Full wwPDB EM Validation Report ⓘ

Mar 12, 2025 – 02:21 AM EDT

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:

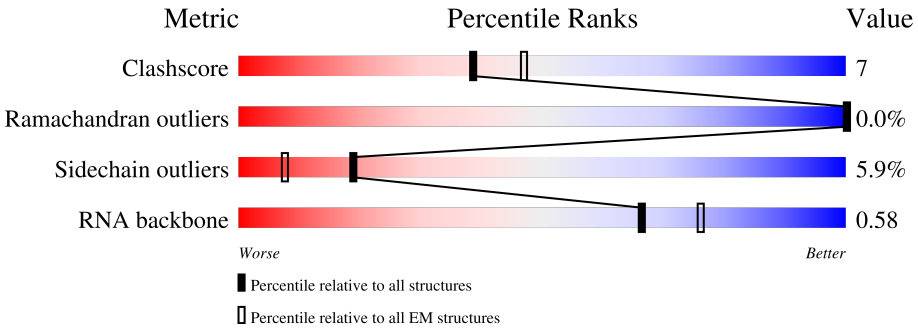
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 <=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	54% 41% 5%
2	SB	241	5% 63% 28% 6%
3	SC	233	62% 26% 12%
4	SD	206	15% 78% 21%
5	SE	167	69% 23% 7%
6	SF	135	14% 51% 23% 21%
7	SG	179	29% 61% 21% 5% 13%

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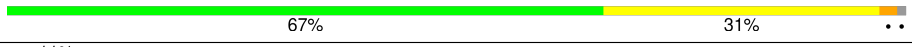
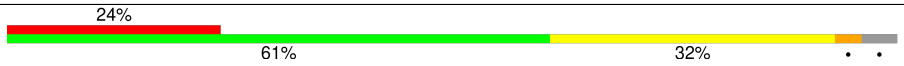
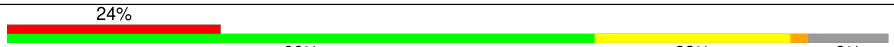
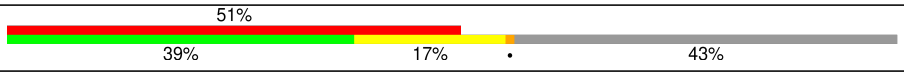
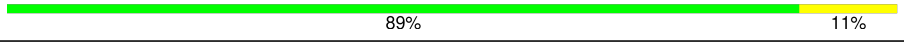
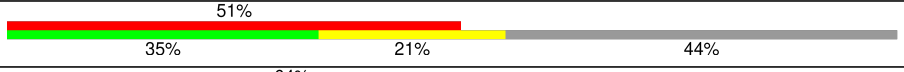
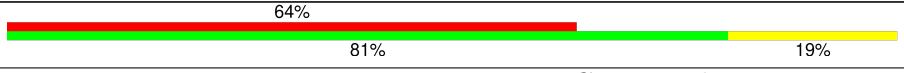
Mol	Chain	Length	Quality of chain
8	SH	130	
9	SI	130	
10	SJ	103	
11	SK	129	
12	SL	124	
13	SM	118	
14	SN	101	
15	SO	89	
16	SP	82	
17	SQ	84	
18	SR	75	
19	SS	92	
20	ST	87	
21	SU	71	
22	mR	60	
23	23	2904	
24	5	120	
25	LA	234	
26	LB	273	
27	LC	209	
28	LD	201	
29	LE	179	
30	LF	177	
31	LG	121	
32	LI	149	

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Mol	Chain	Length	Quality of chain
33	LJ	165	15% 63% 16% 18%
34	LK	142	33% 55% 37% 6%
35	LM	142	84% 16%
36	LN	123	85% 15%
37	LO	144	94% 6%
38	LP	136	85% 15%
39	LQ	127	84% 10% 6%
40	LR	117	80% 18%
41	LS	115	78% 21%
42	LT	118	85% 14%
43	LU	103	78% 22%
44	LV	110	81% 18%
45	LW	100	73% 20% 7%
46	LX	104	90% 8%
47	LY	94	84% 14%
48	La	85	6% 96%
49	Lb	78	96%
50	Lc	63	89% 10%
51	Ld	59	97%
52	Le	70	13% 91%
53	Lf	57	96%
54	Lg	55	89% 9%
55	Lh	46	100%
56	Li	65	95%
57	Lj	38	95% 5%

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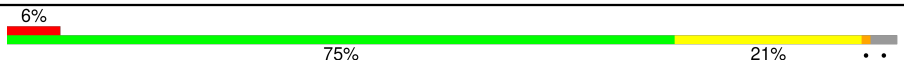
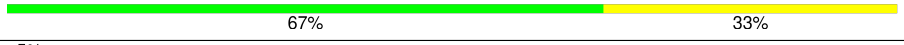
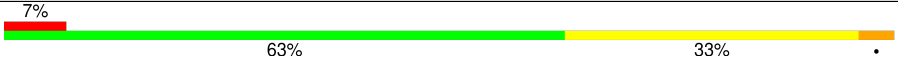
Mol	Chain	Length	Quality of chain
58	EF	704	
59	Pp	3	
60	Pt	76	
61	Dt	76	

2 Entry composition

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
			Total	C	N	O	P		
1	16	1534	32929	14693	6041	10661	1534	0	0

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

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

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

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

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

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

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

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

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

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

- 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 947	C 604	N 192	O 151	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- 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		

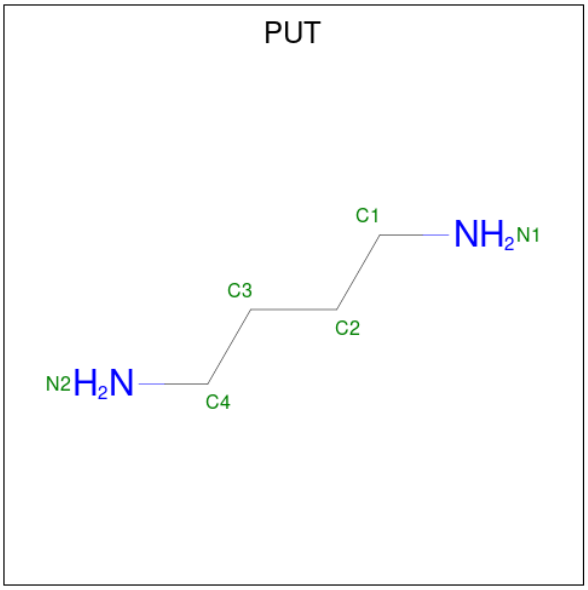
- Molecule 60 is a RNA chain called Chains: Pt.

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: $C_4H_{12}N_2$) (labeled as "Ligand of Interest" by depositor).



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

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

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

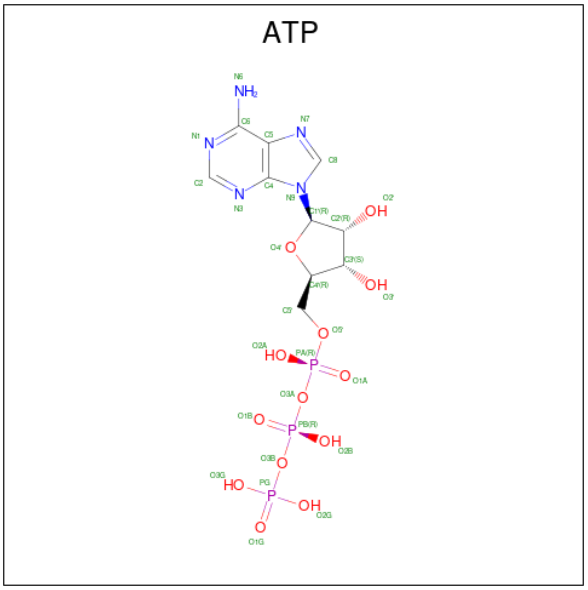
Mol	Chain	Residues	Atoms	AltConf
63	16	40	Total Mg 40 40	0
63	SN	2	Total Mg 2 2	0
63	23	144	Total Mg 144 144	0
63	5	4	Total Mg 4 4	0
63	LB	1	Total Mg 1 1	0
63	LC	1	Total Mg 1 1	0
63	LD	1	Total Mg 1 1	0
63	LQ	1	Total Mg 1 1	0
63	LW	1	Total Mg 1 1	0
63	Lf	1	Total Mg 1 1	0
63	EF	1	Total Mg 1 1	0

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

Interest" by depositor).

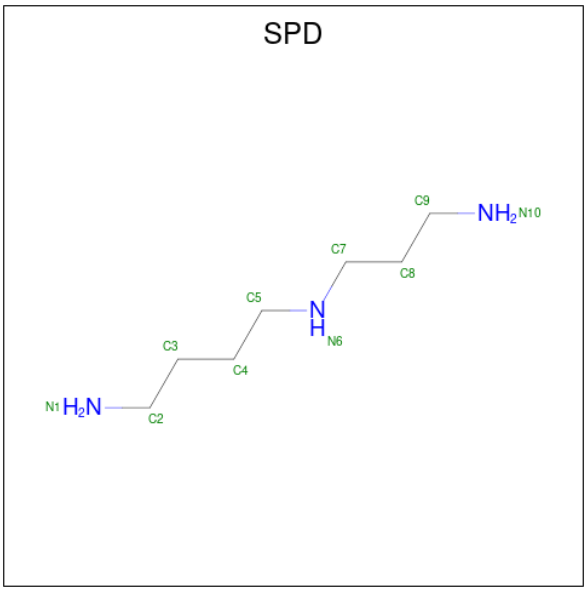
Mol	Chain	Residues	Atoms	AltConf
64	SB	1	Total Zn 1 1	0
64	Le	1	Total Zn 1 1	0
64	Lj	1	Total Zn 1 1	0

- 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).



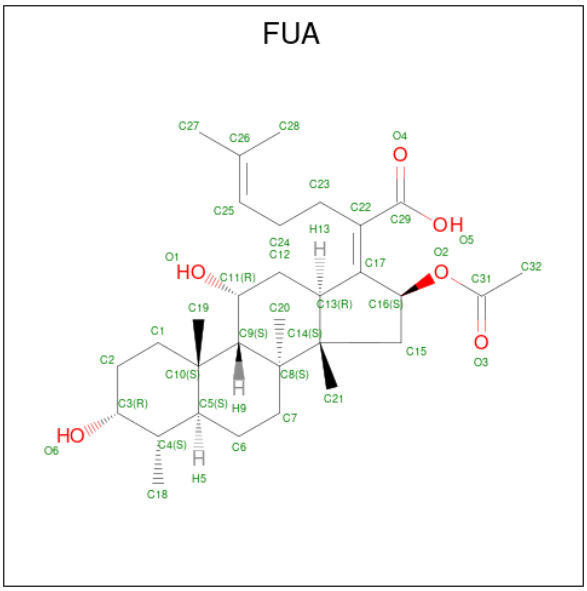
Mol	Chain	Residues	Atoms	AltConf
65	23	1	Total C N O P 31 10 5 13 3	0
65	23	1	Total C N O P 31 10 5 13 3	0

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



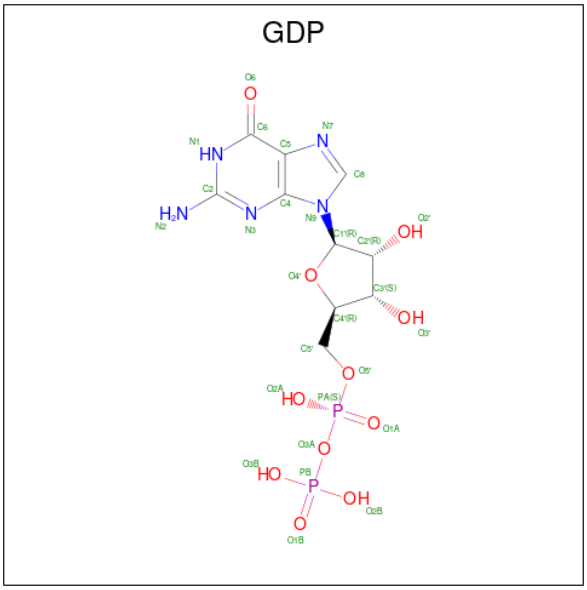
Mol	Chain	Residues	Atoms	AltConf
66	23	1	Total C N 10 7 3	0
66	23	1	Total C N 10 7 3	0
66	23	1	Total C N 10 7 3	0

- 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: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



