	LS	917	0	960	13	0
42	LT	947	0	1019	13	0
43	LU	816	0	839	15	0
44	LV	857	0	922	13	0
45	LW	738	0	807	10	0
46	LX	779	0	831	4	0
47	LY	753	0	780	7	0
48	La	634	0	653	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Lb	625	0	652	0	0
50	Lc	501	0	531	0	0
51	Ld	449	0	488	0	0
52	Le	529	0	527	0	0
53	Lf	444	0	458	0	0
54	Lg	409	0	440	0	0
55	Lh	377	0	418	0	0
56	Li	504	0	572	0	0
57	Lj	302	0	340	0	0
58	EF	4999	0	4781	84	0
59	Pp	28	0	33	0	0
60	Pt	1636	0	840	0	0
61	Dt	1641	0	843	0	0
62	16	12	0	24	1	0
62	23	108	0	216	4	0
62	LC	6	0	12	1	0
63	16	40	0	0	0	0
63	23	144	0	0	0	0
63	5	4	0	0	0	0
63	EF	1	0	0	0	0
63	LB	1	0	0	0	0
63	LC	1	0	0	0	0
63	LD	1	0	0	0	0
63	LQ	1	0	0	0	0
63	LW	1	0	0	0	0
63	Lf	1	0	0	0	0
63	SN	2	0	0	0	0
64	Le	1	0	0	0	0
64	Lj	1	0	0	0	0
64	SB	1	0	0	0	0
65	23	62	0	24	0	0
66	23	30	0	57	0	0
67	EF	37	0	47	15	0
68	EF	28	0	12	0	0
All	All	155157	0	106815	1742	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 7.

All (1742) 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)
23:23:713:G:N2	23:23:718:A:N1	1.92	1.17
6:SF:46:GLN:HA	6:SF:56:LYS:HG2	1.41	1.00
32:LI:147:VAL:HG12	32:LI:149:GLU:HG3	1.43	0.98
29:LE:106:ILE:HG21	29:LE:139:PRO:HD3	1.45	0.97
36:LN:123:LEU:HG	36:LN:123:LEU:O	1.66	0.94
32:LI:147:VAL:CG1	32:LI:149:GLU:HG3	2.04	0.88
2:SB:129:LEU:HB2	2:SB:134:ALA:HB2	1.58	0.85
1:16:267:C:H5'	1:16:267:C:H6	1.42	0.84
26:LB:232:HIS:HA	26:LB:242:LYS:HD2	1.59	0.84
67:EF:802:FUA:H201	67:EF:802:FUA:O1	1.77	0.83
2:SB:108:ARG:O	2:SB:112:LYS:HG3	1.79	0.81
23:23:713:G:N2	23:23:718:A:C2	2.49	0.80
67:EF:802:FUA:H5	67:EF:802:FUA:H202	1.65	0.79
23:23:848:C:H2'	23:23:849:A:H8	1.51	0.75
23:23:1536:C:H4'	23:23:1537:G:H5''	1.70	0.74
13:SM:14:HIS:H	13:SM:44:LYS:HG2	1.51	0.74
16:SP:21:VAL:HG23	16:SP:33:ILE:HB	1.69	0.74
23:23:2153:C:H2'	23:23:2154:A:H8	1.53	0.74
58:EF:431:MET:HB2	58:EF:479:VAL:HG11	1.70	0.73
3:SC:84:VAL:HG13	3:SC:101:ILE:HD11	1.69	0.73
19:SS:36:ARG:HB3	19:SS:72:GLY:HA3	1.71	0.73
1:16:275:G:H5''	1:16:275:G:H8	1.54	0.72
23:23:1087:G:H3'	23:23:1087:G:OP2	1.90	0.72
1:16:34:C:H2'	1:16:35:G:H8	1.52	0.72
58:EF:257:LEU:HD11	58:EF:287:PRO:HB3	1.71	0.71
12:SL:55:VAL:HG21	12:SL:80:ILE:HD11	1.72	0.71
19:SS:45:ILE:HD12	19:SS:64:ASP:HA	1.73	0.71
23:23:1013:C:H2'	23:23:1014:A:H8	1.56	0.71
58:EF:6:PRO:HD2	58:EF:9:ARG:HD3	1.72	0.71
1:16:1522:U:H2'	1:16:1523:G:H8	1.56	0.71
25:LA:48:LEU:HD23	25:LA:50:ILE:H	1.56	0.70
26:LB:162:VAL:HG11	26:LB:174:LEU:HD23	1.72	0.70
9:SI:19:VAL:HA	9:SI:65:ILE:HG22	1.74	0.70
1:16:683:G:H1	1:16:707:U:H3	1.39	0.70
23:23:2064:C:OP2	62:23:3020:PUT:H11	1.92	0.70
23:23:671:C:H6	23:23:671:C:H5''	1.57	0.70
1:16:201:G:H1	1:16:216:U:H3	1.38	0.69
32:LI:129:GLU:HB3	32:LI:141:LYS:HD2	1.73	0.69
58:EF:350:LEU:HD22	58:EF:400:PRO:HA	1.75	0.69
1:16:310:G:H5''	16:SP:31:ARG:HB2	1.74	0.69
5:SE:76:LEU:HD11	5:SE:120:VAL:HG22	1.74	0.69
29:LE:6:ASP:HA	29:LE:9:LYS:HG2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:LY:42:LEU:HD13	47:LY:47:VAL:HG21	1.74	0.69
23:23:45:G:H5''	23:23:46:G:H5'	1.74	0.68
1:16:202:G:HO2'	1:16:468:A:H8	1.40	0.68
23:23:2728:U:HO2'	23:23:2729:G:H8	1.41	0.68
1:16:429:U:H5'	4:SD:9:LEU:HD12	1.75	0.68
23:23:856:G:H2'	23:23:857:G:C8	2.28	0.68
23:23:1478:G:H1	23:23:1513:U:H3	1.39	0.68
1:16:664:G:H22	1:16:741:G:H1	1.41	0.68
23:23:494:G:H4'	44:LV:6:LYS:HB2	1.76	0.68
7:SG:130:ASN:HA	7:SG:135:VAL:HG21	1.76	0.67
1:16:662:U:H2'	1:16:663:A:C8	2.29	0.67
26:LB:21:ASN:HB3	26:LB:24:LEU:HD13	1.75	0.67
1:16:1218:C:H2'	1:16:1219:A:H8	1.60	0.67
1:16:1218:C:H2'	1:16:1219:A:C8	2.28	0.67
8:SH:87:LYS:HE2	8:SH:91:GLU:HB3	1.75	0.67
41:LS:33:VAL:HG22	41:LS:38:LYS:HG2	1.77	0.67
5:SE:74:VAL:HG11	5:SE:144:LEU:HB3	1.76	0.67
67:EF:802:FUA:H152	67:EF:802:FUA:H323	1.77	0.67
6:SF:17:GLN:HE21	6:SF:24:ARG:HH22	1.43	0.67
10:SJ:65:TYR:HB3	14:SN:96:LEU:HD11	1.76	0.67
34:LK:86:ILE:HG13	34:LK:88:SER:H	1.59	0.66
3:SC:186:THR:HG22	3:SC:199:LYS:HG2	1.75	0.66
9:SI:79:ILE:O	9:SI:83:ILE:HG13	1.95	0.66
11:SK:95:SER:HA	11:SK:98:ARG:HD3	1.77	0.66
17:SQ:27:ARG:NH1	17:SQ:42:THR:HG23	2.10	0.66
31:LG:56:VAL:HG22	31:LG:119:VAL:HG22	1.75	0.66
7:SG:148:ASN:HA	7:SG:151:PHE:HB2	1.77	0.66
10:SJ:57:VAL:O	10:SJ:57:VAL:HG22	1.95	0.66
2:SB:43:LEU:HA	2:SB:46:THR:HG22	1.77	0.66
3:SC:124:LEU:HD13	3:SC:196:ILE:HG21	1.78	0.65
11:SK:59:THR:HG22	11:SK:61:PHE:H	1.61	0.65
14:SN:64:CYS:HB2	14:SN:80:SER:HB3	1.76	0.65
23:23:568:U:H1'	23:23:2030:6MZ:H9C1	1.77	0.65
23:23:1105:U:H2'	23:23:1106:G:C8	2.32	0.65
58:EF:618:LYS:HB2	58:EF:685:LEU:HB2	1.78	0.65
26:LB:181:MET:HB2	26:LB:268:VAL:HB	1.76	0.65
7:SG:107:ALA:HA	7:SG:110:LYS:HE3	1.78	0.65
29:LE:158:THR:HG22	29:LE:160:ALA:H	1.60	0.65
1:16:1071:C:H2'	1:16:1072:G:H8	1.61	0.65
1:16:624:C:H4'	16:SP:10:GLY:HA2	1.78	0.65
5:SE:11:LEU:HD13	5:SE:39:VAL:HG13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:LP:75:GLU:HB2	38:LP:90:GLU:HG3	1.78	0.65
14:SN:18:ASP:HA	14:SN:21:PHE:HB2	1.79	0.64
23:23:1434:A:H2'	23:23:1435:G:H8	1.62	0.64
26:LB:24:LEU:HD23	26:LB:83:TYR:HB2	1.79	0.64
23:23:5:A:H2'	23:23:6:A:H8	1.63	0.64
58:EF:94:ASP:HA	58:EF:461:MET:HB2	1.79	0.64
1:16:946:A:H2'	1:16:947:G:C8	2.32	0.63
7:SG:69:VAL:HG11	7:SG:104:ILE:HD11	1.80	0.63
1:16:555:U:H2'	1:16:556:C:C6	2.33	0.63
1:16:1530:G:H2'	1:16:1531:A:H8	1.64	0.63
34:LK:13:VAL:HB	34:LK:42:PHE:HE2	1.62	0.63
8:SH:103:VAL:HG23	8:SH:126:ILE:HB	1.79	0.63
18:SR:21:ILE:O	18:SR:21:ILE:HG13	1.98	0.63
58:EF:640:GLY:HA3	58:EF:658:VAL:HG22	1.78	0.63
67:EF:802:FUA:H211	67:EF:802:FUA:O2	1.98	0.63
1:16:458:U:H2'	1:16:459:A:C8	2.34	0.63
1:16:501:C:H2'	1:16:502:A:H8	1.62	0.62
1:16:1060:U:H2'	1:16:1061:G:H8	1.64	0.62
29:LE:133:ARG:HH11	29:LE:133:ARG:HG3	1.62	0.62
26:LB:175:ARG:HE	26:LB:181:MET:HE1	1.64	0.62
1:16:1409:C:H2'	1:16:1410:A:H8	1.64	0.62
10:SJ:30:LYS:HA	10:SJ:30:LYS:HE2	1.82	0.62
23:23:1028:A:H2'	23:23:1029:A:C8	2.35	0.62
23:23:1433:A:H2'	23:23:1434:A:C8	2.34	0.62
31:LG:69:ILE:HD11	31:LG:87:VAL:HG21	1.80	0.62
1:16:1249:C:H4'	9:SI:75:GLN:HE22	1.65	0.62
1:16:137:U:H6	1:16:137:U:H5''	1.65	0.62
17:SQ:22:VAL:HG22	17:SQ:45:HIS:HD2	1.65	0.62
23:23:143:C:H2'	23:23:144:A:H8	1.65	0.62
23:23:1412:U:H3	23:23:1590:A:H62	1.48	0.62
23:23:2175:C:H2'	23:23:2176:A:H8	1.65	0.62
28:LD:119:ILE:HB	28:LD:187:VAL:HG22	1.82	0.62
1:16:21:G:H2'	1:16:22:G:C8	2.34	0.61
30:LF:98:VAL:HG12	30:LF:103:ILE:HG13	1.82	0.61
9:SI:30:ILE:HG12	9:SI:65:ILE:HD11	1.82	0.61
25:LA:48:LEU:HD22	25:LA:50:ILE:HG12	1.83	0.61
67:EF:802:FUA:O2	67:EF:802:FUA:C29	2.46	0.61
44:LV:59:GLU:HA	44:LV:64:ALA:HA	1.81	0.61
23:23:910:A:H62	38:LP:12:MET:HA	1.66	0.61
41:LS:3:ASN:HA	41:LS:6:LYS:HE3	1.81	0.61
67:EF:802:FUA:O1	67:EF:802:FUA:C20	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:1432:G:H2'	23:23:1433:A:C8	2.36	0.61
23:23:2229:U:H2'	23:23:2230:G:H8	1.64	0.61
19:SS:41:PHE:H	19:SS:44:MET:HE2	1.65	0.61
23:23:5:A:H2'	23:23:6:A:C8	2.36	0.61
1:16:673:A:H2'	1:16:674:G:C8	2.36	0.60
23:23:2175:C:H2'	23:23:2176:A:C8	2.36	0.60
31:LG:73:ARG:HH22	31:LG:80:LEU:HA	1.65	0.60
1:16:691:G:H2'	1:16:692:U:C6	2.36	0.60
1:16:1530:G:H2'	1:16:1531:A:C8	2.36	0.60
8:SH:108:LYS:HG2	8:SH:121:LEU:HD11	1.83	0.60
16:SP:21:VAL:HG11	16:SP:60:TRP:CD1	2.37	0.60
23:23:2547:A:H2'	23:23:2548:U:C6	2.36	0.60
26:LB:107:PRO:HD2	26:LB:110:LEU:HD22	1.83	0.60
1:16:275:G:H5'	1:16:275:G:C8	2.36	0.60
1:16:501:C:H2'	1:16:502:A:C8	2.36	0.60
41:LS:32:VAL:HG12	41:LS:39:ARG:HB2	1.82	0.60
42:LT:109:LEU:HD23	43:LU:49:ILE:HD13	1.84	0.60
45:LW:10:VAL:HG23	45:LW:11:LEU:HD12	1.83	0.60
29:LE:53:ALA:HA	29:LE:150:ARG:HH21	1.66	0.60
1:16:1391:U:H2'	1:16:1392:G:C8	2.37	0.60
23:23:177:G:H3'	23:23:178:G:H8	1.66	0.60
1:16:235:C:H2'	1:16:236:A:H8	1.66	0.60
23:23:286:U:H2'	23:23:287:G:C8	2.37	0.60
44:LV:73:LYS:HB2	44:LV:106:VAL:HB	1.82	0.60
1:16:34:C:H2'	1:16:35:G:C8	2.36	0.60
3:SC:51:SER:HB2	3:SC:115:LEU:HD11	1.84	0.60
34:LK:102:SER:HB3	34:LK:105:GLN:HG3	1.84	0.60
1:16:128:G:H5'	17:SQ:6:ARG:HH12	1.67	0.60
23:23:589:U:H2'	23:23:590:A:H8	1.67	0.60
4:SD:177:LYS:HE2	4:SD:179:GLU:HG2	1.84	0.59
12:SL:77:HIS:CD2	58:EF:428:GLN:HG2	2.37	0.59
33:LJ:64:VAL:HA	33:LJ:67:THR:HG23	1.82	0.59
21:SU:29:LEU:O	21:SU:33:ARG:HG3	2.02	0.59
23:23:639:U:H2'	23:23:640:C:C6	2.37	0.59
23:23:1796:U:H2'	23:23:1797:G:H8	1.66	0.59
1:16:461:A:H2'	1:16:462:G:H8	1.67	0.59
16:SP:18:GLN:HE22	16:SP:35:ARG:HE	1.49	0.59
38:LP:41:LEU:HG	38:LP:96:ILE:HG13	1.85	0.59
13:SM:23:TYR:HE2	13:SM:70:ARG:HG3	1.66	0.59
1:16:492:C:H2'	1:16:493:A:C4	2.37	0.59
9:SI:43:THR:HA	9:SI:46:MET:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SJ:6:ILE:HG13	10:SJ:76:ILE:HB	1.85	0.59
23:23:948:C:H2'	23:23:949:G:H8	1.68	0.59
29:LE:8:TYR:HA	29:LE:12:VAL:HB	1.83	0.59
3:SC:47:LEU:HD12	3:SC:50:ALA:HB2	1.85	0.59
45:LW:54:GLU:HB3	45:LW:88:LYS:HD2	1.85	0.59
1:16:575:G:H4'	1:16:576:C:H5''	1.84	0.59
23:23:1056:G:H4'	23:23:1086:A:H8	1.68	0.59
23:23:2157:G:H1'	23:23:2158:A:H2	1.68	0.59
23:23:1105:U:H2'	23:23:1106:G:H8	1.65	0.59
19:SS:50:ALA:HB1	19:SS:57:HIS:HB3	1.83	0.59
23:23:2291:U:H2'	23:23:2292:U:C6	2.37	0.59
2:SB:5:SER:H	2:SB:8:ASP:HB2	1.68	0.58
1:16:41:G:H2'	1:16:42:G:H8	1.69	0.58
39:LQ:54:LEU:HD11	39:LQ:65:LEU:HD22	1.85	0.58
1:16:1414:U:H2'	1:16:1415:G:H8	1.69	0.58
8:SH:29:SER:HB2	8:SH:59:LEU:HB2	1.85	0.58
8:SH:10:MET:O	8:SH:14:ILE:HG13	2.04	0.58
29:LE:105:THR:O	29:LE:109:PRO:HD2	2.03	0.58
23:23:1796:U:H2'	23:23:1797:G:C8	2.39	0.58
23:23:1802:A:H2'	23:23:1803:A:C8	2.39	0.58
23:23:2220:U:H2'	23:23:2221:G:H8	1.69	0.58
1:16:94:G:H4'	1:16:95:C:H5'	1.85	0.58
1:16:392:C:H2'	1:16:393:A:H8	1.69	0.58
1:16:1518:MA6:H92	1:16:1519:MA6:H93	1.85	0.58
1:16:17:U:H2'	1:16:18:C:C6	2.38	0.58
1:16:513:C:H2'	1:16:514:C:H6	1.68	0.58
1:16:831:A:H4'	2:SB:21:ARG:HH21	1.69	0.58
1:16:1513:A:H2'	1:16:1514:G:C8	2.39	0.58
9:SI:25:ASN:HB3	9:SI:62:ASP:HB3	1.85	0.58
12:SL:89:D2T:O	12:SL:91:PRO:HD3	2.04	0.57
17:SQ:27:ARG:HH12	17:SQ:42:THR:HG23	1.68	0.57
23:23:598:U:H2'	23:23:599:A:H8	1.69	0.57
2:SB:27:MET:HG3	2:SB:189:THR:HA	1.85	0.57
15:SO:7:ALA:O	15:SO:11:ILE:HD12	2.04	0.57
23:23:1038:G:H2'	23:23:1039:A:C8	2.38	0.57
1:16:424:G:H2'	1:16:425:G:C8	2.40	0.57
58:EF:136:PRO:HG2	58:EF:287:PRO:HG3	1.86	0.57
23:23:1353:A:H2'	23:23:1354:A:C8	2.40	0.57
23:23:2165:C:H2'	23:23:2166:U:O4'	2.05	0.57
25:LA:27:ILE:HG23	25:LA:182:ALA:HB1	1.86	0.57
34:LK:78:VAL:HA	34:LK:81:LYS:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:SN:54:ASP:HA	14:SN:59:ARG:HD2	1.86	0.57
25:LA:14:LYS:HD3	25:LA:32:GLU:HG3	1.85	0.57
23:23:927:A:H2'	23:23:928:A:C8	2.40	0.57
1:16:376:G:H2'	1:16:377:G:H8	1.69	0.56
29:LE:94:GLU:H	29:LE:94:GLU:CD	2.08	0.56
58:EF:104:ARG:HH21	58:EF:407:GLU:HB2	1.69	0.56
23:23:1115:G:H2'	23:23:1116:G:H8	1.69	0.56
1:16:477:C:H2'	1:16:478:A:C8	2.40	0.56
40:LR:58:ILE:O	40:LR:58:ILE:HG13	2.05	0.56
58:EF:324:ILE:HG13	58:EF:334:THR:HG23	1.87	0.56
3:SC:108:LYS:HB3	3:SC:111:LEU:HD23	1.87	0.56
33:LJ:52:MET:HB2	33:LJ:81:LEU:HD11	1.86	0.56
1:16:465:A:H2'	1:16:466:A:C8	2.41	0.56
23:23:2801:G:H2'	23:23:2802:G:H8	1.71	0.56
36:LN:63:VAL:HG12	36:LN:107:LEU:HD11	1.87	0.56
3:SC:54:ARG:HB2	3:SC:69:HIS:HB2	1.88	0.56
11:SK:66:ALA:HA	11:SK:69:ARG:HH21	1.70	0.56
1:16:900:A:H2'	1:16:901:A:C8	2.41	0.56
23:23:151:C:H2'	23:23:152:A:H8	1.70	0.56
26:LB:158:ALA:O	26:LB:195:VAL:HG13	2.05	0.56
1:16:902:G:H2'	1:16:903:G:H8	1.69	0.56
23:23:1443:U:H2'	23:23:1444:G:H8	1.71	0.56
1:16:111:G:H1	1:16:330:C:H41	1.53	0.56
1:16:264:C:H4'	17:SQ:65:ARG:HD2	1.87	0.56
23:23:64:A:H2'	23:23:65:U:C6	2.41	0.56
23:23:910:A:H2'	23:23:911:A:C8	2.41	0.56
30:LF:3:ARG:HA	30:LF:6:LYS:HG2	1.87	0.56
19:SS:63:THR:HG22	19:SS:65:GLU:H	1.71	0.56
23:23:1434:A:H2'	23:23:1435:G:C8	2.39	0.56
23:23:2245:U:H5''	23:23:2246:G:H5'	1.88	0.56
40:LR:24:THR:HG22	40:LR:42:PRO:HD3	1.87	0.56
3:SC:156:ARG:H	3:SC:163:ALA:HA	1.70	0.55
32:LI:135:HIS:H	32:LI:138:VAL:HB	1.71	0.55
43:LU:51:VAL:HB	43:LU:52:PRO:HD3	1.88	0.55
58:EF:393:THR:HG21	58:EF:443:PRO:HG3	1.89	0.55
1:16:999:C:H2'	1:16:1000:A:H8	1.71	0.55
2:SB:15:HIS:HB3	2:SB:43:LEU:HD21	1.88	0.55
12:SL:76:GLU:HG3	12:SL:77:HIS:CE1	2.42	0.55
23:23:171:U:H2'	23:23:172:A:H8	1.71	0.55
33:LJ:29:ASP:HB3	33:LJ:107:GLU:HB2	1.88	0.55
5:SE:115:LEU:HD13	5:SE:123:VAL:HG11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:1853:A:H2'	23:23:1854:A:C8	2.41	0.55
58:EF:465:HIS:O	58:EF:469:ILE:HG12	2.07	0.55
1:16:1376:U:H2'	1:16:1377:A:H8	1.72	0.55
17:SQ:60:GLU:HG3	17:SQ:76:VAL:HB	1.87	0.55
35:LM:17:VAL:HG12	35:LM:55:ILE:HB	1.87	0.55
58:EF:492:GLU:OE1	58:EF:564:GLY:HA3	2.06	0.55
29:LE:56:ASP:O	29:LE:60:ILE:HG13	2.05	0.55
1:16:147:G:H2'	1:16:148:G:C8	2.41	0.55
23:23:1353:A:H2'	23:23:1354:A:H8	1.71	0.55
23:23:1411:U:H3	23:23:1591:A:H62	1.54	0.55
23:23:1794:A:H2'	23:23:1795:C:H6	1.71	0.55
1:16:449:G:H2'	1:16:450:G:C8	2.42	0.55
18:SR:13:PHE:HD1	18:SR:18:VAL:HG11	1.71	0.55
19:SS:55:ARG:HG3	19:SS:56:GLN:OE1	2.07	0.55
20:ST:67:ILE:HB	20:ST:71:LYS:HD3	1.89	0.55
23:23:764:A:H5'	26:LB:209:GLY:HA2	1.89	0.55
23:23:2241:A:H2'	23:23:2242:G:C8	2.42	0.55
47:LY:2:PHE:HB3	47:LY:61:LEU:HD13	1.89	0.55
1:16:1163:A:H2'	1:16:1164:G:H8	1.72	0.55
8:SH:35:ALA:O	8:SH:39:VAL:HG23	2.06	0.55
13:SM:23:TYR:CE2	13:SM:70:ARG:HG3	2.41	0.55
23:23:1386:C:H2'	23:23:1387:A:C8	2.42	0.55
26:LB:227:PRO:HA	26:LB:233:GLY:HA2	1.88	0.55
35:LM:45:THR:HB	35:LM:48:VAL:HG12	1.87	0.55
1:16:1409:C:H2'	1:16:1410:A:C8	2.42	0.55
23:23:594:U:H2'	23:23:595:C:C6	2.42	0.54
58:EF:253:ARG:HD3	58:EF:285:TYR:HA	1.90	0.54
8:SH:27:MET:HG3	8:SH:59:LEU:HB3	1.90	0.54
1:16:267:C:H6	1:16:267:C:C5'	2.19	0.54
1:16:269:C:H2'	1:16:270:A:C8	2.43	0.54
23:23:2176:A:H2'	23:23:2177:C:C6	2.42	0.54
46:LX:41:LEU:HD12	46:LX:60:GLU:HB3	1.89	0.54
4:SD:65:TYR:HD2	4:SD:94:LEU:HD13	1.71	0.54
23:23:1846:G:H2'	23:23:1847:A:C8	2.43	0.54
23:23:2081:U:H2'	23:23:2082:A:H8	1.73	0.54
23:23:2537:U:H2'	23:23:2538:C:C6	2.43	0.54
43:LU:63:VAL:HA	43:LU:96:VAL:HG12	1.89	0.54
1:16:236:A:H2'	1:16:237:G:C8	2.42	0.54
1:16:1513:A:H2'	1:16:1514:G:H8	1.71	0.54
23:23:813:U:H2'	23:23:814:C:C6	2.42	0.54
1:16:1437:A:H2'	1:16:1438:G:H8	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SC:39:VAL:O	3:SC:43:LEU:HD13	2.08	0.54
13:SM:25:VAL:HG23	13:SM:29:ARG:HB3	1.88	0.54
23:23:2327:A:H2'	23:23:2328:A:C8	2.43	0.54
1:16:1524:C:H2'	1:16:1525:G:C8	2.42	0.54
8:SH:18:GLN:HG3	8:SH:72:VAL:HB	1.89	0.54
23:23:1278:C:H2'	23:23:1279:G:H8	1.72	0.54
34:LK:22:PRO:HB2	34:LK:23:PRO:HD3	1.90	0.54
1:16:222:C:H2'	1:16:223:A:H8	1.73	0.54
1:16:1412:C:H2'	1:16:1413:A:C8	2.43	0.54
7:SG:69:VAL:HG13	7:SG:100:ALA:HB1	1.90	0.54
1:16:202:G:O2'	1:16:468:A:H8	1.91	0.54
1:16:235:C:H2'	1:16:236:A:C8	2.43	0.54
9:SI:11:ARG:HB3	9:SI:106:ARG:HH21	1.73	0.54
23:23:1405:U:H2'	23:23:1406:U:C6	2.42	0.54
23:23:1469:A:H2'	23:23:1470:A:H8	1.73	0.54
23:23:1469:A:H2'	23:23:1470:A:C8	2.43	0.54
23:23:2305:U:H5''	29:LE:131:GLY:HA3	1.90	0.54
25:LA:6:LYS:HA	25:LA:9:ARG:HG2	1.89	0.54
9:SI:5:GLN:HG2	9:SI:22:LYS:HD3	1.90	0.53
23:23:1429:G:H2'	23:23:1430:G:H8	1.73	0.53
31:LG:90:ALA:HB3	31:LG:91:PRO:HD3	1.90	0.53
1:16:79:G:H21	1:16:80:A:H62	1.56	0.53
1:16:1293:C:H2'	1:16:1294:G:H8	1.73	0.53
1:16:137:U:H5''	1:16:137:U:C6	2.43	0.53
1:16:505:G:H2'	1:16:506:G:C8	2.43	0.53
3:SC:76:VAL:HG23	3:SC:77:ILE:HD12	1.89	0.53
6:SF:5:GLU:HG3	6:SF:90:MET:HB3	1.90	0.53
17:SQ:9:GLN:HE21	17:SQ:58:VAL:HG12	1.73	0.53
23:23:1794:A:H2'	23:23:1795:C:C6	2.43	0.53
26:LB:19:VAL:HG23	26:LB:203:ARG:HB3	1.90	0.53
1:16:1251:A:H2'	1:16:1252:A:C8	2.44	0.53
3:SC:138:VAL:HG11	3:SC:170:GLU:HG3	1.91	0.53
8:SH:105:SER:HB2	8:SH:126:ILE:HD11	1.90	0.53
23:23:1441:G:H2'	23:23:1442:U:C6	2.43	0.53
23:23:2306:C:H5''	23:23:2307:G:H2'	1.90	0.53
23:23:2836:U:H2'	23:23:2837:A:C8	2.43	0.53
26:LB:142:HIS:CD2	26:LB:195:VAL:HB	2.43	0.53
30:LF:107:LEU:HD13	30:LF:152:ARG:HB2	1.89	0.53
40:LR:27:VAL:HA	40:LR:93:ASP:HB3	1.90	0.53
2:SB:164:ILE:O	2:SB:186:ILE:HB	2.08	0.53
23:23:286:U:H2'	23:23:287:G:H8	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:1077:A:H4'	34:LK:94:ASN:HD21	1.73	0.53
23:23:2804:U:H2'	23:23:2805:C:H6	1.74	0.53
40:LR:40:ILE:HG13	40:LR:47:VAL:HG23	1.90	0.53
58:EF:553:VAL:HG12	58:EF:593:PHE:HB3	1.90	0.53
23:23:52:A:H2'	23:23:53:A:C8	2.44	0.53
23:23:589:U:H2'	23:23:590:A:C8	2.43	0.53
23:23:833:A:H2'	23:23:834:G:C8	2.43	0.53
23:23:52:A:H2'	23:23:53:A:H8	1.74	0.53
23:23:1094:U:H1'	23:23:1097:U:H5	1.74	0.53
23:23:2747:G:O6	23:23:2755:C:H5''	2.09	0.53
28:LD:58:LYS:HG3	28:LD:71:GLY:HA2	1.89	0.53
31:LG:57:ILE:HG22	31:LG:93:ALA:HA	1.90	0.53
1:16:1142:G:H3'	1:16:1143:G:H8	1.74	0.53
3:SC:42:TYR:HD1	3:SC:43:LEU:HD12	1.74	0.53
5:SE:40:GLY:HA3	5:SE:46:VAL:HG12	1.91	0.53
13:SM:13:LYS:HD2	13:SM:13:LYS:O	2.08	0.53
23:23:282:A:H2'	23:23:283:G:H8	1.74	0.53
25:LA:45:ALA:HA	25:LA:171:ILE:O	2.09	0.53
26:LB:16:VAL:HG22	26:LB:206:GLY:HA3	1.90	0.53
29:LE:110:ARG:HB2	29:LE:137:ILE:HG13	1.91	0.53
32:LI:83:LYS:HA	32:LI:149:GLU:OXT	2.09	0.53
7:SG:27:VAL:O	7:SG:31:MET:HB2	2.09	0.53
23:23:2394:C:H5''	37:LO:63:LYS:HE2	1.91	0.53
39:LQ:79:LEU:HD23	39:LQ:83:LEU:HD22	1.89	0.53
67:EF:802:FUA:H152	67:EF:802:FUA:C32	2.39	0.53
23:23:689:A:H2'	23:23:690:G:C8	2.43	0.52
24:5:1:U:H2'	24:5:2:G:H8	1.74	0.52
1:16:41:G:H2'	1:16:42:G:C8	2.44	0.52
1:16:131:A:H2'	1:16:132:C:C6	2.43	0.52
1:16:713:G:H2'	1:16:714:G:C8	2.44	0.52
14:SN:64:CYS:HB3	14:SN:68:GLY:H	1.74	0.52
23:23:1569:A:H2'	23:23:1570:A:C8	2.45	0.52
23:23:1911:PSU:H6	23:23:1911:PSU:O5'	1.92	0.52
23:23:2530:A:N7	30:LF:172:LYS:NZ	2.57	0.52
25:LA:47:ASN:OD1	25:LA:211:LYS:HG3	2.09	0.52
58:EF:156:ASN:O	58:EF:160:THR:HG22	2.09	0.52
1:16:1131:G:H1	1:16:1143:G:H21	1.55	0.52
23:23:876:C:H2'	23:23:877:A:O4'	2.10	0.52
23:23:1000:A:H2'	23:23:1001:A:C8	2.44	0.52
23:23:1819:A:H5''	26:LB:160:THR:HG21	1.91	0.52
35:LM:31:GLU:HG2	35:LM:142:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:EF:97:ILE:HD13	58:EF:412:PRO:HD2	1.90	0.52
4:SD:155:VAL:O	4:SD:159:LEU:HG	2.09	0.52
16:SP:4:ILE:HG21	16:SP:71:VAL:HG11	1.92	0.52
23:23:1809:A:H2'	23:23:1810:A:C8	2.44	0.52
29:LE:16:LEU:HD23	29:LE:28:VAL:HG13	1.92	0.52
36:LN:70:ARG:HD2	36:LN:76:VAL:HG22	1.92	0.52
41:LS:22:PRO:HD3	41:LS:50:ILE:HD12	1.91	0.52
1:16:458:U:H2'	1:16:459:A:H8	1.73	0.52
1:16:777:A:H2'	1:16:778:G:C8	2.45	0.52
23:23:675:A:H4'	28:LD:62:GLN:HE21	1.75	0.52
23:23:2801:G:H2'	23:23:2802:G:C8	2.45	0.52
29:LE:108:VAL:HG13	29:LE:114:PHE:CE2	2.44	0.52
41:LS:106:LYS:HA	41:LS:109:ARG:NH1	2.25	0.52
1:16:1386:G:H2'	1:16:1387:G:H8	1.75	0.52
11:SK:45:ALA:N	11:SK:70:CYS:SG	2.83	0.52
13:SM:4:ILE:HD11	13:SM:10:PRO:HG3	1.92	0.52
20:ST:79:LEU:O	20:ST:83:ILE:HG13	2.09	0.52
29:LE:70:ALA:HB3	29:LE:81:GLN:HA	1.92	0.52
1:16:337:G:H2'	1:16:338:A:C8	2.45	0.52
17:SQ:64:CYS:SG	17:SQ:74:THR:HG23	2.49	0.52
23:23:191:A:H2'	23:23:192:C:H6	1.73	0.52
23:23:729:G:O2'	23:23:763:G:H4'	2.10	0.52
23:23:2515:C:H2'	23:23:2516:A:H8	1.75	0.52
45:LW:8:LEU:HD23	45:LW:50:LEU:HD21	1.91	0.52
1:16:1342:C:H2'	1:16:1343:G:C8	2.45	0.52
2:SB:101:LEU:HB2	2:SB:175:GLU:HG2	1.92	0.52
8:SH:102:ALA:HB3	8:SH:113:ASP:HB3	1.92	0.52
23:23:657:U:H2'	23:23:658:U:C6	2.45	0.52
23:23:1056:G:H4'	23:23:1086:A:C8	2.44	0.52
25:LA:212:VAL:HG23	25:LA:224:VAL:HB	1.90	0.52
37:LO:116:VAL:HG11	37:LO:135:ILE:HD13	1.91	0.52
38:LP:20:LEU:HD13	47:LY:81:PRO:HG2	1.92	0.52
40:LR:4:LYS:O	40:LR:8:ILE:HG12	2.10	0.52
1:16:600:A:H2'	1:16:601:G:H8	1.73	0.52
3:SC:12:LEU:HD11	14:SN:91:GLY:HA2	1.91	0.52
23:23:64:A:H2'	23:23:65:U:H6	1.75	0.52
23:23:1438:U:H2'	23:23:1439:A:H8	1.75	0.52
23:23:2557:G:H2'	23:23:2558:C:C6	2.45	0.52
58:EF:666:TYR:CE2	58:EF:670:LEU:HD12	2.45	0.52
3:SC:7:PRO:HA	3:SC:10:ILE:HG22	1.91	0.52
16:SP:20:VAL:HG23	16:SP:35:ARG:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:SQ:47:HIS:HB3	17:SQ:74:THR:HG22	1.92	0.52
23:23:2183:A:H2'	23:23:2184:A:H8	1.74	0.52
58:EF:90:PRO:HB3	67:EF:802:FUA:H211	1.92	0.52
16:SP:4:ILE:HG22	16:SP:71:VAL:HG21	1.91	0.51
29:LE:4:LEU:HD23	29:LE:101:GLU:HB2	1.91	0.51
7:SG:74:GLU:HG2	7:SG:91:VAL:HG13	1.92	0.51
23:23:29:U:H2'	23:23:30:G:C8	2.46	0.51
23:23:813:U:H2'	23:23:814:C:H6	1.76	0.51
23:23:1542:U:H3'	23:23:1543:G:H8	1.75	0.51
23:23:1746:A:H2'	23:23:1747:U:C6	2.45	0.51
23:23:2804:U:H2'	23:23:2805:C:C6	2.45	0.51
1:16:600:A:H2'	1:16:601:G:C8	2.44	0.51
1:16:783:C:H2'	1:16:784:A:H8	1.75	0.51
3:SC:73:PRO:HA	3:SC:76:VAL:HG22	1.92	0.51
4:SD:11:LEU:HD13	4:SD:63:ARG:HG2	1.92	0.51
15:SO:26:GLU:HG3	15:SO:81:LEU:HD12	1.91	0.51
23:23:351:C:H2'	23:23:352:A:H8	1.75	0.51
23:23:2194:U:H2'	23:23:2195:U:H6	1.75	0.51
29:LE:58:ALA:HB2	29:LE:65:PRO:HD3	1.92	0.51
2:SB:100:MET:HA	2:SB:107:VAL:HG21	1.91	0.51
3:SC:66:VAL:HB	3:SC:101:ILE:HG22	1.93	0.51
12:SL:114:ARG:HB3	12:SL:119:VAL:HB	1.92	0.51
23:23:593:U:H2'	23:23:594:U:C6	2.45	0.51
23:23:2074:U:H2'	23:23:2075:U:C6	2.46	0.51
33:LJ:23:LEU:HD12	33:LJ:87:GLU:O	2.10	0.51
34:LK:77:ALA:HA	34:LK:136:MET:HE1	1.92	0.51
58:EF:469:ILE:HD11	67:EF:802:FUA:H22	1.93	0.51
10:SJ:21:ALA:HB1	10:SJ:92:LEU:HD13	1.92	0.51
23:23:1548:A:H2'	23:23:1549:A:C8	2.46	0.51
23:23:1597:A:H5''	23:23:1598:A:H5'	1.91	0.51
58:EF:317:PHE:HA	58:EF:341:GLY:HA3	1.92	0.51
1:16:323:U:H2'	1:16:324:G:O4'	2.09	0.51
1:16:538:G:H2'	1:16:539:A:H8	1.76	0.51
1:16:1042:A:H2'	1:16:1043:G:C8	2.45	0.51
37:LO:29:LYS:HG2	37:LO:29:LYS:O	2.10	0.51
58:EF:89:THR:HB	58:EF:99:VAL:HG22	1.91	0.51
58:EF:337:ARG:HD3	58:EF:339:TYR:HE1	1.76	0.51
1:16:840:C:O2	1:16:840:C:H2'	2.10	0.51
1:16:1034:G:H2'	1:16:1035:A:H8	1.75	0.51
5:SE:105:ILE:HG22	5:SE:123:VAL:HG12	1.92	0.51
6:SF:40:GLU:HB2	6:SF:61:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SK:32:VAL:HG13	11:SK:70:CYS:SG	2.51	0.51
23:23:172:A:H2'	23:23:173:A:C8	2.46	0.51
23:23:2064:C:H2'	23:23:2065:C:C6	2.46	0.51
23:23:2567:G:H2'	23:23:2568:U:C6	2.46	0.51
1:16:777:A:H2'	1:16:778:G:H8	1.75	0.51
23:23:143:C:H2'	23:23:144:A:C8	2.46	0.51
23:23:172:A:H2'	23:23:173:A:H8	1.75	0.51
23:23:632:A:H2'	23:23:633:A:C8	2.46	0.51
23:23:848:C:H2'	23:23:849:A:C8	2.38	0.51
23:23:2097:A:H2'	23:23:2098:U:C6	2.45	0.51
23:23:2290:G:H2'	23:23:2291:U:C6	2.45	0.51
23:23:2514:U:H2'	23:23:2515:C:C6	2.45	0.51
34:LK:16:GLY:H	34:LK:46:THR:HB	1.75	0.51
34:LK:61:VAL:HG22	34:LK:67:PHE:HA	1.93	0.51
1:16:1038:C:H2'	1:16:1039:G:H8	1.76	0.51
1:16:1175:G:H2'	1:16:1176:A:C8	2.46	0.51
2:SB:13:GLY:HA2	2:SB:15:HIS:CE1	2.46	0.51
23:23:645:C:H2'	23:23:647:G:C8	2.46	0.51
23:23:2537:U:H2'	23:23:2538:C:H6	1.76	0.51
27:LC:121:THR:HG21	27:LC:143:PRO:HB3	1.93	0.51
1:16:728:A:H2'	1:16:729:A:C8	2.46	0.51
3:SC:189:ALA:HB3	3:SC:196:ILE:HB	1.93	0.51
8:SH:43:GLU:HG3	8:SH:101:ILE:HG21	1.92	0.51
13:SM:80:LEU:HA	13:SM:83:LEU:HD23	1.93	0.51
23:23:1198:U:H2'	23:23:1199:U:C6	2.46	0.51
23:23:1571:A:H2'	23:23:1572:A:C8	2.46	0.51
29:LE:8:TYR:HB2	29:LE:173:PHE:HZ	1.75	0.51
1:16:522:C:H41	12:SL:50:ARG:HH21	1.58	0.50
11:SK:64:GLN:HE21	11:SK:95:SER:HB2	1.76	0.50
23:23:1028:A:N6	23:23:1125:G:H2'	2.26	0.50
23:23:2233:U:H2'	23:23:2234:G:H8	1.76	0.50
23:23:2328:A:H8	23:23:2328:A:O5'	1.93	0.50
58:EF:175:ALA:H	58:EF:178:HIS:HB2	1.77	0.50
1:16:1064:G:H1'	1:16:1190:G:H21	1.76	0.50
9:SI:91:ASP:O	9:SI:92:GLU:HG3	2.12	0.50
31:LG:104:GLU:O	31:LG:108:LYS:HG3	2.10	0.50
1:16:552:U:H2'	1:16:553:A:H8	1.75	0.50
1:16:677:U:H3	1:16:713:G:H22	1.60	0.50
1:16:1138:G:H3'	1:16:1138:G:N3	2.26	0.50
1:16:1376:U:H2'	1:16:1377:A:C8	2.46	0.50
13:SM:83:LEU:HD12	19:SS:74:PHE:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:SR:9:LYS:HB2	18:SR:46:GLY:HA3	1.94	0.50
23:23:284:U:H2'	23:23:285:G:C8	2.47	0.50
23:23:414:C:H2'	23:23:415:A:H8	1.76	0.50
23:23:639:U:H2'	23:23:640:C:H6	1.75	0.50
23:23:2241:A:H2'	23:23:2242:G:H8	1.77	0.50
44:LV:28:LYS:HA	44:LV:70:LYS:HA	1.93	0.50
1:16:486:U:H6	1:16:486:U:P	2.34	0.50
1:16:1477:U:H2'	1:16:1478:U:C6	2.46	0.50
3:SC:77:ILE:HA	3:SC:84:VAL:HG23	1.93	0.50
13:SM:3:ARG:HG3	13:SM:9:ILE:HG12	1.94	0.50
23:23:1808:A:H3'	23:23:1809:A:C8	2.46	0.50
23:23:2014:A:H2'	23:23:2015:A:C8	2.47	0.50
23:23:2220:U:H2'	23:23:2221:G:C8	2.46	0.50
1:16:840:C:H3'	1:16:842:U:H5''	1.94	0.50
3:SC:116:VAL:HG23	3:SC:200:VAL:HG21	1.93	0.50
9:SI:110:GLN:HG2	9:SI:111:VAL:N	2.26	0.50
23:23:566:U:H5''	37:LO:29:LYS:HE2	1.94	0.50
23:23:1013:C:H2'	23:23:1014:A:C8	2.42	0.50
23:23:1827:U:H2'	23:23:1828:G:O4'	2.11	0.50
23:23:1853:A:N1	23:23:2087:G:H1'	2.27	0.50
23:23:2443:C:H2'	23:23:2444:G:H8	1.76	0.50
41:LS:106:LYS:HG2	41:LS:109:ARG:HH12	1.75	0.50
1:16:222:C:H2'	1:16:223:A:C8	2.47	0.50
1:16:666:G:H5'	1:16:726:C:H1'	1.93	0.50
23:23:1830:C:H2'	23:23:1831:G:H8	1.76	0.50
30:LF:101:ASN:HA	30:LF:117:LEU:HD12	1.93	0.50
1:16:461:A:H2'	1:16:462:G:C8	2.47	0.50
1:16:1395:C:HO2'	1:16:1401:G:HO2'	1.60	0.50
10:SJ:30:LYS:HE2	10:SJ:30:LYS:CA	2.41	0.50
23:23:2649:C:H2'	23:23:2650:U:H6	1.77	0.50
29:LE:30:ARG:H	29:LE:159:THR:HB	1.76	0.50
42:LT:83:LEU:HD12	42:LT:113:ALA:HB2	1.94	0.50
23:23:2086:U:H2'	23:23:2087:G:C8	2.47	0.50
45:LW:7:LEU:HD13	45:LW:46:ALA:HA	1.94	0.50
58:EF:214:LEU:HD23	58:EF:218:TRP:HD1	1.77	0.50
1:16:985:C:H2'	1:16:986:U:C6	2.46	0.50
7:SG:75:VAL:HG13	7:SG:148:ASN:HD21	1.76	0.50
13:SM:75:MET:HA	13:SM:78:LYS:HG2	1.94	0.50
23:23:282:A:H2'	23:23:283:G:C8	2.46	0.50
23:23:1689:A:H2'	23:23:1690:A:H8	1.77	0.50
23:23:2025:C:H2'	23:23:2026:U:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:LQ:73:ASN:HA	39:LQ:76:VAL:HG22	1.94	0.50
58:EF:14:GLY:HA2	58:EF:87:ILE:O	2.12	0.50
1:16:999:C:H2'	1:16:1000:A:C8	2.47	0.49
8:SH:10:MET:HG3	8:SH:27:MET:SD	2.52	0.49
23:23:1666:G:HO2'	36:LN:6:THR:HG1	1.59	0.49
23:23:1689:A:H2'	23:23:1690:A:C8	2.47	0.49
23:23:1742:U:H2'	23:23:1743:G:C8	2.47	0.49
30:LF:91:GLY:HA3	30:LF:94:TYR:CD2	2.47	0.49
58:EF:17:ALA:HB2	58:EF:112:VAL:HB	1.94	0.49
58:EF:309:ARG:HH21	58:EF:316:PRO:HD2	1.76	0.49
67:EF:802:FUA:H202	67:EF:802:FUA:C5	2.41	0.49
1:16:572:A:HO2'	1:16:916:U:HO2'	1.59	0.49
1:16:1486:G:H2'	1:16:1487:G:C8	2.48	0.49
23:23:634:C:H2'	23:23:635:C:C6	2.47	0.49
23:23:1394:U:H2'	23:23:1395:A:O4'	2.12	0.49
1:16:409:U:H2'	1:16:410:G:O4'	2.12	0.49
1:16:459:A:H2'	1:16:460:A:C8	2.47	0.49
6:SF:46:GLN:HA	6:SF:56:LYS:CG	2.29	0.49
23:23:1281:G:H2'	23:23:1282:U:C6	2.47	0.49
23:23:2698:U:H2'	23:23:2699:C:C6	2.47	0.49
23:23:2832:U:H4'	23:23:2833:U:H5'	1.94	0.49
33:LJ:122:GLN:HG3	33:LJ:125:ARG:HE	1.77	0.49
44:LV:83:LYS:HG2	44:LV:95:ARG:HE	1.77	0.49
34:LK:56:PRO:HB2	34:LK:72:LYS:HB2	1.94	0.49
1:16:1011:C:H2'	1:16:1012:A:C8	2.48	0.49
23:23:499:U:H5''	46:LX:43:LYS:HD2	1.95	0.49
23:23:671:C:H5''	23:23:671:C:C6	2.42	0.49
23:23:2845:U:H5''	41:LS:52:ASN:O	2.12	0.49
29:LE:100:PHE:O	29:LE:104:ILE:HG22	2.13	0.49
39:LQ:28:LEU:HD23	39:LQ:48:VAL:HG21	1.94	0.49
58:EF:468:ILE:HD13	67:EF:802:FUA:H11	1.94	0.49
1:16:1531:A:H2'	1:16:1532:U:C6	2.47	0.49
23:23:155:A:H2'	23:23:156:A:C8	2.48	0.49
23:23:1412:U:H3	23:23:1590:A:N6	2.11	0.49
25:LA:46:VAL:HG12	25:LA:171:ILE:HB	1.95	0.49
25:LA:48:LEU:HD21	25:LA:208:TYR:CE1	2.47	0.49
5:SE:60:ILE:O	5:SE:64:MET:HG2	2.13	0.49
23:23:171:U:H2'	23:23:172:A:C8	2.48	0.49
23:23:284:U:H2'	23:23:285:G:H8	1.77	0.49
23:23:594:U:H2'	23:23:595:C:H6	1.77	0.49
23:23:843:G:H2'	23:23:844:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:851:C:H2'	23:23:852:U:C6	2.48	0.49
23:23:1709:U:H2'	23:23:1710:G:H8	1.78	0.49
23:23:2101:A:H2'	23:23:2102:G:H8	1.77	0.49
23:23:2460:U:C2	23:23:2461:A:C8	3.00	0.49
23:23:2639:A:H2'	23:23:2640:G:O4'	2.13	0.49
31:LG:78:LEU:HD21	31:LG:86:LEU:HD21	1.95	0.49
32:LI:84:ALA:HB2	32:LI:90:LEU:HD23	1.94	0.49
1:16:377:G:H2'	1:16:378:G:H8	1.78	0.49
9:SI:28:ILE:HG12	9:SI:35:LEU:HD22	1.95	0.49
23:23:871:U:H2'	23:23:872:U:C6	2.47	0.49
23:23:2148:G:H2'	23:23:2149:U:C6	2.48	0.49
23:23:2286:G:H4'	23:23:2287:A:O4'	2.12	0.49
58:EF:102:SER:O	58:EF:106:LEU:HG	2.13	0.49
58:EF:244:THR:HG23	58:EF:247:GLU:H	1.78	0.49
58:EF:615:PRO:HB2	58:EF:660:LEU:HD23	1.94	0.49
1:16:22:G:H4'	1:16:885:G:C8	2.48	0.49
1:16:393:A:C2	1:16:394:G:C8	3.01	0.49
1:16:494:G:O2'	1:16:496:A:H1'	2.13	0.49
3:SC:46:GLU:HG3	3:SC:47:LEU:HD22	1.95	0.49
11:SK:47:ALA:HB1	11:SK:62:ALA:HB1	1.94	0.49
13:SM:74:SER:HA	13:SM:77:ILE:HG12	1.94	0.49
23:23:1224:U:H2'	23:23:1225:G:C8	2.47	0.49
23:23:1636:U:H2'	23:23:1637:A:C8	2.47	0.49
1:16:459:A:H2'	1:16:460:A:H8	1.78	0.49
1:16:493:A:H2'	1:16:494:G:C4	2.47	0.49
1:16:911:U:H2'	1:16:912:C:C6	2.48	0.49
1:16:1071:C:H2'	1:16:1072:G:C8	2.46	0.49
1:16:1251:A:H2'	1:16:1252:A:H8	1.78	0.49
5:SE:84:PRO:HD2	8:SH:97:ALA:HB2	1.95	0.49
23:23:78:U:H2'	23:23:79:C:C6	2.48	0.49
23:23:1286:A:H1'	23:23:1288:G:OP2	2.13	0.49
23:23:1442:U:H2'	23:23:1443:U:C6	2.47	0.49
23:23:1682:G:H2'	23:23:1683:U:C6	2.47	0.49
23:23:2011:U:H2'	23:23:2012:G:O4'	2.13	0.49
23:23:2687:U:H2'	23:23:2688:G:O4'	2.13	0.49
38:LP:46:ILE:HD12	38:LP:69:PRO:HG3	1.95	0.49
1:16:294:U:H2'	1:16:295:C:C6	2.47	0.48
1:16:355:C:H1'	1:16:388:G:H1'	1.95	0.48
6:SF:88:MET:HB3	18:SR:64:TYR:HE2	1.78	0.48
10:SJ:8:ILE:HD11	10:SJ:87:LEU:HD11	1.94	0.48
19:SS:53:ASN:HB2	19:SS:77:THR:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:1571:A:H2'	23:23:1572:A:H8	1.77	0.48
1:16:1493:A:H2'	23:23:1913:A:C2	2.48	0.48
23:23:6:A:H2'	23:23:7:G:H8	1.78	0.48
23:23:351:C:H2'	23:23:352:A:C8	2.48	0.48
23:23:875:G:H2'	23:23:876:C:C6	2.47	0.48
23:23:1141:U:H4'	23:23:1142:A:O4'	2.13	0.48
23:23:1316:U:H2'	23:23:1317:G:H8	1.78	0.48
30:LF:137:ASP:HB3	30:LF:140:VAL:HB	1.95	0.48
34:LK:62:TYR:H	34:LK:66:SER:HB2	1.78	0.48
7:SG:35:LYS:HB3	7:SG:38:THR:HG22	1.95	0.48
20:ST:4:ILE:HG22	20:ST:6:SER:H	1.77	0.48
20:ST:35:VAL:O	20:ST:39:ILE:HG12	2.11	0.48
23:23:644:A:H2'	23:23:645:C:O4'	2.13	0.48
23:23:967:U:H2'	23:23:968:C:C6	2.48	0.48
23:23:967:U:H2'	23:23:968:C:H6	1.78	0.48
25:LA:48:LEU:HD12	25:LA:196:LEU:HD21	1.96	0.48
1:16:513:C:H2'	1:16:514:C:C6	2.47	0.48
1:16:524:G:H2'	1:16:525:C:C6	2.47	0.48
23:23:296:U:H2'	23:23:297:G:C8	2.48	0.48
43:LU:6:GLN:HB3	43:LU:11:GLN:HG2	1.94	0.48
67:EF:802:FUA:C32	67:EF:802:FUA:C15	2.91	0.48
1:16:399:G:H2'	1:16:400:C:C6	2.48	0.48
1:16:1359:C:O5'	1:16:1359:C:H6	1.96	0.48
16:SP:18:GLN:NE2	16:SP:35:ARG:HE	2.10	0.48
23:23:155:A:H2'	23:23:156:A:H8	1.79	0.48
23:23:2097:A:H2'	23:23:2098:U:H6	1.79	0.48
23:23:2661:G:H5'	58:EF:19:ILE:HD13	1.96	0.48
35:LM:4:PHE:CD2	42:LT:100:VAL:HG11	2.49	0.48
35:LM:114:LEU:O	35:LM:118:MET:HG3	2.13	0.48
1:16:1239:A:H62	1:16:1299:A:H62	1.61	0.48
1:16:1271:A:H2'	1:16:1272:G:H8	1.78	0.48
1:16:1533:C:H4'	1:16:1534:A:C8	2.49	0.48
2:SB:94:HIS:CG	2:SB:95:ARG:H	2.31	0.48
3:SC:22:TRP:HB3	3:SC:59:ARG:H	1.78	0.48
23:23:755:U:H2'	23:23:756:A:C8	2.48	0.48
23:23:2728:U:O2'	23:23:2729:G:H8	1.96	0.48
28:LD:5:LEU:HG	28:LD:120:VAL:HG12	1.94	0.48
43:LU:59:ILE:HG12	43:LU:101:ILE:HG12	1.96	0.48
44:LV:4:ILE:HG13	44:LV:106:VAL:HG22	1.94	0.48
1:16:17:U:H2'	1:16:18:C:H6	1.76	0.48
1:16:56:U:H2'	1:16:57:G:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:16:806:C:H2'	1:16:807:A:H8	1.77	0.48
23:23:296:U:H2'	23:23:297:G:H8	1.78	0.48
23:23:596:U:H2'	23:23:597:G:H8	1.77	0.48
1:16:398:U:H2'	1:16:399:G:H8	1.79	0.48
1:16:539:A:H2'	1:16:540:G:C8	2.48	0.48
1:16:868:C:H2'	1:16:869:G:O4'	2.13	0.48
1:16:1038:C:H2'	1:16:1039:G:C8	2.48	0.48
2:SB:27:MET:O	2:SB:31:ILE:HG12	2.14	0.48
8:SH:32:LEU:O	8:SH:36:ILE:HD12	2.13	0.48
9:SI:71:GLY:O	9:SI:75:GLN:HG3	2.14	0.48
23:23:184:C:H2'	23:23:185:G:H8	1.79	0.48
23:23:365:U:H2'	23:23:366:C:C6	2.49	0.48
23:23:2047:C:H2'	23:23:2048:G:H8	1.79	0.48
28:LD:155:GLU:HG2	28:LD:156:ASN:N	2.28	0.48
1:16:523:A:H61	12:SL:89:D2T:CG	2.26	0.48
1:16:538:G:H2'	1:16:539:A:C8	2.49	0.48
1:16:553:A:H2'	1:16:554:A:C8	2.49	0.48
1:16:1287:A:H2'	1:16:1288:A:C8	2.48	0.48
18:SR:62:ALA:HB1	18:SR:67:LEU:HB2	1.96	0.48
23:23:1497:U:H5''	23:23:1498:C:H5	1.78	0.48
23:23:1771:C:H2'	23:23:1772:A:C8	2.49	0.48
23:23:2364:C:H2'	23:23:2365:G:O4'	2.13	0.48
34:LK:126:THR:HA	34:LK:129:ILE:HG12	1.96	0.48
37:LO:131:ALA:O	37:LO:135:ILE:HG12	2.13	0.48
58:EF:11:ARG:HB2	58:EF:84:ILE:HG12	1.96	0.48
1:16:267:C:H5'	1:16:267:C:C6	2.34	0.48
1:16:490:C:H2'	1:16:491:G:C8	2.49	0.48
1:16:1219:A:H2'	1:16:1220:G:C8	2.49	0.48
1:16:1236:A:H4'	1:16:1304:G:H4'	1.94	0.48
2:SB:90:PHE:CE2	2:SB:154:MET:HA	2.48	0.48
2:SB:91:PHE:HE2	2:SB:93:ASN:HB2	1.79	0.48
4:SD:170:TRP:HB2	4:SD:184:ARG:O	2.14	0.48
23:23:2064:C:H2'	23:23:2065:C:H6	1.79	0.48
23:23:2099:U:H2'	23:23:2100:G:C8	2.49	0.48
23:23:2455:G:H2'	23:23:2456:C:C6	2.49	0.48
29:LE:83:TYR:O	29:LE:85:ILE:HG12	2.14	0.48
58:EF:425:LYS:HD3	58:EF:425:LYS:HA	1.65	0.48
58:EF:643:LYS:HB3	58:EF:643:LYS:HE3	1.43	0.48
1:16:73:C:HO2'	1:16:74:A:H8	1.61	0.47
1:16:821:G:H2'	1:16:822:U:C6	2.49	0.47
1:16:1014:A:C2	1:16:1219:A:H1'	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SC:29:PHE:HE2	14:SN:77:PHE:HD1	1.61	0.47
13:SM:6:GLY:HA2	13:SM:66:GLU:HG2	1.95	0.47
23:23:2812:G:H2'	23:23:2813:A:C8	2.49	0.47
34:LK:72:LYS:HA	34:LK:72:LYS:HD2	1.50	0.47
40:LR:17:LYS:HE3	40:LR:21:LEU:HD11	1.94	0.47
1:16:337:G:H2'	1:16:338:A:H8	1.79	0.47
1:16:413:G:O5'	1:16:414:A:H5'	2.14	0.47
1:16:875:U:O2'	8:SH:15:ARG:HD2	2.14	0.47
3:SC:179:ARG:HD3	3:SC:207:ILE:HG13	1.97	0.47
15:SO:9:ALA:HA	15:SO:12:VAL:HG12	1.95	0.47
15:SO:49:ASP:OD2	15:SO:52:SER:HB2	2.14	0.47
34:LK:12:GLN:HA	34:LK:56:PRO:HA	1.94	0.47
1:16:500:G:H2'	1:16:501:C:C6	2.50	0.47
2:SB:164:ILE:HD11	2:SB:214:LEU:HD21	1.97	0.47
7:SG:86:GLN:O	7:SG:151:PHE:HB3	2.13	0.47
10:SJ:49:PHE:HE2	10:SJ:67:ILE:HG12	1.79	0.47
23:23:721:A:H2'	23:23:722:A:C8	2.50	0.47
23:23:2183:A:H2'	23:23:2184:A:C8	2.49	0.47
23:23:2233:U:H2'	23:23:2234:G:C8	2.49	0.47
23:23:2772:C:H5'	27:LC:173:GLN:HE21	1.79	0.47
26:LB:163:GLN:HB3	26:LB:175:ARG:HB3	1.95	0.47
1:16:56:U:H2'	1:16:57:G:H8	1.79	0.47
1:16:114:U:H2'	1:16:115:G:C8	2.49	0.47
1:16:1097:C:H2'	1:16:1098:C:C6	2.49	0.47
3:SC:156:ARG:HG3	3:SC:160:ALA:O	2.14	0.47
13:SM:57:ARG:HA	13:SM:60:VAL:HG12	1.96	0.47
20:ST:31:PHE:HB3	20:ST:54:MET:HB3	1.96	0.47
20:ST:66:LEU:HD23	20:ST:67:ILE:HG23	1.96	0.47
23:23:414:C:H2'	23:23:415:A:C8	2.48	0.47
23:23:1747:U:H2'	23:23:1748:C:C6	2.50	0.47
23:23:2008:C:H2'	23:23:2009:A:H8	1.78	0.47
23:23:2063:C:OP1	62:23:3020:PUT:H22	2.14	0.47
23:23:2636:C:HO2'	27:LC:45:TYR:HH	1.62	0.47
23:23:2731:G:O2'	23:23:2732:G:H5'	2.13	0.47
26:LB:17:VAL:HB	26:LB:204:VAL:HG22	1.97	0.47
30:LF:60:ASP:HB3	30:LF:64:GLN:HG2	1.96	0.47
47:LY:40:ILE:HD12	47:LY:42:LEU:HD23	1.95	0.47
1:16:618:C:H5'	1:16:619:U:H5''	1.96	0.47
1:16:1096:C:H2'	1:16:1097:C:H6	1.80	0.47
1:16:1510:C:H2'	1:16:1511:G:C8	2.49	0.47
3:SC:33:LEU:HD21	14:SN:93:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:SL:46:ASN:ND2	12:SL:89:D2T:SB	2.87	0.47
23:23:1482:G:H2'	23:23:1483:G:H8	1.80	0.47
23:23:1844:C:H5''	26:LB:256:LYS:HG3	1.96	0.47
23:23:1946:U:H2'	23:23:1947:C:C6	2.49	0.47
30:LF:105:LEU:HB2	30:LF:113:VAL:HB	1.96	0.47
34:LK:13:VAL:HB	34:LK:42:PHE:CE2	2.47	0.47
58:EF:280:ASP:O	58:EF:283:ILE:HG22	2.14	0.47
58:EF:666:TYR:HE2	58:EF:670:LEU:HD12	1.79	0.47
1:16:321:A:H61	1:16:332:G:H1	1.62	0.47
1:16:559:A:H4'	1:16:560:A:H3'	1.97	0.47
1:16:1163:A:H2'	1:16:1164:G:C8	2.49	0.47
11:SK:125:LYS:H	11:SK:125:LYS:HG3	1.48	0.47
18:SR:51:TYR:HA	18:SR:54:GLN:HE21	1.80	0.47
23:23:1316:U:H2'	23:23:1317:G:C8	2.50	0.47
23:23:2636:C:H2'	23:23:2637:U:H6	1.79	0.47
23:23:2788:C:H2'	23:23:2789:C:C6	2.49	0.47
26:LB:91:ILE:HD12	26:LB:103:TYR:CD1	2.49	0.47
32:LI:132:PHE:HB2	32:LI:140:ALA:HB3	1.96	0.47
1:16:216:U:H2'	1:16:217:C:H6	1.79	0.47
1:16:335:C:H2'	1:16:336:A:C8	2.49	0.47
1:16:637:C:H2'	1:16:638:U:C6	2.50	0.47
1:16:1271:A:H2'	1:16:1272:G:C8	2.50	0.47
1:16:1323:G:H2'	1:16:1324:A:C8	2.50	0.47
5:SE:65:GLU:HA	5:SE:68:ARG:HG2	1.97	0.47
16:SP:4:ILE:CD1	16:SP:21:VAL:HG12	2.44	0.47
17:SQ:8:LEU:HD22	17:SQ:73:TRP:CH2	2.49	0.47
18:SR:48:ARG:HD3	18:SR:48:ARG:HA	1.46	0.47
20:ST:54:MET:O	20:ST:57:ILE:HG22	2.14	0.47
23:23:6:A:H2'	23:23:7:G:C8	2.49	0.47
23:23:419:U:H2'	23:23:420:C:C6	2.50	0.47
23:23:909:A:H2'	23:23:912:C:H5	1.80	0.47
23:23:2514:U:H2'	23:23:2515:C:H6	1.79	0.47
23:23:2784:U:H2'	23:23:2785:C:C6	2.50	0.47
25:LA:5:THR:H	25:LA:8:MET:HE3	1.79	0.47
33:LJ:5:LEU:O	33:LJ:9:GLN:HG2	2.15	0.47
46:LX:79:LYS:HE3	46:LX:79:LYS:HB3	1.74	0.47
1:16:460:A:H2'	1:16:461:A:H8	1.80	0.47
1:16:1033:G:H2'	1:16:1034:G:H8	1.80	0.47
13:SM:83:LEU:HD12	19:SS:74:PHE:HE1	1.78	0.47
21:SU:41:PRO:O	21:SU:44:GLU:HG2	2.14	0.47
23:23:81:G:HO2'	23:23:295:G:HO2'	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:1173:U:H2'	23:23:1174:U:H4'	1.97	0.47
35:LM:34:ARG:HG3	35:LM:39:LYS:HB2	1.97	0.47
1:16:109:A:H5'	1:16:110:C:H5	1.80	0.47
1:16:996:A:H2'	1:16:997:U:H6	1.80	0.47
4:SD:170:TRP:CD1	4:SD:186:PRO:HD3	2.50	0.47
15:SO:56:LEU:HD23	15:SO:56:LEU:C	2.35	0.47
23:23:754:U:H2'	23:23:755:U:C6	2.50	0.47
23:23:1636:U:H2'	23:23:1637:A:H8	1.80	0.47
29:LE:8:TYR:O	29:LE:13:VAL:HG23	2.15	0.47
45:LW:39:THR:OG1	45:LW:42:GLU:HG3	2.15	0.47
1:16:537:G:H2'	1:16:538:G:H8	1.80	0.47
4:SD:145:ILE:HG22	4:SD:146:ARG:O	2.15	0.47
6:SF:21:MET:HA	6:SF:24:ARG:CZ	2.45	0.47
7:SG:114:LYS:HD3	7:SG:114:LYS:HA	1.53	0.47
13:SM:79:ARG:O	13:SM:83:LEU:HD23	2.15	0.47
23:23:675:A:OP1	28:LD:71:GLY:HA3	2.15	0.47
23:23:1292:G:H2'	23:23:1293:C:C6	2.50	0.47
23:23:2157:G:H1'	23:23:2158:A:C2	2.48	0.47
23:23:2243:U:H2'	23:23:2244:U:C6	2.50	0.47
29:LE:30:ARG:HE	29:LE:30:ARG:HB3	1.57	0.47
42:LT:87:SER:HB2	43:LU:51:VAL:HG12	1.96	0.47
1:16:236:A:H2'	1:16:237:G:H8	1.80	0.46
23:23:2834:G:H2'	23:23:2879:A:H61	1.79	0.46
28:LD:61:ARG:HH12	28:LD:64:GLY:HA3	1.80	0.46
1:16:1293:C:H2'	1:16:1294:G:C8	2.50	0.46
1:16:1294:G:H2'	1:16:1295:U:C6	2.51	0.46
14:SN:64:CYS:HB3	14:SN:68:GLY:N	2.30	0.46
23:23:177:G:H3'	23:23:178:G:C8	2.48	0.46
23:23:468:G:H5''	28:LD:55:SER:HB3	1.97	0.46
23:23:1532:A:H61	23:23:1540:G:H1'	1.81	0.46
58:EF:15:ILE:HG22	58:EF:23:LYS:HG2	1.96	0.46
58:EF:100:GLU:HG3	58:EF:133:TYR:HE2	1.80	0.46
1:16:25:C:H2'	1:16:26:A:H8	1.80	0.46
1:16:512:U:H2'	1:16:513:C:H6	1.80	0.46
1:16:1254:A:P	10:SJ:45:ARG:HH12	2.38	0.46
1:16:1371:G:O3'	9:SI:71:GLY:HA3	2.15	0.46
1:16:1527:U:H2'	1:16:1528:U:C6	2.50	0.46
11:SK:26:SER:O	11:SK:90:GLY:HA3	2.15	0.46
13:SM:27:LYS:O	13:SM:31:LYS:HG2	2.16	0.46
23:23:1067:A:H2'	23:23:1068:G:C8	2.49	0.46
23:23:1169:A:H2'	23:23:1170:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:1433:A:H2'	23:23:1434:A:H8	1.77	0.46
23:23:2150:C:H2'	23:23:2151:U:C6	2.50	0.46
29:LE:105:THR:O	29:LE:109:PRO:CD	2.63	0.46
34:LK:19:ASN:HB2	34:LK:20:PRO:HD3	1.97	0.46
58:EF:337:ARG:HD3	58:EF:339:TYR:CE1	2.50	0.46
1:16:160:A:H2'	1:16:161:A:O4'	2.15	0.46
1:16:956:U:H6	1:16:956:U:O5'	1.99	0.46
1:16:1175:G:H2'	1:16:1176:A:H8	1.81	0.46
4:SD:172:GLU:HG2	4:SD:181:THR:HB	1.96	0.46
23:23:969:G:H2'	23:23:970:U:C6	2.51	0.46
23:23:1327:A:H2'	23:23:1328:A:O4'	2.15	0.46
23:23:1994:C:H5''	62:LC:301:PUT:H41	1.97	0.46
23:23:2158:A:H8	23:23:2159:G:C4	2.33	0.46
34:LK:15:ALA:HA	34:LK:46:THR:HB	1.96	0.46
43:LU:71:LYS:HA	43:LU:90:ARG:HG2	1.98	0.46
1:16:1060:U:H2'	1:16:1061:G:C8	2.48	0.46
9:SI:17:ALA:HA	9:SI:67:VAL:HG22	1.95	0.46
23:23:151:C:H2'	23:23:152:A:C8	2.48	0.46
23:23:1161:C:H2'	23:23:1162:G:H8	1.80	0.46
38:LP:15:GLY:O	38:LP:16:ARG:HD3	2.15	0.46
43:LU:22:LEU:HD12	43:LU:23:GLU:O	2.15	0.46
6:SF:3:HIS:HB2	6:SF:92:THR:O	2.15	0.46
23:23:4:U:H2'	23:23:5:A:H8	1.80	0.46
23:23:743:A:OP1	27:LC:135:GLY:HA2	2.16	0.46
23:23:2339:C:H2'	23:23:2340:A:C8	2.51	0.46
23:23:2784:U:H2'	23:23:2785:C:H6	1.79	0.46
29:LE:117:LEU:HD12	29:LE:117:LEU:HA	1.75	0.46
30:LF:84:THR:HA	30:LF:133:LEU:O	2.15	0.46
58:EF:495:ARG:NH1	58:EF:611:VAL:HB	2.31	0.46
1:16:908:A:H2'	1:16:909:A:H8	1.81	0.46
1:16:1070:U:H2'	1:16:1071:C:C6	2.50	0.46
1:16:1093:A:P	7:SG:4:ARG:HH12	2.37	0.46
2:SB:214:LEU:HA	2:SB:217:VAL:HG12	1.97	0.46
12:SL:76:GLU:HG3	12:SL:77:HIS:ND1	2.31	0.46
23:23:353:C:H2'	23:23:354:A:C8	2.51	0.46
23:23:521:U:H2'	23:23:522:A:H8	1.81	0.46
23:23:1197:G:H2'	23:23:1198:U:H6	1.81	0.46
23:23:1563:U:H2'	23:23:1564:C:C6	2.51	0.46
23:23:1645:G:H5''	23:23:1646:C:H5'	1.97	0.46
23:23:1683:U:H2'	23:23:1684:G:C8	2.51	0.46
23:23:2700:A:H2'	23:23:2701:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:LR:51:ALA:HB3	40:LR:78:VAL:HB	1.98	0.46
58:EF:170:GLN:HE22	58:EF:277:ALA:HB1	1.81	0.46
58:EF:491:ARG:O	58:EF:612:LEU:HD12	2.16	0.46
1:16:299:G:H2'	1:16:300:A:C8	2.51	0.46
1:16:398:U:H2'	1:16:399:G:C8	2.51	0.46
1:16:460:A:H2'	1:16:461:A:C8	2.50	0.46
1:16:972:C:O2'	10:SJ:57:VAL:HG23	2.16	0.46
1:16:1272:G:H2'	1:16:1273:C:C6	2.50	0.46
2:SB:91:PHE:CE2	2:SB:93:ASN:HB2	2.51	0.46
15:SO:63:ARG:O	15:SO:67:LEU:HD23	2.15	0.46
23:23:418:C:H2'	23:23:419:U:C6	2.51	0.46
23:23:528:A:H5'	35:LM:113:PRO:HG3	1.98	0.46
23:23:849:A:H2'	23:23:850:U:C6	2.50	0.46
23:23:1306:C:H2'	23:23:1307:A:H8	1.79	0.46
23:23:1386:C:H2'	23:23:1387:A:H8	1.80	0.46
23:23:2549:G:H2'	23:23:2550:G:H8	1.81	0.46
24:5:66:A:H61	24:5:107:G:H2'	1.80	0.46
25:LA:23:ILE:HD12	25:LA:189:LEU:HD11	1.98	0.46
31:LG:68:VAL:HG21	31:LG:115:ALA:HB2	1.98	0.46
36:LN:35:VAL:HG11	36:LN:104:THR:CG2	2.46	0.46
44:LV:59:GLU:HA	44:LV:64:ALA:CA	2.46	0.46
1:16:275:G:C8	1:16:275:G:C5'	2.99	0.46
1:16:539:A:H2'	1:16:540:G:H8	1.81	0.46
1:16:958:A:H1'	1:16:985:C:O2'	2.15	0.46
2:SB:68:LEU:HB3	2:SB:161:LEU:HG	1.98	0.46
3:SC:36:ASP:OD1	3:SC:57:ILE:HG13	2.15	0.46
7:SG:157:LEU:H	7:SG:157:LEU:HG	1.33	0.46
23:23:1236:G:N7	62:23:3013:PUT:H31	2.31	0.46
23:23:1564:C:H2'	23:23:1565:C:C6	2.50	0.46
58:EF:594:LYS:HE2	58:EF:594:LYS:HB3	1.48	0.46
1:16:501:C:H1'	1:16:549:C:H1'	1.98	0.46
1:16:1250:A:H2	1:16:1370:G:H1'	1.80	0.46
23:23:7:G:H2'	23:23:8:C:C6	2.51	0.46
23:23:1746:A:H2'	23:23:1747:U:H6	1.81	0.46
23:23:1848:A:H2'	23:23:1849:G:O4'	2.16	0.46
23:23:2304:G:H22	23:23:2312:U:H3	1.64	0.46
23:23:2339:C:H2'	23:23:2340:A:H8	1.80	0.46
23:23:2812:G:H2'	23:23:2813:A:H8	1.80	0.46
26:LB:145:GLU:HB2	26:LB:188:CYS:HB3	1.98	0.46
32:LI:81:ALA:HB1	32:LI:149:GLU:OE1	2.16	0.46
45:LW:44:LYS:O	45:LW:48:GLN:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:EF:413:GLU:H	58:EF:413:GLU:CD	2.20	0.46
23:23:20:C:H2'	23:23:21:A:H8	1.80	0.45
23:23:305:C:H2'	23:23:306:U:C6	2.52	0.45
23:23:1495:A:H2'	23:23:1496:A:C8	2.51	0.45
23:23:1683:U:H2'	23:23:1684:G:H8	1.81	0.45
58:EF:501:VAL:HG22	58:EF:520:ILE:O	2.16	0.45
1:16:111:G:H1	1:16:330:C:N4	2.13	0.45
1:16:373:A:H61	1:16:391:G:H1'	1.80	0.45
1:16:768:A:H4'	1:16:1523:G:N2	2.32	0.45
1:16:1225:A:OP1	13:SM:102:THR:HG22	2.17	0.45
1:16:1246:A:H2'	1:16:1247:U:C6	2.51	0.45
6:SF:72:ASP:O	6:SF:76:THR:HG23	2.17	0.45
12:SL:79:VAL:HG13	12:SL:79:VAL:O	2.17	0.45
15:SO:79:THR:HA	15:SO:82:ILE:HG12	1.98	0.45
23:23:608:A:H2'	23:23:609:A:C8	2.51	0.45
23:23:1684:G:H2'	23:23:1685:C:C6	2.52	0.45
23:23:1772:A:H2'	23:23:1773:A:O3'	2.16	0.45
23:23:2345:G:N3	23:23:2381:A:H2'	2.30	0.45
26:LB:245:VAL:HG12	26:LB:251:GLN:HA	1.98	0.45
36:LN:35:VAL:HG11	36:LN:104:THR:HG22	1.97	0.45
58:EF:171:LEU:HD23	58:EF:172:ALA:N	2.30	0.45
58:EF:330:VAL:HG21	58:EF:371:ARG:HH11	1.80	0.45
1:16:193:C:H2'	1:16:194:C:C6	2.51	0.45
11:SK:116:ILE:HD11	21:SU:31:GLU:HG2	1.97	0.45
23:23:347:A:H2'	23:23:348:A:C8	2.51	0.45
23:23:1709:U:H2'	23:23:1710:G:C8	2.51	0.45
25:LA:187:GLU:H	25:LA:187:GLU:HG2	1.54	0.45
34:LK:75:PRO:HG2	34:LK:78:VAL:HG22	1.98	0.45
34:LK:103:ARG:HG2	34:LK:103:ARG:HH11	1.82	0.45
35:LM:26:GLY:O	35:LM:30:THR:HG23	2.16	0.45
36:LN:114:LYS:O	36:LN:118:LEU:HG	2.17	0.45
40:LR:26:LEU:HA	40:LR:38:GLN:O	2.16	0.45
58:EF:13:ILE:HA	58:EF:108:GLY:O	2.16	0.45
1:16:322:C:H2'	1:16:323:U:C6	2.51	0.45
8:SH:78:VAL:HG21	8:SH:128:TYR:CD1	2.51	0.45
23:23:634:C:H2'	23:23:635:C:H6	1.82	0.45
23:23:1196:C:C2	23:23:1197:G:C8	3.04	0.45
23:23:1854:A:H8	23:23:1854:A:O5'	1.99	0.45
32:LI:4:ILE:HD11	32:LI:18:GLN:HG3	1.99	0.45
4:SD:105:MET:HB3	4:SD:171:LEU:HD13	1.98	0.45
5:SE:99:ALA:HB1	5:SE:103:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SE:137:VAL:O	5:SE:141:ILE:HG12	2.17	0.45
8:SH:64:LYS:HB3	8:SH:71:VAL:HG21	1.98	0.45
9:SI:23:PRO:HA	9:SI:61:LEU:HD13	1.98	0.45
10:SJ:80:THR:HB	10:SJ:83:THR:HG23	1.97	0.45
11:SK:71:ALA:HA	11:SK:74:VAL:HG22	1.98	0.45
23:23:640:C:H2'	23:23:641:U:C6	2.51	0.45
23:23:2799:A:H2'	23:23:2801:G:OP2	2.17	0.45
28:LD:28:VAL:HG13	28:LD:108:ILE:HD11	1.99	0.45
1:16:35:G:H2'	1:16:36:C:C6	2.52	0.45
1:16:429:U:H2'	4:SD:31:LYS:HE3	1.98	0.45
1:16:662:U:H2'	1:16:663:A:H8	1.80	0.45
1:16:1118:U:H2'	1:16:1119:C:C6	2.52	0.45
1:16:1170:A:H2'	1:16:1171:A:O4'	2.16	0.45
3:SC:155:GLY:HA2	3:SC:163:ALA:HB1	1.99	0.45
23:23:588:U:H2'	23:23:589:U:C6	2.51	0.45
23:23:947:A:H2'	23:23:948:C:C6	2.51	0.45
23:23:1494:A:H2'	23:23:1495:A:C8	2.51	0.45
26:LB:175:ARG:NE	26:LB:181:MET:HE1	2.30	0.45
28:LD:61:ARG:NH1	28:LD:64:GLY:HA3	2.30	0.45
1:16:505:G:H2'	1:16:506:G:H8	1.80	0.45
1:16:672:U:H2'	1:16:673:A:C8	2.52	0.45
1:16:894:G:O6	62:16:1602:PUT:H12	2.17	0.45
1:16:985:C:H2'	1:16:986:U:H6	1.80	0.45
1:16:1402:4OC:H2'	1:16:1403:C:O4'	2.17	0.45
7:SG:155:ARG:H	7:SG:155:ARG:HG2	1.48	0.45
10:SJ:42:LEU:HB2	10:SJ:71:LEU:HB2	1.97	0.45
23:23:1278:C:H2'	23:23:1279:G:C8	2.50	0.45
23:23:1987:A:H2'	23:23:1988:G:H8	1.82	0.45
23:23:2803:G:H2'	23:23:2804:U:C6	2.51	0.45
24:5:49:C:H2'	24:5:50:A:C8	2.51	0.45
34:LK:74:PRO:HB2	34:LK:79:LEU:HD21	1.99	0.45
1:16:2:A:H4'	4:SD:83:LYS:HE2	1.97	0.45
1:16:193:C:H4'	20:ST:56:PRO:HB3	1.99	0.45
1:16:1239:A:H1'	1:16:1241:G:C4	2.52	0.45
1:16:1510:C:H2'	1:16:1511:G:H8	1.82	0.45
4:SD:26:ARG:HG2	4:SD:27:ALA:H	1.82	0.45
23:23:598:U:H2'	23:23:599:A:C8	2.48	0.45
23:23:1339:G:P	45:LW:15:HIS:HE2	2.40	0.45
23:23:1447:C:H2'	23:23:1448:G:H8	1.82	0.45
23:23:1569:A:H2'	23:23:1570:A:H8	1.81	0.45
23:23:1946:U:H2'	23:23:1947:C:H6	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:2328:A:H2'	23:23:2329:U:C6	2.52	0.45
23:23:2740:A:H2'	23:23:2741:A:C8	2.52	0.45
31:LG:64:ASN:O	31:LG:68:VAL:HG23	2.17	0.45
40:LR:15:ARG:HD3	40:LR:25:ARG:HH12	1.82	0.45
1:16:416:G:H2'	1:16:417:G:H8	1.82	0.45
1:16:1072:G:H2'	1:16:1073:U:C6	2.52	0.45
1:16:1356:G:H2'	1:16:1357:A:C8	2.52	0.45
13:SM:29:ARG:O	13:SM:33:ILE:HG12	2.17	0.45
23:23:191:A:H2'	23:23:192:C:C6	2.51	0.45
23:23:597:G:H2'	23:23:598:U:C6	2.52	0.45
23:23:1829:A:H3'	23:23:1830:C:H6	1.81	0.45
23:23:2065:C:H2'	23:23:2066:C:H6	1.80	0.45
26:LB:160:THR:HB	26:LB:177:ARG:HG3	1.99	0.45
1:16:512:U:H2'	1:16:513:C:C6	2.52	0.45
1:16:591:U:H2'	1:16:592:G:H8	1.81	0.45
1:16:1308:U:H2'	1:16:1309:G:C8	2.52	0.45
2:SB:166:ALA:HB3	2:SB:191:SER:HB3	1.98	0.45
10:SJ:8:ILE:HG12	10:SJ:100:ILE:HG23	1.98	0.45
23:23:1107:G:H1'	33:LJ:31:ARG:HH12	1.82	0.45
23:23:1771:C:H2'	23:23:1772:A:H8	1.82	0.45
23:23:1831:G:H2'	23:23:1832:C:C6	2.52	0.45
23:23:1849:G:H5''	23:23:1849:G:C8	2.52	0.45
23:23:2124:G:H2'	23:23:2125:G:O4'	2.17	0.45
23:23:2552:OMU:OP2	23:23:2552:OMU:H6	2.17	0.45
26:LB:53:HIS:CE1	26:LB:219:THR:HA	2.51	0.45
29:LE:103:LEU:O	29:LE:104:ILE:C	2.54	0.45
34:LK:75:PRO:O	34:LK:79:LEU:HD23	2.16	0.45
45:LW:6:ARG:O	45:LW:10:VAL:HG13	2.17	0.45
1:16:381:C:H2'	1:16:382:A:O4'	2.17	0.44
1:16:493:A:H2'	1:16:494:G:N9	2.32	0.44
1:16:591:U:H2'	1:16:592:G:C8	2.52	0.44
2:SB:23:TRP:CZ3	2:SB:25:PRO:HA	2.52	0.44
8:SH:75:ILE:HG13	8:SH:129:VAL:HG22	1.98	0.44
8:SH:89:LYS:HB2	8:SH:89:LYS:HE2	1.51	0.44
10:SJ:17:LEU:HD12	10:SJ:17:LEU:O	2.17	0.44
23:23:599:A:H2'	23:23:600:G:H8	1.83	0.44
23:23:674:G:H1'	28:LD:69:ARG:HD3	1.99	0.44
23:23:2038:G:H2'	23:23:2039:U:O4'	2.17	0.44
23:23:2229:U:H2'	23:23:2230:G:C8	2.49	0.44
42:LT:94:ILE:HG21	43:LU:4:VAL:HG11	1.99	0.44
1:16:478:A:H2'	1:16:479:U:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SC:6:HIS:CE1	3:SC:8:ASN:HB3	2.52	0.44
8:SH:50:LYS:HG2	8:SH:60:GLU:HB3	2.00	0.44
10:SJ:66:GLU:HB2	14:SN:99:ALA:HB2	1.98	0.44
14:SN:27:LEU:H	14:SN:27:LEU:HG	1.55	0.44
23:23:1:G:H2'	23:23:2:G:H8	1.81	0.44
23:23:1054:A:H8	23:23:1054:A:H5''	1.81	0.44
23:23:1115:G:H2'	23:23:1116:G:C8	2.51	0.44
23:23:1297:C:H2'	23:23:1298:C:H6	1.83	0.44
23:23:1684:G:H2'	23:23:1685:C:H6	1.82	0.44
23:23:2119:A:H1'	23:23:2172:U:O4	2.18	0.44
23:23:2543:G:H2'	23:23:2544:G:C8	2.51	0.44
23:23:2723:C:H2'	23:23:2724:U:O4'	2.17	0.44
58:EF:24:THR:HA	58:EF:27:THR:HG22	1.99	0.44
58:EF:114:CYS:SG	58:EF:116:VAL:HG22	2.58	0.44
1:16:981:U:H5''	14:SN:6:MET:HE3	1.98	0.44
1:16:1493:A:O2'	1:16:1494:G:H5'	2.17	0.44
3:SC:122:SER:O	3:SC:125:GLU:HG2	2.17	0.44
23:23:784:G:H5'	23:23:785:G:OP1	2.16	0.44
23:23:881:G:H2'	23:23:882:G:C8	2.53	0.44
23:23:1441:G:H2'	23:23:1442:U:H6	1.83	0.44
23:23:1710:G:H2'	23:23:1711:A:C8	2.52	0.44
23:23:2074:U:H2'	23:23:2075:U:H6	1.82	0.44
23:23:2204:G:H4'	26:LB:150:LYS:HD2	1.98	0.44
58:EF:106:LEU:HD23	58:EF:106:LEU:HA	1.82	0.44
1:16:113:G:H2'	1:16:114:U:C6	2.52	0.44
1:16:1107:C:C4	1:16:1108:G:C8	3.05	0.44
16:SP:53:ASP:OD2	16:SP:56:ARG:HG2	2.17	0.44
23:23:686:U:H6	23:23:788:A:N1	2.16	0.44
23:23:2070:A:H2'	23:23:2071:A:O4'	2.17	0.44
23:23:2273:A:H2'	23:23:2274:A:C8	2.52	0.44
23:23:2304:G:H5'	29:LE:121:SER:HB2	1.99	0.44
23:23:2700:A:H2'	23:23:2701:U:H6	1.82	0.44
23:23:2772:C:H5'	27:LC:173:GLN:NE2	2.33	0.44
31:LG:76:THR:HG23	31:LG:78:LEU:H	1.82	0.44
58:EF:125:THR:O	58:EF:129:GLN:HG3	2.17	0.44
58:EF:548:GLU:H	58:EF:548:GLU:HG3	1.53	0.44
1:16:744:C:H2'	1:16:745:G:C8	2.53	0.44
1:16:865:A:H2'	1:16:866:C:C6	2.52	0.44
1:16:1070:U:H2'	1:16:1071:C:H6	1.83	0.44
5:SE:134:ILE:HG23	5:SE:135:ASN:ND2	2.33	0.44
8:SH:106:THR:HB	8:SH:121:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:689:A:H2'	23:23:690:G:H8	1.82	0.44
23:23:878:A:H2'	23:23:879:G:O4'	2.18	0.44
23:23:1440:U:H2'	23:23:1441:G:C8	2.53	0.44
23:23:1914:C:H2'	23:23:1915:3TD:H6	2.00	0.44
23:23:2127:G:H2'	23:23:2128:G:C8	2.53	0.44
23:23:2636:C:H2'	23:23:2637:U:C6	2.51	0.44
26:LB:160:THR:O	26:LB:195:VAL:HG12	2.17	0.44
27:LC:13:ARG:HD2	41:LS:56:HIS:ND1	2.31	0.44
33:LJ:119:PRO:HD2	33:LJ:122:GLN:HB3	1.98	0.44
43:LU:48:LYS:HE3	43:LU:103:ALA:HB1	1.98	0.44
1:16:255:G:H2'	1:16:256:U:C6	2.53	0.44
1:16:613:C:H2'	1:16:614:C:C6	2.52	0.44
1:16:872:A:C4	1:16:874:G:N7	2.86	0.44
1:16:1345:U:C2	1:16:1377:A:C6	3.06	0.44
11:SK:20:VAL:O	11:SK:34:ILE:HA	2.16	0.44
11:SK:42:LEU:HD12	11:SK:77:TYR:CE2	2.53	0.44
18:SR:11:CYS:HB3	18:SR:14:THR:HG22	2.00	0.44
23:23:156:A:H2'	23:23:157:C:C6	2.52	0.44
23:23:593:U:H2'	23:23:594:U:H6	1.83	0.44
58:EF:3:ARG:HA	58:EF:378:ARG:NH1	2.32	0.44
1:16:110:C:C2	1:16:111:G:C8	3.05	0.44
1:16:1127:G:H22	1:16:1145:A:H2	1.66	0.44
5:SE:38:VAL:HG11	5:SE:114:VAL:HG22	1.99	0.44
20:ST:38:ALA:HA	20:ST:41:ALA:HB3	1.98	0.44
23:23:554:U:H2'	23:23:555:G:O4'	2.17	0.44
23:23:559:G:H1'	42:LT:56:GLN:OE1	2.17	0.44
23:23:817:C:H2'	23:23:818:G:O4'	2.18	0.44
23:23:1677:A:H2'	23:23:1678:A:H8	1.83	0.44
23:23:2096:C:H2'	23:23:2097:A:H8	1.82	0.44
23:23:2367:G:C2	23:23:2368:C:C5	3.06	0.44
33:LJ:113:PHE:HB3	33:LJ:116:GLU:HG2	1.99	0.44
37:LO:142:ILE:HD12	37:LO:142:ILE:N	2.33	0.44
42:LT:86:ALA:HB2	42:LT:116:ALA:HB2	2.00	0.44
1:16:279:A:H5''	1:16:281:G:O4'	2.17	0.44
1:16:363:A:C6	12:SL:28:PRO:HD2	2.52	0.44
1:16:769:G:H4'	1:16:1513:A:H4'	2.00	0.44
1:16:792:A:C4	1:16:794:A:C6	3.06	0.44
2:SB:99:GLY:O	2:SB:103:ASN:HB3	2.18	0.44
5:SE:107:ALA:HB2	5:SE:125:ALA:HB3	2.00	0.44
7:SG:76:LYS:HE3	7:SG:76:LYS:HB3	1.76	0.44
11:SK:16:VAL:HG23	11:SK:79:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:SO:17:ARG:H	15:SO:17:ARG:HG2	1.45	0.44
16:SP:69:ASP:OD1	16:SP:69:ASP:N	2.51	0.44
23:23:680:C:H2'	23:23:681:G:C8	2.53	0.44
23:23:755:U:H2'	23:23:756:A:H8	1.82	0.44
23:23:1744:A:H3'	23:23:1745:A:H8	1.82	0.44
23:23:1954:G:N3	23:23:2551:C:H5''	2.32	0.44
23:23:2037:A:H2'	23:23:2038:G:C8	2.53	0.44
23:23:2502:G:H5''	23:23:2503:2MA:H5''	1.99	0.44
24:5:1:U:H2'	24:5:2:G:C8	2.53	0.44
29:LE:4:LEU:HD12	29:LE:173:PHE:CD1	2.53	0.44
29:LE:60:ILE:HA	29:LE:140:GLU:HG3	1.99	0.44
29:LE:170:LEU:HD23	29:LE:170:LEU:HA	1.84	0.44
31:LG:83:ALA:O	31:LG:87:VAL:HG22	2.17	0.44
58:EF:22:GLY:O	58:EF:26:THR:HG23	2.18	0.44
1:16:216:U:H2'	1:16:217:C:C6	2.53	0.44
1:16:553:A:H2'	1:16:554:A:H8	1.82	0.44
1:16:1106:G:H2'	1:16:1107:C:C6	2.53	0.44
1:16:1219:A:H2'	1:16:1220:G:H8	1.82	0.44
3:SC:116:VAL:HG21	3:SC:200:VAL:HG11	1.99	0.44
5:SE:159:LYS:HE2	5:SE:159:LYS:HB3	1.80	0.44
13:SM:40:ALA:HB3	13:SM:43:VAL:HG13	2.00	0.44
14:SN:8:ALA:HA	14:SN:11:VAL:HG12	2.00	0.44
23:23:250:G:H2'	23:23:251:A:C8	2.53	0.44
23:23:1251:C:H5''	42:LT:13:ARG:NH2	2.32	0.44
23:23:2836:U:H2'	23:23:2837:A:H8	1.83	0.44
44:LV:14:ALA:O	44:LV:18:ARG:HG3	2.18	0.44
58:EF:338:VAL:HG12	58:EF:379:ALA:HA	2.00	0.44
58:EF:519:VAL:HB	58:EF:580:PHE:HB3	2.00	0.44
1:16:33:A:H2'	1:16:34:C:C6	2.53	0.43
1:16:1120:C:H2'	1:16:1121:U:C6	2.53	0.43
1:16:1252:A:H61	1:16:1285:A:H61	1.66	0.43
1:16:1479:C:H2'	1:16:1480:A:H8	1.83	0.43
3:SC:135:LYS:O	3:SC:139:GLN:HG2	2.18	0.43
4:SD:124:MET:HA	4:SD:129:VAL:HA	2.00	0.43
12:SL:42:PRO:HB3	12:SL:89:D2T:H5	2.01	0.43
23:23:364:C:H2'	23:23:365:U:H6	1.83	0.43
23:23:879:G:H2'	23:23:880:G:H8	1.83	0.43
23:23:1045:C:H4'	23:23:1047:G:H5''	2.00	0.43
23:23:1383:A:H1'	23:23:1405:U:O2'	2.17	0.43
23:23:1604:C:H2'	23:23:1605:C:C6	2.53	0.43
23:23:2136:G:H1	23:23:2155:U:H3	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:LK:33:VAL:HG22	34:LK:65:ARG:HH22	1.83	0.43
58:EF:90:PRO:HB3	67:EF:802:FUA:C21	2.48	0.43
1:16:502:A:H2'	1:16:503:C:H6	1.83	0.43
1:16:514:C:H2'	1:16:515:G:H8	1.82	0.43
1:16:1369:C:H2'	1:16:1370:G:C8	2.53	0.43
6:SF:70:VAL:O	6:SF:74:LEU:HD23	2.17	0.43
6:SF:106:LYS:HB3	6:SF:106:LYS:HE3	1.86	0.43
19:SS:13:LEU:O	19:SS:17:LYS:HG2	2.17	0.43
23:23:796:C:H2'	23:23:797:G:C8	2.53	0.43
23:23:843:G:H2'	23:23:844:A:H8	1.82	0.43
23:23:948:C:H2'	23:23:949:G:C8	2.50	0.43
23:23:1774:C:O2	23:23:1774:C:H2'	2.18	0.43
23:23:1957:C:H2'	23:23:1958:C:H6	1.83	0.43
23:23:1989:G:H2'	23:23:1990:C:O4'	2.18	0.43
23:23:2473:U:OP1	23:23:2475:C:N4	2.51	0.43
23:23:2649:C:H2'	23:23:2650:U:C6	2.52	0.43
31:LG:58:LEU:HG	31:LG:117:VAL:HG22	2.00	0.43
42:LT:52:GLN:O	42:LT:56:GLN:HG3	2.18	0.43
46:LX:50:PRO:HA	46:LX:54:GLN:HG3	2.00	0.43
1:16:1410:A:H2'	1:16:1411:C:C6	2.53	0.43
1:16:1465:A:H2'	1:16:1466:C:C6	2.52	0.43
2:SB:104:TRP:HE1	2:SB:108:ARG:NH2	2.15	0.43
4:SD:60:LYS:O	4:SD:64:ILE:HD12	2.18	0.43
11:SK:89:PRO:HG3	21:SU:32:VAL:HG11	2.01	0.43
14:SN:3:LYS:HB2	14:SN:6:MET:HB2	1.98	0.43
23:23:828:U:H2'	23:23:829:A:C8	2.53	0.43
23:23:2570:G:H2'	23:23:2571:U:O4'	2.18	0.43
24:5:66:A:N6	24:5:107:G:H2'	2.33	0.43
30:LF:94:TYR:HA	30:LF:106:SER:O	2.18	0.43
35:LM:117:ALA:HA	35:LM:120:ARG:HH11	1.83	0.43
36:LN:1:MET:HE3	36:LN:32:TYR:CE1	2.53	0.43
1:16:109:A:H5'	1:16:110:C:C5	2.53	0.43
1:16:456:A:H2'	1:16:457:G:O4'	2.18	0.43
1:16:1463:U:H2'	1:16:1464:U:C6	2.53	0.43
23:23:590:A:H2'	23:23:591:U:C6	2.53	0.43
23:23:635:C:H2'	23:23:636:G:O4'	2.18	0.43
23:23:851:C:H2'	23:23:852:U:H6	1.83	0.43
23:23:1077:A:H3'	23:23:1078:U:C6	2.54	0.43
23:23:1357:C:H2'	23:23:1358:G:O4'	2.19	0.43
35:LM:17:VAL:HG13	35:LM:137:PRO:HB2	2.00	0.43
1:16:1096:C:H2'	1:16:1097:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:16:1312:G:H5'	19:SS:5:LEU:HD21	2.00	0.43
1:16:1428:A:H2'	1:16:1429:A:O4'	2.18	0.43
2:SB:102:THR:HG23	2:SB:175:GLU:HG3	1.99	0.43
17:SQ:65:ARG:HG3	17:SQ:66:PRO:HD2	2.00	0.43
23:23:4:U:H2'	23:23:5:A:C8	2.53	0.43
23:23:30:G:H2'	23:23:31:C:C6	2.53	0.43
23:23:227:A:C2	23:23:2407:A:H1'	2.53	0.43
23:23:558:U:H2'	23:23:559:G:H8	1.84	0.43
23:23:644:A:C2	23:23:2369:A:H1'	2.54	0.43
23:23:980:A:N7	23:23:1136:G:H5'	2.33	0.43
23:23:1295:C:C2	23:23:1296:G:C8	3.06	0.43
23:23:2172:U:H5''	23:23:2173:A:H5''	2.00	0.43
29:LE:34:ILE:HD12	29:LE:96:MET:HG3	2.00	0.43
31:LG:107:LYS:HE3	31:LG:119:VAL:HG23	1.99	0.43
33:LJ:27:VAL:O	33:LJ:27:VAL:HG13	2.18	0.43
1:16:328:C:H4'	1:16:329:A:H5''	1.99	0.43
1:16:952:U:H2'	1:16:953:G:H8	1.83	0.43
1:16:1521:C:H2'	1:16:1522:U:C6	2.54	0.43
2:SB:226:SER:HA	2:SB:229:LEU:HD12	1.99	0.43
23:23:65:U:H2'	23:23:66:C:H6	1.83	0.43
23:23:77:G:H2'	23:23:78:U:C6	2.53	0.43
23:23:740:C:H5'	23:23:1784:A:H3'	1.99	0.43
23:23:1138:G:H2'	23:23:1139:G:O4'	2.18	0.43
23:23:1182:G:H2'	23:23:1183:U:O4'	2.19	0.43
23:23:1604:C:H2'	23:23:1605:C:H6	1.82	0.43
23:23:2184:A:H2'	23:23:2185:U:C6	2.53	0.43
23:23:2513:A:H2'	23:23:2514:U:C6	2.54	0.43
23:23:2650:U:H2'	23:23:2651:C:H6	1.84	0.43
23:23:2728:U:O2'	23:23:2729:G:H5''	2.19	0.43
27:LC:97:SER:HB3	27:LC:99:GLU:HG3	2.01	0.43
32:LI:68:ARG:O	32:LI:72:ILE:HG12	2.18	0.43
36:LN:25:LEU:HD12	36:LN:38:ILE:HG22	1.99	0.43
1:16:22:G:H2'	1:16:23:C:H6	1.84	0.43
1:16:335:C:H2'	1:16:336:A:H8	1.84	0.43
1:16:725:G:H2'	1:16:726:C:C6	2.54	0.43
1:16:904:U:H2'	1:16:905:U:H6	1.83	0.43
1:16:1140:C:O2	1:16:1140:C:H2'	2.19	0.43
1:16:1472:U:H2'	1:16:1473:G:C8	2.54	0.43
8:SH:18:GLN:HB3	8:SH:70:ALA:HB1	2.01	0.43
23:23:438:G:H2'	23:23:439:A:C8	2.53	0.43
23:23:1680:U:H2'	23:23:1681:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:1821:A:H2'	23:23:1822:C:H6	1.83	0.43
23:23:2443:C:H2'	23:23:2444:G:C8	2.53	0.43
28:LD:148:ILE:HB	28:LD:169:VAL:HG22	2.01	0.43
29:LE:140:GLU:H	29:LE:140:GLU:HG2	1.50	0.43
31:LG:84:LYS:NZ	58:EF:238:LEU:HA	2.33	0.43
33:LJ:75:ALA:O	33:LJ:77:VAL:HG23	2.18	0.43
34:LK:76:ALA:HB2	34:LK:113:LYS:HE2	2.00	0.43
58:EF:68:THR:HA	58:EF:366:MET:HB2	2.01	0.43
58:EF:631:VAL:O	58:EF:635:LEU:HD23	2.18	0.43
1:16:579:A:H2'	1:16:580:C:C6	2.52	0.43
1:16:904:U:H2'	1:16:905:U:C6	2.54	0.43
2:SB:117:LEU:HD12	2:SB:117:LEU:HA	1.86	0.43
23:23:1234:U:H2'	23:23:1235:G:O4'	2.19	0.43
23:23:1443:U:H2'	23:23:1444:G:C8	2.52	0.43
23:23:1511:G:H2'	23:23:1512:C:H6	1.84	0.43
23:23:1770:G:C6	23:23:1983:G:C6	3.07	0.43
23:23:1821:A:H2'	23:23:1822:C:C6	2.53	0.43
23:23:2099:U:H2'	23:23:2100:G:H8	1.82	0.43
23:23:2281:A:O2'	23:23:2282:G:H5'	2.19	0.43
23:23:2373:G:H2'	23:23:2374:C:C6	2.54	0.43
25:LA:69:THR:HG23	25:LA:176:GLY:HA2	2.00	0.43
32:LI:50:ARG:O	32:LI:53:GLU:HG3	2.19	0.43
43:LU:38:VAL:HG12	43:LU:59:ILE:HD12	2.00	0.43
1:16:695:A:H2'	1:16:696:A:C8	2.53	0.43
1:16:1042:A:H2'	1:16:1043:G:H8	1.83	0.43
1:16:1146:A:N3	1:16:1146:A:H2'	2.33	0.43
1:16:1431:A:H2	1:16:1469:C:H41	1.66	0.43
1:16:1436:U:H2'	1:16:1437:A:C8	2.54	0.43
6:SF:1:MET:H3	6:SF:66:ALA:C	2.22	0.43
19:SS:36:ARG:NH2	19:SS:72:GLY:O	2.51	0.43
21:SU:11:PRO:HB2	21:SU:14:VAL:HG12	2.01	0.43
23:23:596:U:H2'	23:23:597:G:C8	2.53	0.43
23:23:1429:G:H2'	23:23:1430:G:C8	2.53	0.43
23:23:1532:A:N6	23:23:1540:G:H1'	2.33	0.43
23:23:2685:G:H2'	23:23:2686:G:H8	1.83	0.43
30:LF:154:PRO:HD3	30:LF:162:VAL:O	2.19	0.43
32:LI:147:VAL:HG11	32:LI:149:GLU:HG3	1.95	0.43
36:LN:58:LEU:HD12	36:LN:87:LEU:O	2.18	0.43
1:16:12:U:H4'	1:16:526:C:H4'	2.01	0.43
1:16:20:U:H2'	1:16:21:G:O4'	2.17	0.43
1:16:827:U:H2'	1:16:870:U:O4	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SI:30:ILE:HD12	9:SI:35:LEU:HA	2.00	0.43
10:SJ:52:LEU:HD23	10:SJ:62:ARG:HG2	2.01	0.43
18:SR:51:TYR:HA	18:SR:54:GLN:NE2	2.33	0.43
23:23:81:G:H2'	23:23:82:U:O4'	2.19	0.43
23:23:396:G:C6	23:23:397:U:C4	3.06	0.43
23:23:959:A:H2'	23:23:960:A:C8	2.54	0.43
23:23:963:U:C2	23:23:964:C:C5	3.06	0.43
23:23:1199:U:H2'	23:23:1200:C:C6	2.53	0.43
23:23:1583:A:HO2'	23:23:1585:C:H5	1.63	0.43
23:23:2036:C:H2'	23:23:2037:A:H8	1.83	0.43
23:23:2096:C:H2'	23:23:2097:A:C8	2.54	0.43
26:LB:155:ALA:HB2	26:LB:162:VAL:HG23	2.01	0.43
29:LE:108:VAL:HG22	29:LE:176:PRO:HG3	2.01	0.43
33:LJ:54:VAL:HG12	33:LJ:81:LEU:HD13	2.01	0.43
36:LN:41:ILE:HD11	36:LN:86:LEU:HD22	2.01	0.43
45:LW:1:MET:HG3	45:LW:42:GLU:HG2	2.00	0.43
1:16:113:G:H2'	1:16:114:U:H6	1.84	0.42
1:16:796:C:OP1	11:SK:128:ARG:N	2.52	0.42
1:16:1001:C:H2'	1:16:1002:G:C8	2.53	0.42
1:16:1090:U:H2'	1:16:1091:U:C6	2.53	0.42
1:16:1092:A:H2'	1:16:1093:A:C8	2.53	0.42
2:SB:49:MET:HE3	2:SB:49:MET:HB3	1.93	0.42
6:SF:11:HIS:CD2	6:SF:13:ASP:HB2	2.54	0.42
10:SJ:12:ALA:HB3	10:SJ:18:ILE:HB	2.00	0.42
23:23:248:G:O5'	23:23:249:C:H5''	2.19	0.42
23:23:1267:U:O2	23:23:1267:U:H2'	2.18	0.42
23:23:1677:A:H2'	23:23:1678:A:C8	2.53	0.42
23:23:1710:G:H2'	23:23:1711:A:H8	1.85	0.42
23:23:2050:C:H2'	23:23:2051:A:O4'	2.18	0.42
23:23:2266:A:H4'	23:23:2267:A:N3	2.33	0.42
58:EF:17:ALA:N	58:EF:23:LYS:HD3	2.34	0.42
58:EF:19:ILE:H	58:EF:19:ILE:HD12	1.83	0.42
1:16:93:U:H2'	1:16:95:C:C5	2.54	0.42
1:16:645:G:C2	1:16:646:G:C8	3.07	0.42
1:16:921:U:H2'	1:16:922:G:O4'	2.19	0.42
1:16:1095:U:H2'	1:16:1096:C:C6	2.53	0.42
1:16:1273:C:H2'	1:16:1274:A:O4'	2.18	0.42
20:ST:51:PHE:HA	20:ST:54:MET:HG3	2.01	0.42
23:23:78:U:H2'	23:23:79:C:H6	1.84	0.42
23:23:352:A:H3'	23:23:353:C:H5''	2.01	0.42
23:23:742:A:H2'	23:23:743:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:963:U:H2'	23:23:964:C:H6	1.84	0.42
23:23:1496:A:H2'	23:23:1498:C:C5	2.55	0.42
24:5:95:U:H2'	24:5:96:G:H8	1.84	0.42
58:EF:18:HIS:ND1	58:EF:122:GLN:HB2	2.34	0.42
58:EF:172:ALA:HB2	58:EF:266:CYS:SG	2.59	0.42
1:16:82:G:H1	1:16:89:U:H1'	1.84	0.42
1:16:617:G:N1	1:16:624:C:N3	2.67	0.42
1:16:834:U:H2'	1:16:835:U:C6	2.53	0.42
1:16:996:A:H2'	1:16:997:U:C6	2.54	0.42
1:16:1456:A:H2'	1:16:1457:G:O4'	2.19	0.42
7:SG:108:ALA:HA	7:SG:123:GLU:HG3	2.01	0.42
9:SI:36:GLU:HA	9:SI:45:ARG:HD3	2.00	0.42
23:23:1585:C:H2'	23:23:1586:A:O4'	2.19	0.42
23:23:2112:G:H2'	23:23:2113:U:C6	2.53	0.42
23:23:2197:U:H1'	23:23:2198:A:C8	2.55	0.42
23:23:2377:A:H2'	23:23:2378:A:C8	2.55	0.42
23:23:2816:G:H5''	39:LQ:99:LYS:HE3	2.01	0.42
30:LF:67:THR:O	30:LF:71:LEU:HD23	2.18	0.42
1:16:620:C:C2	4:SD:132:ILE:HG21	2.54	0.42
1:16:735:C:H5'	18:SR:60:LYS:HD3	2.00	0.42
1:16:1136:C:O2	1:16:1136:C:O4'	2.34	0.42
1:16:1345:U:H5''	9:SI:122:ARG:HH21	1.84	0.42
4:SD:98:LEU:O	4:SD:101:VAL:HG22	2.19	0.42
7:SG:70:ARG:HA	7:SG:100:ALA:HB2	2.01	0.42
13:SM:23:TYR:HB3	13:SM:66:GLU:HA	2.02	0.42
17:SQ:22:VAL:HG22	17:SQ:45:HIS:CD2	2.51	0.42
23:23:3:U:H2'	23:23:4:U:C6	2.53	0.42
23:23:1511:G:H2'	23:23:1512:C:C6	2.54	0.42
23:23:2246:G:H2'	23:23:2247:A:C8	2.54	0.42
25:LA:7:ARG:O	25:LA:11:ILE:HG13	2.19	0.42
30:LF:27:LYS:HG2	30:LF:32:GLU:HG2	2.02	0.42
32:LI:64:ALA:O	32:LI:68:ARG:HG2	2.19	0.42
32:LI:81:ALA:HB1	32:LI:149:GLU:CD	2.39	0.42
58:EF:469:ILE:CD1	67:EF:802:FUA:H22	2.49	0.42
67:EF:802:FUA:O1	67:EF:802:FUA:H12	2.20	0.42
1:16:1437:A:H2'	1:16:1438:G:C8	2.52	0.42
2:SB:208:ARG:O	2:SB:212:LEU:HD23	2.19	0.42
9:SI:9:THR:H	9:SI:85:ARG:HD2	1.85	0.42
15:SO:35:GLN:O	15:SO:39:LEU:HD23	2.19	0.42
16:SP:67:ILE:HD12	16:SP:67:ILE:N	2.34	0.42
26:LB:76:ALA:HB2	26:LB:96:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:LV:11:ARG:HA	44:LV:11:ARG:HD2	1.75	0.42
1:16:317:U:H2'	1:16:318:G:H8	1.83	0.42
1:16:470:C:H2'	1:16:471:U:C6	2.54	0.42
1:16:908:A:H2'	1:16:909:A:C8	2.55	0.42
1:16:1464:U:H2'	1:16:1465:A:H8	1.84	0.42
3:SC:70:THR:O	3:SC:106:VAL:HG22	2.19	0.42
5:SE:82:GLN:HG2	5:SE:147:MET:HE2	2.00	0.42
7:SG:70:ARG:HA	7:SG:71:PRO:HD3	1.91	0.42
16:SP:58:ALA:HA	16:SP:61:VAL:HG12	2.01	0.42
16:SP:74:LEU:O	16:SP:78:VAL:HG12	2.20	0.42
23:23:285:G:C6	23:23:356:G:C6	3.07	0.42
23:23:364:C:H2'	23:23:365:U:C6	2.54	0.42
23:23:492:A:H2'	23:23:493:G:O4'	2.20	0.42
23:23:670:A:H4'	23:23:671:C:H5'	2.01	0.42
23:23:1198:U:H2'	23:23:1199:U:H6	1.84	0.42
23:23:1231:U:H2'	23:23:1232:G:H8	1.84	0.42
23:23:1737:G:H8	23:23:1737:G:O5'	2.02	0.42
23:23:2147:A:C2	23:23:2148:G:C8	3.07	0.42
29:LE:4:LEU:HD12	29:LE:173:PHE:HD1	1.84	0.42
33:LJ:97:LYS:HA	33:LJ:97:LYS:HD2	1.85	0.42
39:LQ:56:LYS:HE2	39:LQ:87:PHE:O	2.18	0.42
58:EF:167:VAL:HA	58:EF:168:PRO:HD3	1.89	0.42
58:EF:639:ARG:NH1	58:EF:691:PRO:HG2	2.35	0.42
1:16:123:U:C2	1:16:124:C:C5	3.07	0.42
1:16:649:A:H2'	1:16:650:G:O4'	2.20	0.42
1:16:1227:A:H5''	19:SS:83:HIS:HD2	1.85	0.42
11:SK:126:LYS:HE3	21:SU:38:TYR:O	2.20	0.42
14:SN:48:LEU:HD23	14:SN:48:LEU:HA	1.84	0.42
15:SO:40:GLN:HE22	23:23:715:A:H2	1.67	0.42
18:SR:9:LYS:H	18:SR:9:LYS:HG2	1.65	0.42
19:SS:45:ILE:HD13	19:SS:62:VAL:HG12	2.02	0.42
23:23:608:A:H2'	23:23:609:A:H8	1.85	0.42
23:23:760:G:H2'	23:23:761:A:O4'	2.19	0.42
23:23:801:G:C8	28:LD:50:ALA:HB2	2.54	0.42
23:23:1410:G:H2'	23:23:1411:U:C6	2.55	0.42
23:23:1490:A:N3	23:23:1490:A:H2'	2.35	0.42
23:23:1993:U:H4'	27:LC:133:THR:OG1	2.20	0.42
58:EF:29:ARG:HA	58:EF:29:ARG:HE	1.85	0.42
58:EF:501:VAL:HG21	58:EF:522:MET:HE3	2.02	0.42
1:16:519:C:H2'	1:16:520:A:O4'	2.20	0.42
1:16:721:G:H4'	1:16:722:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:16:902:G:H2'	1:16:903:G:C8	2.53	0.42
1:16:1386:G:H2'	1:16:1387:G:C8	2.54	0.42
1:16:1472:U:H2'	1:16:1473:G:H8	1.85	0.42
1:16:1515:G:H2'	1:16:1516:2MG:C8	2.55	0.42
2:SB:207:ILE:O	2:SB:211:THR:HG23	2.19	0.42
3:SC:57:ILE:HG23	3:SC:64:ILE:HD11	2.01	0.42
10:SJ:51:VAL:HG13	14:SN:81:ARG:HG3	2.00	0.42
16:SP:56:ARG:HA	16:SP:56:ARG:HH11	1.85	0.42
19:SS:17:LYS:HE2	19:SS:17:LYS:HB3	1.91	0.42
23:23:521:U:H2'	23:23:522:A:C8	2.54	0.42
23:23:1317:G:H2'	23:23:1318:U:C6	2.54	0.42
23:23:1540:G:H2'	23:23:1541:C:C6	2.54	0.42
23:23:2131:U:O4	23:23:2158:A:H2'	2.20	0.42
23:23:2194:U:H2'	23:23:2195:U:C6	2.54	0.42
23:23:2872:A:H2'	23:23:2873:A:H5''	2.02	0.42
25:LA:69:THR:HA	25:LA:176:GLY:HA2	2.02	0.42
26:LB:69:ARG:HB3	26:LB:129:THR:HG21	2.01	0.42
35:LM:57:LEU:HD23	35:LM:128:ASN:O	2.19	0.42
36:LN:53:LYS:HE3	36:LN:53:LYS:HB2	1.82	0.42
58:EF:168:PRO:HG2	58:EF:218:TRP:CZ3	2.54	0.42
1:16:160:A:H2'	1:16:161:A:C8	2.55	0.42
1:16:551:U:H2'	1:16:552:U:C6	2.54	0.42
1:16:1372:U:H2'	1:16:1373:G:O4'	2.19	0.42
3:SC:42:TYR:OH	3:SC:90:VAL:HG21	2.20	0.42
8:SH:5:ASP:OD2	8:SH:81:PRO:HD3	2.20	0.42
11:SK:20:VAL:HG23	11:SK:37:ARG:NH1	2.34	0.42
23:23:20:C:H2'	23:23:21:A:C8	2.55	0.42
23:23:419:U:H2'	23:23:420:C:H6	1.84	0.42
23:23:1224:U:H4'	43:LU:88:GLY:O	2.20	0.42
23:23:1782:U:H1'	23:23:2609:U:H5''	2.02	0.42
23:23:2369:A:H2'	23:23:2370:G:H8	1.83	0.42
23:23:2591:C:H2'	23:23:2592:G:C8	2.55	0.42
33:LJ:41:LEU:HD23	33:LJ:41:LEU:HA	1.93	0.42
1:16:90:C:H6	1:16:90:C:H2'	1.68	0.42
1:16:147:G:H2'	1:16:148:G:H8	1.83	0.42
1:16:472:U:H2'	1:16:473:U:C6	2.54	0.42
1:16:579:A:H2'	1:16:580:C:H6	1.85	0.42
1:16:728:A:H2'	1:16:729:A:H8	1.84	0.42
1:16:1308:U:H2'	1:16:1309:G:H8	1.84	0.42
2:SB:54:LEU:HD12	2:SB:54:LEU:HA	1.83	0.42
4:SD:70:ARG:HD2	4:SD:70:ARG:HA	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SJ:47:GLU:OE1	14:SN:76:LYS:HE2	2.20	0.42
14:SN:73:PHE:CZ	14:SN:78:GLY:HA2	2.55	0.42
17:SQ:46:VAL:HG21	17:SQ:61:ILE:HG21	2.02	0.42
23:23:713:G:H22	23:23:718:A:H2	1.67	0.42
23:23:884:U:H2'	23:23:885:C:O4'	2.20	0.42
23:23:903:C:H2'	23:23:904:G:H8	1.84	0.42
23:23:1171:G:H2'	23:23:1172:C:C6	2.55	0.42
23:23:1707:G:C8	23:23:1756:G:C5	3.08	0.42
23:23:2114:A:H3'	23:23:2115:G:C8	2.55	0.42
23:23:2813:A:H2'	23:23:2814:A:H8	1.84	0.42
23:23:2815:C:C2	23:23:2816:G:C8	3.07	0.42
29:LE:8:TYR:HB2	29:LE:173:PHE:CZ	2.54	0.42
31:LG:73:ARG:NH2	31:LG:80:LEU:HA	2.33	0.42
38:LP:33:LEU:HD13	38:LP:117:PHE:HB3	2.02	0.42
47:LY:80:HIS:CD2	47:LY:83:LYS:H	2.38	0.42
1:16:154:U:H2'	1:16:155:A:H8	1.85	0.41
1:16:737:C:H2'	1:16:738:C:C6	2.55	0.41
4:SD:170:TRP:O	4:SD:171:LEU:HD23	2.20	0.41
10:SJ:78:GLU:HA	10:SJ:79:PRO:HD3	1.83	0.41
23:23:208:C:H2'	23:23:209:C:H6	1.84	0.41
23:23:1153:C:H2'	23:23:1154:G:O4'	2.20	0.41
23:23:1387:A:H5'	23:23:1469:A:H1'	2.02	0.41
23:23:1901:A:OP2	23:23:1901:A:H4'	2.20	0.41
23:23:2111:U:O4'	23:23:2118:U:H1'	2.20	0.41
23:23:2251:OMG:H1'	23:23:2251:OMG:HM23	1.64	0.41
23:23:2342:C:O2'	23:23:2374:C:H5''	2.20	0.41
27:LC:122:VAL:HG21	27:LC:129:THR:HG22	2.02	0.41
31:LG:65:LYS:O	31:LG:69:ILE:HG12	2.20	0.41
34:LK:40:LYS:HB2	34:LK:40:LYS:HE2	1.84	0.41
43:LU:85:LYS:HE2	43:LU:85:LYS:HB2	1.77	0.41
44:LV:79:GLY:H	44:LV:101:SER:HA	1.85	0.41
1:16:629:A:H2'	1:16:630:A:O4'	2.20	0.41
1:16:757:U:H2'	1:16:758:C:O4'	2.20	0.41
1:16:1095:U:H2'	1:16:1096:C:H6	1.84	0.41
6:SF:66:ALA:HB1	6:SF:70:VAL:HG21	2.03	0.41
7:SG:50:LEU:C	7:SG:50:LEU:HD23	2.40	0.41
15:SO:62:GLN:O	15:SO:66:LEU:HG	2.19	0.41
23:23:29:U:H2'	23:23:30:G:H8	1.84	0.41
23:23:863:A:H2'	23:23:864:G:C8	2.55	0.41
23:23:1028:A:H2'	23:23:1029:A:H8	1.80	0.41
23:23:2461:A:H2'	23:23:2462:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LA:195:ALA:O	25:LA:198:LYS:HG3	2.19	0.41
30:LF:164:TYR:HB2	30:LF:167:GLU:HB2	2.01	0.41
1:16:636:U:H2'	1:16:637:C:C6	2.55	0.41
1:16:643:C:H2'	1:16:644:U:H6	1.85	0.41
1:16:847:G:H2'	1:16:848:C:C6	2.55	0.41
2:SB:166:ALA:HB2	2:SB:187:VAL:HG12	2.02	0.41
5:SE:91:GLY:O	5:SE:130:SER:N	2.50	0.41
6:SF:47:LEU:HD12	6:SF:47:LEU:HA	1.85	0.41
7:SG:86:GLN:H	7:SG:86:GLN:HG3	1.58	0.41
20:ST:32:ILE:H	20:ST:32:ILE:HD12	1.85	0.41
23:23:128:C:H2'	23:23:129:C:C6	2.55	0.41
23:23:306:U:H2'	23:23:307:G:O4'	2.19	0.41
23:23:861:A:OP2	62:23:3010:PUT:N1	2.53	0.41
23:23:1164:C:H2'	23:23:1165:A:H8	1.85	0.41
23:23:1747:U:H2'	23:23:1748:C:H6	1.86	0.41
23:23:2369:A:H2'	23:23:2370:G:C8	2.55	0.41
43:LU:73:LYS:HB3	43:LU:73:LYS:HE2	1.77	0.41
58:EF:322:PHE:HA	58:EF:393:THR:HA	2.02	0.41
1:16:377:G:H2'	1:16:378:G:C8	2.54	0.41
1:16:401:C:H2'	1:16:402:G:C8	2.55	0.41
1:16:826:C:H2'	1:16:827:U:C6	2.55	0.41
1:16:1032:G:C5	1:16:1033:G:H1'	2.55	0.41
1:16:1397:C:H4'	1:16:1398:A:OP2	2.20	0.41
1:16:1477:U:H2'	1:16:1478:U:H6	1.85	0.41
2:SB:62:SER:HA	2:SB:228:ASP:OD1	2.20	0.41
7:SG:86:GLN:HE21	7:SG:86:GLN:HB2	1.51	0.41
13:SM:7:ILE:H	13:SM:7:ILE:HG13	1.49	0.41
16:SP:18:GLN:HE22	16:SP:35:ARG:HH21	1.68	0.41
17:SQ:21:ILE:HG13	17:SQ:46:VAL:HB	2.02	0.41
23:23:303:G:H2'	23:23:304:U:C6	2.55	0.41
23:23:570:G:H2'	23:23:2030:6MZ:N7	2.35	0.41
23:23:579:G:H2'	23:23:580:U:C6	2.56	0.41
23:23:699:A:H2'	23:23:700:G:O4'	2.20	0.41
23:23:926:G:H2'	23:23:927:A:C8	2.56	0.41
23:23:1183:U:H2'	23:23:1184:U:C6	2.55	0.41
23:23:1435:G:H2'	23:23:1436:G:H8	1.86	0.41
23:23:2166:U:H3	23:23:2171:A:N6	2.17	0.41
23:23:2294:G:H2'	23:23:2295:C:H6	1.85	0.41
32:LI:57:LYS:HA	32:LI:60:GLU:HG3	2.01	0.41
41:LS:31:TRP:CE2	41:LS:40:LEU:HD21	2.55	0.41
43:LU:50:GLY:HA3	43:LU:53:PHE:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:LW:34:VAL:HG23	45:LW:81:LYS:HB3	2.02	0.41
1:16:647:C:H2'	1:16:648:A:C8	2.55	0.41
1:16:696:A:H2'	1:16:697:U:C6	2.56	0.41
1:16:768:A:H4'	1:16:1523:G:H21	1.85	0.41
1:16:1225:A:H2'	1:16:1226:C:C5	2.55	0.41
1:16:1524:C:H2'	1:16:1525:G:H8	1.85	0.41
16:SP:70:ARG:HD3	16:SP:70:ARG:HA	1.85	0.41
23:23:175:G:H2'	23:23:176:A:C8	2.56	0.41
23:23:656:G:H2'	23:23:657:U:C6	2.55	0.41
23:23:1223:G:C6	23:23:1227:G:C6	3.08	0.41
23:23:1720:U:H2'	23:23:1721:G:O4'	2.21	0.41
23:23:2840:C:H5''	39:LQ:53:THR:OG1	2.20	0.41
26:LB:242:LYS:HE3	26:LB:242:LYS:HB3	1.90	0.41
29:LE:106:ILE:H	29:LE:106:ILE:HG12	1.72	0.41
30:LF:52:PHE:CZ	30:LF:72:LEU:HD22	2.55	0.41
44:LV:29:VAL:HA	44:LV:32:ALA:HB3	2.03	0.41
1:16:144:G:H2'	1:16:145:G:H8	1.85	0.41
1:16:436:C:H2'	1:16:437:U:C6	2.55	0.41
1:16:626:G:H2'	1:16:627:G:C8	2.55	0.41
1:16:632:U:H4'	1:16:633:G:O5'	2.20	0.41
1:16:958:A:N1	19:SS:55:ARG:HG2	2.35	0.41
1:16:1270:G:C2	1:16:1271:A:C5	3.09	0.41
1:16:1385:G:H2'	1:16:1386:G:H8	1.85	0.41
11:SK:24:HIS:O	11:SK:30:THR:HA	2.20	0.41
12:SL:10:LYS:HE2	12:SL:10:LYS:HB3	1.69	0.41
15:SO:4:SER:O	15:SO:8:THR:HG23	2.21	0.41
23:23:239:C:H2'	23:23:240:C:O4'	2.19	0.41
23:23:580:U:H2'	23:23:581:C:C6	2.55	0.41
23:23:966:G:H2'	23:23:967:U:C6	2.56	0.41
23:23:1034:G:H2'	23:23:1035:U:O4'	2.20	0.41
23:23:1435:G:H2'	23:23:1436:G:C8	2.56	0.41
23:23:1672:A:C2	23:23:2582:G:H5'	2.56	0.41
23:23:2190:G:H2'	23:23:2191:A:C8	2.54	0.41
23:23:2794:C:H2'	23:23:2795:C:C6	2.56	0.41
24:5:60:C:H2'	24:5:61:G:C8	2.56	0.41
29:LE:11:GLU:HA	29:LE:14:LYS:HG2	2.03	0.41
58:EF:345:SER:OG	58:EF:361:GLY:HA2	2.20	0.41
1:16:123:U:H5''	1:16:311:C:O2'	2.20	0.41
1:16:205:A:N3	1:16:205:A:H2'	2.36	0.41
1:16:545:C:H5'	4:SD:69:GLU:HB2	2.02	0.41
1:16:553:A:H5''	12:SL:21:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:16:563:A:H2'	1:16:567:G:C8	2.56	0.41
1:16:946:A:H2'	1:16:947:G:H8	1.80	0.41
1:16:967:5MC:H2'	1:16:968:A:C8	2.56	0.41
4:SD:37:ALA:O	4:SD:42:GLY:HA3	2.21	0.41
4:SD:78:GLU:O	4:SD:82:LEU:HG	2.20	0.41
5:SE:84:PRO:HB3	5:SE:97:GLN:HG3	2.03	0.41
7:SG:126:ASP:HA	7:SG:129:GLU:HG2	2.03	0.41
11:SK:23:ILE:HD12	11:SK:96:THR:HG21	2.03	0.41
18:SR:71:THR:HG23	18:SR:73:ARG:H	1.86	0.41
23:23:1398:C:C2	23:23:1399:C:C5	3.09	0.41
23:23:1676:A:H2'	23:23:1677:A:O4'	2.21	0.41
23:23:1704:C:H2'	23:23:1705:A:H8	1.86	0.41
23:23:2583:G:H2'	23:23:2584:U:O4'	2.21	0.41
24:5:28:C:P	40:LR:34:HIS:HD2	2.44	0.41
25:LA:49:GLY:HA3	25:LA:207:VAL:O	2.21	0.41
27:LC:148:GLN:HB2	27:LC:152:PRO:HG3	2.02	0.41
38:LP:3:GLN:HE21	38:LP:92:TRP:HE1	1.69	0.41
40:LR:7:ARG:HG2	40:LR:7:ARG:HH11	1.86	0.41
47:LY:16:ALA:HA	47:LY:19:ARG:HE	1.86	0.41
1:16:45:G:H5''	1:16:307:C:O2'	2.20	0.41
1:16:123:U:H2'	1:16:124:C:H6	1.85	0.41
1:16:285:C:H2'	1:16:286:C:C6	2.56	0.41
1:16:550:G:H2'	1:16:551:U:C6	2.55	0.41
1:16:821:G:H2'	1:16:822:U:H6	1.85	0.41
1:16:1029:U:H1'	1:16:1033:G:N2	2.36	0.41
1:16:1062:U:H2'	1:16:1063:C:C6	2.55	0.41
1:16:1384:C:H2'	1:16:1385:G:H8	1.84	0.41
1:16:1391:U:H2'	1:16:1392:G:H8	1.81	0.41
23:23:221:A:H61	23:23:428:A:H62	1.68	0.41
23:23:703:U:H2'	23:23:704:G:O4'	2.21	0.41
23:23:1447:C:H2'	23:23:1448:G:C8	2.56	0.41
23:23:1812:U:H2'	23:23:1813:G:C8	2.56	0.41
23:23:2065:C:H2'	23:23:2066:C:C6	2.55	0.41
23:23:2853:C:H2'	23:23:2854:G:H8	1.85	0.41
24:5:39:A:H2'	24:5:40:U:C6	2.56	0.41
27:LC:8:LYS:HB2	27:LC:201:LEU:HD11	2.02	0.41
34:LK:20:PRO:C	34:LK:22:PRO:HD3	2.41	0.41
38:LP:38:ARG:HB3	38:LP:98:PRO:HD3	2.01	0.41
39:LQ:48:VAL:O	39:LQ:51:LEU:HB2	2.20	0.41
41:LS:31:TRP:CD1	41:LS:82:ASP:HB2	2.55	0.41
47:LY:30:ILE:HG12	47:LY:91:PHE:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:16:510:A:N3	1:16:543:U:H1'	2.36	0.41
1:16:580:C:H2'	1:16:581:G:O4'	2.21	0.41
1:16:1001:C:H2'	1:16:1002:G:H8	1.85	0.41
1:16:1095:U:P	1:16:1108:G:H1	2.43	0.41
1:16:1354:U:H2'	1:16:1355:G:H8	1.86	0.41
2:SB:122:GLN:HE21	2:SB:122:GLN:HB3	1.50	0.41
3:SC:61:ALA:C	3:SC:62:LYS:HD2	2.41	0.41
4:SD:28:ILE:HG13	4:SD:29:ASP:N	2.36	0.41
8:SH:89:LYS:HA	8:SH:92:LEU:HD23	2.03	0.41
9:SI:25:ASN:HB3	9:SI:62:ASP:CB	2.49	0.41
13:SM:56:LEU:HD23	13:SM:56:LEU:HA	1.85	0.41
21:SU:20:LYS:O	21:SU:23:CYS:HB2	2.20	0.41
23:23:39:G:H2'	23:23:40:U:C6	2.55	0.41
23:23:146:A:H2'	23:23:147:C:C6	2.56	0.41
23:23:401:A:H2'	23:23:402:A:C8	2.56	0.41
23:23:443:A:N7	28:LD:40:ARG:HG2	2.36	0.41
23:23:580:U:O3'	42:LT:31:VAL:HG13	2.21	0.41
23:23:858:G:N3	23:23:2268:A:H2'	2.36	0.41
23:23:1011:G:C6	23:23:1151:A:C6	3.08	0.41
23:23:1156:A:C8	42:LT:51:ARG:HG2	2.56	0.41
23:23:1315:C:H2'	23:23:1316:U:C6	2.56	0.41
23:23:1321:A:C4	23:23:1322:A:C8	3.08	0.41
23:23:1704:C:H2'	23:23:1705:A:C8	2.56	0.41
23:23:1932:A:H2'	23:23:1933:G:O4'	2.21	0.41
23:23:2081:U:H2'	23:23:2082:A:C8	2.53	0.41
23:23:2128:G:H2'	23:23:2129:C:H6	1.86	0.41
23:23:2415:G:H2'	23:23:2416:C:H6	1.84	0.41
23:23:2745:C:H2'	23:23:2746:U:C6	2.56	0.41
25:LA:46:VAL:HB	25:LA:212:VAL:HG12	2.03	0.41
28:LD:194:LYS:O	28:LD:197:GLU:HG3	2.21	0.41
58:EF:140:PHE:HA	58:EF:265:THR:O	2.21	0.41
58:EF:490:TYR:HB3	58:EF:612:LEU:HD11	2.02	0.41
58:EF:495:ARG:HG2	58:EF:609:LYS:O	2.21	0.41
1:16:131:A:H2'	1:16:132:C:H6	1.86	0.41
1:16:1512:U:H2'	1:16:1513:A:C8	2.56	0.41
10:SJ:57:VAL:O	10:SJ:57:VAL:CG2	2.64	0.41
12:SL:53:CYS:SG	12:SL:67:ILE:HD11	2.60	0.41
16:SP:52:LEU:HD11	16:SP:57:ILE:HD11	2.02	0.41
23:23:150:U:H2'	23:23:151:C:C6	2.55	0.41
23:23:685:A:N1	23:23:787:C:H1'	2.36	0.41
23:23:849:A:H2'	23:23:850:U:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:863:A:H2'	23:23:864:G:H8	1.86	0.41
23:23:1297:C:H2'	23:23:1298:C:C6	2.56	0.41
23:23:1322:A:C5	23:23:1323:C:C5	3.09	0.41
23:23:2554:U:H2'	23:23:2555:U:C6	2.56	0.41
23:23:2809:A:H2'	23:23:2810:A:C8	2.56	0.41
24:5:112:G:H2'	24:5:113:C:C6	2.55	0.41
25:LA:27:ILE:CG2	25:LA:182:ALA:HB1	2.51	0.41
25:LA:57:GLN:HE21	25:LA:203:GLN:HG3	1.86	0.41
37:LO:55:MET:SD	37:LO:56:PRO:HD2	2.61	0.41
58:EF:488:VAL:HG21	58:EF:661:SER:HB3	2.03	0.41
1:16:1384:C:H2'	1:16:1385:G:C8	2.56	0.40
1:16:1465:A:H2'	1:16:1466:C:H6	1.84	0.40
3:SC:130:PHE:O	3:SC:134:MET:HG3	2.21	0.40
4:SD:60:LYS:HG2	4:SD:64:ILE:HD11	2.03	0.40
17:SQ:25:ILE:HB	17:SQ:42:THR:OG1	2.22	0.40
17:SQ:80:GLU:C	17:SQ:81:LYS:HD3	2.42	0.40
23:23:2:G:H2'	23:23:3:U:C6	2.55	0.40
23:23:638:G:H2'	23:23:639:U:C6	2.56	0.40
23:23:1178:C:H6	23:23:1178:C:H2'	1.69	0.40
23:23:2114:A:H2'	23:23:2115:G:O4'	2.22	0.40
23:23:2148:G:C2	23:23:2149:U:C4	3.09	0.40
23:23:2216:G:H2'	23:23:2217:G:H8	1.86	0.40
25:LA:203:GLN:O	25:LA:205:LYS:HG2	2.21	0.40
26:LB:144:VAL:HG11	26:LB:174:LEU:HD21	2.03	0.40
32:LI:4:ILE:HD13	32:LI:4:ILE:HA	1.90	0.40
35:LM:110:PRO:O	35:LM:115:GLY:HA3	2.21	0.40
42:LT:5:LYS:HB3	42:LT:5:LYS:HE2	1.66	0.40
58:EF:473:MET:HE2	58:EF:473:MET:HB2	1.84	0.40
1:16:171:A:H2'	1:16:172:A:C8	2.56	0.40
1:16:647:C:H2'	1:16:648:A:H8	1.86	0.40
1:16:1065:U:H5''	1:16:1190:G:N2	2.36	0.40
1:16:1164:G:H2'	1:16:1165:U:C6	2.56	0.40
1:16:1316:G:N2	1:16:1318:A:H3'	2.35	0.40
1:16:1410:A:H2'	1:16:1411:C:H6	1.87	0.40
2:SB:64:LYS:HA	2:SB:225:ARG:HH12	1.85	0.40
5:SE:77:ASN:HB2	5:SE:82:GLN:CD	2.42	0.40
8:SH:96:MET:HG3	8:SH:99:LEU:HB2	2.03	0.40
13:SM:17:ILE:H	13:SM:17:ILE:HD12	1.86	0.40
14:SN:87:ALA:HB1	14:SN:92:GLU:HB2	2.03	0.40
19:SS:21:LYS:HA	19:SS:24:GLU:HG3	2.02	0.40
23:23:152:A:H2'	23:23:153:U:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:175:G:H2'	23:23:176:A:H8	1.86	0.40
23:23:1383:A:H2'	23:23:1384:A:C8	2.56	0.40
23:23:2071:A:H2'	23:23:2072:C:C6	2.56	0.40
23:23:2521:C:C2	23:23:2545:G:N2	2.90	0.40
41:LS:9:GLU:O	41:LS:13:MET:HG3	2.20	0.40
44:LV:10:ALA:N	44:LV:101:SER:O	2.53	0.40
58:EF:253:ARG:O	58:EF:257:LEU:HD23	2.22	0.40
1:16:502:A:H2'	1:16:503:C:C6	2.57	0.40
1:16:643:C:C2	1:16:644:U:C5	3.10	0.40
1:16:1097:C:H2'	1:16:1098:C:H6	1.85	0.40
1:16:1136:C:H5''	1:16:1137:C:C4	2.56	0.40
1:16:1355:G:H2'	1:16:1356:G:C8	2.56	0.40
1:16:1435:G:H2'	1:16:1436:U:C6	2.56	0.40
6:SF:22:ILE:O	6:SF:26:THR:HG23	2.21	0.40
7:SG:78:ARG:HD3	7:SG:78:ARG:HA	1.85	0.40
7:SG:124:LEU:HD23	7:SG:124:LEU:HA	1.92	0.40
16:SP:6:LEU:HD23	16:SP:17:TYR:CG	2.56	0.40
23:23:822:G:H2'	23:23:823:C:C6	2.56	0.40
23:23:2292:U:H2'	23:23:2293:G:H8	1.85	0.40
23:23:2538:C:H2'	23:23:2539:C:H6	1.86	0.40
29:LE:107:ALA:HA	29:LE:137:ILE:HD11	2.03	0.40
32:LI:29:PHE:HD2	32:LI:30:LEU:HD23	1.85	0.40
35:LM:46:PRO:HD3	42:LT:60:LEU:HD13	2.02	0.40
44:LV:13:SER:O	44:LV:17:VAL:HG23	2.21	0.40
1:16:52:C:H2'	1:16:53:A:C8	2.57	0.40
1:16:202:G:H21	1:16:466:A:H61	1.69	0.40
1:16:824:G:H2'	1:16:825:A:H8	1.86	0.40
1:16:831:A:H5''	2:SB:21:ARG:HE	1.86	0.40
1:16:966:2MG:H2'	1:16:967:5MC:C6	2.56	0.40
1:16:1086:U:H3	1:16:1099:G:H22	1.68	0.40
1:16:1102:A:H2'	1:16:1103:C:C6	2.56	0.40
1:16:1342:C:H4'	9:SI:127:PHE:O	2.22	0.40
3:SC:112:ASP:OD2	3:SC:115:LEU:HD23	2.22	0.40
6:SF:101:PRO:HG2	18:SR:25:ASP:HA	2.03	0.40
17:SQ:49:GLU:OE1	17:SQ:50:ASN:HB2	2.22	0.40
23:23:184:C:H2'	23:23:185:G:C8	2.56	0.40
23:23:1438:U:H2'	23:23:1439:A:C8	2.54	0.40
23:23:2238:G:H2'	23:23:2238:G:N3	2.36	0.40
23:23:2704:C:H2'	23:23:2705:A:O4'	2.20	0.40
23:23:2774:C:H2'	23:23:2775:G:O4'	2.21	0.40
23:23:2785:C:H2'	23:23:2786:U:H6	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LA:21:TYR:CD2	25:LA:222:VAL:HG13	2.56	0.40
25:LA:50:ILE:HD12	25:LA:57:GLN:O	2.21	0.40
25:LA:197:LYS:NZ	25:LA:209:ILE:HG13	2.36	0.40
32:LI:99:ILE:O	32:LI:103:VAL:HG23	2.21	0.40
41:LS:63:LYS:HE2	41:LS:65:SER:HB2	2.02	0.40
41:LS:78:SER:OG	41:LS:80:VAL:HG22	2.21	0.40
1:16:1041:G:H2'	1:16:1042:A:C8	2.56	0.40
1:16:1318:A:H4'	19:SS:10:PHE:CD2	2.56	0.40
5:SE:83:HIS:CE1	5:SE:147:MET:HA	2.56	0.40
7:SG:71:PRO:HD3	7:SG:100:ALA:HB2	2.04	0.40
23:23:532:A:N1	23:23:2020:A:H1'	2.37	0.40
23:23:680:C:H2'	23:23:681:G:H8	1.87	0.40
23:23:2078:C:H2'	23:23:2079:U:C6	2.56	0.40
23:23:2813:A:H2'	23:23:2814:A:C8	2.56	0.40
27:LC:24:VAL:HG12	27:LC:178:VAL:HG21	2.03	0.40
27:LC:25:THR:HG21	27:LC:193:VAL:HG22	2.02	0.40
33:LJ:108:VAL:HG21	33:LJ:123:ILE:HD13	2.03	0.40
58:EF:202:PHE:CD1	58:EF:202:PHE:N	2.82	0.40
58:EF:332:ASN:O	58:EF:386:ILE:HA	2.21	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 PDB entries followed by that with respect to all EM entries.