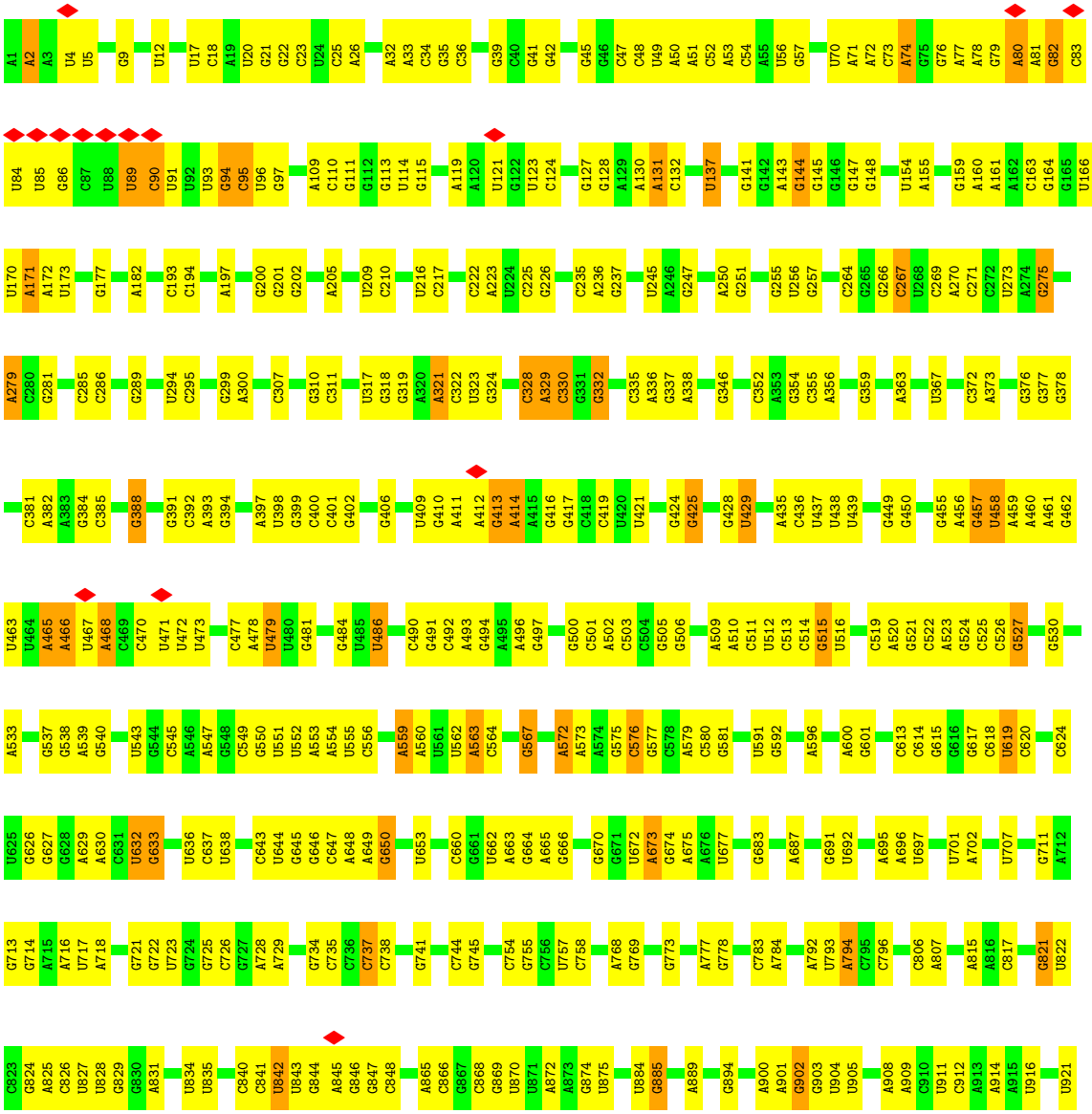
Mol	Chain	Residues	Atoms					AltConf
68	EF	1	Total	C	N	O	P	0
			28	10	5	11	2	

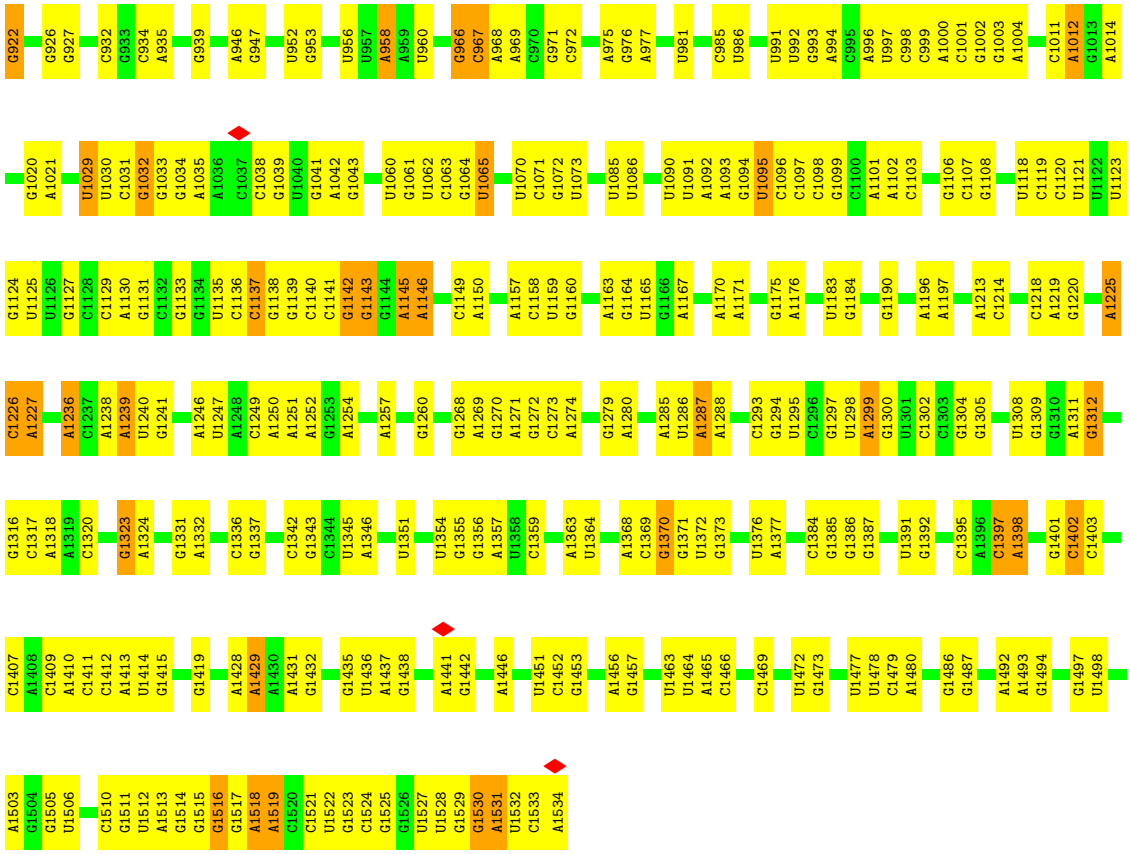
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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

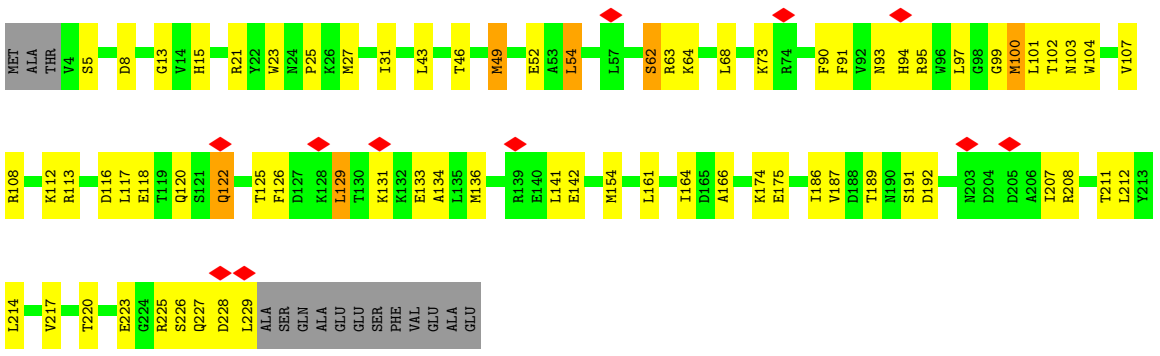
Chain 16:





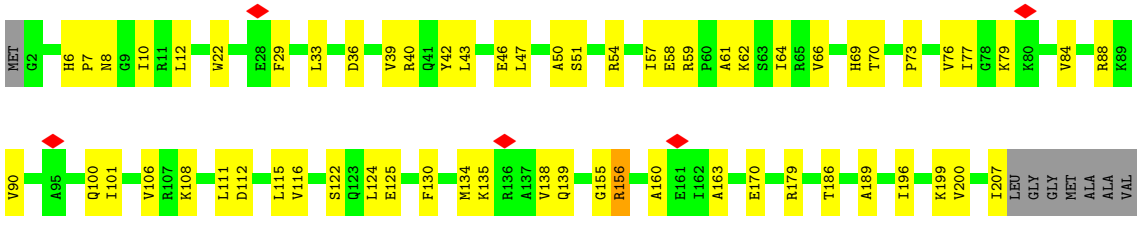
• Molecule 2: 30S ribosomal protein S2

Chain SB:



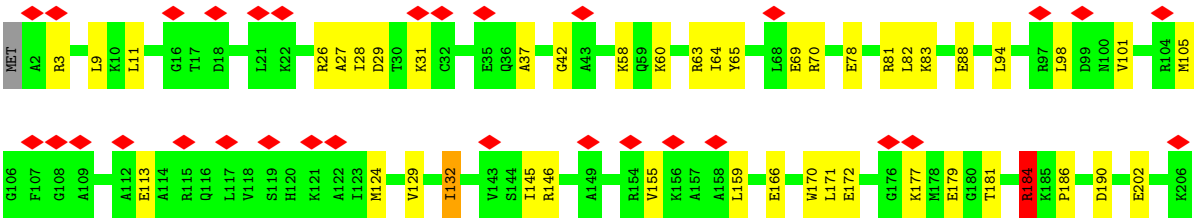
• Molecule 3: 30S ribosomal protein S3

Chain SC:



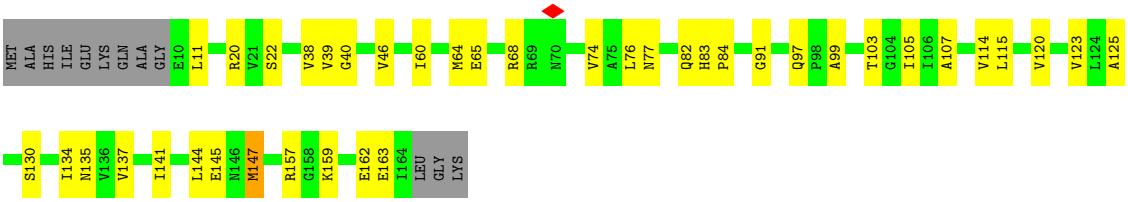
• Molecule 4: 30S ribosomal protein S4

Chain SD:



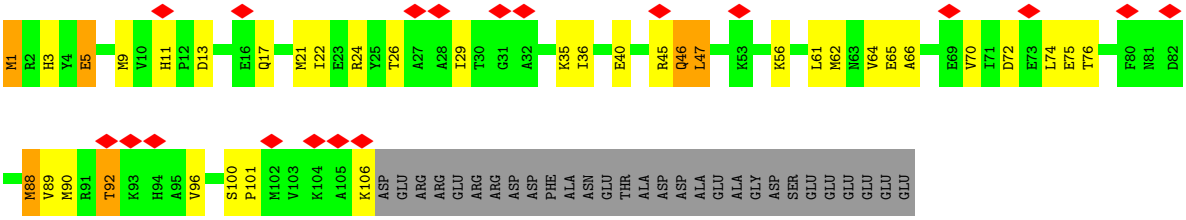
• Molecule 5: 30S ribosomal protein S5

Chain SE:



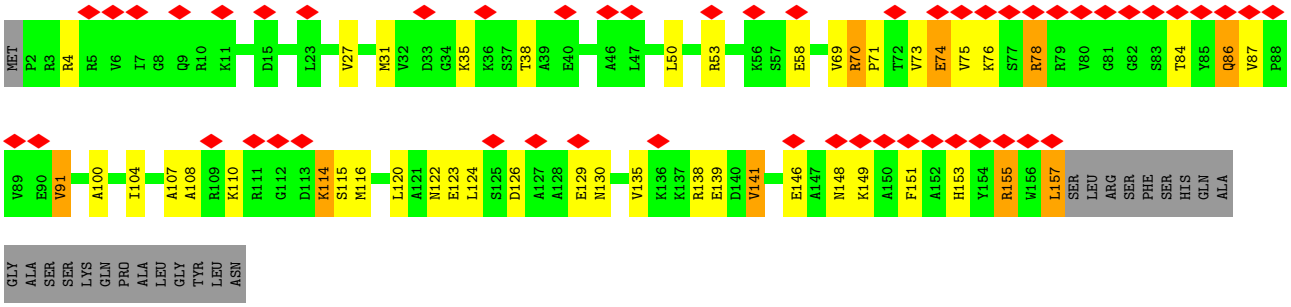
• Molecule 6: 30S ribosomal protein S6

Chain SF:



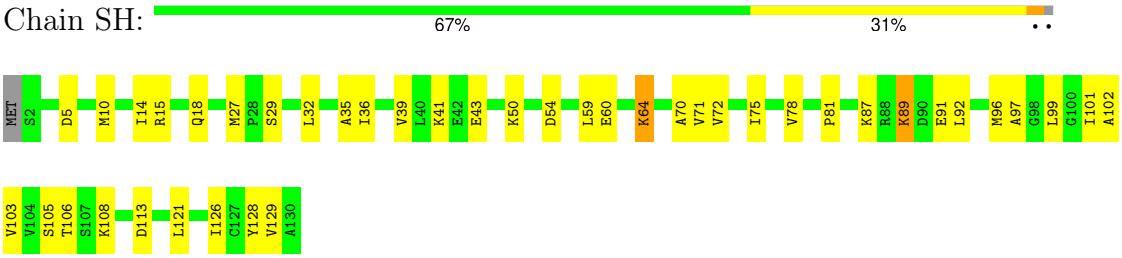
• Molecule 7: 30S ribosomal protein S7

Chain SG:



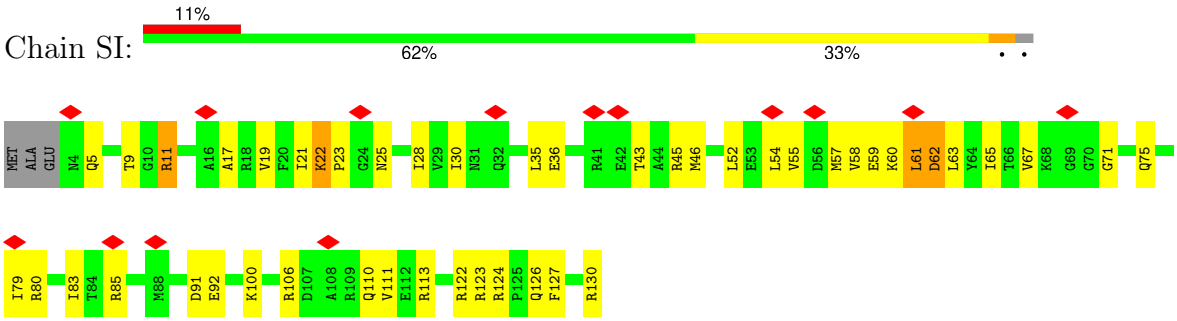
• Molecule 8: 30S ribosomal protein S8

Chain SH:



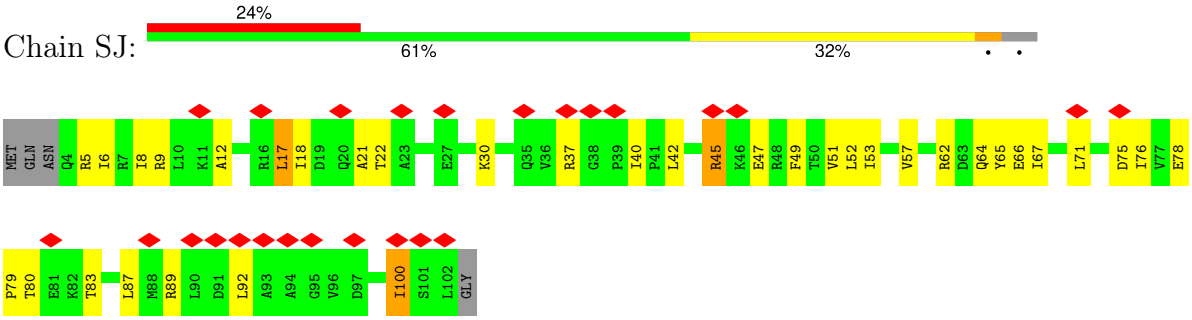
• Molecule 9: 30S ribosomal protein S9

Chain SI:



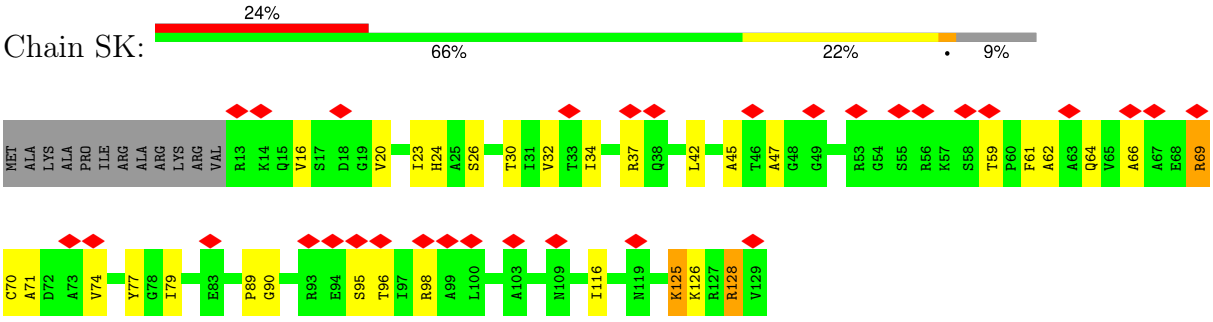
• Molecule 10: 30S ribosomal protein S10

Chain SJ:



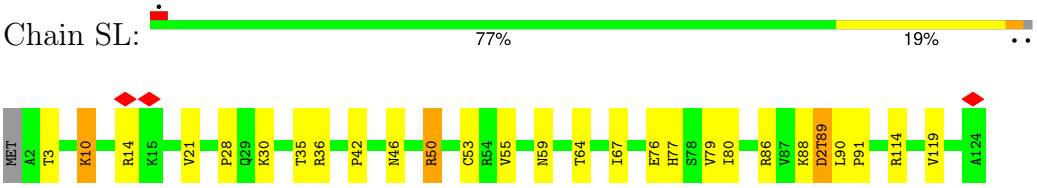
• Molecule 11: 30S ribosomal protein S11

Chain SK:



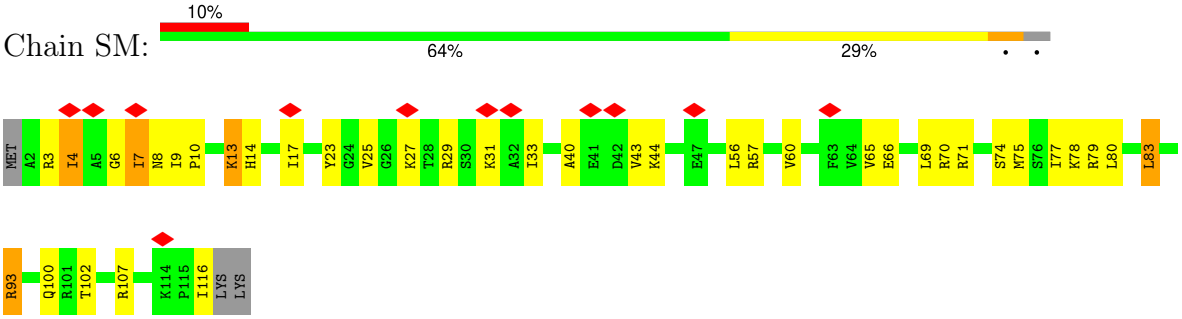
• Molecule 12: 30S ribosomal protein S12

Chain SL:



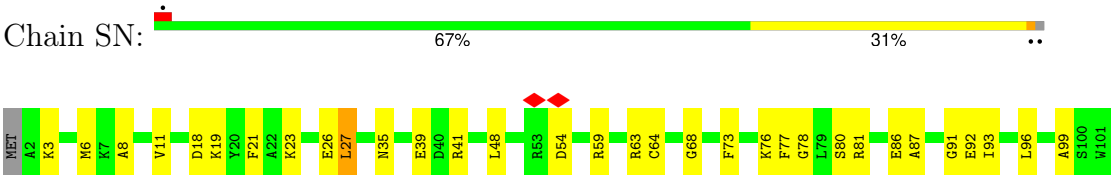
• Molecule 13: 30S ribosomal protein S13

Chain SM:



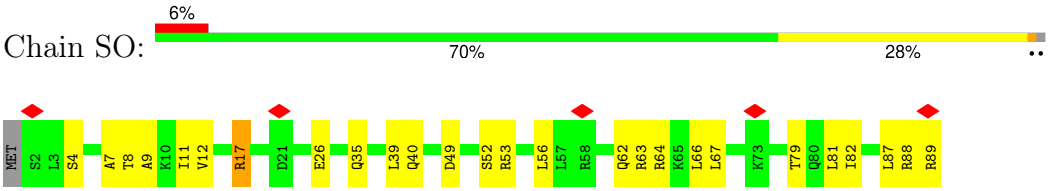
• Molecule 14: 30S ribosomal protein S14

Chain SN:



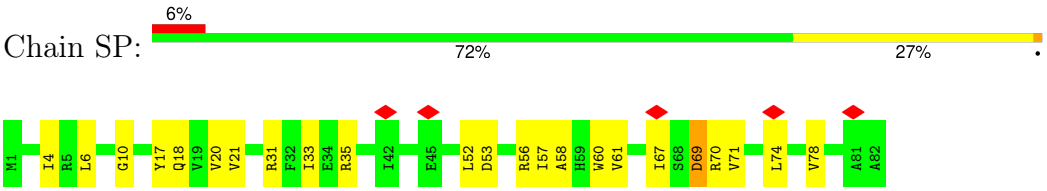
• Molecule 15: 30S ribosomal protein S15

Chain SO:



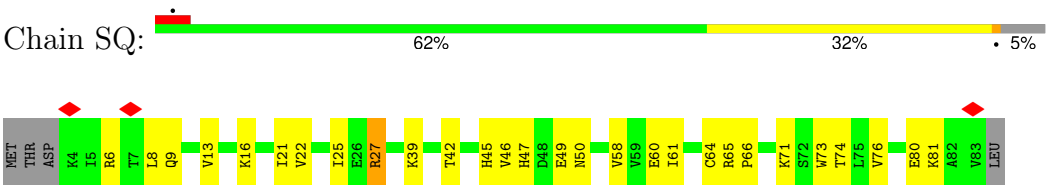
• Molecule 16: 30S ribosomal protein S16

Chain SP:



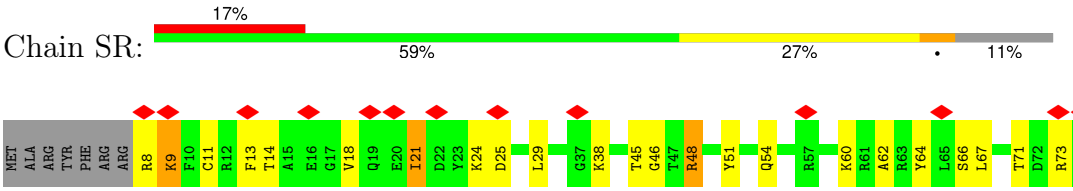
• Molecule 17: 30S ribosomal protein S17

Chain SQ:



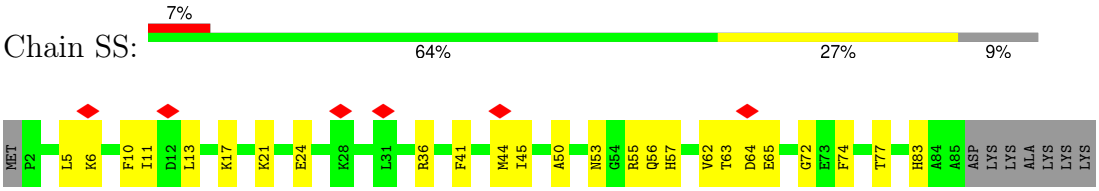
• Molecule 18: 30S ribosomal protein S18

Chain SR:



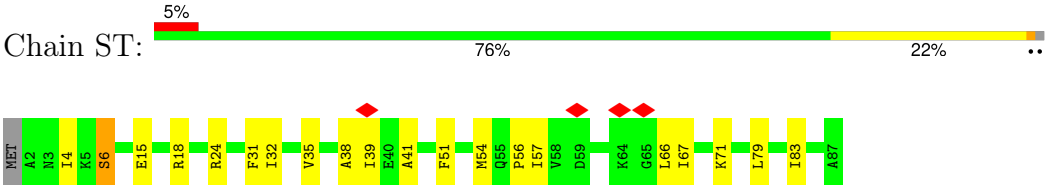
• Molecule 19: 30S ribosomal protein S19

Chain SS:



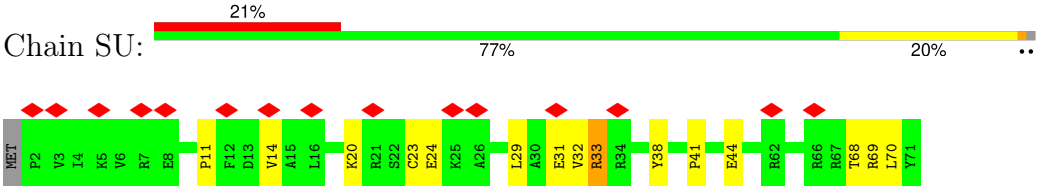
• Molecule 20: 30S ribosomal protein S20

Chain ST:



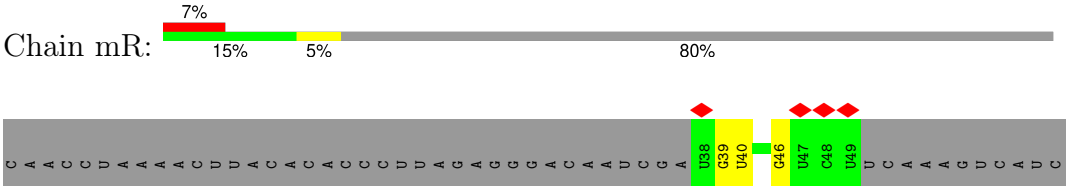
• Molecule 21: 30S ribosomal protein S21

Chain SU:



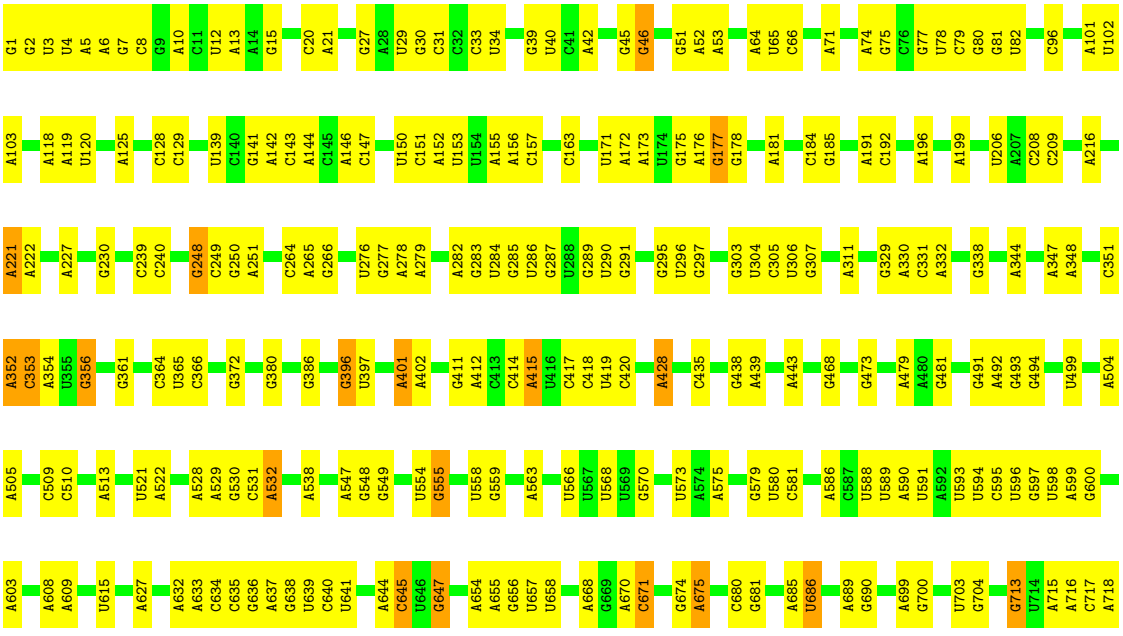
• Molecule 22: Chains: mR

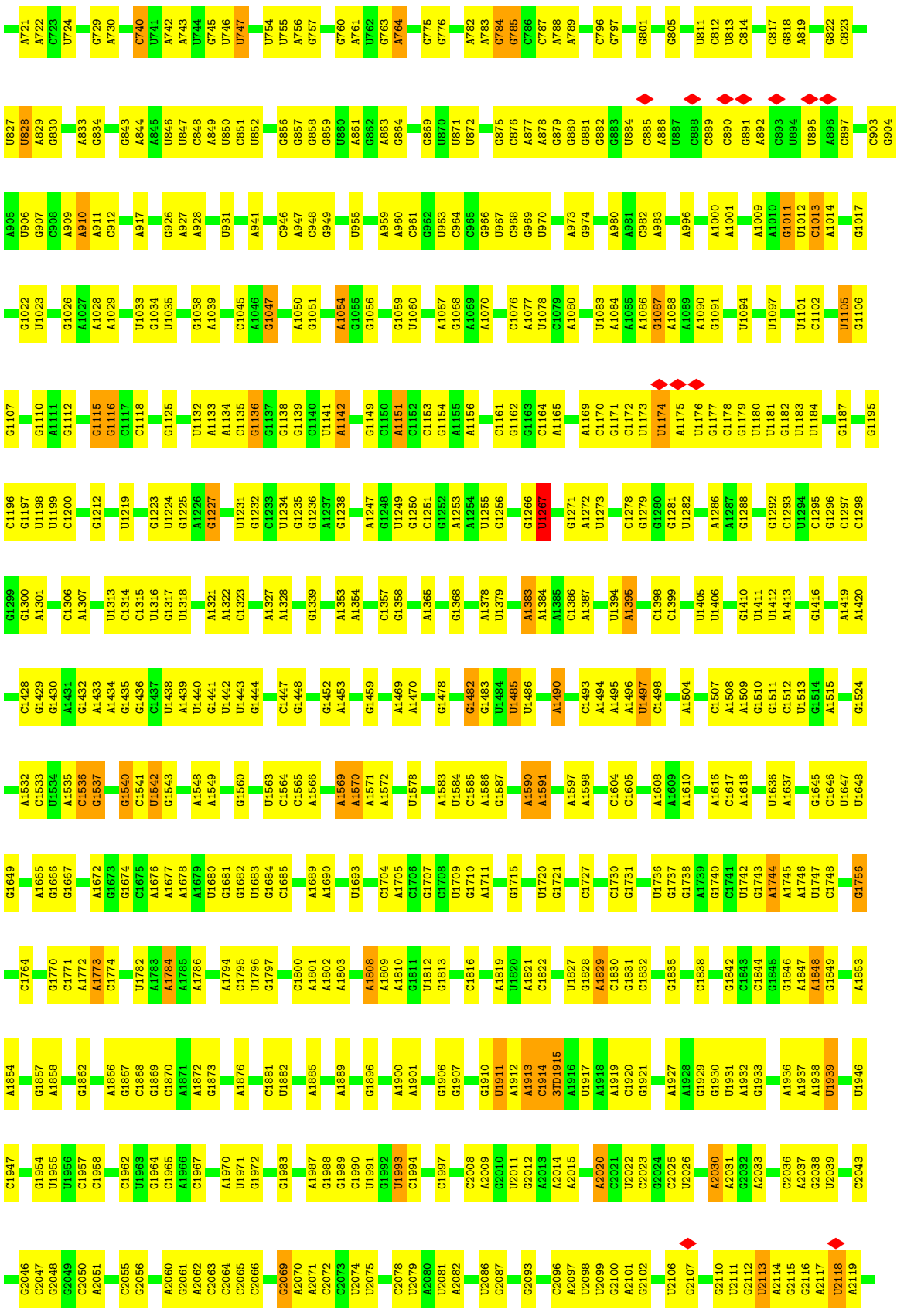
Chain mR:

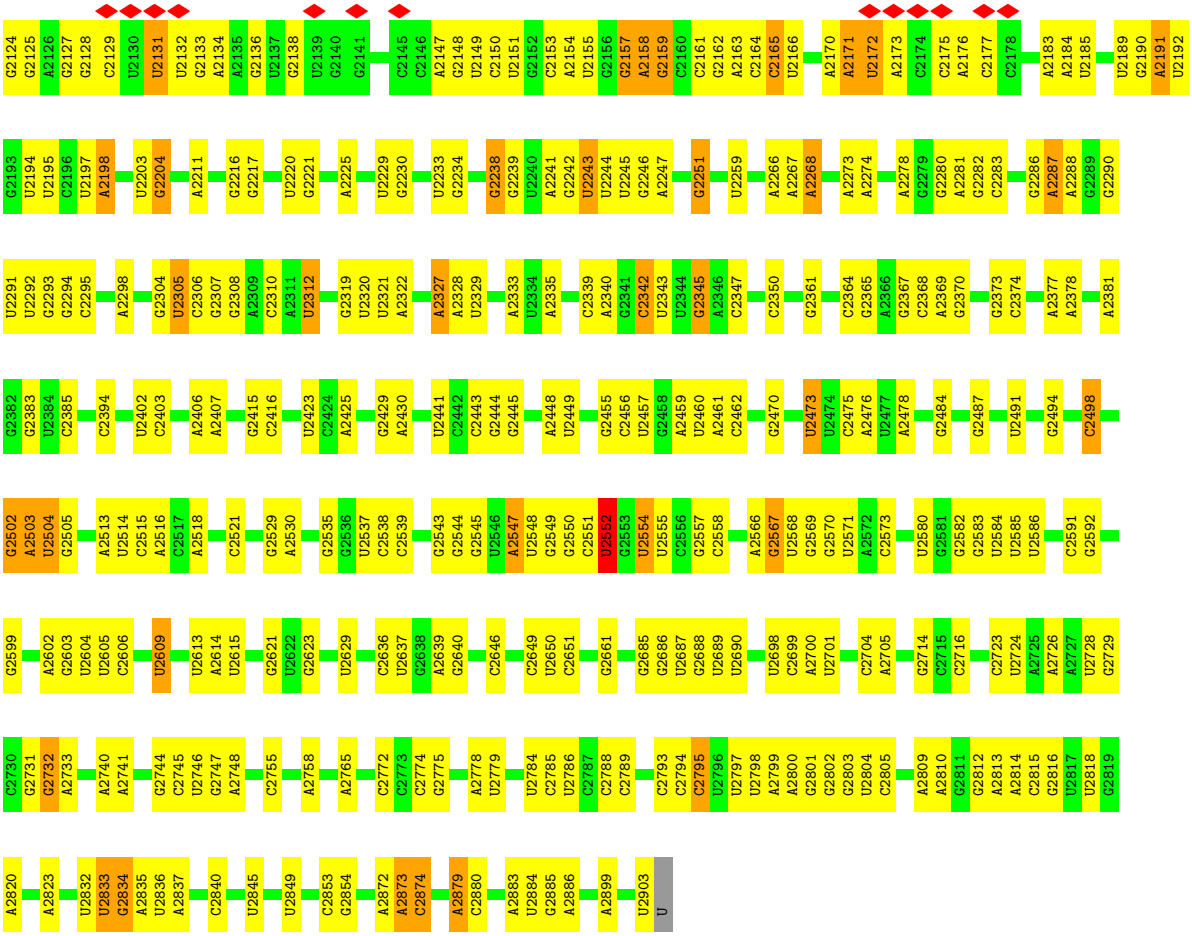


• Molecule 23: 23S rRNA

Chain 23:

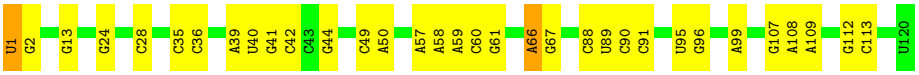



A721 A722 C723 U724 G729 A730 C740 U741 A742 A743 U744 G745 U746 U747 U754 U755 A756 G757 G760 A761 U762 G763 A764 G775 G776 A782 A783 G784 G785 C786 C787 A788 A789 C796 G797 G801 G805 U811 C812 U813 C814 C817 G818 A819 G822 C823
U827 U828 A829 G830 A833 G834 G843 A844 A845 U846 U847 C848 A849 U850 C851 U852 G856 G857 G858 G859 U860 A861 G862 A863 G864 G869 U870 U871 U872 G875 C876 A877 A878 G879 G880 G881 G882 G883 U884 C885 A886 U887 C888 C889 C890 G891 A892 C893 U894 U895 A896 C897 C903 G904
A905 U906 G907 C908 A909 A910 A911 C912 A917 G926 A927 A928 U931 A941 C946 A947 C948 G949 U955 A959 A960 C961 G962 U963 C964 G965 G966 U967 C968 G969 U970 A973 G974 A980 A981 C982 A983 A996 A1000 A1001 A1009 A1010 G1011 U1012 C1013 A1014 G1017
G1022 U1023 G1026 A1027 A1028 A1029 U1033 G1034 U1035 G1038 A1039 C1045 A1046 G1047 A1050 G1051 A1054 G1055 G1056 G1059 U1060 A1067 G1068 A1069 A1070 C1076 A1077 U1078 C1079 A1080 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1091 U1094 U1097 U1101 C1102 U1105 G1106
G1107 G1110 A1111 G1112 G1115 G1116 C1117 C1118 G1125 U1132 A1133 A1134 C1135 G1136 G1137 G1138 G1139 C1140 U1141 A1142 G1149 C1150 A1151 C1152 C1153 G1154 A1155 A1156 C1161 G1162 G1163 C1164 A1165 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 U1183 U1184 G1187 G1195
C1196 G1197 U1198 U1199 C1200 G1212 U1219 G1223 U1224 G1225 A1226 G1227 U1231 G1232 C1233 U1234 G1235 G1236 A1237 G1238 A1247 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 G1266 U1267 G1271 A1272 U1273 C1278 G1279 G1280 G1281 U1282 A1286 A1287 G1288 G1292 C1293 U1294 C1295 G1296 C1297 C1298
G1299 G1300 A1301 C1306 A1307 U1313 C1314 C1315 U1316 G1317 U1318 A1321 A1322 C1323 A1327 A1328 G1339 A1353 A1354 C1357 G1358 A1365 G1368 A1378 U1379 A1383 A1384 A1385 C1386 A1387 U1394 A1395 C1398 C1399 U1405 U1406 G1410 U1411 U1412 A1413 G1416 A1419 A1420
C1428 G1429 G1430 A1431 G1432 A1433 A1434 G1435 G1436 C1437 U1438 A1439 U1440 G1441 U1442 U1443 G1444 C1447 G1448 G1452 A1453 G1459 A1469 A1470 G1478 G1482 G1483 U1484 U1485 U1486 A1490 C1493 A1494 A1495 A1496 U1497 C1498 A1504 C1507 A1508 A1509 G1510 G1511 C1512 U1513 G1514 A1515 G1524
A1532 C1533 U1534 A1535 C1536 G1537 G1540 C1541 U1542 G1543 A1548 A1549 G1560 U1563 C1564 C1565 A1566 A1569 A1570 A1571 A1572 U1578 A1583 U1584 C1585 A1586 G1587 A1590 A1591 A1597 A1598 C1604 C1605 A1608 A1609 A1610 A1616 C1617 A1618 U1636 A1637 G1645 C1646 U1647 U1648
G1649 A1665 G1666 G1667 A1672 G1673 G1674 C1675 A1676 A1677 A1678 A1679 U1680 G1681 G1682 U1683 G1684 C1685 A1689 A1690 U1693 C1704 A1705 C1706 G1707 C1708 U1709 G1710 A1711 G1715 U1720 G1721 C1727 C1730 G1731 U1736 G1737 G1738 A1739 G1740 C1741 U1742 G1743 A1744 A1745 A1746 U1747 C1748 G1756
C1764 G1770 C1771 A1772 A1773 C1774 U1782 A1783 A1784 A1785 A1786 A1794 C1795 U1796 G1797 C1800 A1801 A1802 A1803 A1808 A1809 A1810 G1811 U1812 G1813 C1816 A1819 U1820 A1821 C1822 U1827 G1828 A1829 C1830 G1831 C1832 G1835 C1838 G1842 C1843 C1844 G1845 G1846 A1847 A1848 G1849 A1853
A1854 G1857 A1858 G1862 A1866 G1867 C1868 G1869 C1870 A1871 A1872 G1873 A1876 C1881 U1882 A1885 A1889 G1896 A1900 A1901 G1906 G1907 G1910 U1911 A1912 A1913 C1914 3TD1915 A1916 U1917 A1918 A1919 C1920 G1921 A1927 A1928 G1929 G1930 U1931 A1932 G1933 A1936 A1937 A1938 U1939 U1946
C1947 G1954 U1955 U1956 C1957 C1958 C1962 U1963 G1964 C1965 A1966 C1967 A1970 U1971 G1972 G1983 A1987 G1988 G1989 C1990 U1991 G1992 U1993 C1994 C1997 C2008 A2009 G2010 U2011 G2012 A2013 A2014 A2015 A2020 C2021 U2022 C2023 G2024 C2025 U2026 A2030 A2031 G2032 A2033 C2036 A2037 G2038 U2039 C2043
G2046 C2047 G2048 G2049 C2050 A2051 C2055 G2056 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2069 A2070 A2071 C2072 C2073 U2074 U2075 C2078 U2079 A2080 U2081 A2082 U2086 G2087 G2093 C2096 A2097 U2098 U2099 G2100 A2101 G2102 U2106 G2107 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119