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	SB	224/241 (93%)	209 (93%)	15 (7%)	0	100	100
3	SC	204/233 (88%)	198 (97%)	6 (3%)	0	100	100
4	SD	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
5	SE	153/167 (92%)	147 (96%)	6 (4%)	0	100	100
6	SF	104/135 (77%)	96 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	SG	154/179 (86%)	145 (94%)	9 (6%)	0	100	100
8	SH	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
9	SI	125/130 (96%)	112 (90%)	13 (10%)	0	100	100
10	SJ	97/103 (94%)	92 (95%)	5 (5%)	0	100	100
11	SK	115/129 (89%)	106 (92%)	9 (8%)	0	100	100
12	SL	120/124 (97%)	112 (93%)	8 (7%)	0	100	100
13	SM	113/118 (96%)	106 (94%)	7 (6%)	0	100	100
14	SN	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
15	SO	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
16	SP	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
17	SQ	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
18	SR	65/75 (87%)	62 (95%)	3 (5%)	0	100	100
19	SS	82/92 (89%)	78 (95%)	4 (5%)	0	100	100
20	ST	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	SU	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
25	LA	130/234 (56%)	127 (98%)	3 (2%)	0	100	100
26	LB	269/273 (98%)	259 (96%)	10 (4%)	0	100	100
27	LC	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
28	LD	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
29	LE	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
30	LF	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
31	LG	66/121 (54%)	61 (92%)	5 (8%)	0	100	100
32	LI	147/149 (99%)	137 (93%)	10 (7%)	0	100	100
33	LJ	133/165 (81%)	122 (92%)	11 (8%)	0	100	100
34	LK	132/142 (93%)	110 (83%)	21 (16%)	1 (1%)	16	36
35	LM	140/142 (99%)	140 (100%)	0	0	100	100
36	LN	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
37	LO	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
38	LP	133/136 (98%)	133 (100%)	0	0	100	100
39	LQ	118/127 (93%)	115 (98%)	3 (2%)	0	100	100
40	LR	114/117 (97%)	109 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	LS	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
42	LT	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
43	LU	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
44	LV	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
45	LW	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
46	LX	100/104 (96%)	91 (91%)	9 (9%)	0	100	100
47	LY	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
48	La	82/85 (96%)	81 (99%)	1 (1%)	0	100	100
49	Lb	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
50	Lc	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
51	Ld	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
52	Le	65/70 (93%)	54 (83%)	11 (17%)	0	100	100
53	Lf	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
54	Lg	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
55	Lh	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
56	Li	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
57	Lj	36/38 (95%)	36 (100%)	0	0	100	100
58	EF	681/704 (97%)	646 (95%)	35 (5%)	0	100	100
59	Pp	1/3 (33%)	1 (100%)	0	0	100	100
All	All	6763/7282 (93%)	6447 (95%)	315 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
34	LK	22	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	SB	188/199 (94%)	162 (86%)	26 (14%)	3	6
3	SC	170/190 (90%)	164 (96%)	6 (4%)	31	58
4	SD	172/173 (99%)	162 (94%)	10 (6%)	17	37
5	SE	118/126 (94%)	111 (94%)	7 (6%)	16	37
6	SF	92/116 (79%)	75 (82%)	17 (18%)	1	3
7	SG	129/147 (88%)	106 (82%)	23 (18%)	1	3
8	SH	104/105 (99%)	100 (96%)	4 (4%)	28	55
9	SI	105/107 (98%)	86 (82%)	19 (18%)	1	3
10	SJ	87/90 (97%)	77 (88%)	10 (12%)	4	10
11	SK	90/99 (91%)	87 (97%)	3 (3%)	33	61
12	SL	102/103 (99%)	90 (88%)	12 (12%)	4	10
13	SM	93/96 (97%)	81 (87%)	12 (13%)	3	8
14	SN	83/84 (99%)	74 (89%)	9 (11%)	5	12
15	SO	76/77 (99%)	72 (95%)	4 (5%)	19	42
16	SP	65/65 (100%)	64 (98%)	1 (2%)	60	82
17	SQ	74/78 (95%)	69 (93%)	5 (7%)	13	31
18	SR	58/65 (89%)	49 (84%)	9 (16%)	2	5
19	SS	72/79 (91%)	70 (97%)	2 (3%)	38	66
20	ST	65/66 (98%)	61 (94%)	4 (6%)	15	34
21	SU	60/61 (98%)	56 (93%)	4 (7%)	13	31
25	LA	110/181 (61%)	102 (93%)	8 (7%)	11	27
26	LB	216/218 (99%)	211 (98%)	5 (2%)	45	73
27	LC	164/164 (100%)	162 (99%)	2 (1%)	67	85
28	LD	165/165 (100%)	165 (100%)	0	100	100
29	LE	148/150 (99%)	141 (95%)	7 (5%)	22	47
30	LF	137/138 (99%)	136 (99%)	1 (1%)	81	92
31	LG	47/85 (55%)	45 (96%)	2 (4%)	25	50
32	LI	114/114 (100%)	110 (96%)	4 (4%)	31	58
33	LJ	103/123 (84%)	91 (88%)	12 (12%)	4	10
34	LK	103/110 (94%)	80 (78%)	23 (22%)	1	2
35	LM	116/116 (100%)	115 (99%)	1 (1%)	75	89
36	LN	104/104 (100%)	103 (99%)	1 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	LO	103/103 (100%)	102 (99%)	1 (1%)	73	88
38	LP	108/108 (100%)	105 (97%)	3 (3%)	38	66
39	LQ	100/103 (97%)	100 (100%)	0	100	100
40	LR	86/87 (99%)	83 (96%)	3 (4%)	31	58
41	LS	99/100 (99%)	96 (97%)	3 (3%)	36	64
42	LT	89/90 (99%)	86 (97%)	3 (3%)	32	59
43	LU	84/84 (100%)	83 (99%)	1 (1%)	67	85
44	LV	93/93 (100%)	91 (98%)	2 (2%)	47	74
45	LW	80/84 (95%)	77 (96%)	3 (4%)	28	55
46	LX	83/85 (98%)	82 (99%)	1 (1%)	67	85
47	LY	78/78 (100%)	75 (96%)	3 (4%)	28	55
48	La	62/63 (98%)	61 (98%)	1 (2%)	58	81
49	Lb	67/68 (98%)	65 (97%)	2 (3%)	36	64
50	Lc	54/55 (98%)	49 (91%)	5 (9%)	7	17
51	Ld	48/49 (98%)	48 (100%)	0	100	100
52	Le	60/62 (97%)	57 (95%)	3 (5%)	20	44
53	Lf	47/48 (98%)	47 (100%)	0	100	100
54	Lg	45/49 (92%)	44 (98%)	1 (2%)	47	74
55	Lh	38/38 (100%)	38 (100%)	0	100	100
56	Li	51/52 (98%)	49 (96%)	2 (4%)	27	54
57	Lj	34/34 (100%)	32 (94%)	2 (6%)	16	37
58	EF	480/578 (83%)	446 (93%)	34 (7%)	12	29
59	Pp	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	5522/5908 (94%)	5195 (94%)	327 (6%)	19	37