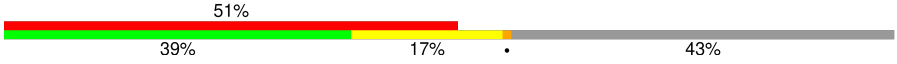
• Molecule 24: 5S rRNA

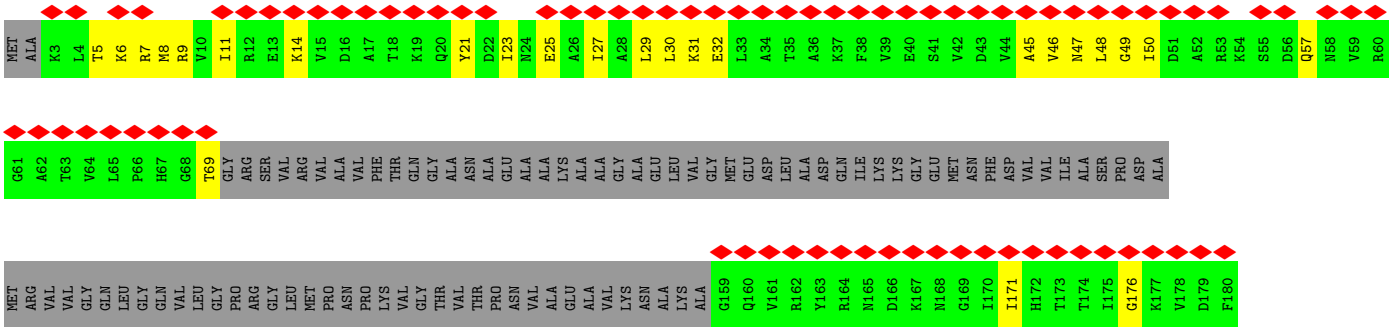
Chain 5:



• Molecule 25: 50S ribosomal protein L1

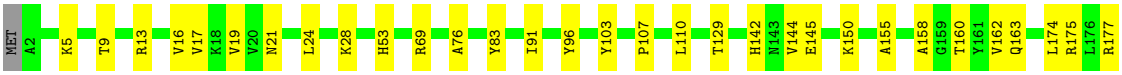
Chain LA:

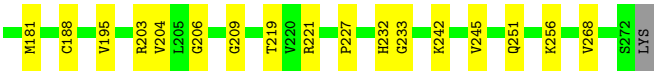




• Molecule 26: 50S ribosomal protein L2

Chain LB:



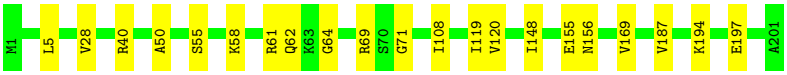


• Molecule 27: 50S ribosomal protein L3

Chain LC:

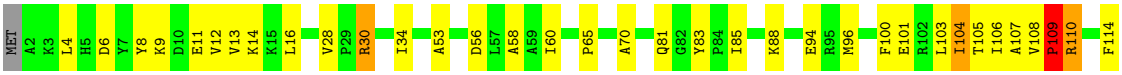
• Molecule 28: 50S ribosomal protein L4

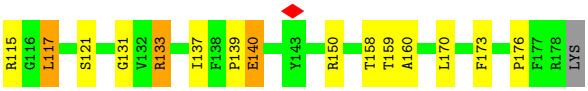
Chain LD:



• Molecule 29: 50S ribosomal protein L5

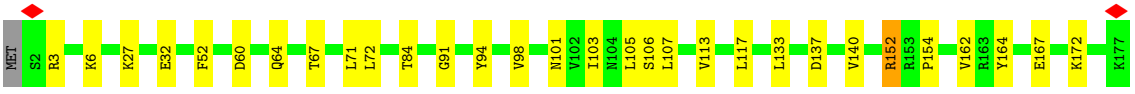
Chain LE:





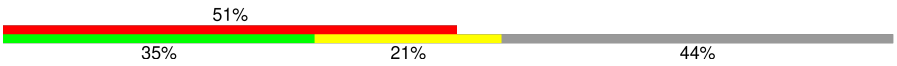
• Molecule 30: 50S ribosomal protein L6

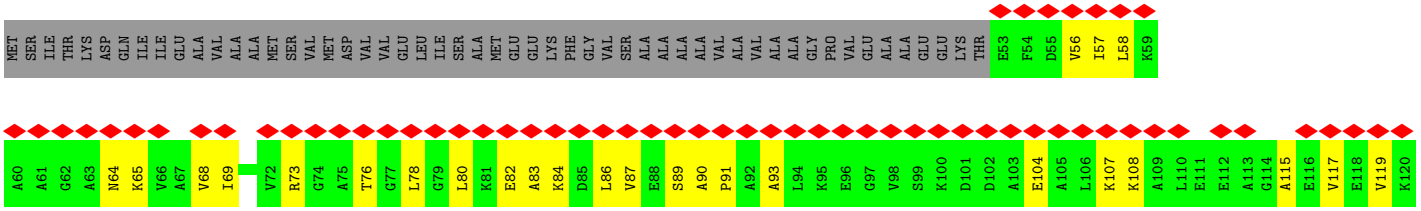
Chain LF:



• Molecule 31: 50S ribosomal protein L7/L12

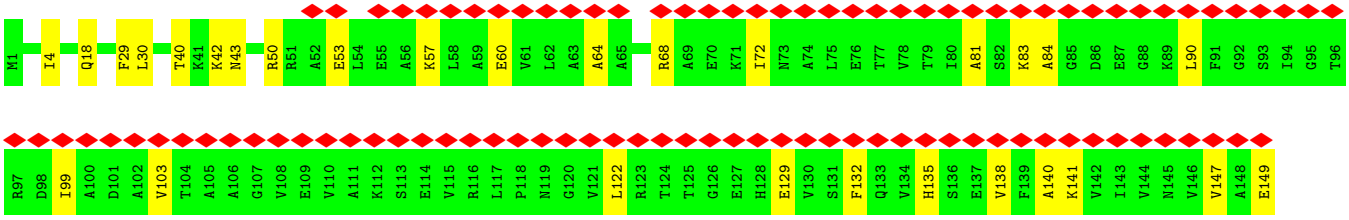
Chain LG:





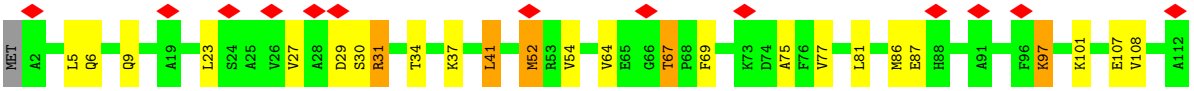
• Molecule 32: 50S ribosomal protein L9

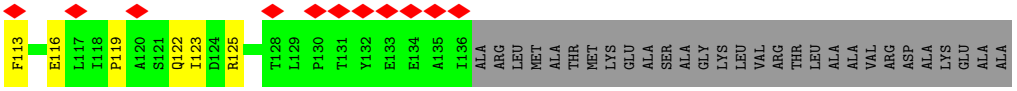
Chain LI:



• Molecule 33: 50S ribosomal protein L10

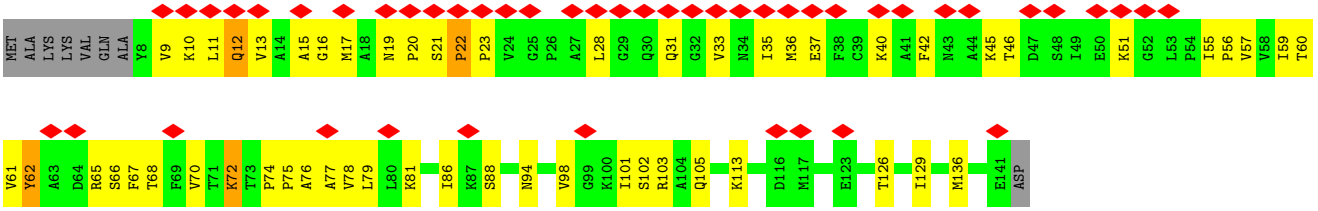
Chain LJ:





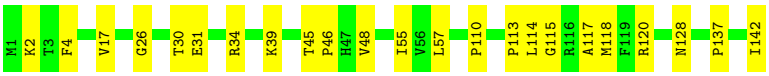
• Molecule 34: 50S ribosomal protein L11

Chain LK:



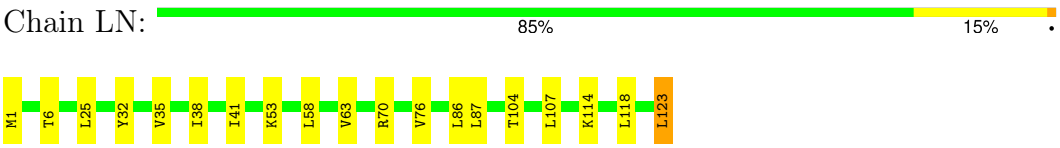
• Molecule 35: 50S ribosomal protein L13

Chain LM:



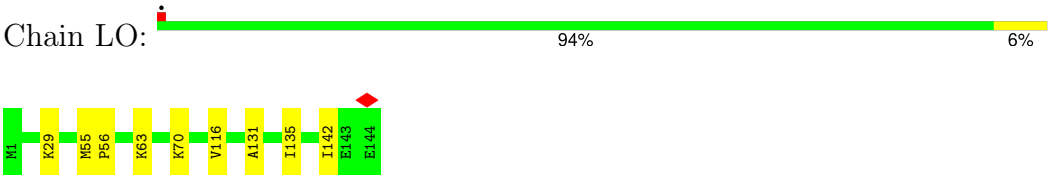
• Molecule 36: 50S ribosomal protein L14

Chain LN:



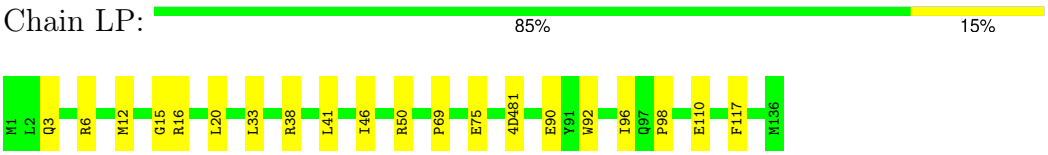
• Molecule 37: 50S ribosomal protein L15

Chain LO:



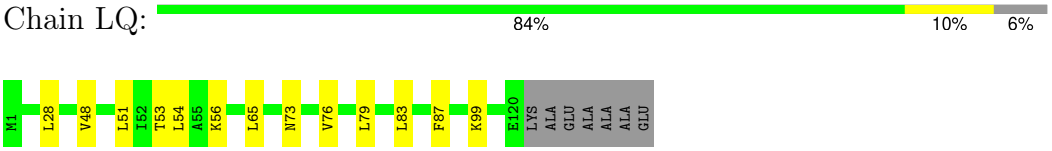
• Molecule 38: 50S ribosomal protein L16

Chain LP:



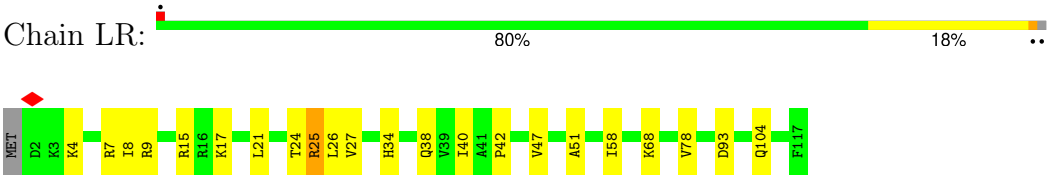
• Molecule 39: 50S ribosomal protein L17

Chain LQ:



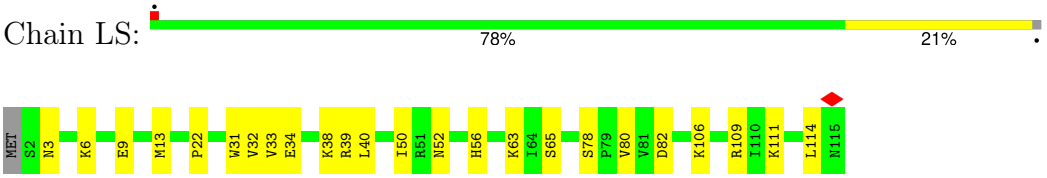
• Molecule 40: 50S ribosomal protein L18

Chain LR:



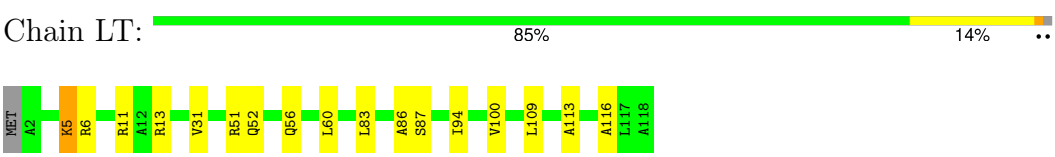
• Molecule 41: 50S ribosomal protein L19

Chain LS:



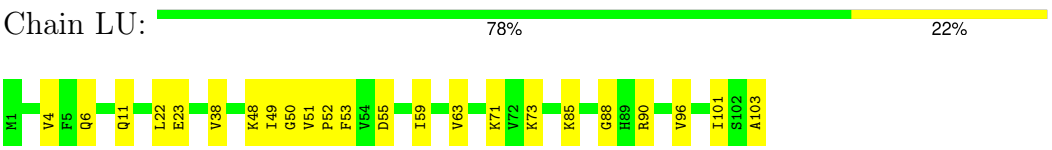
• Molecule 42: 50S ribosomal protein L20