All (327) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SB	49	MET
2	SB	52	GLU
2	SB	54	LEU
2	SB	62	SER
2	SB	63	ARG
2	SB	73	LYS

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Mol	Chain	Res	Type
2	SB	97	LEU
2	SB	100	MET
2	SB	113	ARG
2	SB	116	ASP
2	SB	118	GLU
2	SB	120	GLN
2	SB	122	GLN
2	SB	125	THR
2	SB	126	PHE
2	SB	129	LEU
2	SB	131	LYS
2	SB	133	GLU
2	SB	136	MET
2	SB	141	LEU
2	SB	142	GLU
2	SB	174	LYS
2	SB	192	ASP
2	SB	220	THR
2	SB	223	GLU
2	SB	227	GLN
3	SC	40	ARG
3	SC	58	GLU
3	SC	79	LYS
3	SC	88	ARG
3	SC	100	GLN
3	SC	156	ARG
4	SD	3	ARG
4	SD	58	LYS
4	SD	81	ARG
4	SD	88	GLU
4	SD	113	GLU
4	SD	132	ILE
4	SD	166	GLU
4	SD	184	ARG
4	SD	190	ASP
4	SD	202	GLU
5	SE	20	ARG
5	SE	22	SER
5	SE	145	GLU
5	SE	147	MET
5	SE	157	ARG
5	SE	162	GLU

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Mol	Chain	Res	Type
5	SE	163	GLU
6	SF	1	MET
6	SF	5	GLU
6	SF	9	MET
6	SF	29	ILE
6	SF	35	LYS
6	SF	36	ILE
6	SF	46	GLN
6	SF	47	LEU
6	SF	62	MET
6	SF	64	VAL
6	SF	65	GLU
6	SF	75	GLU
6	SF	88	MET
6	SF	89	VAL
6	SF	92	THR
6	SF	96	VAL
6	SF	100	SER
7	SG	53	ARG
7	SG	58	GLU
7	SG	70	ARG
7	SG	73	VAL
7	SG	74	GLU
7	SG	78	ARG
7	SG	84	THR
7	SG	86	GLN
7	SG	87	VAL
7	SG	91	VAL
7	SG	114	LYS
7	SG	115	SER
7	SG	116	MET
7	SG	120	LEU
7	SG	122	ASN
7	SG	138	ARG
7	SG	139	GLU
7	SG	141	VAL
7	SG	146	GLU
7	SG	149	LYS
7	SG	153	HIS
7	SG	155	ARG
7	SG	157	LEU
8	SH	41	LYS

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Mol	Chain	Res	Type
8	SH	54	ASP
8	SH	64	LYS
8	SH	89	LYS
9	SI	11	ARG
9	SI	21	ILE
9	SI	22	LYS
9	SI	52	LEU
9	SI	54	LEU
9	SI	55	VAL
9	SI	57	MET
9	SI	58	VAL
9	SI	59	GLU
9	SI	60	LYS
9	SI	61	LEU
9	SI	62	ASP
9	SI	63	LEU
9	SI	80	ARG
9	SI	100	LYS
9	SI	123	ARG
9	SI	124	ARG
9	SI	126	GLN
9	SI	130	ARG
10	SJ	5	ARG
10	SJ	9	ARG
10	SJ	17	LEU
10	SJ	22	THR
10	SJ	40	ILE
10	SJ	45	ARG
10	SJ	53	ILE
10	SJ	64	GLN
10	SJ	75	ASP
10	SJ	100	ILE
11	SK	69	ARG
11	SK	125	LYS
11	SK	128	ARG
12	SL	3	THR
12	SL	10	LYS
12	SL	14	ARG
12	SL	30	LYS
12	SL	35	THR
12	SL	36	ARG
12	SL	50	ARG

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Mol	Chain	Res	Type
12	SL	59	ASN
12	SL	64	THR
12	SL	86	ARG
12	SL	88	LYS
12	SL	90	LEU
13	SM	4	ILE
13	SM	7	ILE
13	SM	8	ASN
13	SM	13	LYS
13	SM	65	VAL
13	SM	69	LEU
13	SM	71	ARG
13	SM	83	LEU
13	SM	93	ARG
13	SM	100	GLN
13	SM	107	ARG
13	SM	116	ILE
14	SN	19	LYS
14	SN	23	LYS
14	SN	26	GLU
14	SN	27	LEU
14	SN	35	ASN
14	SN	39	GLU
14	SN	41	ARG
14	SN	63	ARG
14	SN	86	GLU
15	SO	17	ARG
15	SO	64	ARG
15	SO	87	LEU
15	SO	88	ARG
16	SP	69	ASP
17	SQ	13	VAL
17	SQ	16	LYS
17	SQ	27	ARG
17	SQ	39	LYS
17	SQ	71	LYS
18	SR	8	ARG
18	SR	9	LYS
18	SR	21	ILE
18	SR	24	LYS
18	SR	29	LEU
18	SR	38	LYS

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Mol	Chain	Res	Type
18	SR	45	THR
18	SR	48	ARG
18	SR	66	SER
19	SS	6	LYS
19	SS	11	ILE
20	ST	6	SER
20	ST	15	GLU
20	ST	18	ARG
20	ST	24	ARG
21	SU	24	GLU
21	SU	68	THR
21	SU	69	ARG
21	SU	70	LEU
25	LA	25	GLU
25	LA	29	LEU
25	LA	30	LEU
25	LA	31	LYS
25	LA	187	GLU
25	LA	198	LYS
25	LA	211	LYS
25	LA	215	SER
26	LB	5	LYS
26	LB	9	THR
26	LB	13	ARG
26	LB	28	LYS
26	LB	221	ARG
27	LC	1	MET
27	LC	141	ARG
29	LE	30	ARG
29	LE	88	LYS
29	LE	104	ILE
29	LE	109	PRO
29	LE	115	ARG
29	LE	117	LEU
29	LE	140	GLU
30	LF	152	ARG
31	LG	82	GLU
31	LG	89	SER
32	LI	40	THR
32	LI	42	LYS
32	LI	43	ASN
32	LI	122	LEU

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Mol	Chain	Res	Type
33	LJ	6	GLN
33	LJ	30	SER
33	LJ	31	ARG
33	LJ	34	THR
33	LJ	37	LYS
33	LJ	41	LEU
33	LJ	52	MET
33	LJ	67	THR
33	LJ	69	PHE
33	LJ	86	MET
33	LJ	97	LYS
33	LJ	101	LYS
34	LK	9	VAL
34	LK	10	LYS
34	LK	11	LEU
34	LK	12	GLN
34	LK	17	MET
34	LK	21	SER
34	LK	28	LEU
34	LK	31	GLN
34	LK	35	ILE
34	LK	36	MET
34	LK	37	GLU
34	LK	45	LYS
34	LK	51	LYS
34	LK	55	ILE
34	LK	57	VAL
34	LK	59	ILE
34	LK	60	THR
34	LK	62	TYR
34	LK	68	THR
34	LK	70	VAL
34	LK	72	LYS
34	LK	98	VAL
34	LK	101	ILE
35	LM	2	LYS
36	LN	123	LEU
37	LO	70	LYS
38	LP	6	ARG
38	LP	50	ARG
38	LP	110	GLU
40	LR	25	ARG

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Mol	Chain	Res	Type
40	LR	68	LYS
40	LR	104	GLN
41	LS	34	GLU
41	LS	111	LYS
41	LS	114	LEU
42	LT	5	LYS
42	LT	6	ARG
42	LT	11	ARG
43	LU	55	ASP
44	LV	11	ARG
44	LV	98	LYS
45	LW	64	LYS
45	LW	92	ASN
45	LW	93	LEU
46	LX	81	ASP
47	LY	51	GLN
47	LY	59	GLU
47	LY	93	ARG
48	La	3	HIS
49	Lb	11	ARG
49	Lb	54	LYS
50	Lc	10	SER
50	Lc	11	VAL
50	Lc	13	GLU
50	Lc	14	LEU
50	Lc	58	ASN
52	Le	39	LYS
52	Le	62	LYS
52	Le	66	ILE
54	Lg	6	ARG
56	Li	30	ARG
56	Li	52	LYS
57	Lj	2	LYS
57	Lj	12	ARG
58	EF	4	THR
58	EF	29	ARG
58	EF	37	ASN
58	EF	78	GLN
58	EF	80	GLU
58	EF	104	ARG
58	EF	161	ARG
58	EF	201	THR

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Mol	Chain	Res	Type
58	EF	202	PHE
58	EF	301	ASP
58	EF	352	SER
58	EF	363	ILE
58	EF	401	ASP
58	EF	404	ILE
58	EF	405	ILE
58	EF	435	LEU
58	EF	442	ASP
58	EF	473	MET
58	EF	507	LYS
58	EF	518	VAL
58	EF	538	ASN
58	EF	539	ASP
58	EF	540	ILE
58	EF	548	GLU
58	EF	553	VAL
58	EF	576	ILE
58	EF	582	SER
58	EF	587	ASP
58	EF	594	LYS
58	EF	595	LEU
58	EF	642	LEU
58	EF	643	LYS
58	EF	645	GLN
58	EF	669	GLN
59	Pp	3	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
2	SB	122	GLN
2	SB	168	HIS
4	SD	100	ASN
5	SE	82	GLN
5	SE	122	ASN
6	SF	17	GLN
6	SF	37	HIS
7	SG	52	GLN
7	SG	86	GLN
7	SG	130	ASN
7	SG	148	ASN

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Mol	Chain	Res	Type
11	SK	64	GLN
12	SL	73	ASN
12	SL	77	HIS
13	SM	100	GLN
14	SN	49	GLN
16	SP	79	ASN
17	SQ	9	GLN
17	SQ	47	HIS
27	LC	150	GLN
29	LE	81	GLN
32	LI	43	ASN
34	LK	94	ASN
43	LU	66	HIS
47	LY	80	HIS
48	La	46	HIS
49	Lb	34	HIS
50	Lc	45	GLN
52	Le	6	HIS
58	EF	37	ASN
58	EF	82	HIS
58	EF	170	GLN
58	EF	428	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16	1530/1534 (99%)	281 (18%)	14 (0%)
22	mR	11/60 (18%)	3 (27%)	0
23	23	2898/2904 (99%)	484 (16%)	12 (0%)
24	5	119/120 (99%)	19 (15%)	2 (1%)
60	Pt	73/76 (96%)	14 (19%)	0
61	Dt	73/76 (96%)	22 (30%)	0
All	All	4704/4770 (98%)	823 (17%)	28 (0%)

All (823) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16	2	A
1	16	4	U
1	16	5	U
1	16	9	G

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Mol	Chain	Res	Type
1	16	32	A
1	16	39	G
1	16	47	C
1	16	48	C
1	16	49	U
1	16	50	A
1	16	51	A
1	16	54	C
1	16	71	A
1	16	72	A
1	16	74	A
1	16	76	G
1	16	77	A
1	16	78	A
1	16	80	A
1	16	81	A
1	16	82	G
1	16	83	C
1	16	84	U
1	16	85	U
1	16	86	G
1	16	89	U
1	16	90	C
1	16	91	U
1	16	94	G
1	16	95	C
1	16	96	U
1	16	97	G
1	16	119	A
1	16	121	U
1	16	127	G
1	16	130	A
1	16	131	A
1	16	137	U
1	16	141	G
1	16	143	A
1	16	144	G
1	16	159	G
1	16	163	C
1	16	164	G
1	16	166	U
1	16	170	U

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Mol	Chain	Res	Type
1	16	171	A
1	16	173	U
1	16	177	G
1	16	182	A
1	16	197	A
1	16	200	G
1	16	209	U
1	16	210	C
1	16	225	C
1	16	226	G
1	16	245	U
1	16	247	G
1	16	250	A
1	16	251	G
1	16	257	G
1	16	266	G
1	16	267	C
1	16	271	C
1	16	273	U
1	16	275	G
1	16	279	A
1	16	289	G
1	16	319	G
1	16	321	A
1	16	328	C
1	16	329	A
1	16	330	C
1	16	332	G
1	16	346	G
1	16	352	C
1	16	354	G
1	16	356	A
1	16	359	G
1	16	367	U
1	16	372	C
1	16	384	G
1	16	385	C
1	16	388	G
1	16	397	A
1	16	406	G
1	16	411	A
1	16	412	A

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Mol	Chain	Res	Type
1	16	413	G
1	16	414	A
1	16	421	U
1	16	429	U
1	16	435	A
1	16	438	U
1	16	439	U
1	16	455	G
1	16	457	G
1	16	458	U
1	16	463	U
1	16	465	A
1	16	466	A
1	16	467	U
1	16	468	A
1	16	479	U
1	16	481	G
1	16	484	G
1	16	486	U
1	16	497	G
1	16	509	A
1	16	511	C
1	16	515	G
1	16	521	G
1	16	527	G7M
1	16	530	G
1	16	533	A
1	16	547	A
1	16	559	A
1	16	562	U
1	16	563	A
1	16	564	C
1	16	567	G
1	16	572	A
1	16	573	A
1	16	576	C
1	16	577	G
1	16	596	A
1	16	615	G
1	16	619	U
1	16	632	U
1	16	633	G

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Mol	Chain	Res	Type
1	16	650	G
1	16	653	U
1	16	660	C
1	16	665	A
1	16	670	G
1	16	673	A
1	16	675	A
1	16	687	A
1	16	701	U
1	16	702	A
1	16	711	G
1	16	716	A
1	16	717	U
1	16	718	A
1	16	723	U
1	16	734	G
1	16	737	C
1	16	755	G
1	16	773	G
1	16	793	U
1	16	794	A
1	16	815	A
1	16	817	C
1	16	821	G
1	16	828	U
1	16	829	G
1	16	841	C
1	16	842	U
1	16	843	U
1	16	844	G
1	16	845	A
1	16	846	G
1	16	885	G
1	16	889	A
1	16	902	G
1	16	914	A
1	16	922	G
1	16	926	G
1	16	927	G
1	16	932	C
1	16	934	C
1	16	935	A

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Mol	Chain	Res	Type
1	16	939	G
1	16	958	A
1	16	960	U
1	16	969	A
1	16	971	G
1	16	975	A
1	16	976	G
1	16	977	A
1	16	991	U
1	16	992	U
1	16	993	G
1	16	994	A
1	16	1003	G
1	16	1004	A
1	16	1012	A
1	16	1020	G
1	16	1021	A
1	16	1029	U
1	16	1030	U
1	16	1031	C
1	16	1032	G
1	16	1065	U
1	16	1085	U
1	16	1094	G
1	16	1095	U
1	16	1101	A
1	16	1123	U
1	16	1124	G
1	16	1125	U
1	16	1129	C
1	16	1130	A
1	16	1133	G
1	16	1135	U
1	16	1137	C
1	16	1139	G
1	16	1141	C
1	16	1142	G
1	16	1143	G
1	16	1145	A
1	16	1146	A
1	16	1149	C
1	16	1150	A

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Mol	Chain	Res	Type
1	16	1157	A
1	16	1158	C
1	16	1159	U
1	16	1160	G
1	16	1167	A
1	16	1183	U
1	16	1184	G
1	16	1196	A
1	16	1197	A
1	16	1213	A
1	16	1214	C
1	16	1225	A
1	16	1226	C
1	16	1227	A
1	16	1236	A
1	16	1238	A
1	16	1239	A
1	16	1240	U
1	16	1257	A
1	16	1260	G
1	16	1268	G
1	16	1269	A
1	16	1279	G
1	16	1280	A
1	16	1286	U
1	16	1287	A
1	16	1297	G
1	16	1298	U
1	16	1299	A
1	16	1300	G
1	16	1302	C
1	16	1305	G
1	16	1311	A
1	16	1312	G
1	16	1317	C
1	16	1320	C
1	16	1323	G
1	16	1331	G
1	16	1332	A
1	16	1336	C
1	16	1337	G
1	16	1346	A

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Mol	Chain	Res	Type
1	16	1351	U
1	16	1363	A
1	16	1364	U
1	16	1368	A
1	16	1370	G
1	16	1397	C
1	16	1398	A
1	16	1419	G
1	16	1429	A
1	16	1432	G
1	16	1441	A
1	16	1442	G
1	16	1446	A
1	16	1451	U
1	16	1452	C
1	16	1453	G
1	16	1492	A
1	16	1497	G
1	16	1503	A
1	16	1505	G
1	16	1506	U
1	16	1517	G
1	16	1529	G
1	16	1530	G
1	16	1531	A
22	mR	39	G
22	mR	40	U
22	mR	46	G
23	23	10	A
23	23	13	A
23	23	15	G
23	23	27	G
23	23	33	C
23	23	34	U
23	23	42	A
23	23	46	G
23	23	51	G
23	23	71	A
23	23	74	A
23	23	75	G
23	23	80	G
23	23	96	C

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Mol	Chain	Res	Type
23	23	101	A
23	23	102	U
23	23	103	A
23	23	118	A
23	23	119	A
23	23	120	U
23	23	125	A
23	23	139	U
23	23	141	G
23	23	142	A
23	23	163	C
23	23	177	G
23	23	181	A
23	23	196	A
23	23	199	A
23	23	206	U
23	23	216	A
23	23	221	A
23	23	222	A
23	23	230	G
23	23	248	G
23	23	264	C
23	23	265	A
23	23	266	G
23	23	276	U
23	23	277	G
23	23	278	A
23	23	279	A
23	23	289	G
23	23	290	U
23	23	291	G
23	23	311	A
23	23	329	G
23	23	330	A
23	23	331	C
23	23	332	A
23	23	338	G
23	23	344	A
23	23	352	A
23	23	353	C
23	23	356	G
23	23	361	G

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Mol	Chain	Res	Type
23	23	372	G
23	23	380	G
23	23	386	G
23	23	396	G
23	23	401	A
23	23	411	G
23	23	412	A
23	23	415	A
23	23	417	C
23	23	428	A
23	23	435	C
23	23	473	G
23	23	479	A
23	23	481	G
23	23	491	G
23	23	504	A
23	23	505	A
23	23	509	C
23	23	510	C
23	23	513	A
23	23	529	A
23	23	530	G
23	23	531	C
23	23	532	A
23	23	538	A
23	23	547	A
23	23	548	G
23	23	549	G
23	23	555	G
23	23	563	A
23	23	573	U
23	23	575	A
23	23	586	A
23	23	603	A
23	23	615	U
23	23	627	A
23	23	637	A
23	23	645	C
23	23	647	G
23	23	654	A
23	23	655	A
23	23	668	A