Chain LT:



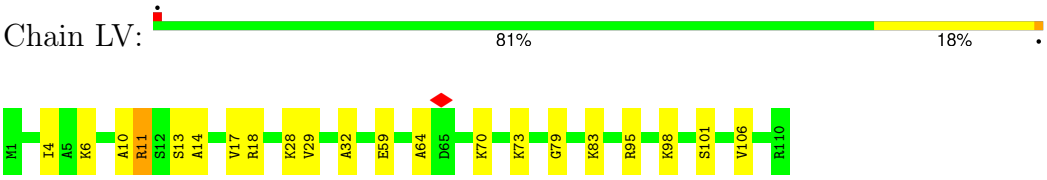
• Molecule 43: 50S ribosomal protein L21

Chain LU:



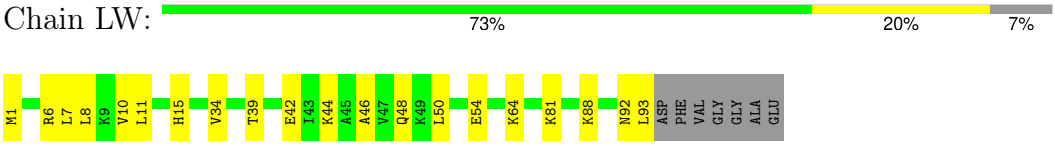
• Molecule 44: 50S ribosomal protein L22

Chain LV:



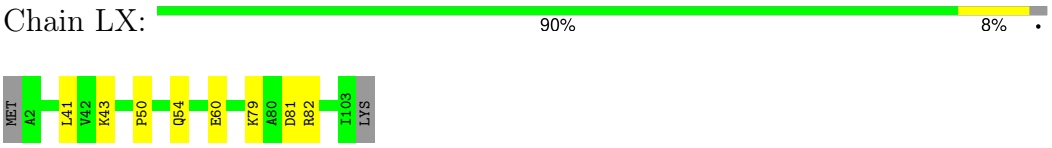
• Molecule 45: 50S ribosomal protein L23

Chain LW:



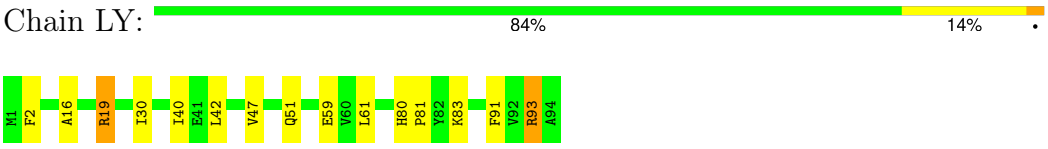
• Molecule 46: 50S ribosomal protein L24

Chain LX:



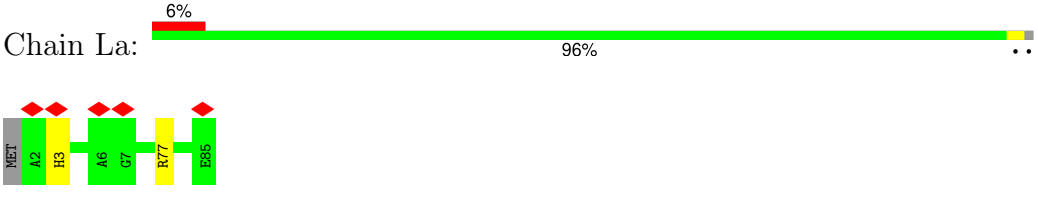
• Molecule 47: 50S ribosomal protein L25

Chain LY:



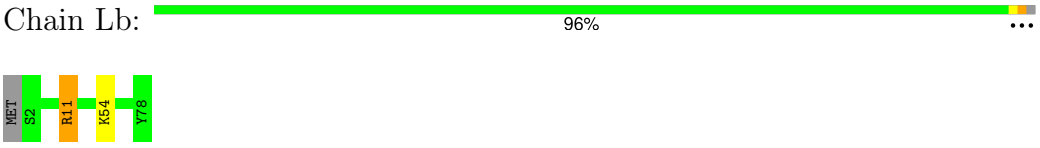
• Molecule 48: 50S ribosomal protein L27

Chain La:



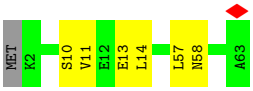
• Molecule 49: 50S ribosomal protein L28

Chain Lb:



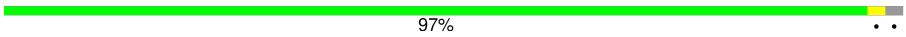
• Molecule 50: 50S ribosomal protein L29

Chain Lc:



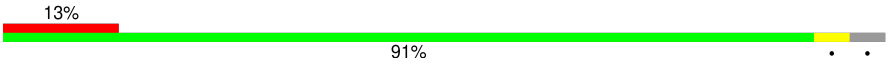
• Molecule 51: 50S ribosomal protein L30

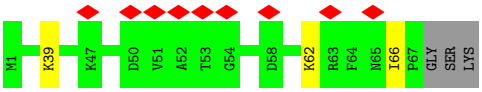
Chain Ld:



• Molecule 52: 50S ribosomal protein L31

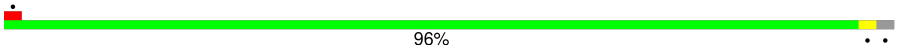
Chain Le:

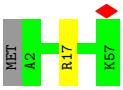




• Molecule 53: 50S ribosomal protein L32

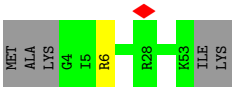
Chain Lf:





• Molecule 54: 50S ribosomal protein L33

Chain Lg:



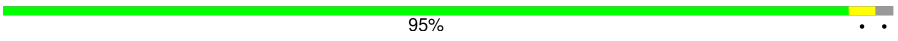
• Molecule 55: 50S ribosomal protein L34

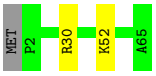
Chain Lh:

There are no outlier residues recorded for this chain.

• Molecule 56: 50S ribosomal protein L35

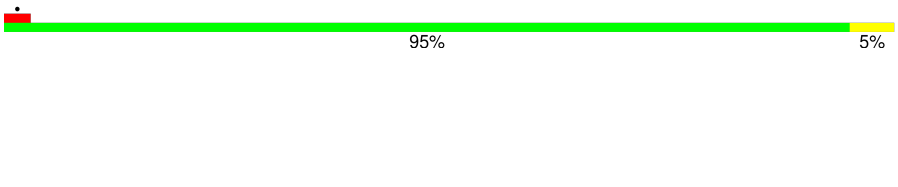
Chain Li:





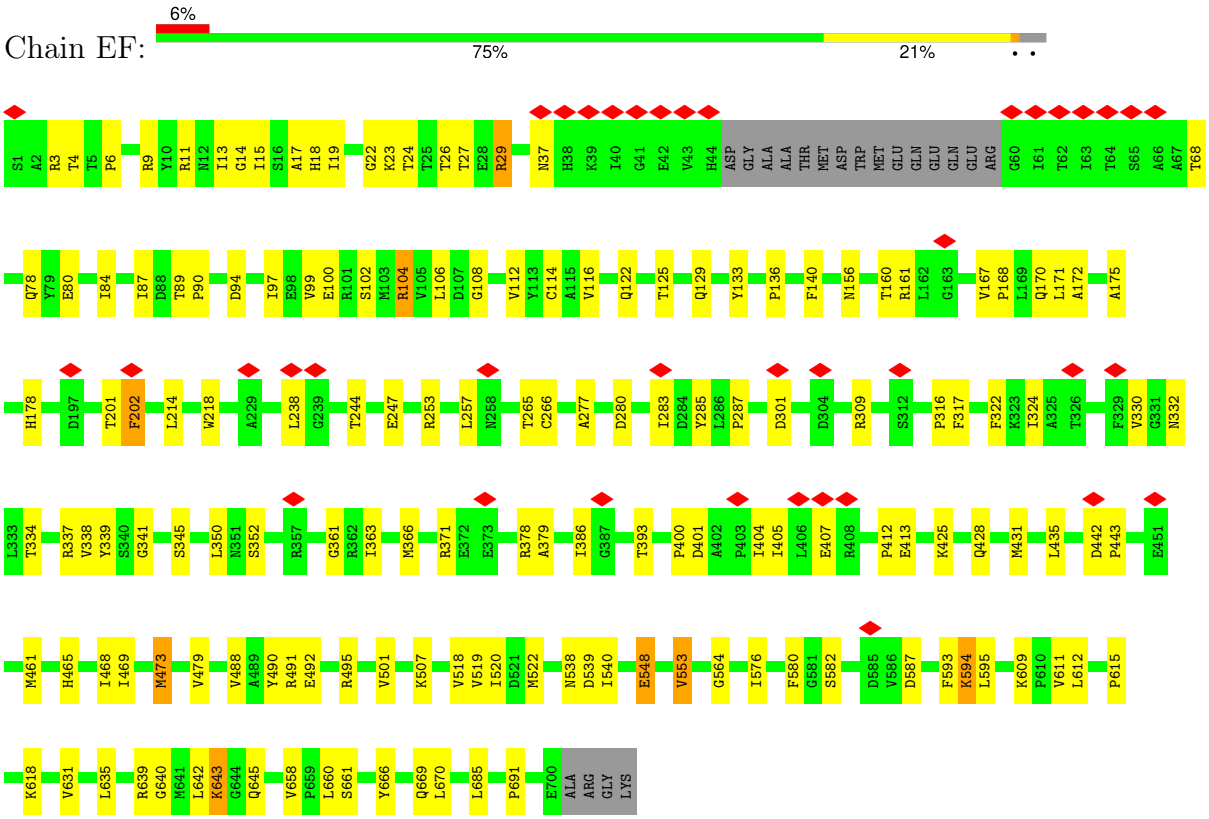
• Molecule 57: 50S ribosomal protein L36

Chain Lj:



• Molecule 58: Elongation factor G

Chain EF:

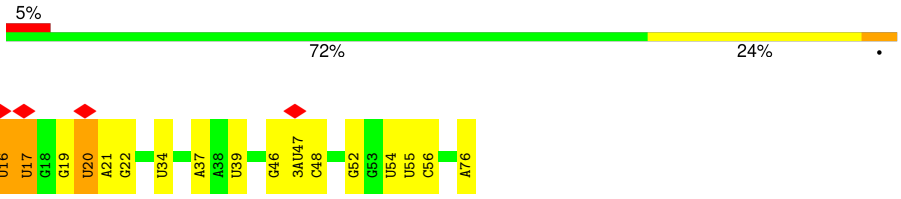


• Molecule 59: Polypeptide

Chain Pp:

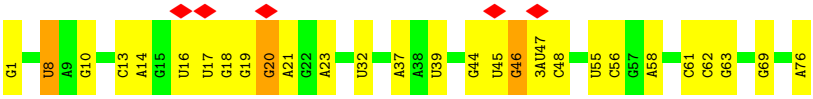
• Molecule 60: Chains: Pt

Chain Pt:



• Molecule 61: tRNA

Chain Dt:


G1
U8
A9
G10
C13
A14
G15
U16
U17
G18
G19
G20
A21
G22
A23
U32
A37
A38
U39
G44
U45
G46
3AU47
C48
U55
C56
G57
A58
C61
C62
G63
G69
A76

4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	610.55994, 610.55994, 610.55994	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Continued on next page...

Continued from previous page...

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (i)

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 (i)