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Mol	Chain	Res	Type
23	23	671	C
23	23	675	A
23	23	686	U
23	23	713	G
23	23	716	A
23	23	717	C
23	23	724	U
23	23	730	A
23	23	740	C
23	23	747	5MU
23	23	757	G
23	23	764	A
23	23	775	G
23	23	776	G
23	23	782	A
23	23	783	A
23	23	784	G
23	23	785	G
23	23	789	A
23	23	805	G
23	23	811	U
23	23	812	C
23	23	819	A
23	23	827	U
23	23	828	U
23	23	830	G
23	23	846	U
23	23	847	U
23	23	859	G
23	23	869	G
23	23	886	A
23	23	889	C
23	23	890	C
23	23	891	G
23	23	892	A
23	23	895	U
23	23	897	C
23	23	906	U
23	23	907	G
23	23	910	A
23	23	917	A
23	23	931	U

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Mol	Chain	Res	Type
23	23	941	A
23	23	946	C
23	23	961	C
23	23	973	A
23	23	974	G
23	23	983	A
23	23	996	A
23	23	1009	A
23	23	1011	G
23	23	1012	U
23	23	1013	C
23	23	1017	G
23	23	1022	G
23	23	1023	U
23	23	1026	G
23	23	1033	U
23	23	1047	G
23	23	1050	A
23	23	1051	G
23	23	1054	A
23	23	1059	G
23	23	1060	U
23	23	1070	A
23	23	1076	C
23	23	1080	A
23	23	1083	U
23	23	1084	A
23	23	1087	G
23	23	1088	A
23	23	1090	A
23	23	1091	G
23	23	1101	U
23	23	1102	C
23	23	1105	U
23	23	1110	G
23	23	1112	G
23	23	1115	G
23	23	1116	G
23	23	1118	C
23	23	1132	U
23	23	1133	A
23	23	1134	A

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Mol	Chain	Res	Type
23	23	1135	C
23	23	1136	G
23	23	1142	A
23	23	1149	G
23	23	1151	A
23	23	1174	U
23	23	1175	A
23	23	1176	U
23	23	1177	G
23	23	1179	G
23	23	1180	U
23	23	1181	U
23	23	1195	G
23	23	1212	G
23	23	1219	U
23	23	1227	G
23	23	1238	G
23	23	1247	A
23	23	1249	U
23	23	1250	G
23	23	1253	A
23	23	1255	U
23	23	1256	G
23	23	1266	G
23	23	1267	U
23	23	1271	G
23	23	1272	A
23	23	1273	U
23	23	1300	G
23	23	1301	A
23	23	1365	A
23	23	1368	G
23	23	1378	A
23	23	1379	U
23	23	1383	A
23	23	1395	A
23	23	1413	A
23	23	1416	G
23	23	1419	A
23	23	1420	A
23	23	1428	C
23	23	1452	G

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Mol	Chain	Res	Type
23	23	1453	A
23	23	1459	G
23	23	1482	G
23	23	1485	U
23	23	1486	U
23	23	1490	A
23	23	1493	C
23	23	1497	U
23	23	1504	A
23	23	1507	C
23	23	1509	A
23	23	1510	G
23	23	1515	A
23	23	1524	G
23	23	1533	C
23	23	1535	A
23	23	1536	C
23	23	1537	G
23	23	1540	G
23	23	1542	U
23	23	1560	G
23	23	1566	A
23	23	1569	A
23	23	1570	A
23	23	1578	U
23	23	1584	U
23	23	1587	G
23	23	1590	A
23	23	1591	A
23	23	1608	A
23	23	1610	A
23	23	1616	A
23	23	1617	C
23	23	1647	U
23	23	1648	U
23	23	1649	G
23	23	1665	A
23	23	1667	G
23	23	1674	G
23	23	1693	U
23	23	1715	G
23	23	1727	C

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Mol	Chain	Res	Type
23	23	1730	C
23	23	1731	G
23	23	1736	U
23	23	1738	G
23	23	1740	G
23	23	1744	A
23	23	1756	G
23	23	1764	C
23	23	1773	A
23	23	1784	A
23	23	1786	A
23	23	1800	C
23	23	1801	A
23	23	1808	A
23	23	1816	C
23	23	1829	A
23	23	1838	C
23	23	1842	G
23	23	1848	A
23	23	1857	G
23	23	1858	A
23	23	1862	G
23	23	1866	A
23	23	1867	G
23	23	1868	C
23	23	1869	G
23	23	1870	C
23	23	1872	A
23	23	1873	G
23	23	1876	A
23	23	1881	C
23	23	1882	U
23	23	1885	A
23	23	1889	A
23	23	1896	G
23	23	1900	A
23	23	1906	G
23	23	1907	G
23	23	1910	G
23	23	1912	A
23	23	1913	A
23	23	1914	C

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Mol	Chain	Res	Type
23	23	1919	A
23	23	1920	C
23	23	1921	G
23	23	1927	A
23	23	1929	G
23	23	1930	G
23	23	1931	U
23	23	1936	A
23	23	1937	A
23	23	1938	A
23	23	1939	5MU
23	23	1955	U
23	23	1964	G
23	23	1965	C
23	23	1967	C
23	23	1970	A
23	23	1971	U
23	23	1972	G
23	23	1991	U
23	23	1993	U
23	23	1997	C
23	23	2020	A
23	23	2022	U
23	23	2023	C
23	23	2031	A
23	23	2033	A
23	23	2043	C
23	23	2046	G
23	23	2055	C
23	23	2056	G
23	23	2060	A
23	23	2061	G
23	23	2062	A
23	23	2069	G7M
23	23	2093	G
23	23	2106	U
23	23	2107	G
23	23	2110	G
23	23	2113	U
23	23	2116	G
23	23	2117	A
23	23	2118	U

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Mol	Chain	Res	Type
23	23	2132	U
23	23	2133	G
23	23	2134	A
23	23	2138	G
23	23	2157	G
23	23	2158	A
23	23	2159	G
23	23	2161	C
23	23	2162	G
23	23	2163	A
23	23	2164	C
23	23	2165	C
23	23	2170	A
23	23	2171	A
23	23	2172	U
23	23	2189	U
23	23	2191	A
23	23	2192	U
23	23	2198	A
23	23	2203	U
23	23	2204	G
23	23	2211	A
23	23	2225	A
23	23	2238	G
23	23	2239	G
23	23	2243	U
23	23	2259	U
23	23	2268	A
23	23	2278	A
23	23	2280	G
23	23	2283	C
23	23	2287	A
23	23	2288	A
23	23	2298	A
23	23	2305	U
23	23	2308	G
23	23	2310	C
23	23	2312	U
23	23	2319	G
23	23	2320	U
23	23	2321	U
23	23	2322	A

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Mol	Chain	Res	Type
23	23	2327	A
23	23	2333	A
23	23	2335	A
23	23	2342	C
23	23	2343	U
23	23	2345	G
23	23	2347	C
23	23	2350	C
23	23	2361	G
23	23	2383	G
23	23	2385	C
23	23	2402	U
23	23	2403	C
23	23	2406	A
23	23	2423	U
23	23	2425	A
23	23	2429	G
23	23	2430	A
23	23	2441	U
23	23	2448	A
23	23	2459	A
23	23	2470	G
23	23	2473	U
23	23	2476	A
23	23	2478	A
23	23	2484	G
23	23	2487	G
23	23	2491	U
23	23	2494	G
23	23	2498	OMC
23	23	2502	G
23	23	2504	PSU
23	23	2505	G
23	23	2518	A
23	23	2529	G
23	23	2535	G
23	23	2547	A
23	23	2552	OMU
23	23	2554	U
23	23	2566	A
23	23	2567	G
23	23	2569	G

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Mol	Chain	Res	Type
23	23	2573	C
23	23	2585	U
23	23	2586	U
23	23	2599	G
23	23	2602	A
23	23	2603	G
23	23	2606	C
23	23	2609	U
23	23	2613	U
23	23	2614	A
23	23	2615	U
23	23	2621	G
23	23	2623	G
23	23	2629	U
23	23	2646	C
23	23	2689	U
23	23	2690	U
23	23	2714	G
23	23	2716	C
23	23	2726	A
23	23	2732	G
23	23	2733	A
23	23	2744	G
23	23	2748	A
23	23	2758	A
23	23	2765	A
23	23	2778	A
23	23	2779	U
23	23	2793	C
23	23	2795	C
23	23	2797	U
23	23	2798	U
23	23	2800	A
23	23	2818	U
23	23	2820	A
23	23	2823	A
23	23	2833	U
23	23	2834	G
23	23	2835	A
23	23	2849	U
23	23	2873	A
23	23	2874	C

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Mol	Chain	Res	Type
23	23	2879	A
23	23	2880	C
23	23	2883	A
23	23	2884	U
23	23	2885	G
23	23	2886	A
23	23	2899	A
23	23	2903	U
24	5	13	G
24	5	24	G
24	5	35	C
24	5	36	C
24	5	41	G
24	5	42	C
24	5	44	G
24	5	57	A
24	5	58	A
24	5	59	A
24	5	66	A
24	5	67	G
24	5	88	C
24	5	89	U
24	5	90	C
24	5	91	C
24	5	99	A
24	5	108	A
24	5	109	A
60	Pt	7	U
60	Pt	13	C
60	Pt	15	G
60	Pt	16	H2U
60	Pt	17	H2U
60	Pt	19	G
60	Pt	20	H2U
60	Pt	21	A
60	Pt	22	G
60	Pt	46	G
60	Pt	48	C
60	Pt	52	G
60	Pt	56	C
60	Pt	76	A
61	Dt	8	4SU

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Mol	Chain	Res	Type
61	Dt	10	G
61	Dt	13	C
61	Dt	14	A
61	Dt	16	U
61	Dt	17	U
61	Dt	18	G
61	Dt	19	G
61	Dt	20	G
61	Dt	21	A
61	Dt	23	A
61	Dt	44	G
61	Dt	45	U
61	Dt	46	G7M
61	Dt	48	C
61	Dt	56	C
61	Dt	58	A
61	Dt	61	C
61	Dt	62	C
61	Dt	63	G
61	Dt	69	G
61	Dt	76	A

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	16	70	U
1	16	251	G
1	16	428	G
1	16	632	U
1	16	884	U
1	16	926	G
1	16	993	G
1	16	1124	G
1	16	1145	A
1	16	1157	A
1	16	1299	A
1	16	1331	G
1	16	1397	C
1	16	1452	C
23	23	12	U
23	23	177	G
23	23	784	G

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Mol	Chain	Res	Type
23	23	889	C
23	23	982	C
23	23	1176	U
23	23	1508	A
23	23	1730	C
23	23	2131	U
23	23	2158	A
23	23	2430	A
23	23	2778	A
24	5	66	A
24	5	108	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
60	H2U	Pt	16	60	18,21,22	1.03	2 (11%)	19,30,33	1.09	2 (10%)
23	PSU	23	2580	23	18,21,22	1.41	3 (16%)	21,30,33	2.08	4 (19%)
23	PSU	23	1917	23	18,21,22	6.15	12 (66%)	21,30,33	2.04	5 (23%)
61	PSU	Dt	39	61	18,21,22	1.37	2 (11%)	21,30,33	2.05	4 (19%)
23	OMG	23	2251	23,60	19,26,27	1.18	2 (10%)	21,38,41	0.83	1 (4%)
1	MA6	16	1519	1	19,26,27	1.14	2 (10%)	18,38,41	2.03	4 (22%)
23	5MU	23	1939	23	19,22,23	1.43	5 (26%)	27,32,35	2.35	6 (22%)
23	5MC	23	1962	23	19,22,23	1.54	3 (15%)	26,32,35	1.12	2 (7%)
23	2MG	23	1835	23	18,26,27	0.90	1 (5%)	16,38,41	1.32	3 (18%)
38	4D4	LP	81	38	9,11,12	2.19	2 (22%)	7,13,15	2.07	3 (42%)
23	PSU	23	2504	23	18,21,22	1.39	3 (16%)	21,30,33	2.09	3 (14%)
23	1MG	23	745	23	19,26,27	0.99	1 (5%)	18,39,42	1.57	3 (16%)
1	PSU	16	516	1	18,21,22	1.42	3 (16%)	21,30,33	2.09	4 (19%)
60	3AU	Pt	47	60	24,28,29	1.03	0	30,40,43	1.57	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	MIA	Dt	37	61	24,31,32	2.30	3 (12%)	22,44,47	2.78	7 (31%)
60	H2U	Pt	20	60	18,21,22	1.07	2 (11%)	19,30,33	1.33	4 (21%)
23	3TD	23	1915	23	19,22,23	1.38	2 (10%)	23,32,35	2.31	4 (17%)
61	4SU	Dt	8	61	18,21,22	1.96	4 (22%)	25,30,33	2.25	6 (24%)
1	G7M	16	527	1	20,26,27	2.60	4 (20%)	16,39,42	1.27	2 (12%)
60	U8U	Pt	34	22,60	20,24,25	1.50	3 (15%)	22,34,37	1.25	3 (13%)
60	5MU	Pt	54	60	19,22,23	1.39	6 (31%)	27,32,35	2.08	6 (22%)
23	6MZ	23	1618	23	17,25,26	0.93	1 (5%)	15,36,39	2.20	4 (26%)
23	2MG	23	2445	23	18,26,27	0.91	1 (5%)	16,38,41	1.27	2 (12%)
23	OMU	23	2552	23	19,22,23	1.24	3 (15%)	25,31,34	1.86	5 (20%)
1	2MG	16	1516	1	18,26,27	0.90	1 (5%)	16,38,41	1.36	3 (18%)
23	PSU	23	2604	23	18,21,22	1.50	4 (22%)	21,30,33	2.20	4 (19%)
60	H2U	Pt	17	60	18,21,22	0.97	2 (11%)	19,30,33	0.99	2 (10%)
1	2MG	16	966	1	18,26,27	1.01	1 (5%)	16,38,41	1.33	2 (12%)
23	6MZ	23	2030	23	17,25,26	0.88	1 (5%)	15,36,39	2.41	4 (26%)
23	G7M	23	2069	23	20,26,27	2.79	5 (25%)	16,39,42	2.11	4 (25%)
1	4OC	16	1402	1	20,23,24	0.76	0	25,32,35	0.94	1 (4%)
23	5MU	23	747	23	19,22,23	1.40	5 (26%)	27,32,35	2.12	6 (22%)
23	PSU	23	955	23	18,21,22	1.40	3 (16%)	21,30,33	2.12	4 (19%)
23	H2U	23	2449	23	18,21,22	1.09	3 (16%)	19,30,33	1.02	1 (5%)
1	5MC	16	967	1	19,22,23	1.58	3 (15%)	26,32,35	1.21	3 (11%)
23	PSU	23	2457	23	18,21,22	1.41	2 (11%)	21,30,33	2.12	5 (23%)
60	PSU	Pt	39	60	18,21,22	1.40	2 (11%)	21,30,33	2.01	4 (19%)
12	D2T	SL	89	12	8,9,10	2.44	1 (12%)	6,11,13	2.91	4 (66%)
23	2MA	23	2503	23,63	17,25,26	1.03	0	16,37,40	1.29	3 (18%)
60	T6A	Pt	37	60	26,34,35	0.97	1 (3%)	28,49,52	1.71	5 (17%)
60	PSU	Pt	55	60	18,21,22	1.36	2 (11%)	21,30,33	2.08	4 (19%)
61	PSU	Dt	32	61	18,21,22	1.37	2 (11%)	21,30,33	2.02	3 (14%)
61	G7M	Dt	46	61	20,26,27	2.60	4 (20%)	16,39,42	1.27	2 (12%)
23	OMC	23	2498	23,63	19,22,23	0.81	0	25,31,34	0.91	1 (4%)
1	MA6	16	1518	1	19,26,27	1.30	3 (15%)	18,38,41	2.25	6 (33%)
23	PSU	23	2605	23	18,21,22	1.40	4 (22%)	21,30,33	2.02	4 (19%)
1	UR3	16	1498	1	19,22,23	0.96	0	26,32,35	1.72	2 (7%)
61	3AU	Dt	47	61	24,28,29	1.02	0	30,40,43	1.60	4 (13%)
23	PSU	23	746	23,63	18,21,22	1.40	3 (16%)	21,30,33	1.99	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	16	1407	1	19,22,23	1.59	3 (15%)	26,32,35	1.12	3 (11%)
23	PSU	23	1911	23	18,21,22	6.15	13 (72%)	21,30,33	1.98	5 (23%)
61	PSU	Dt	55	61	18,21,22	1.43	2 (11%)	21,30,33	2.20	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	H2U	Pt	16	60	-	3/7/38/39	0/2/2/2
23	PSU	23	2580	23	-	0/7/25/26	0/2/2/2
23	PSU	23	1917	23	-	0/7/25/26	0/2/2/2
61	PSU	Dt	39	61	-	2/7/25/26	0/2/2/2
23	OMG	23	2251	23,60	-	1/5/27/28	0/3/3/3
1	MA6	16	1519	1	-	4/7/29/30	0/3/3/3
23	5MU	23	1939	23	-	2/7/25/26	0/2/2/2
23	5MC	23	1962	23	-	4/7/25/26	0/2/2/2
23	2MG	23	1835	23	-	0/5/27/28	0/3/3/3
38	4D4	LP	81	38	-	4/11/12/14	-
23	PSU	23	2504	23	-	2/7/25/26	0/2/2/2
23	1MG	23	745	23	-	0/3/25/26	0/3/3/3
1	PSU	16	516	1	-	0/7/25/26	0/2/2/2
60	3AU	Pt	47	60	-	2/16/34/35	0/2/2/2
61	MIA	Dt	37	61	-	5/11/33/34	0/3/3/3
60	H2U	Pt	20	60	-	5/7/38/39	0/2/2/2
23	3TD	23	1915	23	-	0/7/25/26	0/2/2/2
61	4SU	Dt	8	61	-	3/7/25/26	0/2/2/2
1	G7M	16	527	1	-	2/3/25/26	0/3/3/3
60	U8U	Pt	34	22,60	-	4/10/28/29	0/2/2/2
60	5MU	Pt	54	60	-	0/7/25/26	0/2/2/2
23	6MZ	23	1618	23	-	0/5/27/28	0/3/3/3
23	2MG	23	2445	23	-	1/5/27/28	0/3/3/3
23	OMU	23	2552	23	-	2/9/27/28	0/2/2/2
1	2MG	16	1516	1	-	0/5/27/28	0/3/3/3
23	PSU	23	2604	23	-	0/7/25/26	0/2/2/2
60	H2U	Pt	17	60	-	3/7/38/39	0/2/2/2
1	2MG	16	966	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	6MZ	23	2030	23	-	2/5/27/28	0/3/3/3
23	G7M	23	2069	23	-	0/3/25/26	0/3/3/3
1	4OC	16	1402	1	-	0/9/29/30	0/2/2/2
23	5MU	23	747	23	-	0/7/25/26	0/2/2/2
23	PSU	23	955	23	-	0/7/25/26	0/2/2/2
23	H2U	23	2449	23	-	0/7/38/39	0/2/2/2
1	5MC	16	967	1	-	0/7/25/26	0/2/2/2
23	PSU	23	2457	23	-	0/7/25/26	0/2/2/2
60	PSU	Pt	39	60	-	0/7/25/26	0/2/2/2
12	D2T	SL	89	12	-	3/7/12/14	-
23	2MA	23	2503	23,63	-	0/3/25/26	0/3/3/3
60	T6A	Pt	37	60	-	10/19/41/42	0/3/3/3
60	PSU	Pt	55	60	-	0/7/25/26	0/2/2/2
61	PSU	Dt	32	61	-	0/7/25/26	0/2/2/2
61	G7M	Dt	46	61	-	1/3/25/26	0/3/3/3
23	OMC	23	2498	23,63	-	2/9/27/28	0/2/2/2
1	MA6	16	1518	1	-	1/7/29/30	0/3/3/3
23	PSU	23	2605	23	-	2/7/25/26	0/2/2/2
1	UR3	16	1498	1	-	0/7/25/26	0/2/2/2
61	3AU	Dt	47	61	-	9/16/34/35	0/2/2/2
23	PSU	23	746	23,63	-	4/7/25/26	0/2/2/2
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2
23	PSU	23	1911	23	-	0/7/25/26	0/2/2/2
61	PSU	Dt	55	61	-	0/7/25/26	0/2/2/2

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	1911	PSU	C6-C5	12.36	1.49	1.35
23	23	1917	PSU	C6-C5	12.25	1.48	1.35
23	23	1911	PSU	C2-N1	12.18	1.52	1.36
23	23	1917	PSU	C2-N1	12.18	1.52	1.36
23	23	1917	PSU	O4'-C1'	10.45	1.58	1.43
23	23	1911	PSU	O4'-C1'	10.36	1.58	1.43
23	23	1917	PSU	C2-N3	8.61	1.51	1.37
23	23	1911	PSU	C2-N3	8.56	1.51	1.37
23	23	2069	G7M	C8-N9	7.83	1.47	1.33
61	Dt	37	MIA	C2-S10	-7.68	1.69	1.75
1	16	527	G7M	C8-N9	7.49	1.46	1.33
23	23	1911	PSU	C3'-C2'	-7.18	1.33	1.53
61	Dt	46	G7M	C8-N9	7.17	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	1917	PSU	C3'-C2'	-7.15	1.34	1.53
61	Dt	46	G7M	C8-N7	7.13	1.46	1.33
23	23	2069	G7M	C8-N7	6.95	1.45	1.33
1	16	527	G7M	C8-N7	6.88	1.45	1.33
61	Dt	37	MIA	C13-C14	6.72	1.52	1.32
23	23	1911	PSU	C6-N1	6.52	1.47	1.36
23	23	1917	PSU	C6-N1	6.38	1.46	1.36
12	SL	89	D2T	CB-CA	-6.34	1.52	1.54
23	23	1917	PSU	O4'-C4'	-6.19	1.31	1.45
23	23	1911	PSU	O4'-C4'	-6.12	1.31	1.45
1	16	1407	5MC	C5-C4	5.78	1.48	1.44
1	16	967	5MC	C5-C4	5.51	1.48	1.44
23	23	1962	5MC	C5-C4	5.47	1.48	1.44
61	Dt	8	4SU	C4-S4	-5.16	1.59	1.68
38	LP	81	4D4	CZ-NE	5.11	1.43	1.33
60	Pt	34	U8U	C2-S2	-4.99	1.59	1.67
23	23	2069	G7M	C5-C4	4.49	1.48	1.39
23	23	1917	PSU	C4-N3	4.37	1.47	1.38
23	23	1911	PSU	C4-N3	4.34	1.47	1.38
23	23	1917	PSU	C1'-C5	-4.14	1.40	1.50
1	16	527	G7M	C5-C4	4.07	1.47	1.39
23	23	1911	PSU	C1'-C5	-4.06	1.41	1.50
23	23	1915	3TD	C6-C5	4.06	1.39	1.35
61	Dt	46	G7M	C5-C4	3.98	1.47	1.39
61	Dt	8	4SU	C4-N3	-3.88	1.33	1.37
23	23	1917	PSU	C3'-C4'	3.68	1.62	1.53
23	23	1911	PSU	C3'-C4'	3.65	1.62	1.53
61	Dt	55	PSU	C6-C5	3.48	1.39	1.35
38	LP	81	4D4	CZ-NH2	3.44	1.44	1.32
23	23	2069	G7M	O4'-C1'	3.38	1.45	1.40
23	23	2604	PSU	C6-C5	3.21	1.38	1.35
60	Pt	55	PSU	C6-C5	3.19	1.38	1.35
61	Dt	39	PSU	C6-C5	3.17	1.38	1.35
60	Pt	39	PSU	C6-C5	3.12	1.38	1.35
1	16	516	PSU	C6-C5	3.10	1.38	1.35
61	Dt	32	PSU	C6-C5	3.07	1.38	1.35
23	23	2504	PSU	C6-C5	3.06	1.38	1.35
61	Dt	8	4SU	C5-C4	-3.05	1.38	1.42
23	23	746	PSU	C6-C5	3.03	1.38	1.35
23	23	2251	OMG	C8-N7	-3.02	1.30	1.34
23	23	2580	PSU	C6-C5	2.99	1.38	1.35
23	23	955	PSU	C6-C5	2.98	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16	1518	MA6	C6-C5	2.97	1.49	1.44
23	23	2604	PSU	C4-N3	-2.95	1.33	1.38
23	23	2457	PSU	C6-C5	2.94	1.38	1.35
23	23	1917	PSU	C4-C5	2.88	1.52	1.44
60	Pt	20	H2U	C2-N3	-2.87	1.33	1.38
23	23	955	PSU	C4-N3	-2.86	1.33	1.38
23	23	2457	PSU	C4-N3	-2.86	1.33	1.38
23	23	1939	5MU	C4-N3	-2.84	1.33	1.38
23	23	2504	PSU	C4-N3	-2.82	1.33	1.38
23	23	1911	PSU	C4-C5	2.82	1.52	1.44
23	23	747	5MU	C4-N3	-2.82	1.33	1.38
61	Dt	55	PSU	C4-N3	-2.81	1.33	1.38
60	Pt	39	PSU	C4-N3	-2.81	1.33	1.38
23	23	2580	PSU	C4-N3	-2.81	1.33	1.38
23	23	2552	OMU	C4-N3	-2.80	1.33	1.38
23	23	746	PSU	C4-N3	-2.79	1.33	1.38
23	23	2605	PSU	C6-C5	2.78	1.38	1.35
23	23	2449	H2U	C2-N3	-2.78	1.33	1.38
61	Dt	46	G7M	C6-N1	-2.76	1.33	1.37
23	23	1915	3TD	C2-N1	-2.76	1.33	1.37
23	23	2605	PSU	C4-N3	-2.75	1.33	1.38
60	Pt	55	PSU	C4-N3	-2.73	1.33	1.38
1	16	967	5MC	C6-C5	2.72	1.39	1.34
61	Dt	32	PSU	C4-N3	-2.67	1.33	1.38
61	Dt	39	PSU	C4-N3	-2.67	1.33	1.38
60	Pt	54	5MU	C4-N3	-2.65	1.33	1.38
23	23	2445	2MG	C6-N1	-2.63	1.33	1.37
60	Pt	16	H2U	C2-N3	-2.62	1.33	1.38
60	Pt	54	5MU	C6-C5	2.61	1.38	1.34
60	Pt	34	U8U	C4-N3	-2.60	1.34	1.38
1	16	516	PSU	C4-N3	-2.60	1.34	1.38
1	16	1407	5MC	C6-C5	2.60	1.38	1.34
23	23	1911	PSU	O2'-C2'	2.59	1.49	1.43
1	16	1519	MA6	C6-C5	2.58	1.48	1.44
60	Pt	20	H2U	C4-N3	-2.57	1.33	1.37
23	23	1917	PSU	O2'-C2'	2.57	1.49	1.43
60	Pt	17	H2U	C2-N3	-2.56	1.33	1.38
23	23	1939	5MU	C6-N1	-2.56	1.33	1.38
60	Pt	34	U8U	C6-N1	-2.55	1.33	1.38
23	23	2251	OMG	C5-C6	-2.55	1.42	1.47
23	23	747	5MU	C6-C5	2.54	1.38	1.34
23	23	2449	H2U	C4-N3	-2.54	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	1962	5MC	C6-C5	2.53	1.38	1.34
23	23	747	5MU	C6-N1	-2.51	1.33	1.38
23	23	1835	2MG	C6-N1	-2.51	1.34	1.37
23	23	1939	5MU	C2-N3	-2.50	1.33	1.38
23	23	1962	5MC	C6-N1	-2.47	1.33	1.38
61	Dt	37	MIA	C6-C5	2.44	1.48	1.44
1	16	1516	2MG	C6-N1	-2.43	1.34	1.37
61	Dt	8	4SU	C2-N3	-2.43	1.33	1.38
1	16	527	G7M	C6-N1	-2.41	1.34	1.37
23	23	1939	5MU	C6-C5	2.39	1.38	1.34
1	16	966	2MG	C6-N1	-2.39	1.34	1.37
23	23	2552	OMU	C2-N3	-2.35	1.33	1.38
1	16	1518	MA6	C6-N6	2.34	1.42	1.37
23	23	2069	G7M	C6-N1	-2.34	1.34	1.37
1	16	1519	MA6	O4'-C1'	2.33	1.44	1.40
23	23	747	5MU	C2-N3	-2.33	1.33	1.38
1	16	967	5MC	C6-N1	-2.32	1.34	1.38
60	Pt	54	5MU	C6-N1	-2.28	1.34	1.38
1	16	516	PSU	O4'-C1'	-2.26	1.40	1.43
1	16	1407	5MC	C6-N1	-2.26	1.34	1.38
60	Pt	54	5MU	C4-C5	2.20	1.48	1.44
23	23	1939	5MU	C4-C5	2.16	1.48	1.44
23	23	2552	OMU	C5-C4	-2.16	1.39	1.43
23	23	1618	6MZ	C6-C5	2.15	1.48	1.44
60	Pt	54	5MU	C2-N1	2.15	1.41	1.38
23	23	745	1MG	C2-N1	2.14	1.41	1.37
60	Pt	54	5MU	C2-N3	-2.14	1.34	1.38
60	Pt	37	T6A	C6-C5	2.14	1.48	1.44
1	16	1518	MA6	O4'-C1'	2.13	1.43	1.40
23	23	955	PSU	C2-N3	-2.13	1.34	1.37
23	23	2604	PSU	C2-N1	-2.12	1.33	1.36
60	Pt	17	H2U	C4-N3	-2.12	1.34	1.37
23	23	747	5MU	C4-C5	2.11	1.48	1.44
23	23	2605	PSU	C2-N3	-2.09	1.34	1.37
23	23	2504	PSU	C2-N3	-2.08	1.34	1.37
23	23	746	PSU	C2-N3	-2.07	1.34	1.37
23	23	2030	6MZ	C6-C5	2.07	1.48	1.44
60	Pt	16	H2U	C4-N3	-2.07	1.34	1.37
23	23	2604	PSU	C2-N3	-2.06	1.34	1.37
23	23	1911	PSU	O4-C4	-2.05	1.19	1.23
23	23	2580	PSU	C2-N3	-2.04	1.34	1.37
23	23	2449	H2U	C2-N1	-2.04	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	2605	PSU	C2-N1	-2.01	1.34	1.36

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	Dt	37	MIA	C12-C13-C14	-9.04	110.78	127.01
23	23	1915	3TD	N1-C2-N3	8.10	122.02	116.13
1	16	1498	UR3	C4-N3-C2	-6.80	119.11	124.58
23	23	2604	PSU	N1-C2-N3	6.73	122.27	115.17
61	Dt	55	PSU	N1-C2-N3	6.71	122.25	115.17
23	23	955	PSU	N1-C2-N3	6.63	122.16	115.17
23	23	2580	PSU	N1-C2-N3	6.59	122.12	115.17
23	23	2457	PSU	N1-C2-N3	6.58	122.11	115.17
23	23	2504	PSU	N1-C2-N3	6.54	122.07	115.17
1	16	516	PSU	N1-C2-N3	6.50	122.02	115.17
60	Pt	55	PSU	N1-C2-N3	6.47	122.00	115.17
61	Dt	39	PSU	N1-C2-N3	6.44	121.96	115.17
23	23	2030	6MZ	C2-N1-C6	6.44	121.60	116.60
60	Pt	37	T6A	C2-N1-C6	6.40	121.57	116.60
61	Dt	32	PSU	N1-C2-N3	6.35	121.87	115.17
23	23	746	PSU	N1-C2-N3	6.28	121.79	115.17
60	Pt	39	PSU	N1-C2-N3	6.26	121.77	115.17
23	23	1618	6MZ	C2-N1-C6	6.24	121.45	116.60
23	23	2605	PSU	N1-C2-N3	6.23	121.74	115.17
1	16	1518	MA6	C2-N1-C6	6.21	122.93	116.84
61	Dt	8	4SU	C4-N3-C2	-5.94	121.62	127.31
23	23	1939	5MU	C4-N3-C2	-5.79	119.75	127.34
60	Pt	47	3AU	C4-N3-C2	-5.44	118.27	124.66
61	Dt	8	4SU	C5-C4-N3	5.43	119.80	114.75
23	23	1939	5MU	N3-C2-N1	5.22	121.69	114.89
23	23	747	5MU	C4-N3-C2	-5.15	120.58	127.34
61	Dt	47	3AU	C4-N3-C2	-5.15	118.61	124.66
1	16	1519	MA6	C2-N1-C6	5.11	121.85	116.84
60	Pt	54	5MU	C4-N3-C2	-5.06	120.70	127.34
23	23	1915	3TD	C4-N3-C2	-5.03	119.29	124.61
23	23	1939	5MU	C5-C4-N3	4.99	119.66	115.32
23	23	747	5MU	N3-C2-N1	4.97	121.36	114.89
23	23	2552	OMU	C4-N3-C2	-4.92	120.51	126.61
60	Pt	54	5MU	N3-C2-N1	4.88	121.25	114.89
23	23	1917	PSU	C4-N3-C2	-4.88	119.64	126.37
61	Dt	37	MIA	C11-S10-C2	-4.87	98.60	102.25
23	23	1911	PSU	C4-N3-C2	-4.75	119.83	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	1917	PSU	N1-C2-N3	4.55	119.96	115.17
23	23	1939	5MU	C5-C6-N1	-4.51	118.41	123.31
23	23	1911	PSU	N1-C2-N3	4.47	119.89	115.17
23	23	2069	G7M	O4'-C1'-N9	4.44	114.64	108.75
23	23	747	5MU	C5-C4-N3	4.44	119.18	115.32
60	Pt	54	5MU	C5-C4-N3	4.43	119.17	115.32
23	23	2030	6MZ	C9-N6-C6	-4.39	118.78	122.85
12	SL	89	D2T	CB-CA-N	4.37	117.95	109.10
23	23	2552	OMU	N3-C2-N1	4.33	120.53	114.89
23	23	955	PSU	C4-N3-C2	-4.29	120.46	126.37
23	23	2457	PSU	C4-N3-C2	-4.27	120.49	126.37
23	23	2069	G7M	O4'-C4'-C3'	-4.24	96.75	105.15
23	23	2504	PSU	C4-N3-C2	-4.22	120.56	126.37
23	23	746	PSU	C4-N3-C2	-4.20	120.58	126.37
23	23	1939	5MU	O4-C4-C5	-4.19	120.12	124.92
60	Pt	55	PSU	C4-N3-C2	-4.19	120.60	126.37
61	Dt	55	PSU	C4-N3-C2	-4.18	120.61	126.37
61	Dt	37	MIA	C16-C14-C13	-4.17	110.13	122.66
60	Pt	39	PSU	C4-N3-C2	-4.15	120.65	126.37
61	Dt	39	PSU	C4-N3-C2	-4.15	120.66	126.37
23	23	2069	G7M	O3'-C3'-C4'	4.10	122.86	111.08
23	23	2604	PSU	C4-N3-C2	-4.09	120.74	126.37
23	23	2580	PSU	C4-N3-C2	-4.07	120.76	126.37
23	23	747	5MU	O4-C4-C5	-4.03	120.31	124.92
61	Dt	8	4SU	N3-C2-N1	4.02	120.12	114.89
1	16	516	PSU	O2-C2-N1	-4.01	118.66	122.79
1	16	516	PSU	C4-N3-C2	-4.01	120.85	126.37
60	Pt	54	5MU	O4-C4-C5	-4.01	120.33	124.92
61	Dt	32	PSU	C4-N3-C2	-3.99	120.88	126.37
23	23	2605	PSU	C4-N3-C2	-3.94	120.95	126.37
23	23	2552	OMU	C5-C4-N3	3.91	120.27	114.80
61	Dt	37	MIA	C15-C14-C13	-3.89	110.99	122.66
23	23	2457	PSU	O2-C2-N1	-3.84	118.83	122.79
23	23	2580	PSU	O2-C2-N1	-3.79	118.88	122.79
61	Dt	55	PSU	O2-C2-N1	-3.78	118.89	122.79
61	Dt	8	4SU	C5-C4-S4	-3.75	120.02	124.31
23	23	955	PSU	O2-C2-N1	-3.74	118.94	122.79
23	23	747	5MU	C5-C6-N1	-3.73	119.26	123.31
23	23	745	1MG	O4'-C1'-N9	3.73	113.69	108.75
23	23	2605	PSU	O2-C2-N1	-3.71	118.96	122.79
23	23	2504	PSU	O2-C2-N1	-3.68	118.99	122.79
23	23	2030	6MZ	N3-C2-N1	-3.67	123.69	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	Pt	55	PSU	O2-C2-N1	-3.66	119.01	122.79
60	Pt	37	T6A	N3-C2-N1	-3.65	123.71	128.67
61	Dt	39	PSU	O2-C2-N1	-3.65	119.02	122.79
61	Dt	32	PSU	O2-C2-N1	-3.65	119.03	122.79
38	LP	81	4D4	NE-CZ-NH2	-3.61	114.48	120.67
23	23	1917	PSU	C6-C5-C4	3.60	120.60	118.17
23	23	1618	6MZ	N3-C2-N1	-3.59	123.80	128.67
1	16	1519	MA6	N3-C2-N1	-3.58	123.81	128.67
1	16	1518	MA6	C4-C5-N7	-3.58	105.56	109.34
23	23	746	PSU	O2-C2-N1	-3.56	119.11	122.79
23	23	2604	PSU	O2-C2-N1	-3.53	119.15	122.79
60	Pt	54	5MU	C5-C6-N1	-3.53	119.48	123.31
23	23	1618	6MZ	C9-N6-C6	-3.49	119.61	122.85
23	23	1911	PSU	C6-N1-C2	-3.49	119.45	122.69
12	SL	89	D2T	CB1-SB-CB	3.48	108.63	102.36
23	23	1962	5MC	C5-C6-N1	-3.47	119.55	123.31
1	16	1518	MA6	N3-C2-N1	-3.46	123.98	128.67
60	Pt	39	PSU	O2-C2-N1	-3.28	119.41	122.79
38	LP	81	4D4	NH1-CZ-NE	3.27	126.70	119.27
1	16	1498	UR3	C5-C4-N3	3.24	119.31	115.04
23	23	1939	5MU	O2-C2-N1	-3.23	118.59	122.80
23	23	1917	PSU	C6-N1-C2	-3.22	119.70	122.69
60	Pt	47	3AU	C5-C4-N3	3.19	120.05	115.64
1	16	967	5MC	C5-C6-N1	-3.17	119.87	123.31
1	16	527	G7M	O4'-C1'-N9	3.17	112.94	108.75
1	16	1407	5MC	C5-C6-N1	-3.16	119.89	123.31
61	Dt	47	3AU	C5-C4-N3	3.13	119.97	115.64
1	16	1519	MA6	C4-C5-N7	-3.13	106.03	109.34
23	23	2552	OMU	O4-C4-C5	-3.10	119.81	125.16
12	SL	89	D2T	OD2-CG-CB	3.10	119.84	113.15
23	23	1911	PSU	C6-C5-C4	3.04	120.23	118.17
60	Pt	34	U8U	O4-C4-C5	-2.99	119.69	124.71
23	23	2503	2MA	C8-N7-C5	2.98	107.62	102.55
23	23	2604	PSU	C3'-C2'-C1'	2.98	105.20	101.69
23	23	2069	G7M	CN7-N7-C8	-2.92	111.36	125.43
61	Dt	46	G7M	O4'-C1'-N9	2.91	112.61	108.75
23	23	2030	6MZ	C4-C5-N7	-2.89	106.29	109.34
23	23	2445	2MG	C8-N7-C5	2.88	107.45	102.55
1	16	966	2MG	C8-N7-C5	2.87	107.44	102.55
60	Pt	16	H2U	C5-C6-N1	-2.87	102.84	111.52
1	16	527	G7M	CN7-N7-C8	-2.87	111.63	125.43
60	Pt	47	3AU	C10-N3-C2	2.86	121.86	117.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	1835	2MG	C8-N7-C5	2.84	107.39	102.55
1	16	1516	2MG	C8-N7-C5	2.84	107.39	102.55
61	Dt	47	3AU	C10-N3-C2	2.83	121.81	117.64
60	Pt	17	H2U	C5-C6-N1	-2.83	102.97	111.52
61	Dt	37	MIA	C4-C5-N7	-2.83	106.35	109.34
1	16	1519	MA6	C4'-O4'-C1'	2.80	112.49	109.92
1	16	1518	MA6	C10-N6-C6	-2.80	111.69	119.40
61	Dt	46	G7M	CN7-N7-C8	-2.79	111.99	125.43
23	23	2503	2MA	C4-N3-C2	-2.79	121.16	123.30
23	23	745	1MG	C8-N7-C5	2.78	107.29	102.55
60	Pt	16	H2U	C5-C4-N3	2.76	119.62	116.69
1	16	967	5MC	C5-C4-N3	-2.75	118.94	121.75
61	Dt	47	3AU	C3'-C2'-C1'	2.73	106.63	101.46
61	Dt	8	4SU	C3'-C2'-C1'	2.73	106.63	101.46
60	Pt	20	H2U	O4'-C1'-N1	2.68	112.95	109.30
1	16	1407	5MC	C5-C4-N3	-2.66	119.03	121.75
23	23	1962	5MC	C5-C4-N3	-2.66	119.03	121.75
61	Dt	37	MIA	C2-N1-C6	2.63	122.10	117.42
60	Pt	37	T6A	N6-C10-N11	2.60	117.35	113.77
23	23	745	1MG	C5-C6-N1	2.56	117.66	113.96
60	Pt	37	T6A	N6-C6-N1	2.53	121.56	118.71
23	23	2449	H2U	C5-C6-N1	-2.52	103.90	111.52
23	23	2552	OMU	O2-C2-N1	-2.51	119.53	122.80
23	23	1917	PSU	O2-C2-N1	-2.47	120.24	122.79
23	23	2251	OMG	O6-C6-C5	2.46	129.20	124.32
23	23	1618	6MZ	C4-C5-N7	-2.45	106.75	109.34
60	Pt	47	3AU	C3'-C2'-C1'	2.42	106.04	101.46
12	SL	89	D2T	O-C-CA	-2.41	118.57	124.77
1	16	1518	MA6	C4'-O4'-C1'	2.40	112.12	109.92
23	23	747	5MU	O2-C2-N1	-2.34	119.75	122.80
61	Dt	55	PSU	C3'-C2'-C1'	2.34	104.44	101.69
60	Pt	20	H2U	C3'-C2'-C1'	2.28	105.77	101.46
23	23	1915	3TD	C1'-C5-C4	2.27	121.06	117.61
23	23	2498	OMC	O2-C2-N3	-2.27	118.75	122.33
60	Pt	20	H2U	C5-C6-N1	-2.27	104.64	111.52
38	LP	81	4D4	O-C-CA	-2.27	118.94	124.77
23	23	1915	3TD	C4'-O4'-C1'	2.26	114.11	108.44
23	23	2503	2MA	C5-C6-N1	2.24	118.30	114.12
60	Pt	37	T6A	C4-C5-N7	-2.23	106.98	109.34
60	Pt	34	U8U	C5-C4-N3	2.23	118.60	115.21
60	Pt	39	PSU	C5-C6-N1	-2.22	119.06	122.14
60	Pt	54	5MU	O2-C2-N1	-2.22	119.91	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	Dt	37	MIA	N3-C2-N1	-2.21	122.98	127.03
1	16	1516	2MG	N1-C2-N2	2.21	118.82	116.56
23	23	1911	PSU	O2-C2-N1	-2.21	120.51	122.79
1	16	1402	4OC	C6-C5-C4	2.21	119.66	117.00
23	23	2457	PSU	C5-C6-N1	-2.20	119.09	122.14
60	Pt	34	U8U	C1'-N1-C6	-2.19	117.55	121.15
1	16	516	PSU	O4'-C1'-C2'	2.18	108.16	105.15
1	16	1518	MA6	O4'-C1'-N9	2.17	111.62	108.75
23	23	955	PSU	C5-C6-N1	-2.16	119.14	122.14
1	16	1407	5MC	O2-C2-N3	-2.14	118.96	122.33
23	23	2445	2MG	C5-C6-N1	2.13	118.14	114.07
23	23	1835	2MG	C5-C6-N1	2.12	118.11	114.07
60	Pt	17	H2U	C5-C4-N3	2.12	118.94	116.69
1	16	966	2MG	C5-C6-N1	2.12	118.11	114.07
60	Pt	55	PSU	C5-C6-N1	-2.10	119.23	122.14
23	23	746	PSU	C5-C6-N1	-2.09	119.23	122.14
61	Dt	39	PSU	C5-C6-N1	-2.09	119.24	122.14
1	16	1516	2MG	C5-C6-N1	2.09	118.05	114.07
23	23	2580	PSU	O4'-C1'-C2'	2.08	108.03	105.15
1	16	967	5MC	O2-C2-N3	-2.07	119.07	122.33
23	23	2457	PSU	O4'-C1'-C2'	2.06	108.01	105.15
23	23	2605	PSU	O4'-C1'-C2'	2.05	107.99	105.15
23	23	1835	2MG	CM2-N2-C2	-2.03	119.28	123.65
60	Pt	47	3AU	O2-C2-N1	-2.03	118.25	122.78
61	Dt	8	4SU	C6-N1-C2	-2.03	118.53	121.00
60	Pt	20	H2U	O4-C4-N3	2.01	123.40	120.30