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	$\#\|Z\| > 2$
23	2MA	23	2503	63,23	18,25,26	0.68	0	20,37,40	1.99	4 (20%)
60	H2U	Pt	20	60	18,21,22	1.07	2 (11%)	19,30,33	1.33	4 (21%)
61	PSU	Dt	39	61	18,21,22	1.37	2 (11%)	21,30,33	2.05	4 (19%)
23	PSU	23	2605	23	18,21,22	1.40	4 (22%)	21,30,33	2.02	4 (19%)
60	3AU	Pt	47	60	24,28,29	1.03	0	30,40,43	1.57	5 (16%)
23	2MG	23	1835	23	18,26,27	0.90	1 (5%)	16,38,41	1.32	3 (18%)
23	PSU	23	2504	23	18,21,22	1.39	3 (16%)	21,30,33	2.09	3 (14%)
1	MA6	16	1518	1	19,26,27	1.30	3 (15%)	18,38,41	2.25	6 (33%)
23	PSU	23	955	23	18,21,22	1.40	3 (16%)	21,30,33	2.12	4 (19%)
61	PSU	Dt	32	61	18,21,22	1.37	2 (11%)	21,30,33	2.02	3 (14%)
60	H2U	Pt	17	60	18,21,22	0.97	2 (11%)	19,30,33	0.99	2 (10%)
61	MIA	Dt	37	61	24,31,32	2.30	3 (12%)	22,44,47	2.78	7 (31%)
60	5MU	Pt	54	60	19,22,23	1.39	6 (31%)	27,32,35	2.08	6 (22%)
61	G7M	Dt	46	61	20,26,27	2.60	4 (20%)	16,39,42	1.27	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	OMC	23	2498	63,23	19,22,23	0.81	0	25,31,34	0.91	1 (4%)
23	PSU	23	746	63,23	18,21,22	1.40	3 (16%)	21,30,33	1.99	4 (19%)
23	6MZ	23	1618	23	17,25,26	0.93	1 (5%)	15,36,39	2.20	4 (26%)
23	G7M	23	2069	23	20,26,27	2.79	5 (25%)	16,39,42	2.11	4 (25%)
60	U8U	Pt	34	60,22	20,24,25	1.50	3 (15%)	22,34,37	1.25	3 (13%)
38	4D4	LP	81	38	9,11,12	2.19	2 (22%)	7,13,15	2.07	3 (42%)
61	PSU	Dt	55	61	18,21,22	1.43	2 (11%)	21,30,33	2.20	4 (19%)
1	2MG	16	1516	1	18,26,27	0.90	1 (5%)	16,38,41	1.36	3 (18%)
1	PSU	16	516	1	18,21,22	1.42	3 (16%)	21,30,33	2.09	4 (19%)
61	3AU	Dt	47	61	24,28,29	1.02	0	30,40,43	1.60	4 (13%)
23	OMG	23	2251	60,23	19,26,27	1.18	2 (10%)	21,38,41	0.83	1 (4%)
60	T6A	Pt	37	60	26,34,35	0.97	1 (3%)	28,49,52	1.71	5 (17%)
61	4SU	Dt	8	61	18,21,22	1.96	4 (22%)	25,30,33	2.25	6 (24%)
12	D2T	SL	89	12	8,9,10	2.44	1 (12%)	6,11,13	2.91	4 (66%)
23	PSU	23	1911	23	18,21,22	6.15	13 (72%)	21,30,33	1.98	5 (23%)
1	4OC	16	1402	1	20,23,24	0.76	0	25,32,35	0.94	1 (4%)
23	H2U	23	2449	23	18,21,22	1.09	3 (16%)	19,30,33	1.02	1 (5%)
23	5MU	23	747	23	19,22,23	1.40	5 (26%)	27,32,35	2.12	6 (22%)
23	6MZ	23	2030	23	17,25,26	0.88	1 (5%)	15,36,39	2.41	4 (26%)
23	OMU	23	2552	23	19,22,23	1.24	3 (15%)	25,31,34	1.86	5 (20%)
23	PSU	23	2580	23	18,21,22	1.41	3 (16%)	21,30,33	2.08	4 (19%)
60	PSU	Pt	39	60	18,21,22	1.40	2 (11%)	21,30,33	2.01	4 (19%)
23	PSU	23	1917	23	18,21,22	6.15	12 (66%)	21,30,33	2.04	5 (23%)
1	5MC	16	1407	1	19,22,23	1.59	3 (15%)	26,32,35	1.12	3 (11%)
1	2MG	16	966	1	18,26,27	1.01	1 (5%)	16,38,41	1.33	2 (12%)
1	UR3	16	1498	1	19,22,23	0.96	0	26,32,35	1.72	2 (7%)
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	1MG	23	745	23	19,26,27	0.99	1 (5%)	18,39,42	1.57	3 (16%)
23	PSU	23	2604	23	18,21,22	1.50	4 (22%)	21,30,33	2.20	4 (19%)
23	3TD	23	1915	23	19,22,23	1.38	2 (10%)	23,32,35	2.31	4 (17%)
23	2MG	23	2445	23	18,26,27	0.91	1 (5%)	16,38,41	1.27	2 (12%)
1	G7M	16	527	1	20,26,27	2.60	4 (20%)	16,39,42	1.27	2 (12%)
60	H2U	Pt	16	60	18,21,22	1.03	2 (11%)	19,30,33	1.09	2 (10%)
60	PSU	Pt	55	60	18,21,22	1.36	2 (11%)	21,30,33	2.08	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	5MC	23	1962	23	19,22,23	1.54	3 (15%)	26,32,35	1.12	2 (7%)
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%)

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
23	2MA	23	2503	63,23	-	0/3/25/26	0/3/3/3
60	H2U	Pt	20	60	-	5/7/38/39	0/2/2/2
61	PSU	Dt	39	61	-	2/7/25/26	0/2/2/2
23	PSU	23	2605	23	-	2/7/25/26	0/2/2/2
60	3AU	Pt	47	60	-	2/16/34/35	0/2/2/2
23	2MG	23	1835	23	-	0/5/27/28	0/3/3/3
23	PSU	23	2504	23	-	2/7/25/26	0/2/2/2
1	MA6	16	1518	1	-	1/7/29/30	0/3/3/3
23	PSU	23	955	23	-	0/7/25/26	0/2/2/2
61	PSU	Dt	32	61	-	0/7/25/26	0/2/2/2
60	H2U	Pt	17	60	-	3/7/38/39	0/2/2/2
61	MIA	Dt	37	61	-	5/11/33/34	0/3/3/3
60	5MU	Pt	54	60	-	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	63,23	-	2/9/27/28	0/2/2/2
23	PSU	23	746	63,23	-	4/7/25/26	0/2/2/2
23	6MZ	23	1618	23	-	0/5/27/28	0/3/3/3
23	G7M	23	2069	23	-	0/3/25/26	0/3/3/3
60	U8U	Pt	34	60,22	-	4/10/28/29	0/2/2/2
38	4D4	LP	81	38	-	4/11/12/14	-
61	PSU	Dt	55	61	-	0/7/25/26	0/2/2/2
1	2MG	16	1516	1	-	0/5/27/28	0/3/3/3
1	PSU	16	516	1	-	0/7/25/26	0/2/2/2
61	3AU	Dt	47	61	-	9/16/34/35	0/2/2/2
23	OMG	23	2251	60,23	-	1/5/27/28	0/3/3/3
60	T6A	Pt	37	60	-	10/19/41/42	0/3/3/3
61	4SU	Dt	8	61	-	3/7/25/26	0/2/2/2
12	D2T	SL	89	12	-	3/7/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	23	1911	23	-	0/7/25/26	0/2/2/2
1	4OC	16	1402	1	-	0/9/29/30	0/2/2/2
23	H2U	23	2449	23	-	0/7/38/39	0/2/2/2
23	5MU	23	747	23	-	0/7/25/26	0/2/2/2
23	6MZ	23	2030	23	-	2/5/27/28	0/3/3/3
23	OMU	23	2552	23	-	2/9/27/28	0/2/2/2
23	PSU	23	2580	23	-	0/7/25/26	0/2/2/2
60	PSU	Pt	39	60	-	0/7/25/26	0/2/2/2
23	PSU	23	1917	23	-	0/7/25/26	0/2/2/2
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2
1	2MG	16	966	1	-	0/5/27/28	0/3/3/3
1	UR3	16	1498	1	-	0/7/25/26	0/2/2/2
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	1MG	23	745	23	-	0/3/25/26	0/3/3/3
23	PSU	23	2604	23	-	0/7/25/26	0/2/2/2
23	3TD	23	1915	23	-	0/7/25/26	0/2/2/2
23	2MG	23	2445	23	-	1/5/27/28	0/3/3/3
1	G7M	16	527	1	-	2/3/25/26	0/3/3/3
60	H2U	Pt	16	60	-	3/7/38/39	0/2/2/2
60	PSU	Pt	55	60	-	0/7/25/26	0/2/2/2
23	5MC	23	1962	23	-	4/7/25/26	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

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 (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
23	23	2503	2MA	C2-N3-C4	7.06	121.16	115.46
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	1911	PSU	C4-N3-C2	-4.75	119.83	126.37
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	2030	6MZ	N3-C2-N1	-3.67	123.69	128.67
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	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(^{o})	Ideal(^{o})
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
23	23	2503	2MA	C4-C5-N7	-2.82	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	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	2503	2MA	C2-N1-C6	2.57	122.06	118.10
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
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(^{o})	Ideal(^{o})
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
23	23	2503	2MA	C5-C6-N1	-2.15	118.30	120.84
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

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Mol	Chain	Res	Type	Atoms
60	Pt	17	H2U	O4'-C1'-N1-C6
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

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Mol	Chain	Res	Type	Atoms
60	Pt	37	T6A	O4'-C4'-C5'-O5'
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	2503	2MA	1	0
1	16	1518	MA6	1	0
1	16	1516	2MG	1	0
23	23	2251	OMG	1	0
12	SL	89	D2T	4	0
23	23	1911	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	16	1402	4OC	1	0
23	23	2030	6MZ	2	0
23	23	2552	OMU	1	0
1	16	966	2MG	1	0
1	16	1519	MA6	1	0
23	23	1915	3TD	1	0
1	16	967	5MC	2	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	3010	-	5,5,5	0.10	0	4,4,4	0.13	0
62	PUT	23	3018	-	5,5,5	0.11	0	4,4,4	0.13	0
62	PUT	23	3013	-	5,5,5	0.10	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	3009	-	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	3016	-	5,5,5	0.09	0	4,4,4	0.13	0
62	PUT	16	1601	-	5,5,5	0.12	0	4,4,4	0.12	0
62	PUT	23	3008	-	5,5,5	0.10	0	4,4,4	0.14	0
66	SPD	23	3023	-	9,9,9	0.16	0	8,8,8	0.23	0
62	PUT	23	3006	-	5,5,5	0.09	0	4,4,4	0.13	0
66	SPD	23	3021	-	9,9,9	0.32	0	8,8,8	0.91	0
62	PUT	23	3007	-	5,5,5	0.10	0	4,4,4	0.12	0
62	PUT	LC	301	-	5,5,5	0.10	0	4,4,4	0.13	0
62	PUT	23	3014	-	5,5,5	0.10	0	4,4,4	0.12	0
62	PUT	23	3011	-	5,5,5	0.09	0	4,4,4	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
62	PUT	23	3020	-	5,5,5	0.16	0	4,4,4	0.20	0
62	PUT	23	3005	-	5,5,5	0.11	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	23	3017	-	5,5,5	0.12	0	4,4,4	0.13	0
62	PUT	23	3015	-	5,5,5	0.14	0	4,4,4	0.19	0
68	GDP	EF	803	63	25,30,30	0.97	1 (4%)	30,47,47	1.16	3 (10%)
62	PUT	16	1602	-	5,5,5	0.15	0	4,4,4	0.22	0
62	PUT	23	3019	-	5,5,5	0.12	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%)
62	PUT	23	3004	-	5,5,5	0.10	0	4,4,4	0.12	0
66	SPD	23	3022	-	9,9,9	0.32	0	8,8,8	0.89	0
62	PUT	23	3012	-	5,5,5	0.11	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	3010	-	-	1/3/3/3	-
62	PUT	23	3018	-	-	1/3/3/3	-
62	PUT	23	3013	-	-	0/3/3/3	-
62	PUT	23	3003	-	-	0/3/3/3	-
62	PUT	23	3009	-	-	0/3/3/3	-
65	ATP	23	3002	-	-	5/18/38/38	0/3/3/3
62	PUT	23	3016	-	-	1/3/3/3	-
62	PUT	16	1601	-	-	0/3/3/3	-
62	PUT	23	3008	-	-	0/3/3/3	-
66	SPD	23	3023	-	-	2/7/7/7	-
62	PUT	23	3006	-	-	0/3/3/3	-
66	SPD	23	3021	-	-	2/7/7/7	-
62	PUT	23	3007	-	-	1/3/3/3	-
62	PUT	LC	301	-	-	1/3/3/3	-
62	PUT	23	3014	-	-	1/3/3/3	-
62	PUT	23	3011	-	-	1/3/3/3	-
62	PUT	23	3020	-	-	0/3/3/3	-
62	PUT	23	3005	-	-	0/3/3/3	-
65	ATP	23	3001	-	-	5/18/38/38	0/3/3/3
62	PUT	23	3017	-	-	1/3/3/3	-
62	PUT	23	3015	-	-	1/3/3/3	-
68	GDP	EF	803	63	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	PUT	16	1602	-	-	2/3/3/3	-
62	PUT	23	3019	-	-	0/3/3/3	-
67	FUA	EF	802	63	-	5/16/92/92	0/4/4/4
62	PUT	23	3004	-	-	0/3/3/3	-
66	SPD	23	3022	-	-	0/7/7/7	-
62	PUT	23	3012	-	-	0/3/3/3	-

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(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
67	EF	802	FUA	C5-C10-C9	2.69	114.50	108.19
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

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Mol	Chain	Res	Type	Atoms
68	EF	803	GDP	O4'-C4'-C5'-O5'
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

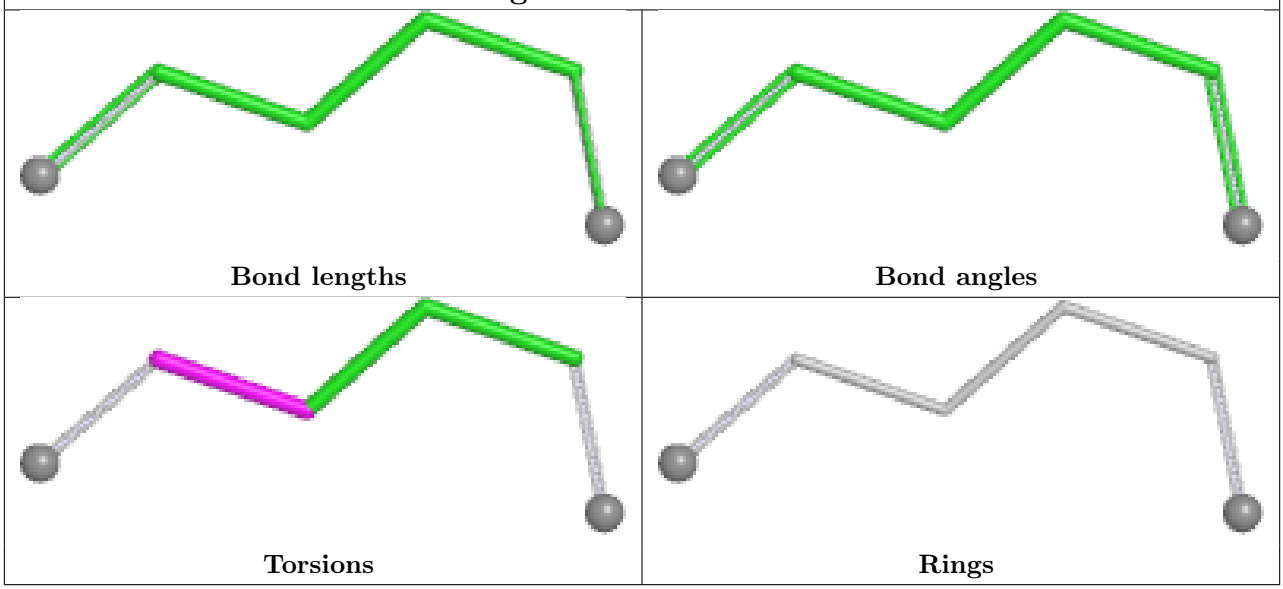
There are no ring outliers.