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16	1519	MA6	O4'-C4'-C5'-O5'
12	SL	89	D2T	CG-CB-SB-CB1
23	23	746	PSU	C2'-C1'-C5-C4
23	23	746	PSU	C2'-C1'-C5-C6
23	23	2251	OMG	C1'-C2'-O2'-CM2
23	23	2605	PSU	C2'-C1'-C5-C4
38	LP	81	4D4	CA-CB-CG-CD
60	Pt	16	H2U	O4'-C1'-N1-C2
60	Pt	16	H2U	O4'-C1'-N1-C6
60	Pt	17	H2U	C4'-C5'-O5'-P
60	Pt	17	H2U	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
60	Pt	20	H2U	O4'-C4'-C5'-O5'
60	Pt	20	H2U	O4'-C1'-N1-C6
60	Pt	34	U8U	N-C-C5-C4
60	Pt	37	T6A	O10-C10-N6-C6
60	Pt	37	T6A	N11-C10-N6-C6
60	Pt	37	T6A	N11-C12-C14-O14
60	Pt	37	T6A	N11-C12-C14-C15
60	Pt	37	T6A	C13-C12-C14-O14
60	Pt	37	T6A	C13-C12-C14-C15
60	Pt	47	3AU	O4'-C4'-C5'-O5'
61	Dt	37	MIA	N6-C12-C13-C14
61	Dt	37	MIA	C12-C13-C14-C15
61	Dt	47	3AU	C2'-C1'-N1-C2
61	Dt	47	3AU	C2'-C1'-N1-C6
61	Dt	47	3AU	C10-C11-C12-C13
61	Dt	47	3AU	C10-C11-C12-N40
61	Dt	47	3AU	O4'-C4'-C5'-O5'
1	16	527	G7M	O4'-C4'-C5'-O5'
1	16	527	G7M	C3'-C4'-C5'-O5'
1	16	1519	MA6	C3'-C4'-C5'-O5'
23	23	2552	OMU	C3'-C4'-C5'-O5'
23	23	2552	OMU	O4'-C4'-C5'-O5'
60	Pt	20	H2U	C3'-C4'-C5'-O5'
60	Pt	47	3AU	C3'-C4'-C5'-O5'
61	Dt	8	4SU	O4'-C4'-C5'-O5'
61	Dt	37	MIA	N3-C2-S10-C11
23	23	1939	5MU	O4'-C4'-C5'-O5'
23	23	2030	6MZ	O4'-C4'-C5'-O5'
23	23	2498	OMC	C3'-C4'-C5'-O5'
23	23	2498	OMC	O4'-C4'-C5'-O5'
23	23	2504	PSU	O4'-C4'-C5'-O5'
61	Dt	8	4SU	C3'-C4'-C5'-O5'
61	Dt	39	PSU	C3'-C4'-C5'-O5'
61	Dt	39	PSU	O4'-C4'-C5'-O5'
61	Dt	47	3AU	C3'-C4'-C5'-O5'
60	Pt	20	H2U	O4'-C1'-N1-C2
23	23	2030	6MZ	C3'-C4'-C5'-O5'
38	LP	81	4D4	OB-CB-CG-CD
60	Pt	37	T6A	C3'-C4'-C5'-O5'
61	Dt	37	MIA	N1-C2-S10-C11
1	16	1519	MA6	N1-C6-N6-C10
60	Pt	37	T6A	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
60	Pt	34	U8U	C3'-C4'-C5'-O5'
60	Pt	34	U8U	O4'-C4'-C5'-O5'
23	23	1962	5MC	C2'-C1'-N1-C6
23	23	2445	2MG	C3'-C4'-C5'-O5'
60	Pt	17	H2U	O4'-C1'-N1-C2
61	Dt	47	3AU	N3-C10-C11-C12
12	SL	89	D2T	SB-CB-CG-OD1
60	Pt	20	H2U	C4'-C5'-O5'-P
23	23	1939	5MU	C3'-C4'-C5'-O5'
23	23	2605	PSU	C3'-C4'-C5'-O5'
23	23	746	PSU	O4'-C1'-C5-C4
23	23	1962	5MC	O4'-C1'-N1-C6
61	Dt	47	3AU	O4'-C1'-N1-C6
1	16	1518	MA6	N1-C6-N6-C10
38	LP	81	4D4	CG-CD-NE-CZ
23	23	2504	PSU	C3'-C4'-C5'-O5'
61	Dt	37	MIA	C12-C13-C14-C16
61	Dt	46	G7M	C4'-C5'-O5'-P
60	Pt	37	T6A	N11-C12-C13-ODA
60	Pt	37	T6A	N11-C12-C13-ODB
1	16	1519	MA6	C4'-C5'-O5'-P
61	Dt	47	3AU	O4'-C1'-N1-C2
12	SL	89	D2T	SB-CB-CG-OD2
23	23	746	PSU	O4'-C1'-C5-C6
60	Pt	34	U8U	N-C-C5-C6
23	23	1962	5MC	O4'-C1'-N1-C2
61	Dt	8	4SU	C4'-C5'-O5'-P
38	LP	81	4D4	O-C-CA-CB
60	Pt	16	H2U	C2'-C1'-N1-C6
23	23	1962	5MC	C2'-C1'-N1-C2

There are no ring outliers.

13 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	23	2251	OMG	1	0
1	16	1519	MA6	1	0
23	23	1915	3TD	1	0
23	23	2552	OMU	1	0
1	16	1516	2MG	1	0
1	16	966	2MG	1	0
23	23	2030	6MZ	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	16	1402	4OC	1	0
1	16	967	5MC	2	0
12	SL	89	D2T	4	0
23	23	2503	2MA	1	0
1	16	1518	MA6	1	0
23	23	1911	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 228 ligands modelled in this entry, 200 are monoatomic - leaving 28 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	$\# Z > 2$
62	PUT	23	3009	-	5,5,5	0.09	0	4,4,4	0.13	0
62	PUT	23	3003	-	5,5,5	0.15	0	4,4,4	0.22	0
62	PUT	23	3016	-	5,5,5	0.09	0	4,4,4	0.13	0
62	PUT	23	3013	-	5,5,5	0.10	0	4,4,4	0.13	0
65	ATP	23	3001	-	28,33,33	0.64	0	34,52,52	0.58	1 (2%)
62	PUT	16	1602	-	5,5,5	0.15	0	4,4,4	0.22	0
62	PUT	23	3010	-	5,5,5	0.10	0	4,4,4	0.13	0
62	PUT	LC	301	-	5,5,5	0.10	0	4,4,4	0.13	0
62	PUT	23	3015	-	5,5,5	0.14	0	4,4,4	0.19	0
62	PUT	23	3004	-	5,5,5	0.10	0	4,4,4	0.12	0
62	PUT	23	3020	-	5,5,5	0.16	0	4,4,4	0.20	0
62	PUT	23	3006	-	5,5,5	0.09	0	4,4,4	0.13	0
65	ATP	23	3002	-	28,33,33	0.64	0	34,52,52	0.58	1 (2%)
62	PUT	23	3008	-	5,5,5	0.10	0	4,4,4	0.14	0
62	PUT	23	3017	-	5,5,5	0.12	0	4,4,4	0.13	0
62	PUT	23	3018	-	5,5,5	0.11	0	4,4,4	0.13	0
68	GDP	EF	803	63	25,30,30	0.97	1 (4%)	30,47,47	1.16	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
62	PUT	23	3007	-	5,5,5	0.10	0	4,4,4	0.12	0
62	PUT	16	1601	-	5,5,5	0.12	0	4,4,4	0.12	0
62	PUT	23	3014	-	5,5,5	0.10	0	4,4,4	0.12	0
62	PUT	23	3012	-	5,5,5	0.11	0	4,4,4	0.13	0
66	SPD	23	3022	-	9,9,9	0.32	0	8,8,8	0.89	0
66	SPD	23	3023	-	9,9,9	0.16	0	8,8,8	0.23	0
62	PUT	23	3005	-	5,5,5	0.11	0	4,4,4	0.13	0
67	FUA	EF	802	63	39,40,40	2.06	13 (33%)	50,64,64	2.79	19 (38%)
66	SPD	23	3021	-	9,9,9	0.32	0	8,8,8	0.91	0
62	PUT	23	3019	-	5,5,5	0.12	0	4,4,4	0.13	0
62	PUT	23	3011	-	5,5,5	0.09	0	4,4,4	0.13	0

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
62	PUT	23	3009	-	-	0/3/3/3	-
62	PUT	23	3003	-	-	0/3/3/3	-
62	PUT	23	3016	-	-	1/3/3/3	-
62	PUT	23	3013	-	-	0/3/3/3	-
65	ATP	23	3001	-	-	5/18/38/38	0/3/3/3
62	PUT	16	1602	-	-	2/3/3/3	-
62	PUT	23	3010	-	-	1/3/3/3	-
62	PUT	LC	301	-	-	1/3/3/3	-
62	PUT	23	3015	-	-	1/3/3/3	-
62	PUT	23	3004	-	-	0/3/3/3	-
62	PUT	23	3020	-	-	0/3/3/3	-
62	PUT	23	3006	-	-	0/3/3/3	-
65	ATP	23	3002	-	-	5/18/38/38	0/3/3/3
62	PUT	23	3008	-	-	0/3/3/3	-
62	PUT	23	3017	-	-	1/3/3/3	-
62	PUT	23	3018	-	-	1/3/3/3	-
68	GDP	EF	803	63	-	4/12/32/32	0/3/3/3
62	PUT	23	3007	-	-	1/3/3/3	-
62	PUT	16	1601	-	-	0/3/3/3	-
62	PUT	23	3014	-	-	1/3/3/3	-
62	PUT	23	3012	-	-	0/3/3/3	-
66	SPD	23	3022	-	-	0/7/7/7	-
66	SPD	23	3023	-	-	2/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	PUT	23	3005	-	-	0/3/3/3	-
67	FUA	EF	802	63	-	5/16/92/92	0/4/4/4
66	SPD	23	3021	-	-	2/7/7/7	-
62	PUT	23	3019	-	-	0/3/3/3	-
62	PUT	23	3011	-	-	1/3/3/3	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	EF	802	FUA	C9-C11	5.22	1.61	1.54
67	EF	802	FUA	C10-C5	-4.17	1.48	1.56
67	EF	802	FUA	C28-C26	4.06	1.61	1.50
67	EF	802	FUA	C20-C8	-3.80	1.47	1.54
67	EF	802	FUA	C27-C26	2.83	1.58	1.50
67	EF	802	FUA	C4-C3	2.81	1.61	1.53
67	EF	802	FUA	C15-C14	-2.72	1.49	1.54
67	EF	802	FUA	C25-C26	-2.72	1.24	1.32
67	EF	802	FUA	C14-C8	2.45	1.63	1.59
67	EF	802	FUA	C4-C5	-2.37	1.49	1.54
68	EF	803	GDP	C6-N1	-2.35	1.34	1.37
67	EF	802	FUA	C32-C31	-2.19	1.42	1.49
67	EF	802	FUA	C18-C4	-2.18	1.49	1.53
67	EF	802	FUA	C10-C9	2.11	1.60	1.57

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	EF	802	FUA	C18-C4-C3	-7.63	102.42	111.35
67	EF	802	FUA	C28-C26-C27	-6.86	98.79	114.59
67	EF	802	FUA	C21-C14-C8	6.34	117.49	112.23
67	EF	802	FUA	C27-C26-C25	5.56	139.33	122.66
67	EF	802	FUA	C10-C5-C4	4.91	119.16	113.20
67	EF	802	FUA	C6-C5-C10	4.66	117.25	111.66
67	EF	802	FUA	C19-C10-C5	-4.62	104.97	111.18
67	EF	802	FUA	O5-C29-O4	-4.22	113.86	123.90
67	EF	802	FUA	C24-C23-C22	4.14	121.54	112.72
67	EF	802	FUA	O5-C29-C22	3.75	126.69	115.83
67	EF	802	FUA	O2-C16-C17	-3.61	97.74	108.30
67	EF	802	FUA	C18-C4-C5	3.07	117.92	112.95
67	EF	802	FUA	C21-C14-C13	-2.92	105.50	112.91
68	EF	803	GDP	C8-N7-C5	2.90	107.49	102.55
67	EF	802	FUA	C5-C10-C9	2.69	114.50	108.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	EF	802	FUA	C1-C2-C3	2.65	116.56	111.59
67	EF	802	FUA	C8-C9-C10	-2.48	113.75	116.42
67	EF	802	FUA	C21-C14-C15	-2.48	101.99	108.66
67	EF	802	FUA	O1-C11-C9	-2.46	104.58	111.11
68	EF	803	GDP	O4'-C1'-N9	2.43	111.97	108.75
65	23	3002	ATP	C5-C6-N6	2.32	123.85	120.31
65	23	3001	ATP	C5-C6-N6	2.31	123.83	120.31
68	EF	803	GDP	C5-C6-N1	2.07	118.01	114.07
67	EF	802	FUA	C7-C6-C5	2.04	116.60	113.14

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
65	23	3001	ATP	C5'-O5'-PA-O3A
65	23	3002	ATP	PB-O3B-PG-O3G
65	23	3002	ATP	O4'-C4'-C5'-O5'
67	EF	802	FUA	C23-C22-C29-O5
67	EF	802	FUA	O3-C31-O2-C16
68	EF	803	GDP	C5'-O5'-PA-O3A
68	EF	803	GDP	C5'-O5'-PA-O1A
68	EF	803	GDP	C5'-O5'-PA-O2A
67	EF	802	FUA	C32-C31-O2-C16
62	23	3015	PUT	C1-C2-C3-C4
65	23	3002	ATP	C3'-C4'-C5'-O5'
67	EF	802	FUA	C22-C23-C24-C25
66	23	3023	SPD	C3-C4-C5-N6
67	EF	802	FUA	C23-C22-C29-O4
62	16	1602	PUT	C2-C3-C4-N2
66	23	3023	SPD	C7-C8-C9-N10
65	23	3001	ATP	PG-O3B-PB-O3A
62	23	3007	PUT	N1-C1-C2-C3
62	23	3010	PUT	N1-C1-C2-C3
62	LC	301	PUT	C1-C2-C3-C4
62	23	3016	PUT	C1-C2-C3-C4
66	23	3021	SPD	C7-C8-C9-N10
65	23	3002	ATP	PG-O3B-PB-O2B
66	23	3021	SPD	C8-C7-N6-C5
65	23	3002	ATP	PG-O3B-PB-O1B
62	23	3011	PUT	C1-C2-C3-C4
62	23	3017	PUT	C1-C2-C3-C4
68	EF	803	GDP	O4'-C4'-C5'-O5'

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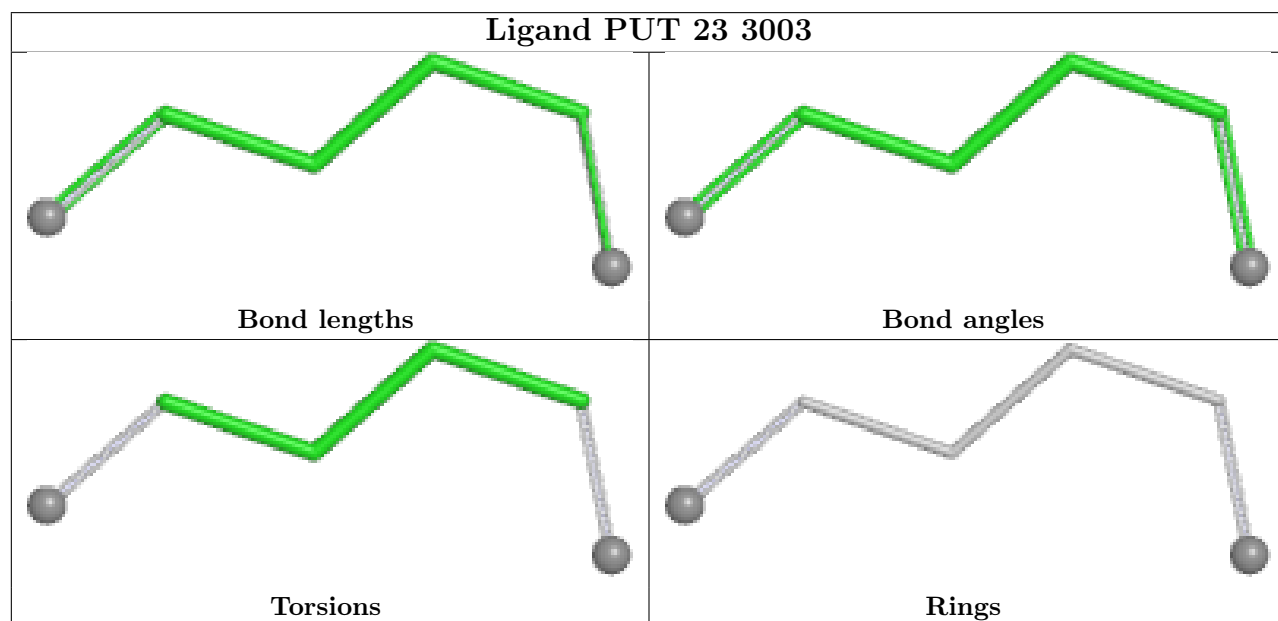
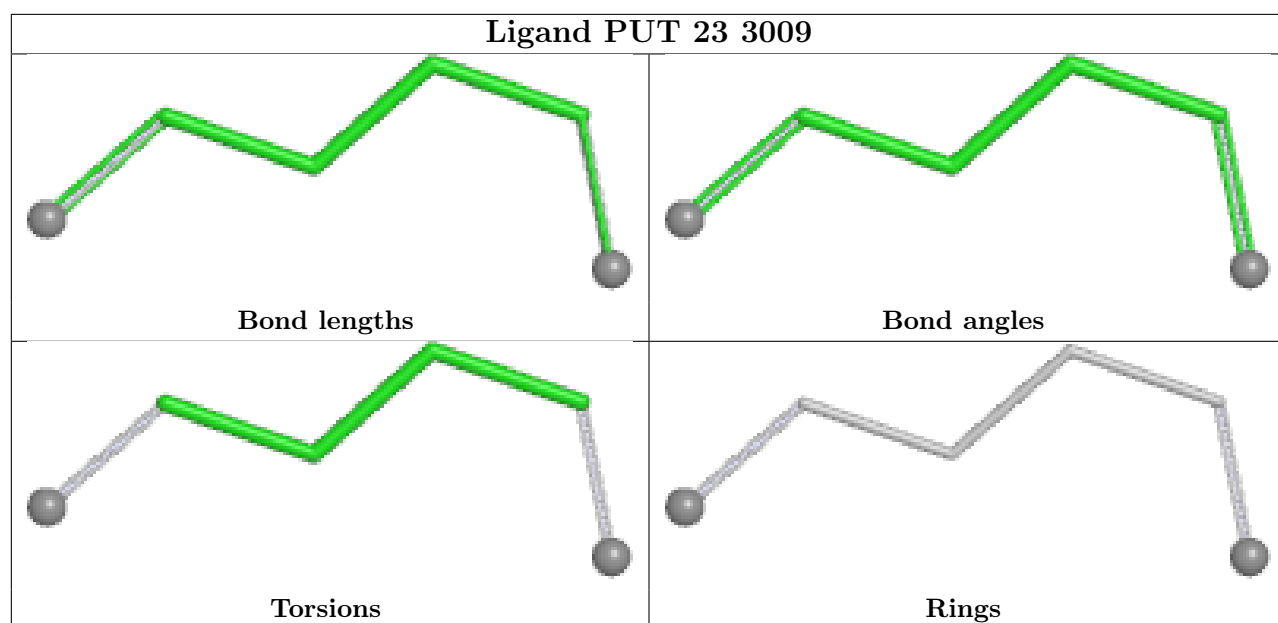
Mol	Chain	Res	Type	Atoms
65	23	3001	ATP	PG-O3B-PB-O1B
62	23	3014	PUT	C1-C2-C3-C4
62	23	3018	PUT	C1-C2-C3-C4
62	16	1602	PUT	C1-C2-C3-C4
65	23	3001	ATP	PG-O3B-PB-O2B
65	23	3001	ATP	PB-O3A-PA-O2A

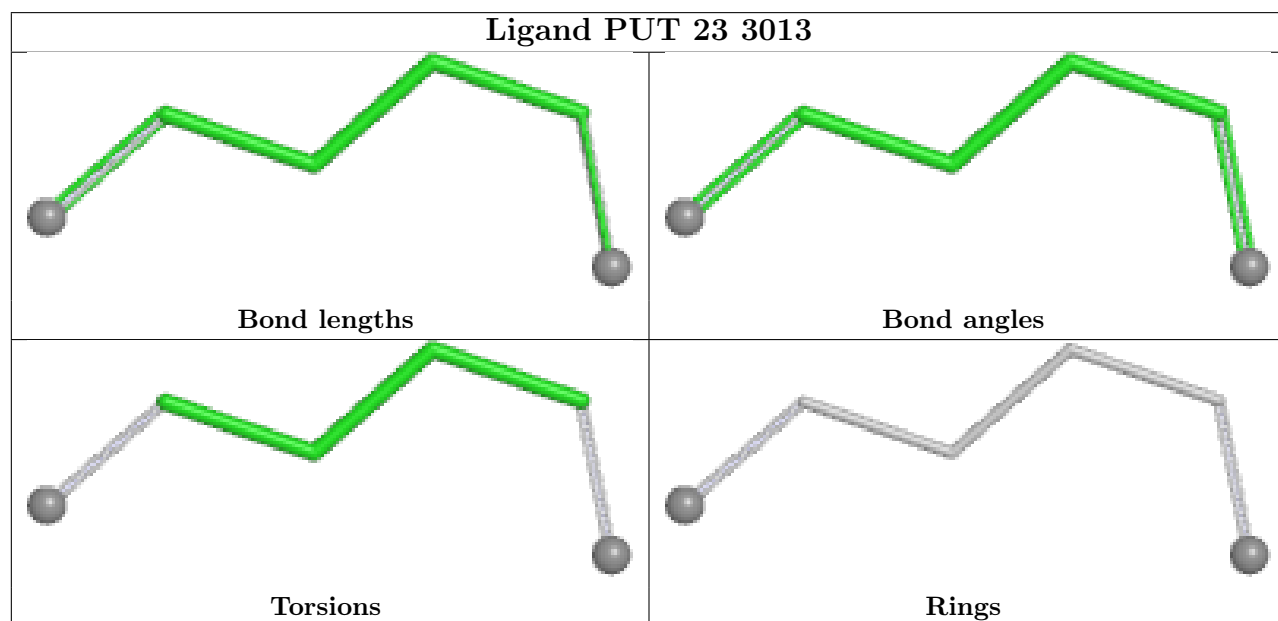
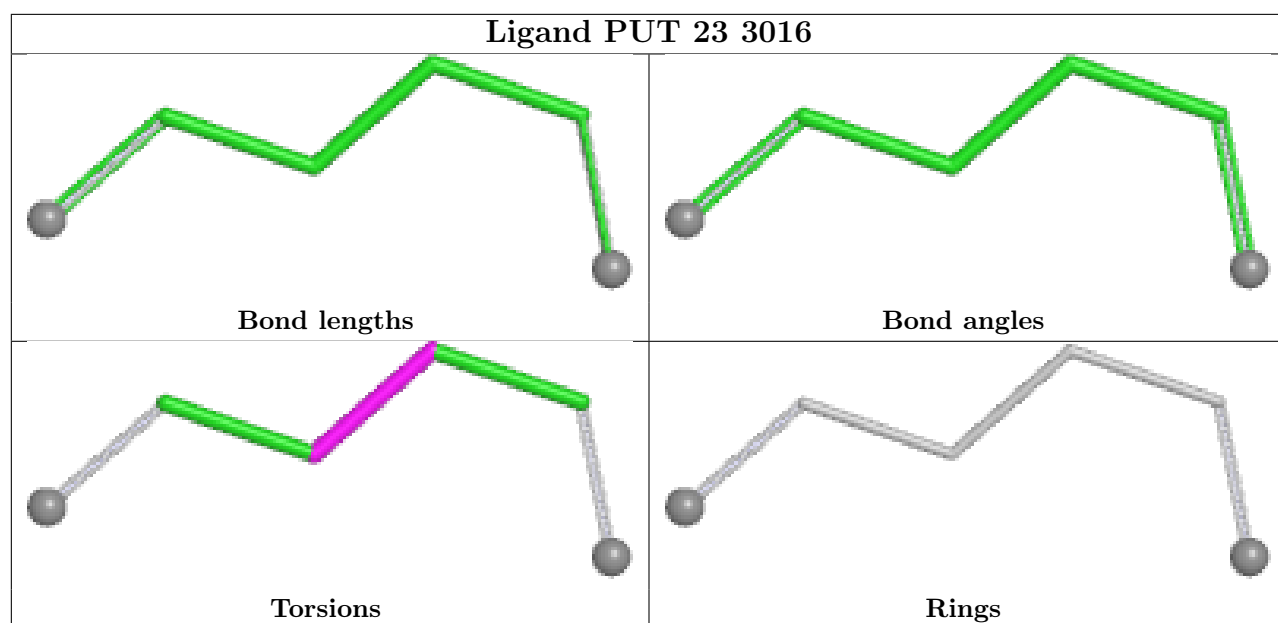
There are no ring outliers.

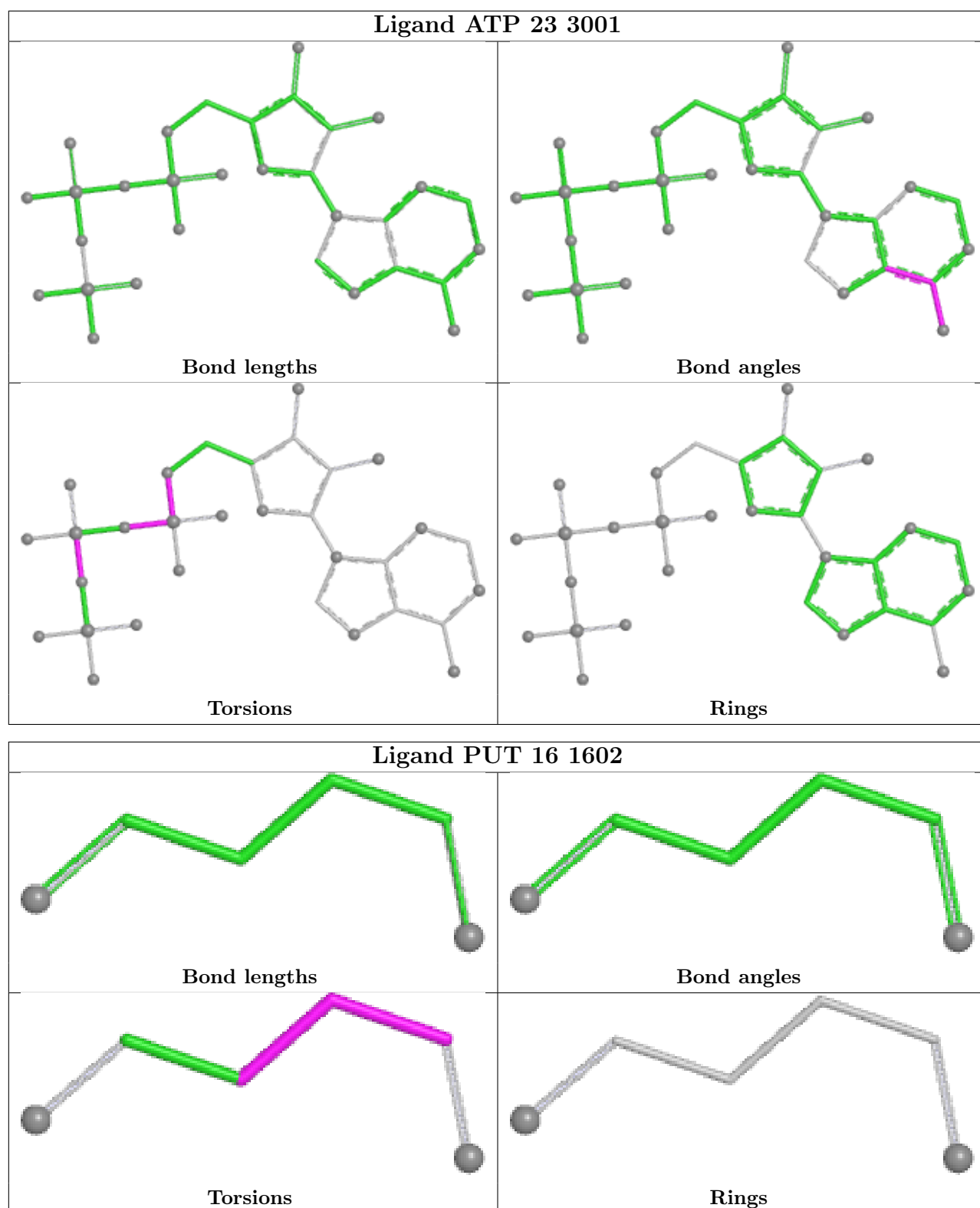
6 monomers are involved in 21 short contacts:

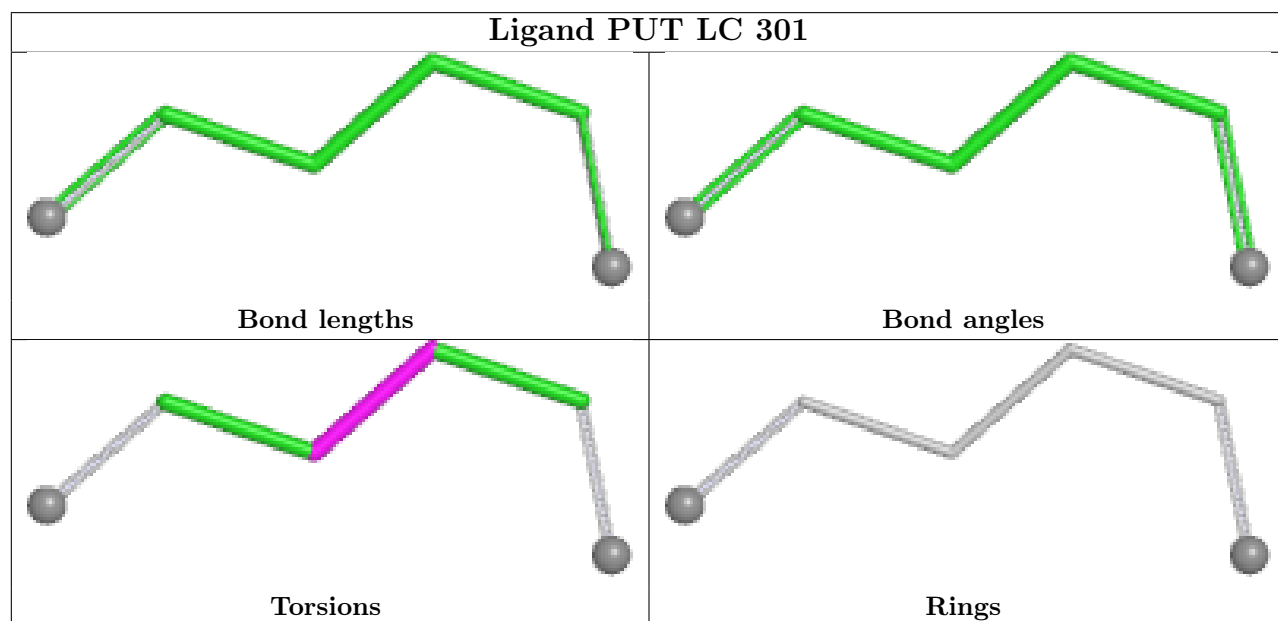
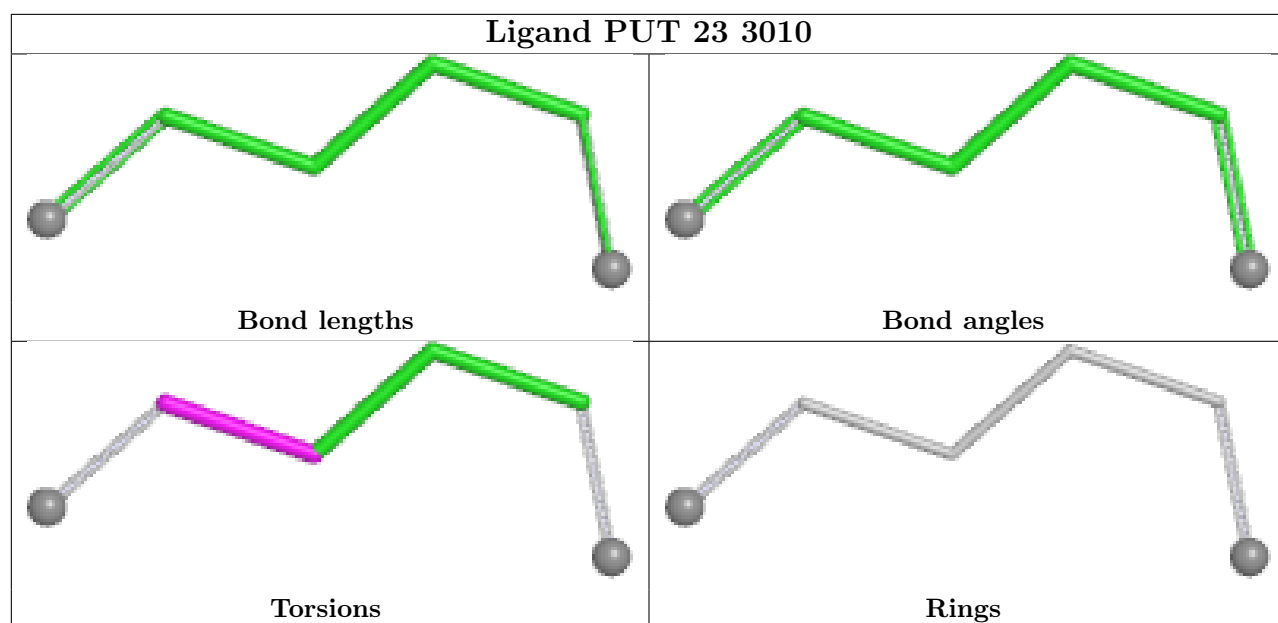
Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	23	3013	PUT	1	0
62	16	1602	PUT	1	0
62	23	3010	PUT	1	0
62	LC	301	PUT	1	0
62	23	3020	PUT	2	0
67	EF	802	FUA	15	0

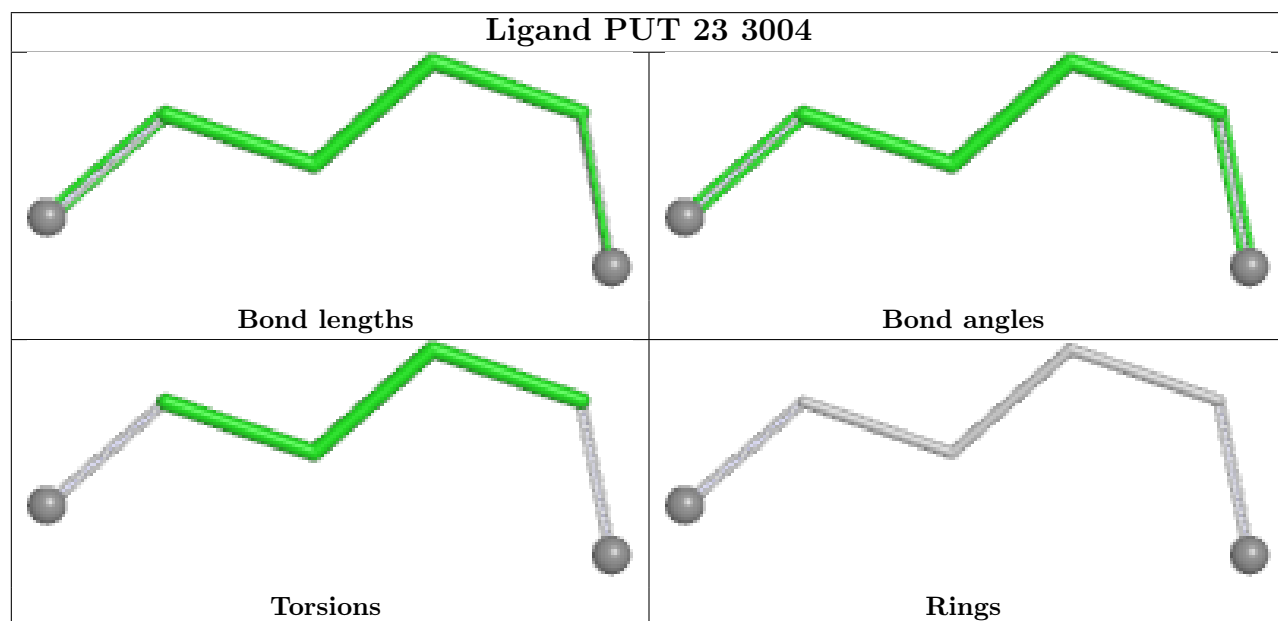
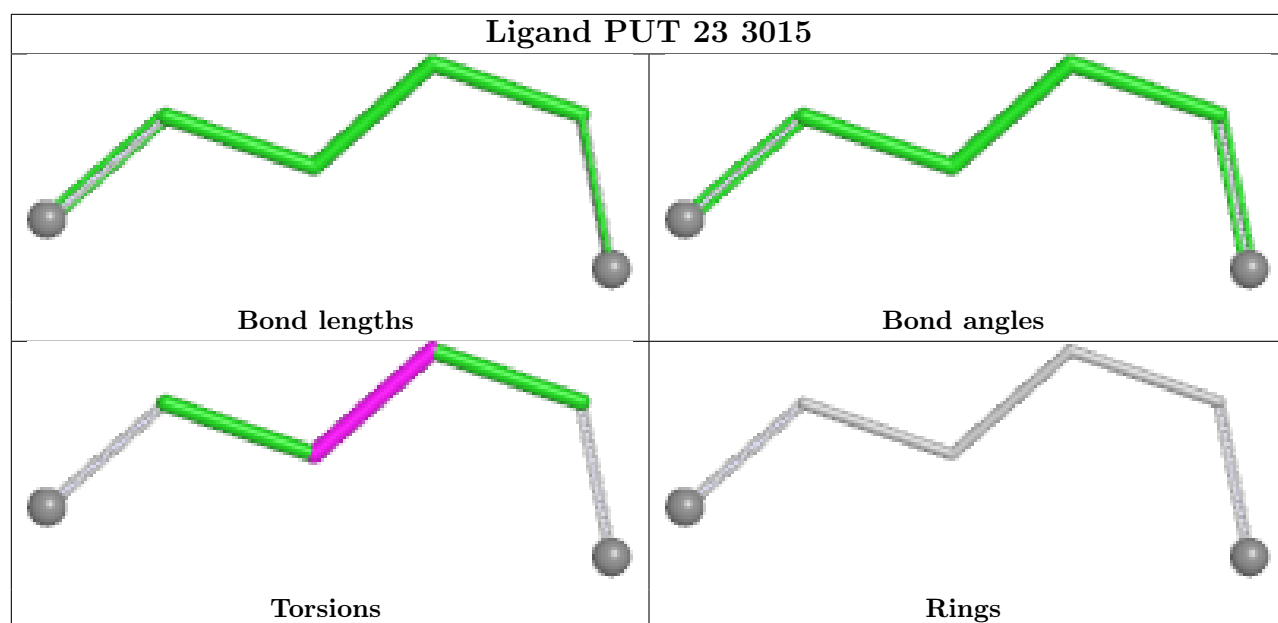
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

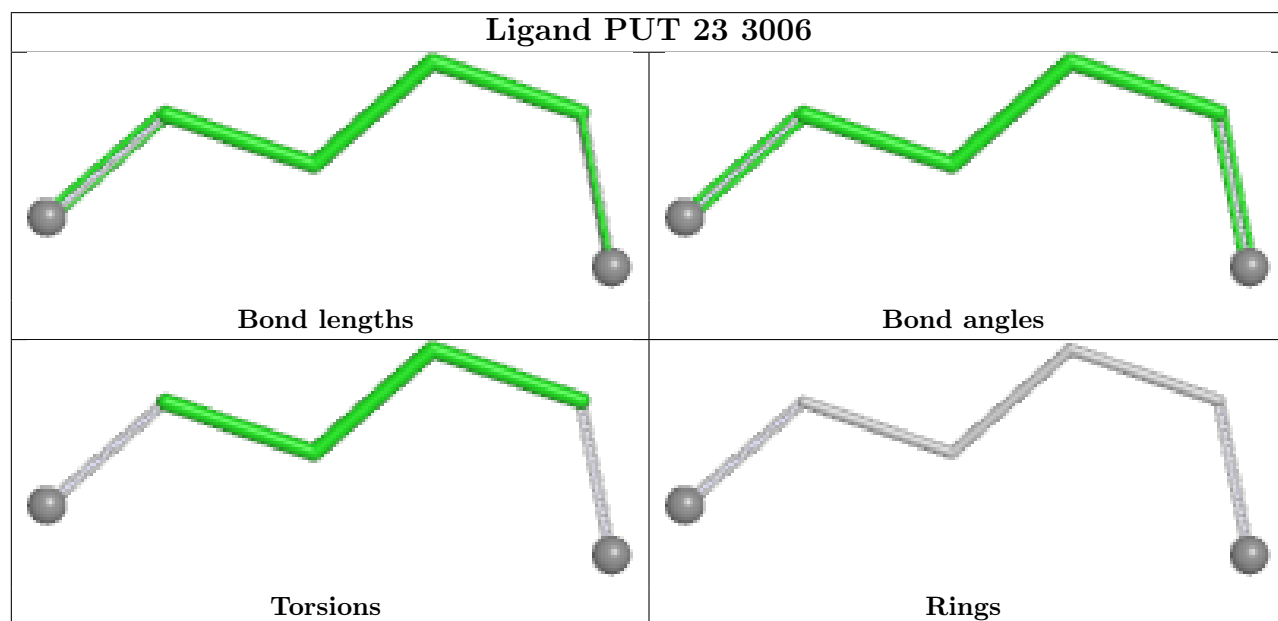
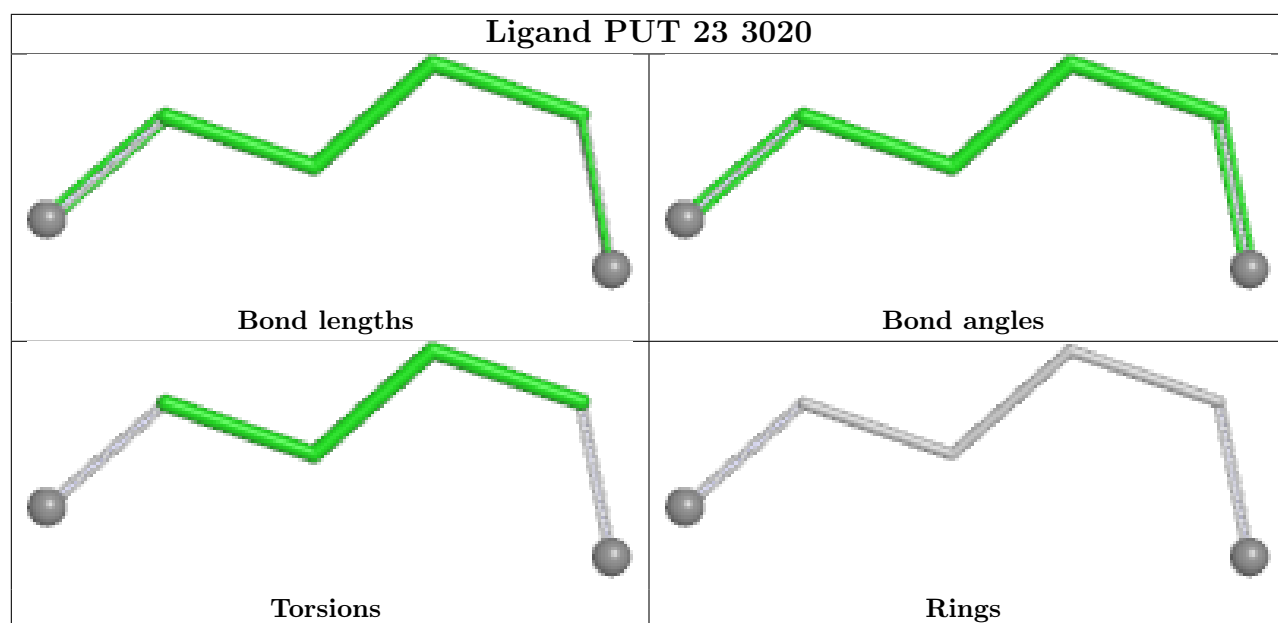




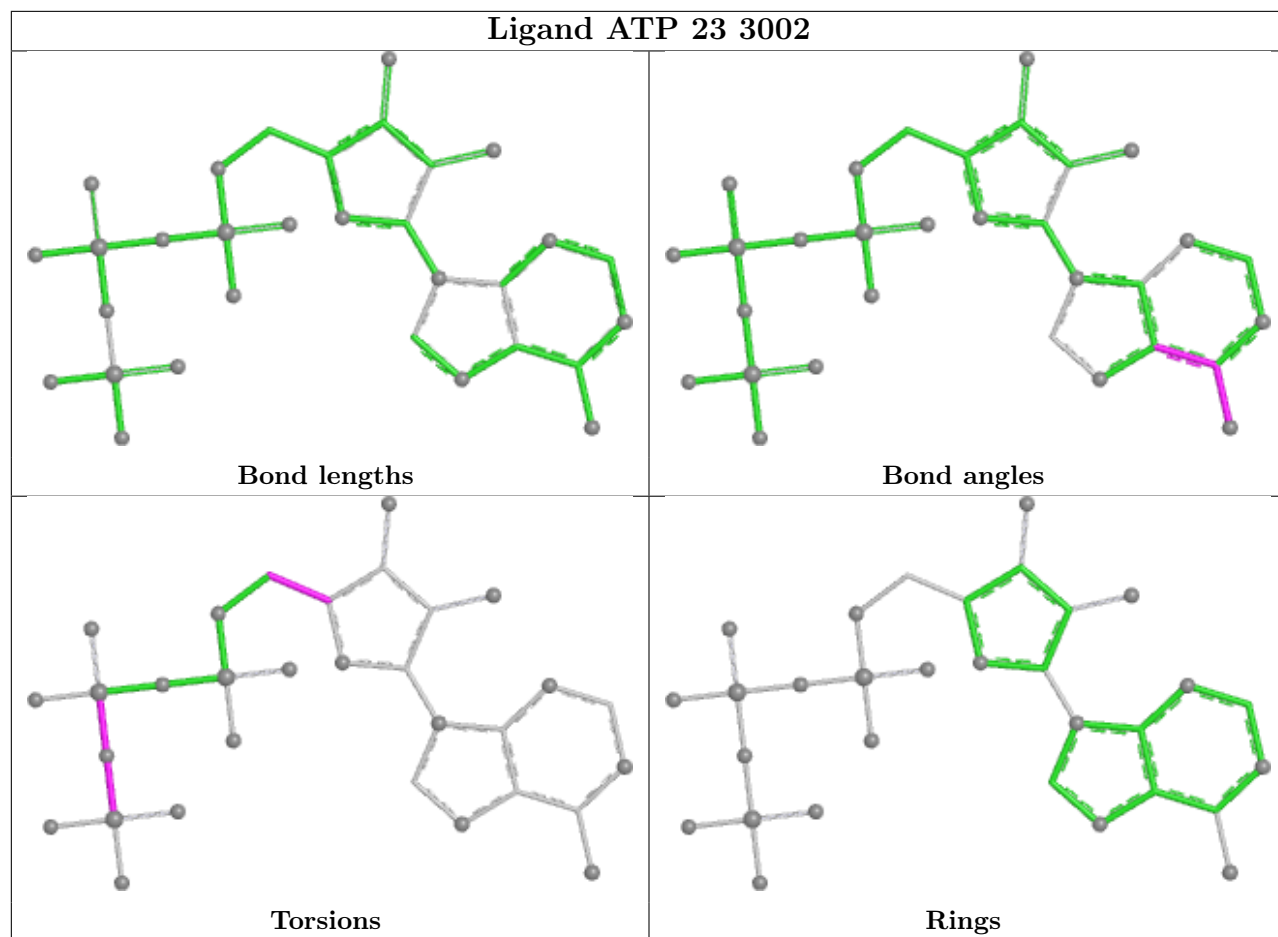




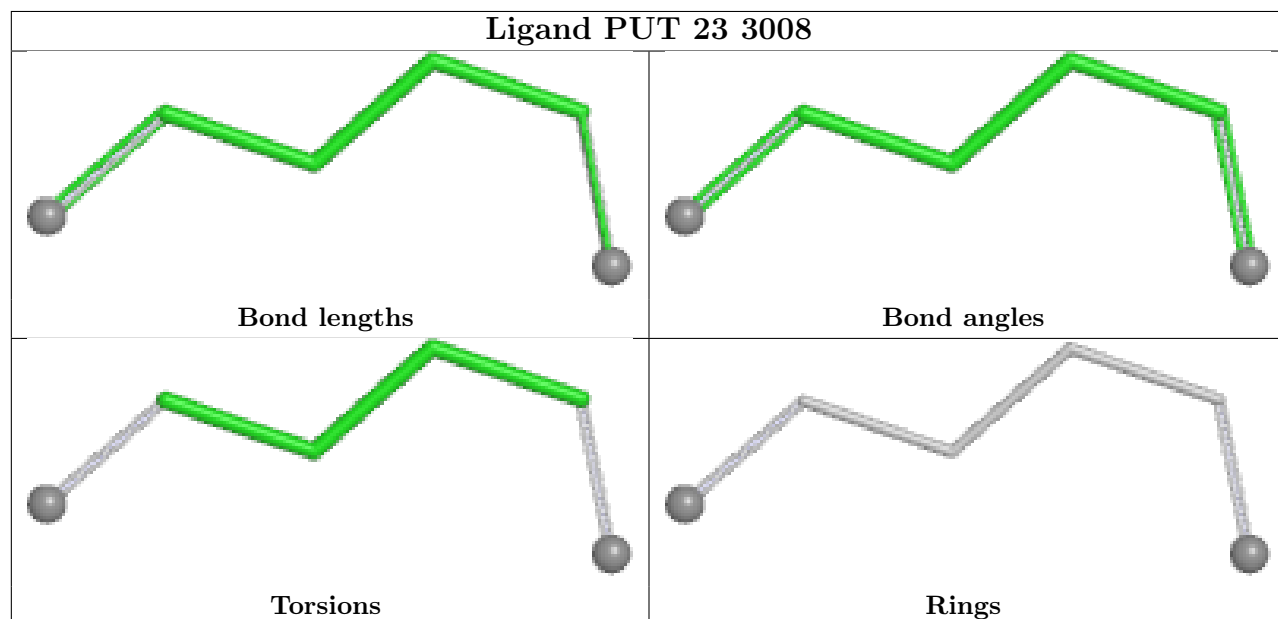


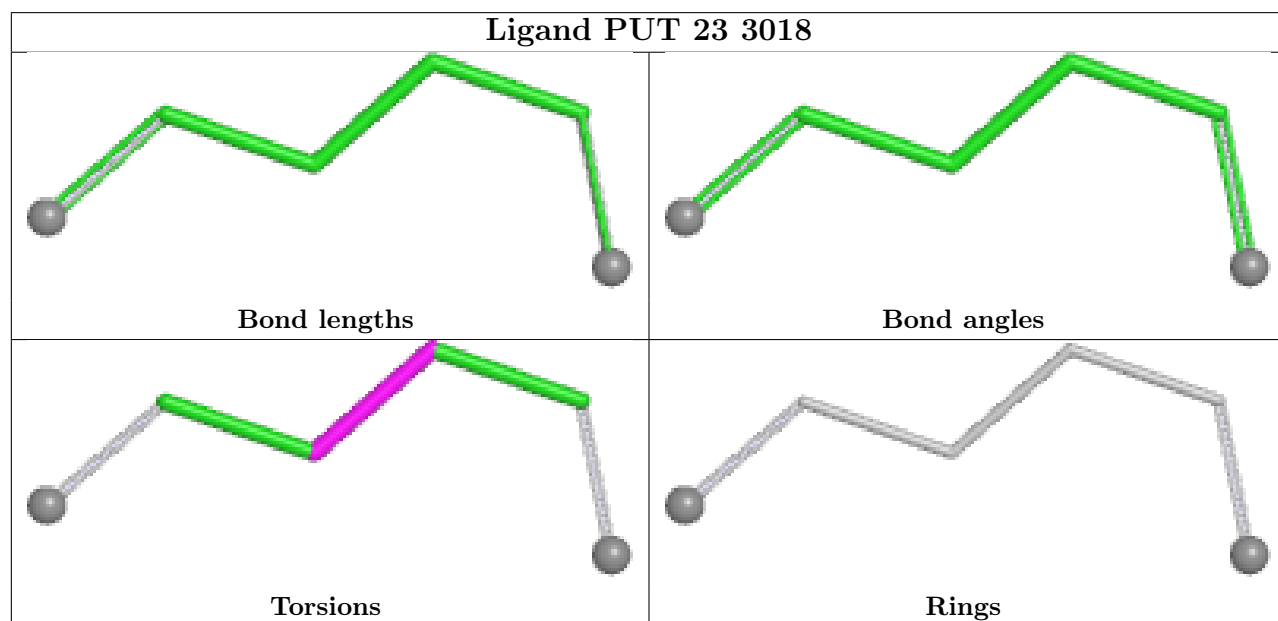
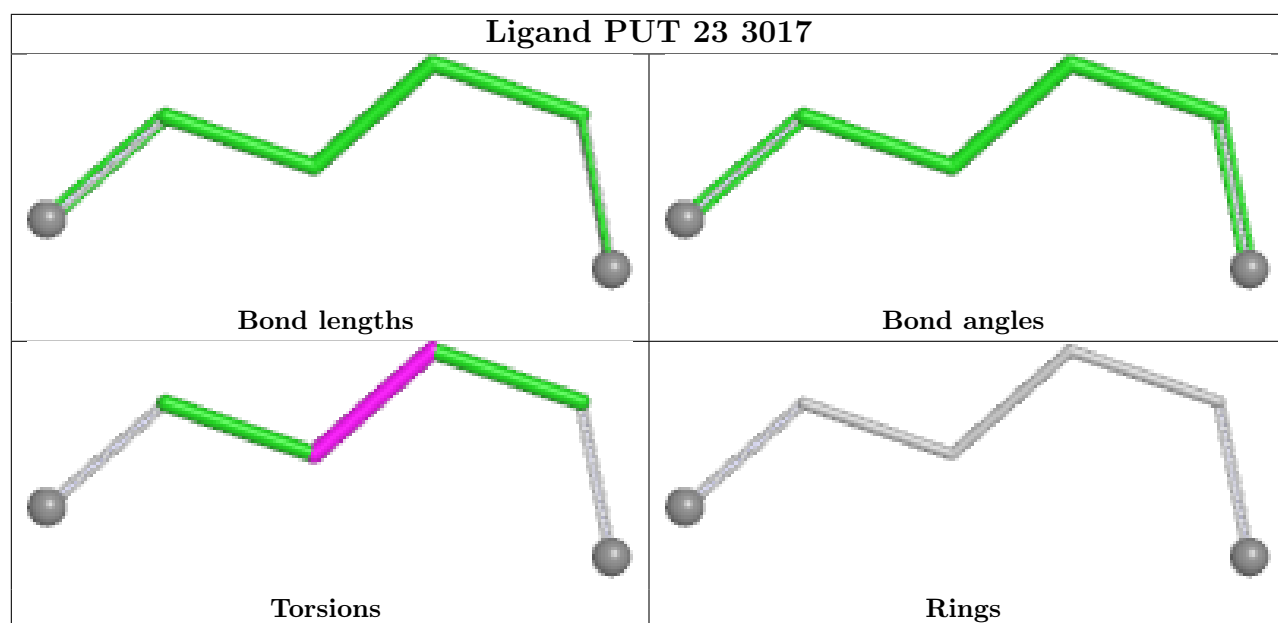


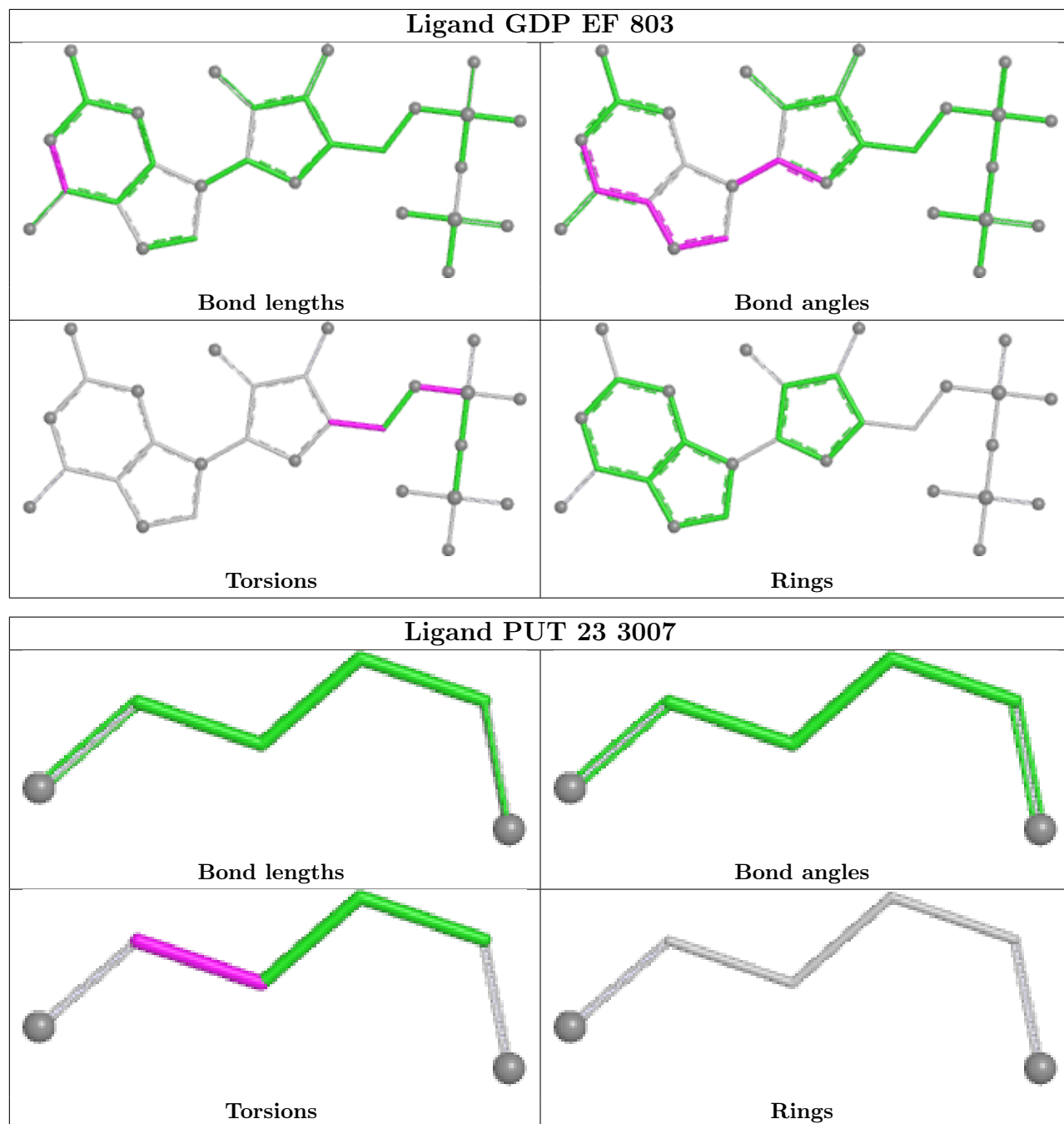
Ligand ATP 23 3002

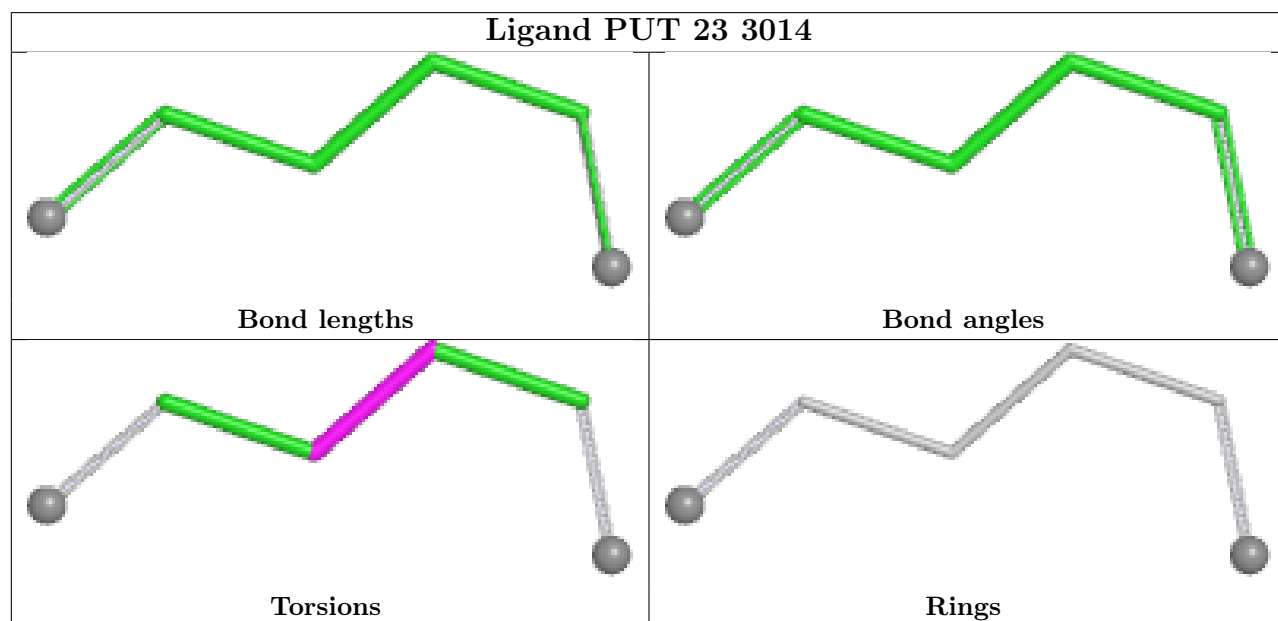
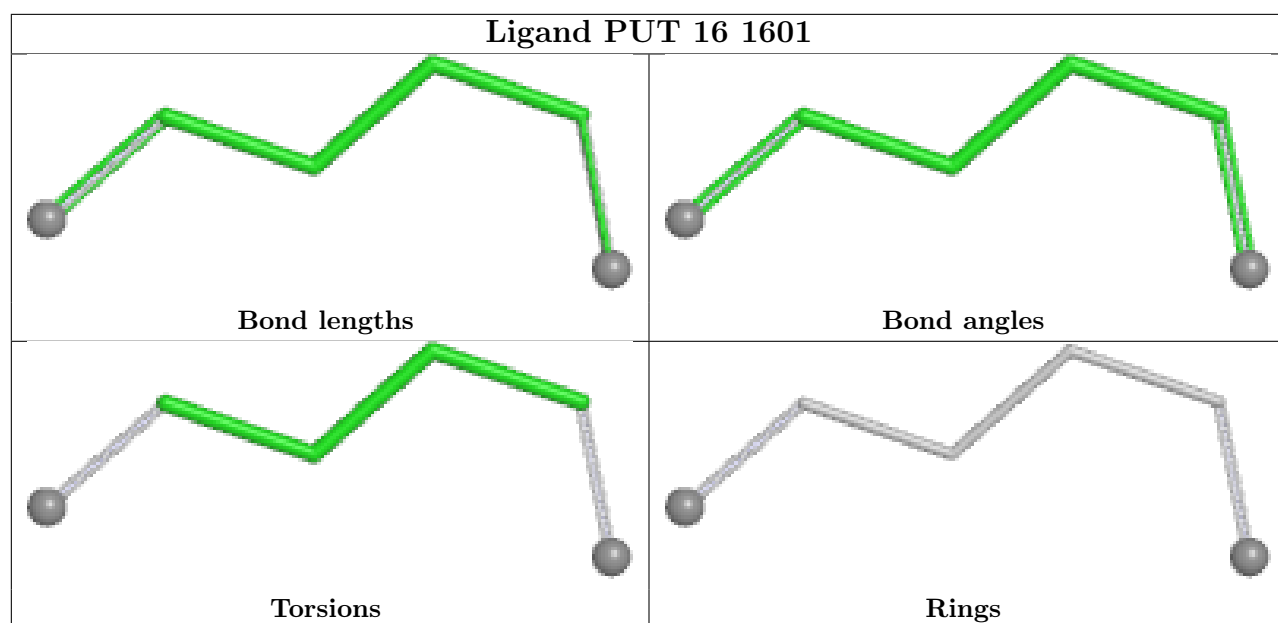


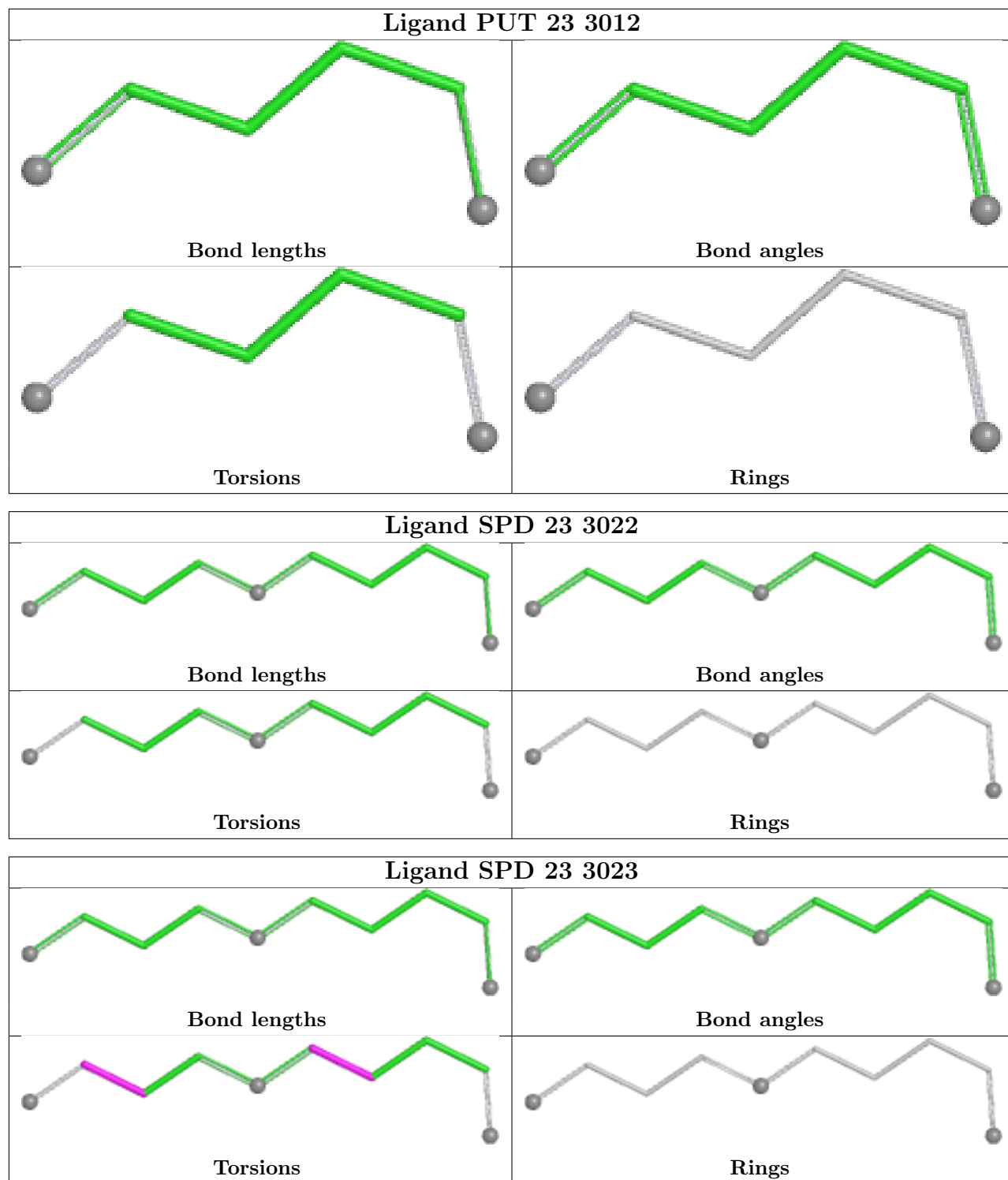
Ligand PUT 23 3008

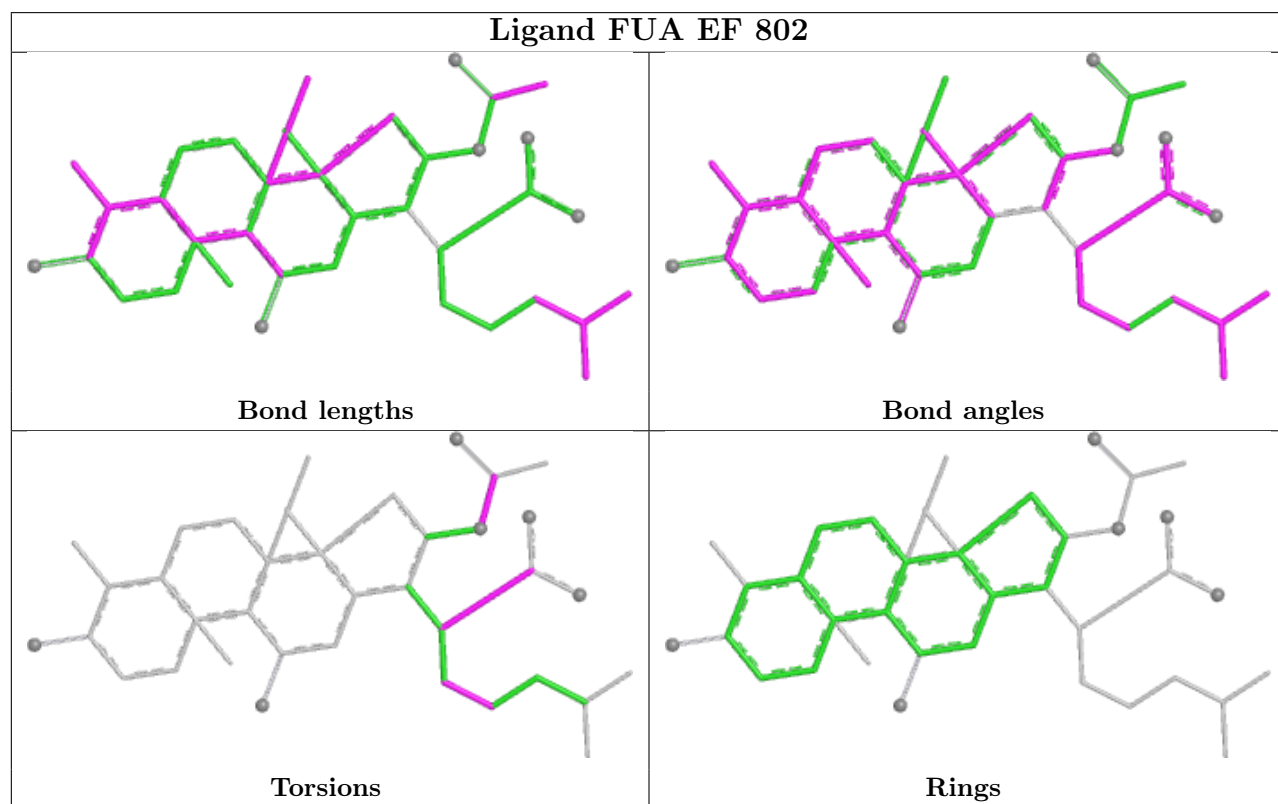
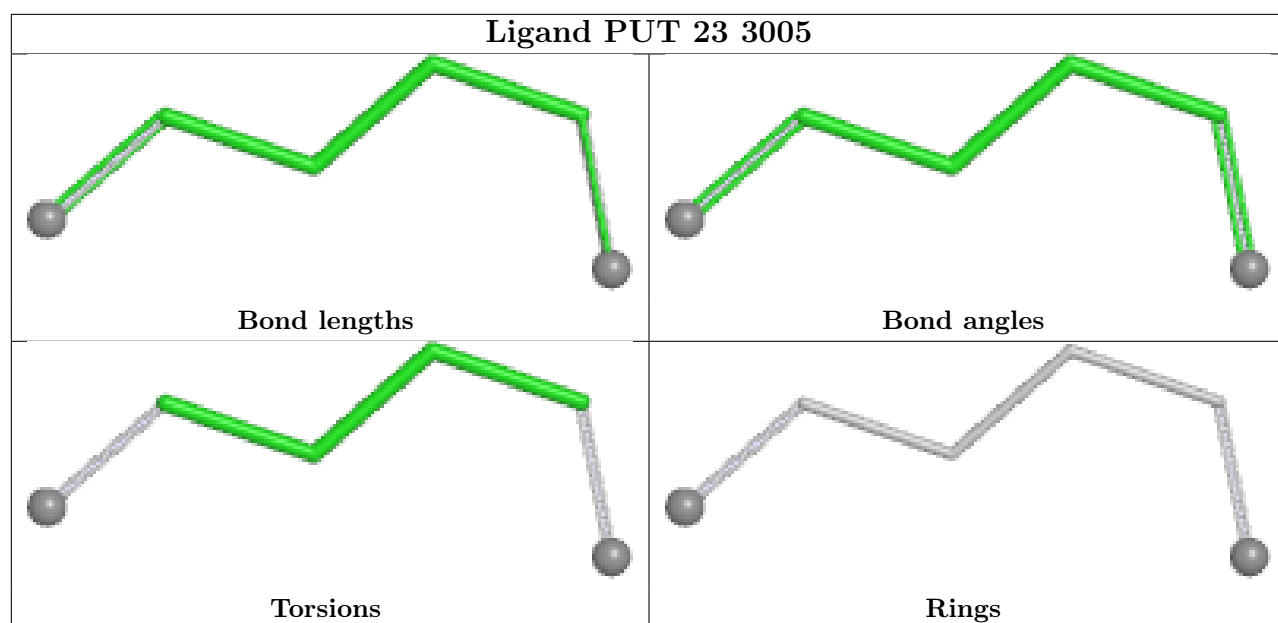


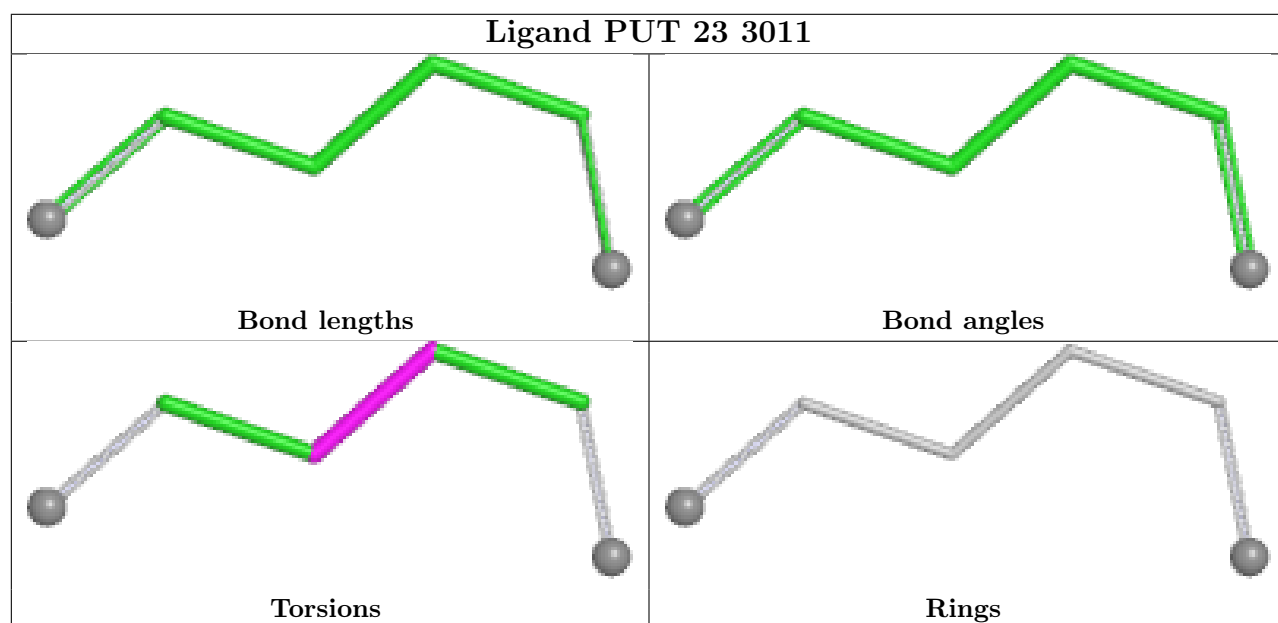
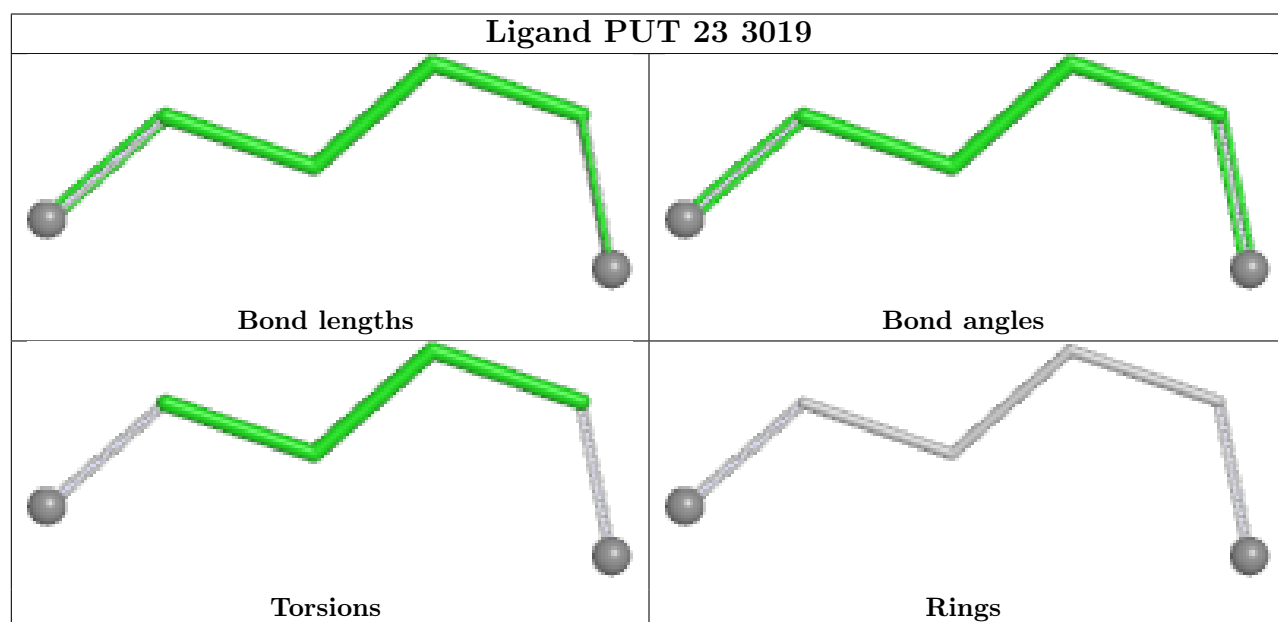
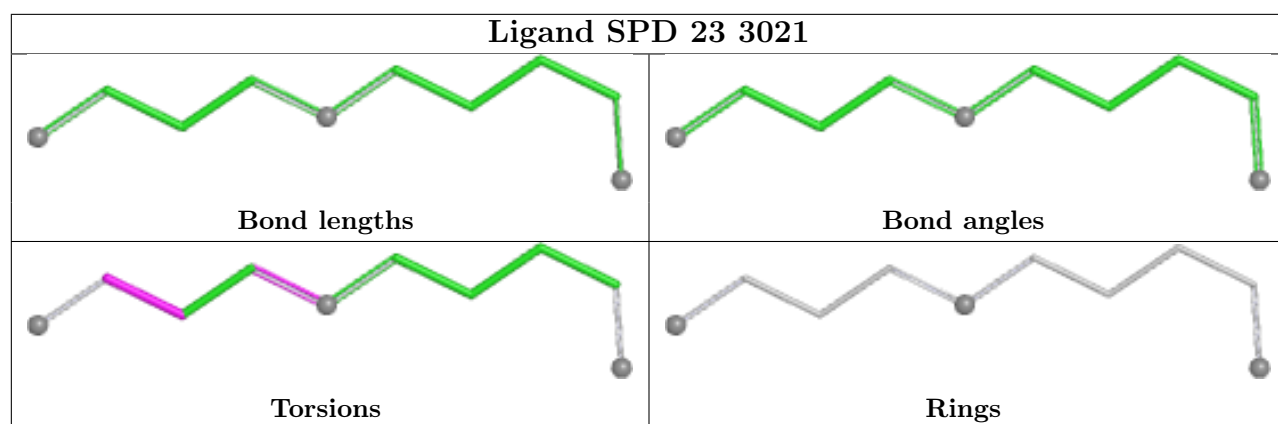












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

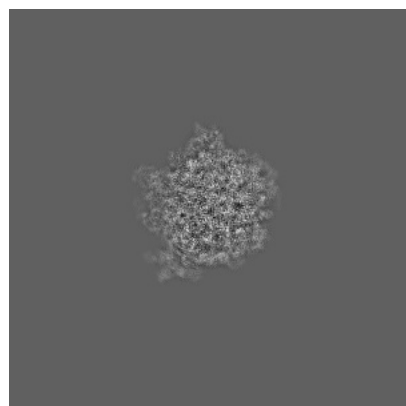
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24132. These allow visual inspection of the internal detail of the map and identification of artifacts.

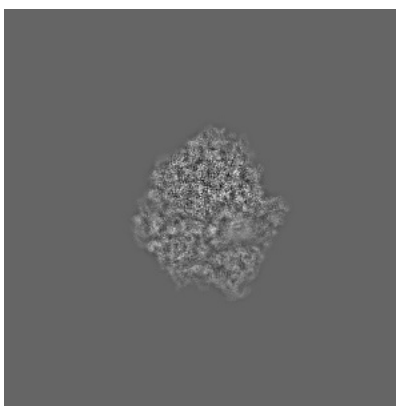
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

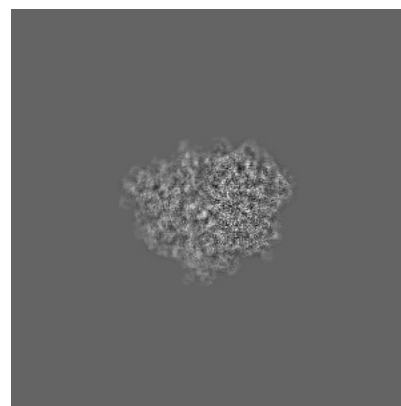
6.1.1 Primary map



X

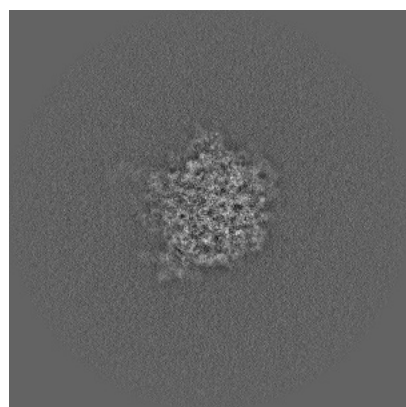


Y

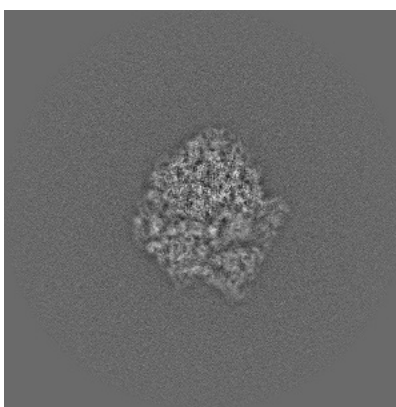


Z

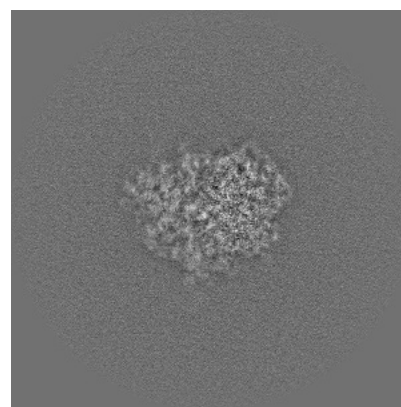
6.1.2 Raw map



X



Y

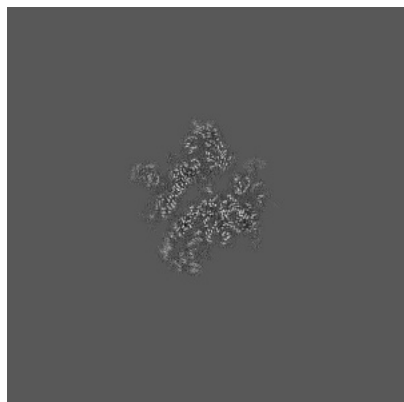


Z

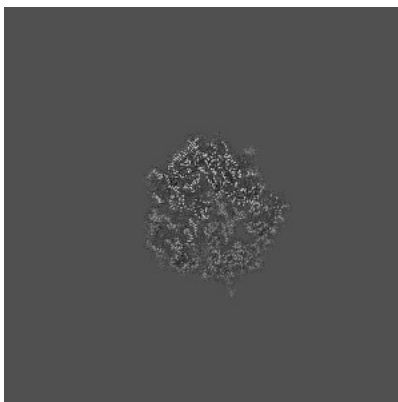
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

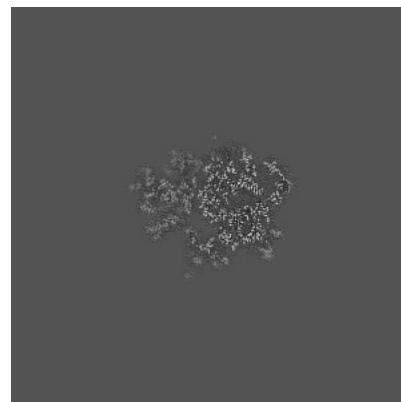
6.2.1 Primary map



X Index: 288

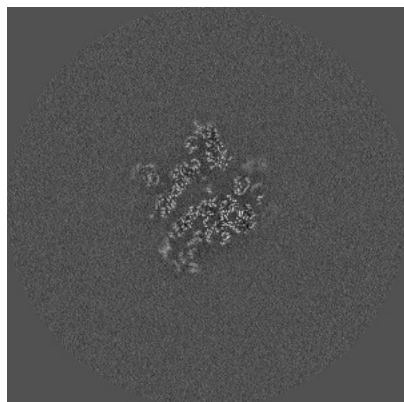


Y Index: 288

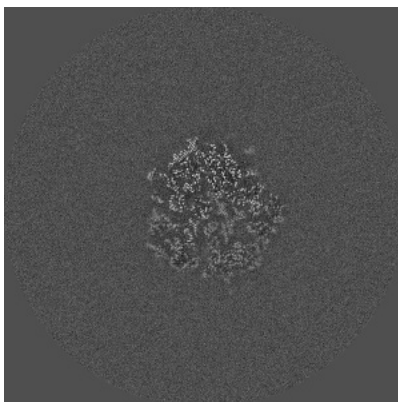


Z Index: 288

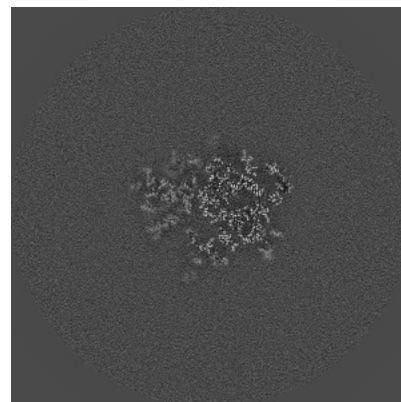
6.2.2 Raw map



X Index: 288



Y Index: 288

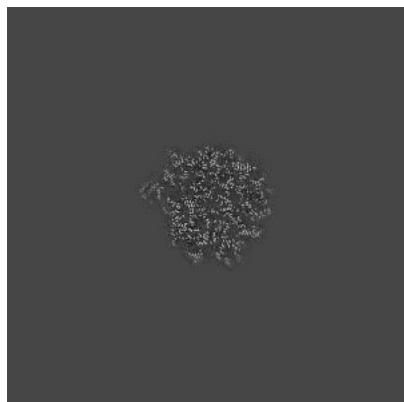


Z Index: 288

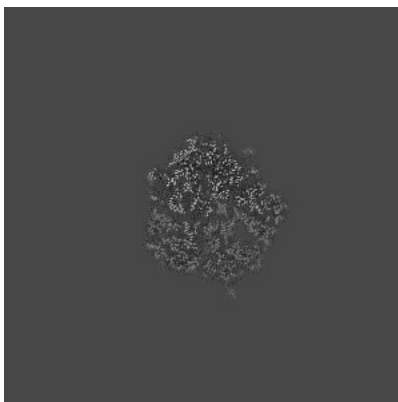
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

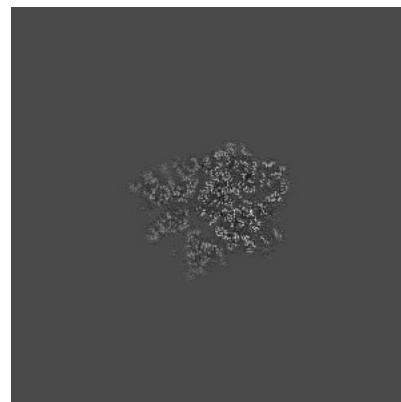
6.3.1 Primary map



X Index: 315

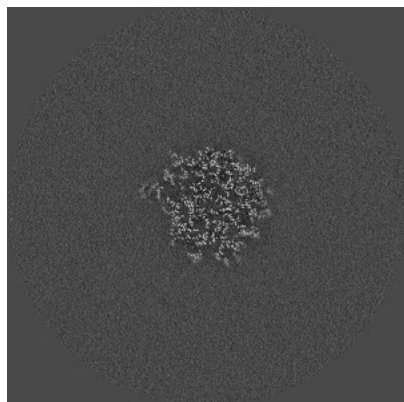


Y Index: 290

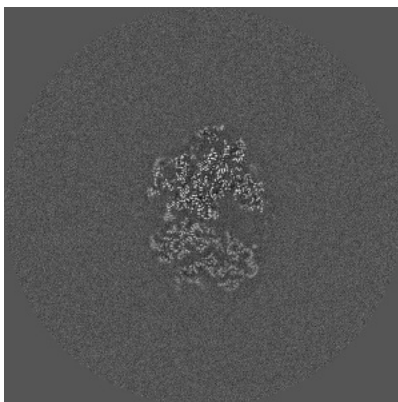


Z Index: 282

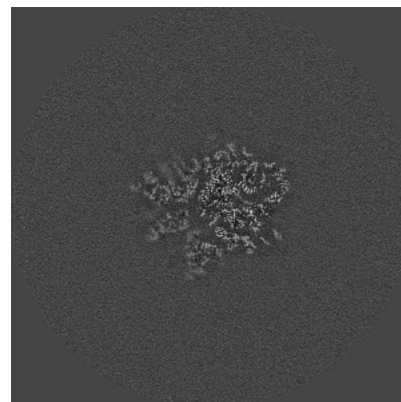
6.3.2 Raw map



X Index: 315



Y Index: 312

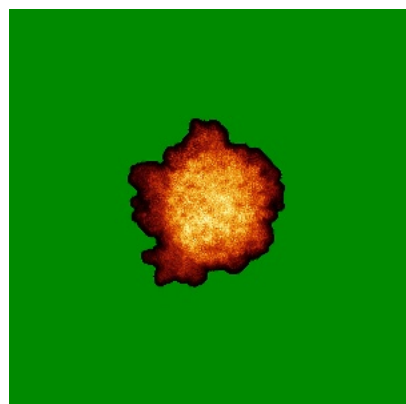


Z Index: 282

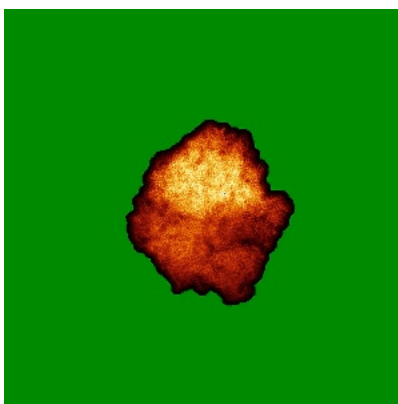
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

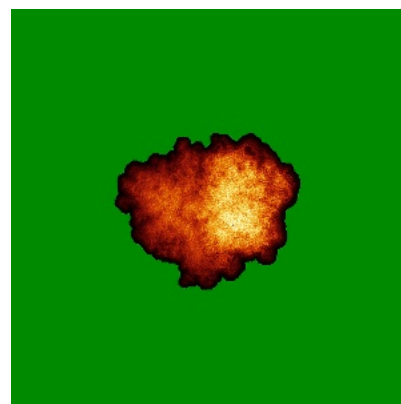
6.4.1 Primary map



X

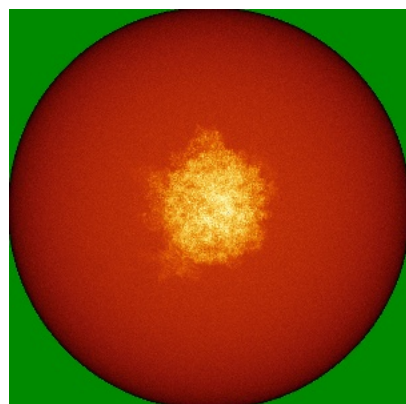


Y

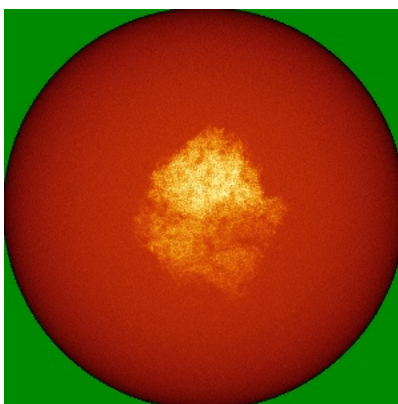


Z

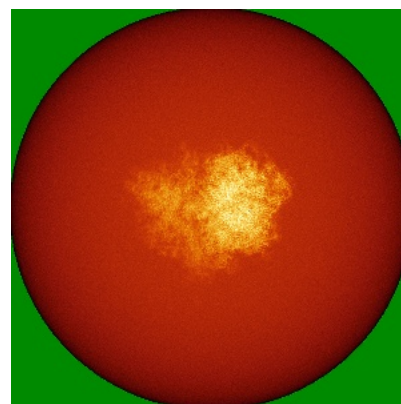
6.4.2 Raw map



X



Y

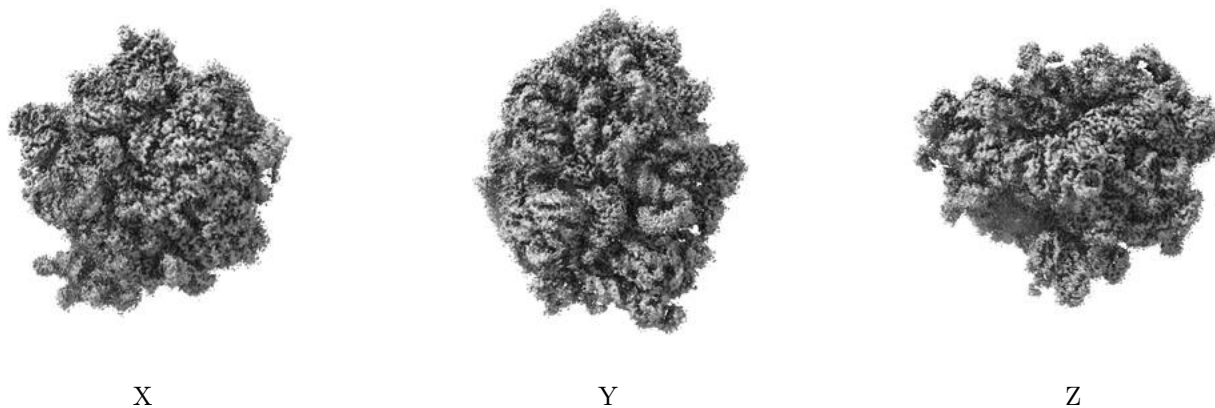


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

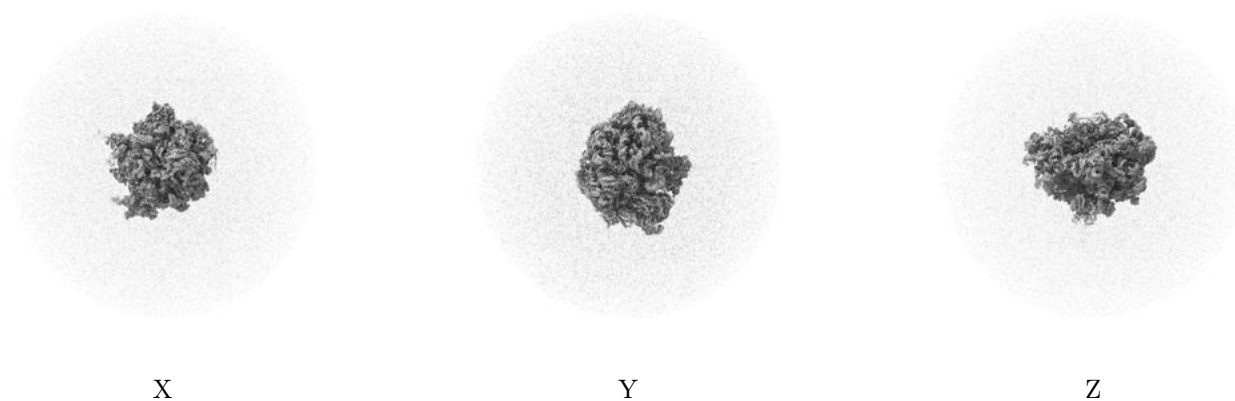
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

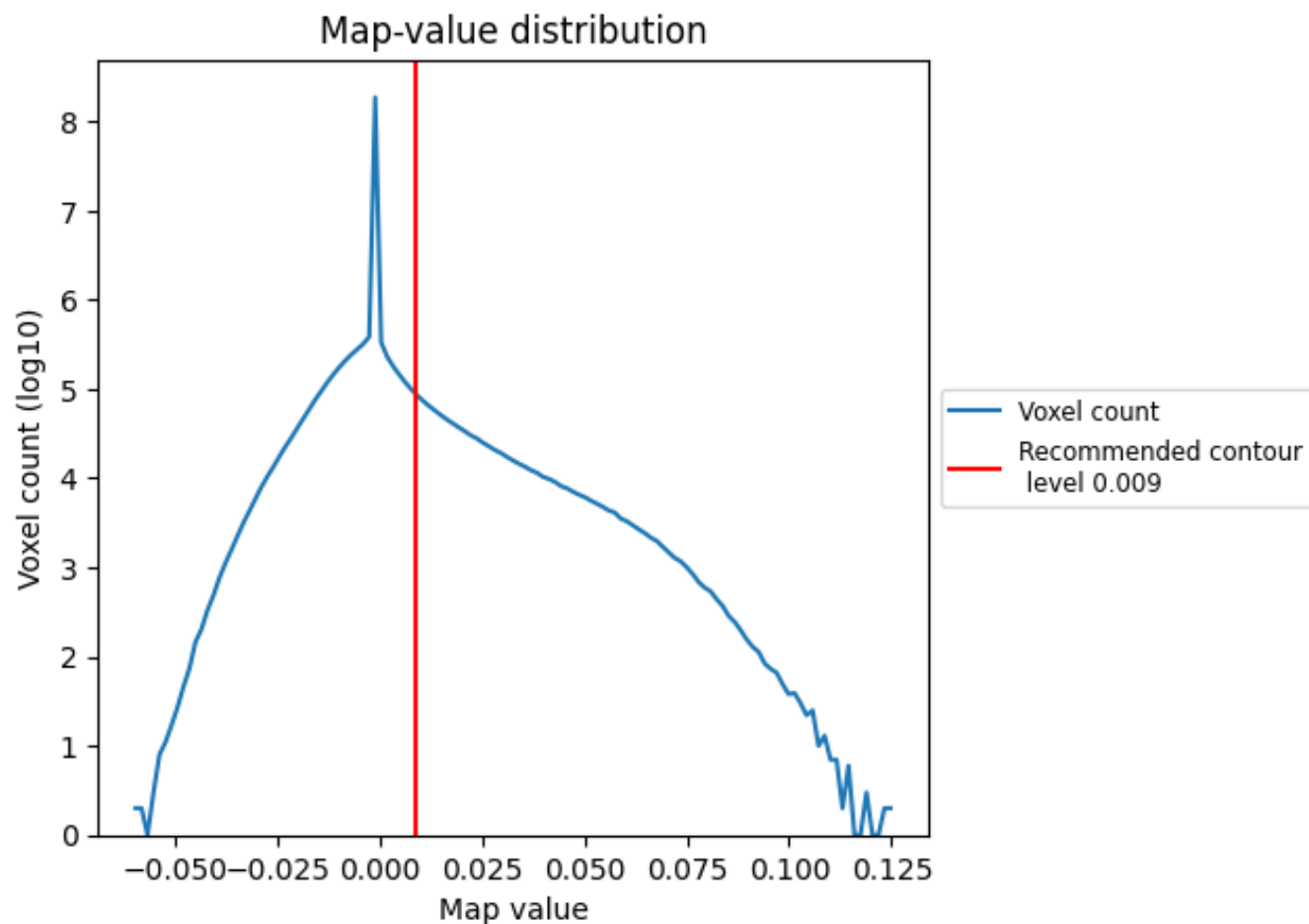
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

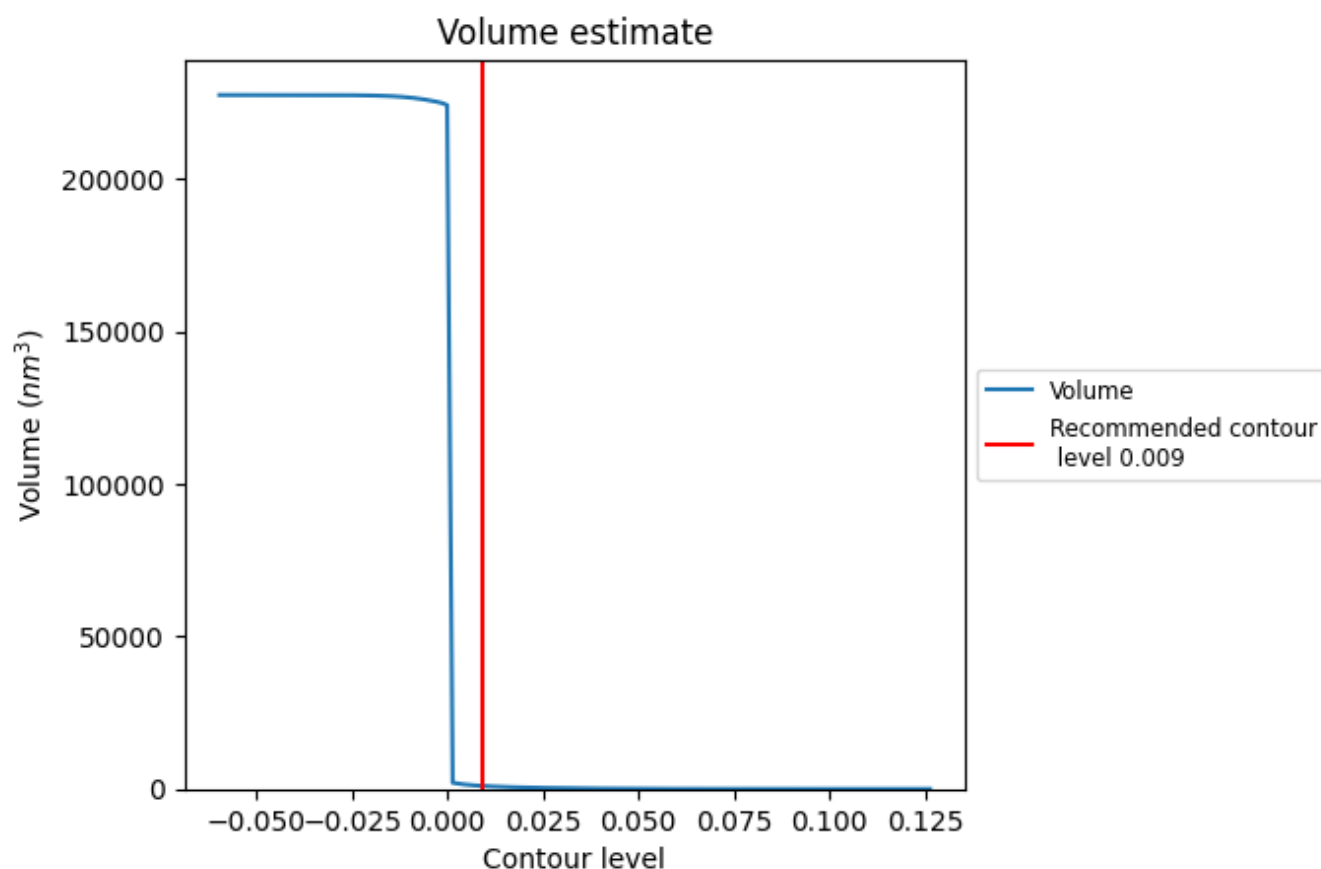
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

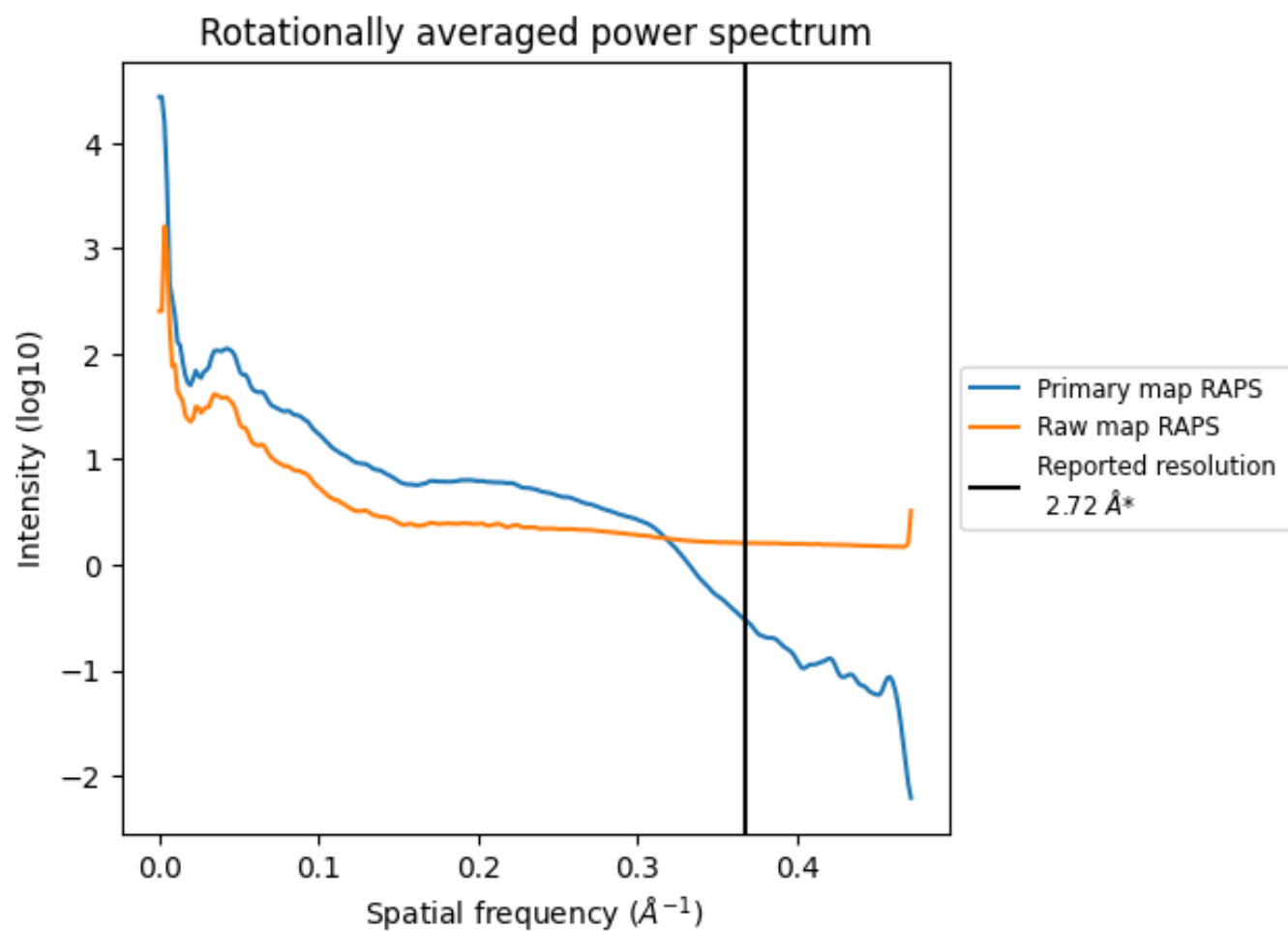
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1017 nm^3 ; this corresponds to an approximate mass of 919 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

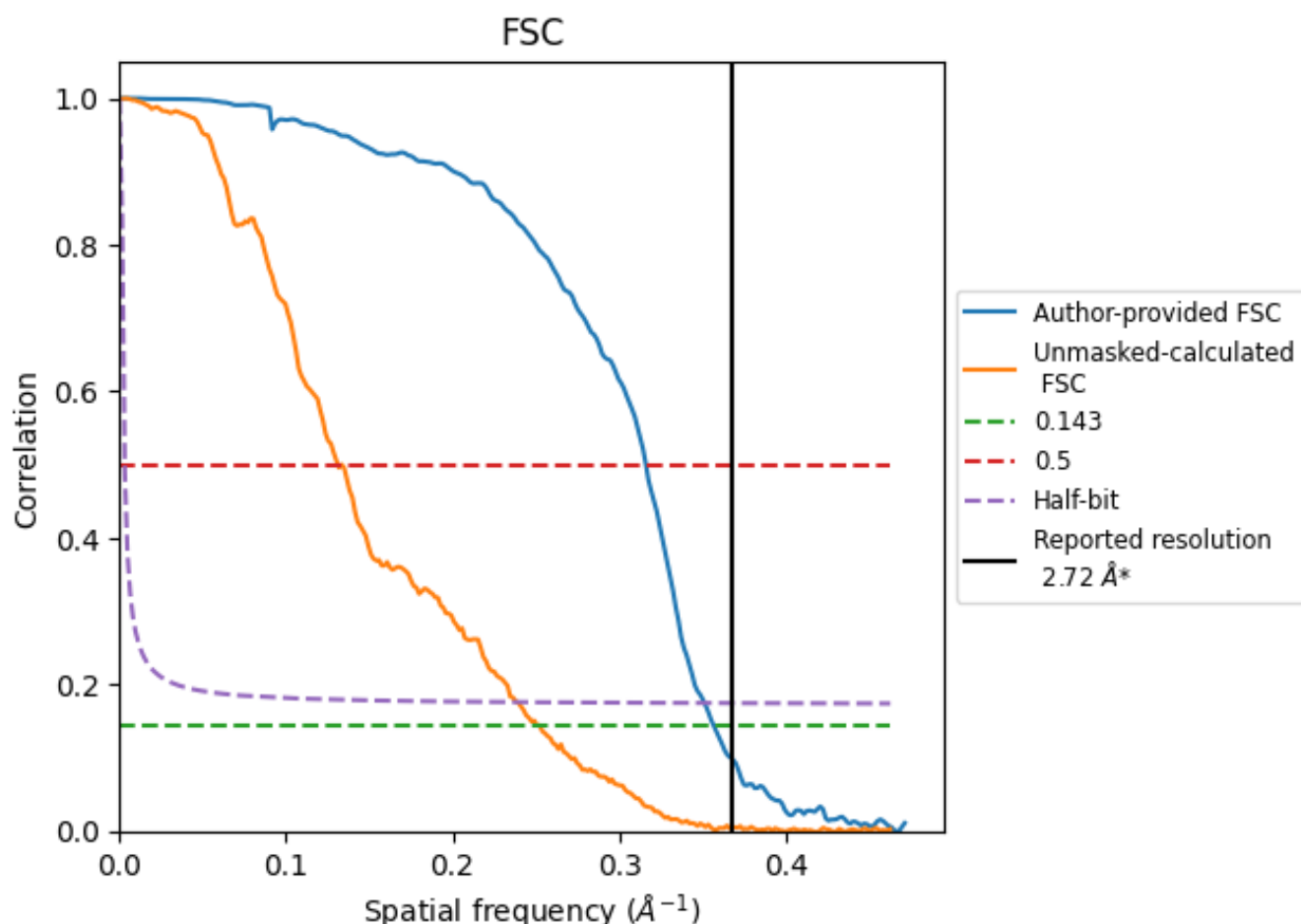


*Reported resolution corresponds to spatial frequency of 0.368 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.368 Å⁻¹

8.2 Resolution estimates [i](#)

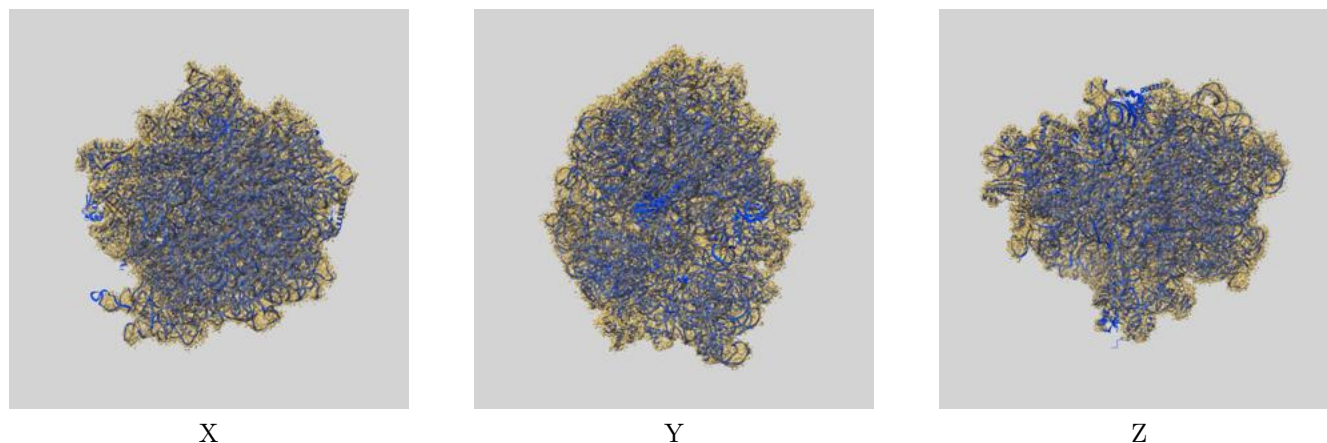
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	2.80	3.16	2.85
Unmasked-calculated*	3.96	7.63	4.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.96 differs from the reported value 2.72 by more than 10 %

9 Map-model fit [i](#)

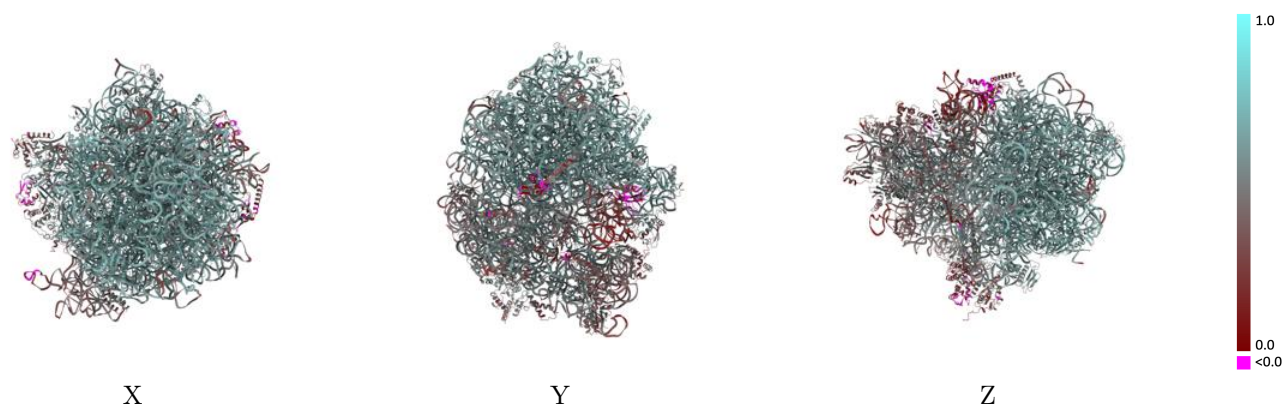
This section contains information regarding the fit between EMDB map EMD-24132 and PDB model 7N2C. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



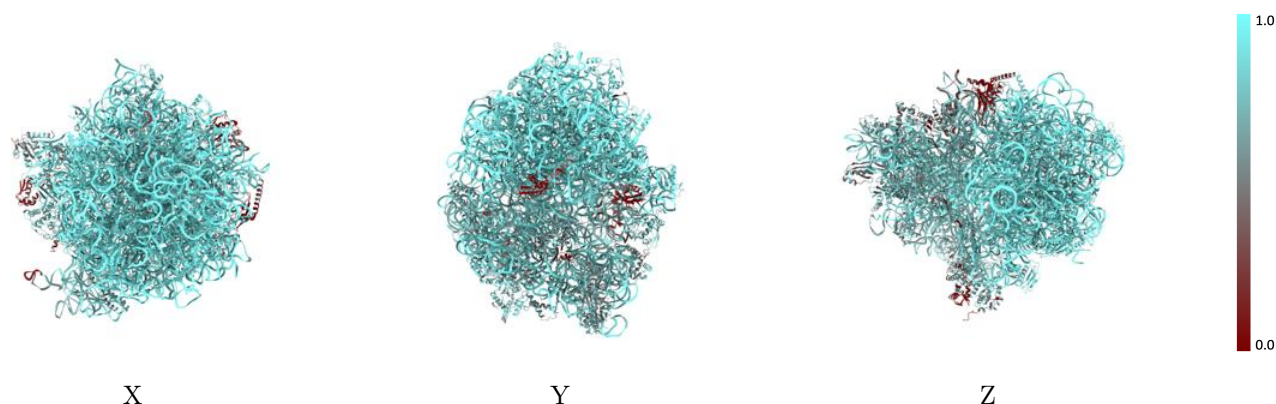
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



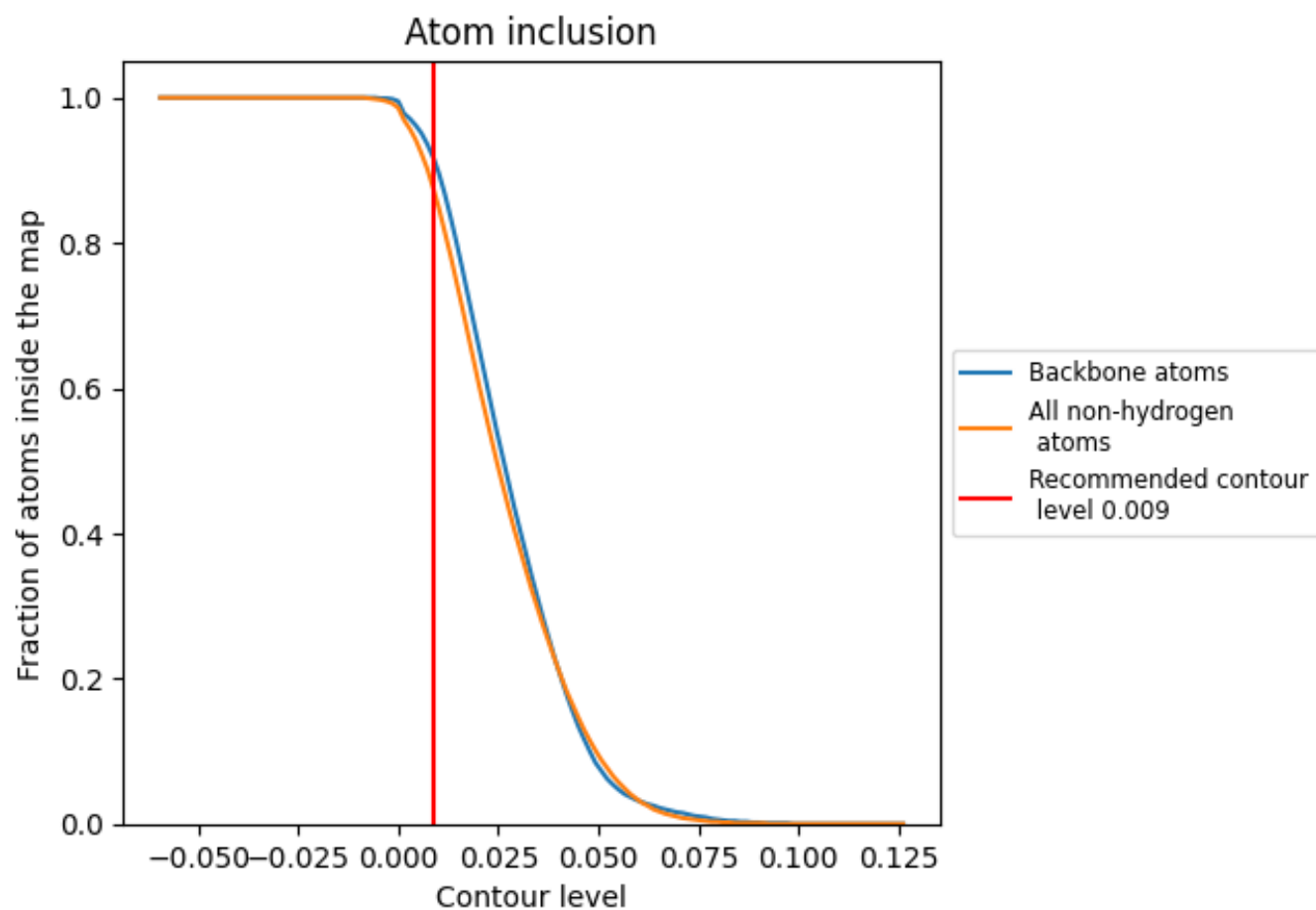
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.009).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ























































The table lists the average atom inclusion at the recommended contour level (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8700	 0.5330
16	 0.8780	 0.4890
23	 0.9590	 0.5920
5	 0.9630	 0.5780
Dt	 0.8430	 0.4490
EF	 0.7550	 0.4750
LA	 0.1540	 0.1230
LB	 0.9220	 0.6190
LC	 0.9350	 0.6220
LD	 0.8990	 0.5890
LE	 0.7650	 0.4910
LF	 0.8420	 0.5400
LG	 0.0910	 0.0660
LI	 0.3390	 0.2440
LJ	 0.5900	 0.3430
LK	 0.4850	 0.2890
LM	 0.9370	 0.6240
LN	 0.9150	 0.6140
LO	 0.9070	 0.6040
LP	 0.9270	 0.6130
LQ	 0.9580	 0.6330
LR	 0.8520	 0.5540
LS	 0.9090	 0.5930
LT	 0.9330	 0.6270
LU	 0.9130	 0.6020
LV	 0.9160	 0.6150
LW	 0.8820	 0.5900
LX	 0.9060	 0.5750
LY	 0.8960	 0.5750
La	 0.8720	 0.6080
Lb	 0.9320	 0.6070
Lc	 0.8610	 0.5440
Ld	 0.9450	 0.6140
Le	 0.6760	 0.3740
Lf	 0.9280	 0.6290



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Chain	Atom inclusion	Q-score
Lg	 0.8480	 0.5720
Lh	 0.9320	 0.6330
Li	 0.9370	 0.6280
Lj	 0.8800	 0.6010
Pp	 0.6790	 0.4830
Pt	 0.8470	 0.4840
SB	 0.6980	 0.4340
SC	 0.7520	 0.4810
SD	 0.6430	 0.3970
SE	 0.7880	 0.5010
SF	 0.5830	 0.3690
SG	 0.4650	 0.2960
SH	 0.7810	 0.5200
SI	 0.6330	 0.4330
SJ	 0.5710	 0.3950
SK	 0.5850	 0.4270
SL	 0.8040	 0.5380
SM	 0.6660	 0.3980
SN	 0.7130	 0.4730
SO	 0.7360	 0.4690
SP	 0.7180	 0.4760
SQ	 0.7180	 0.4660
SR	 0.5920	 0.4250
SS	 0.7120	 0.4760
ST	 0.7190	 0.4460
SU	 0.5800	 0.3660
mR	 0.6270	 0.3910