6 monomers are involved in 21 short contacts:

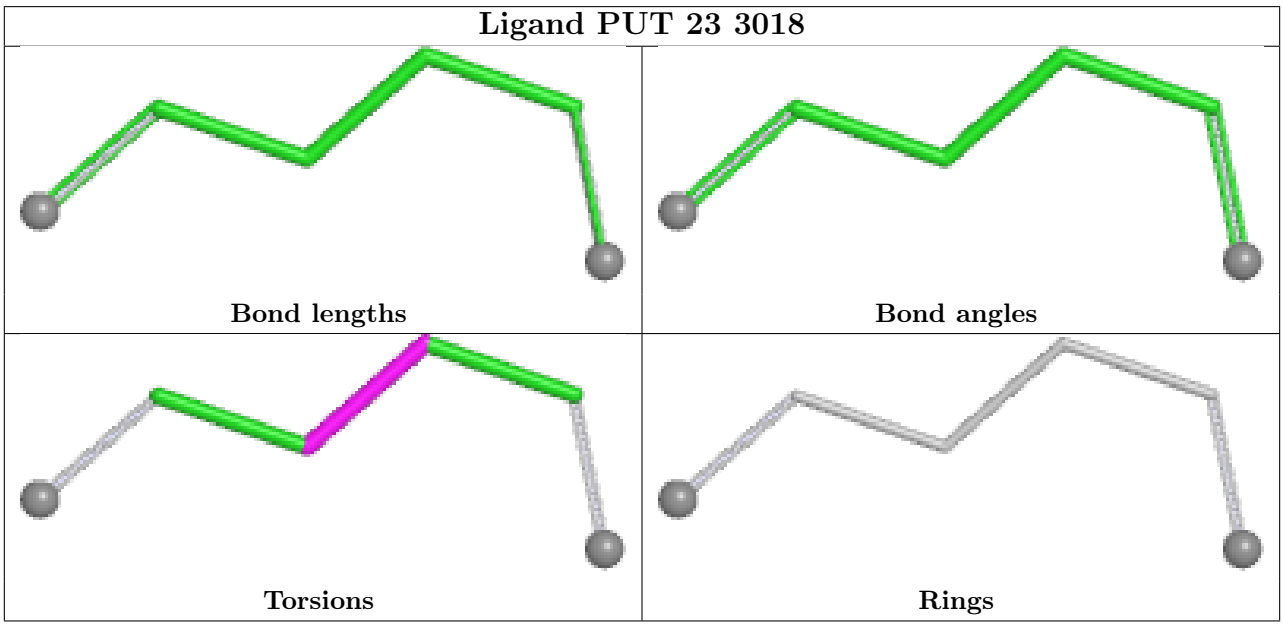
Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	23	3010	PUT	1	0
62	23	3013	PUT	1	0
62	LC	301	PUT	1	0
62	23	3020	PUT	2	0
62	16	1602	PUT	1	0
67	EF	802	FUA	15	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PUT 23 3010



Ligand PUT 23 3018



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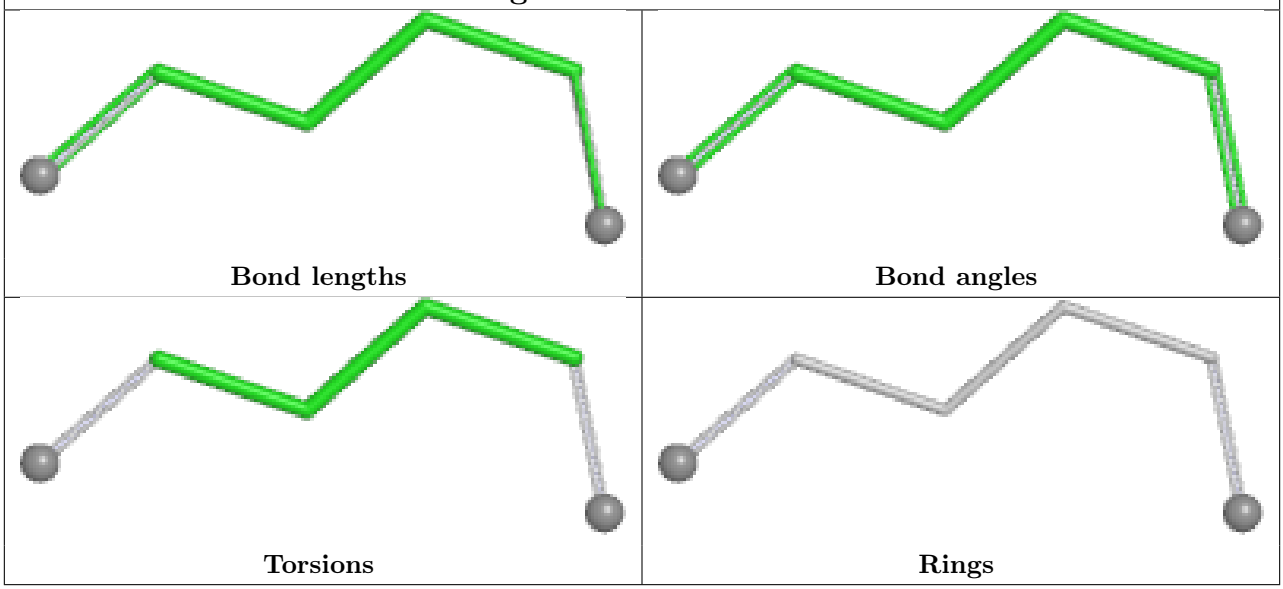

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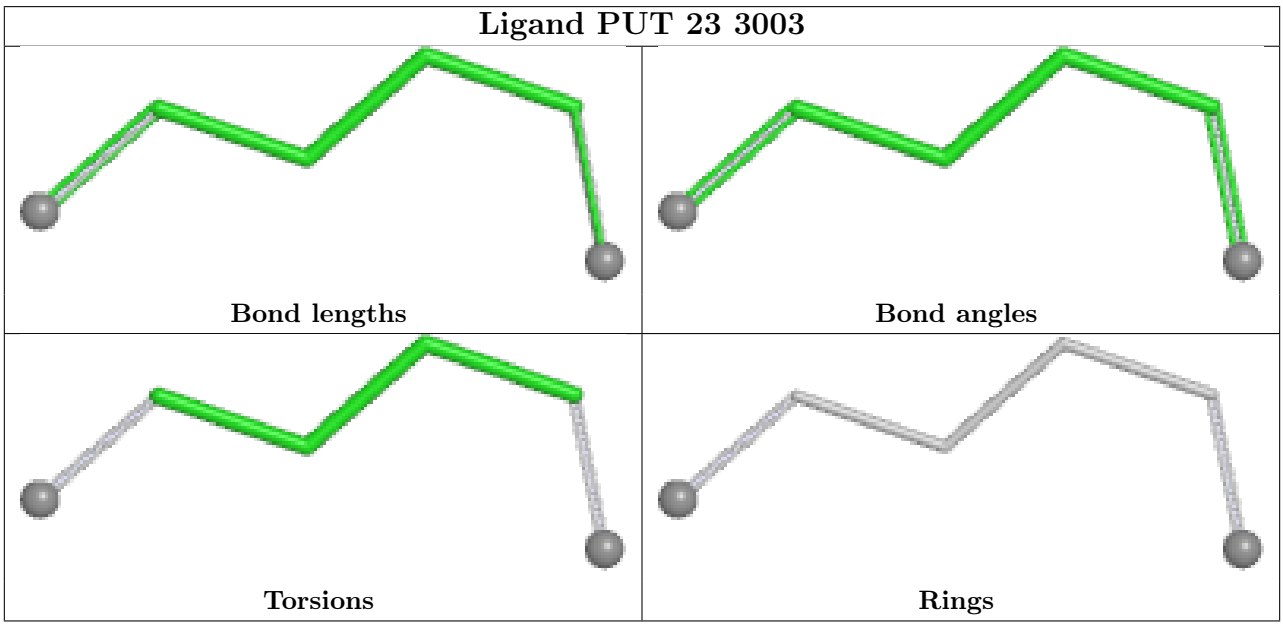
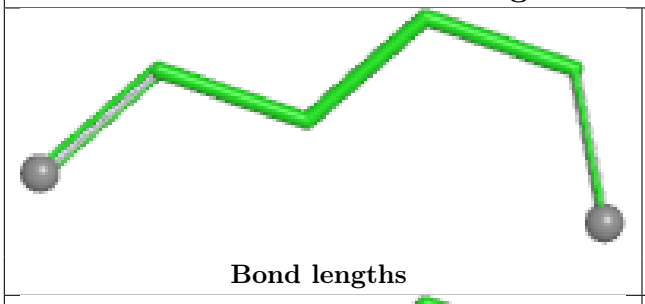
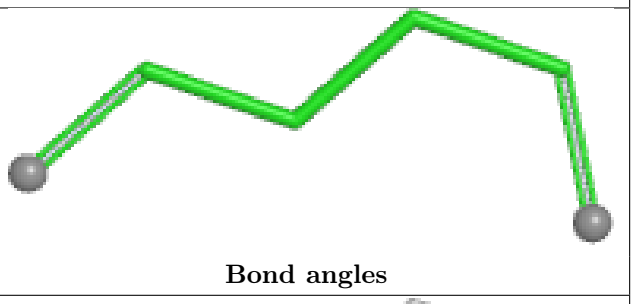


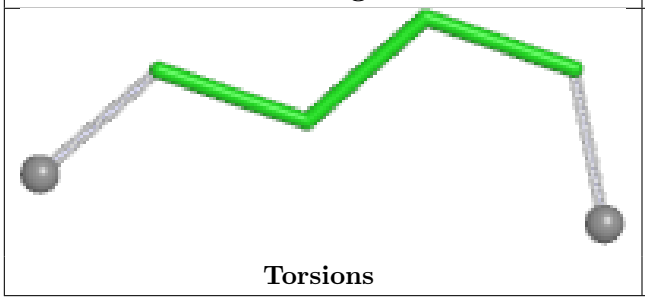
Ligand PUT 23 3009



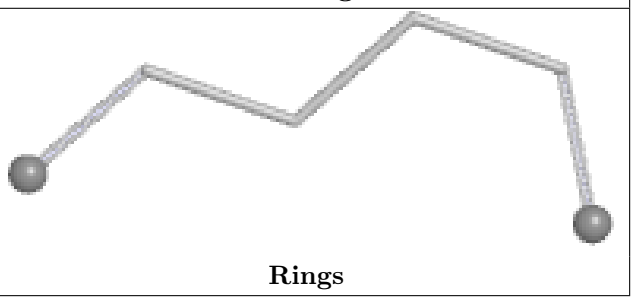
Bond lengths



Bond angles

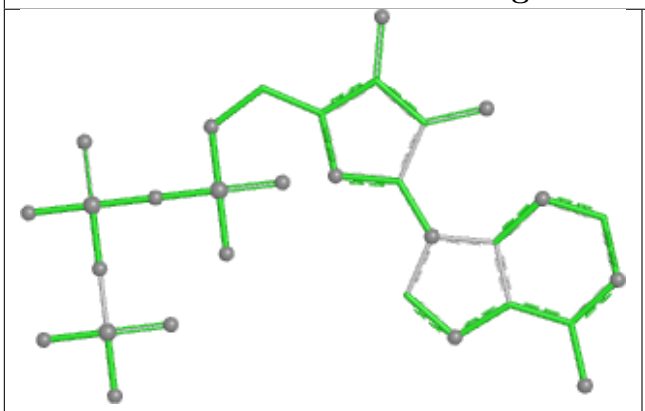


Torsions

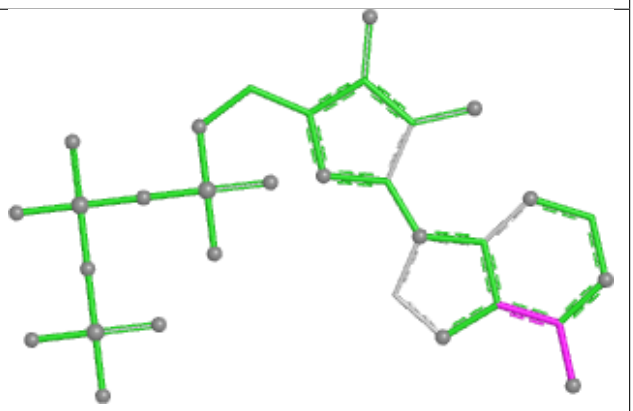


Rings

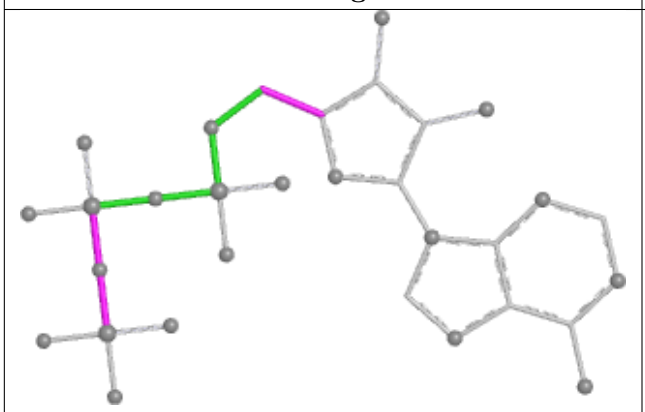
Ligand ATP 23 3002



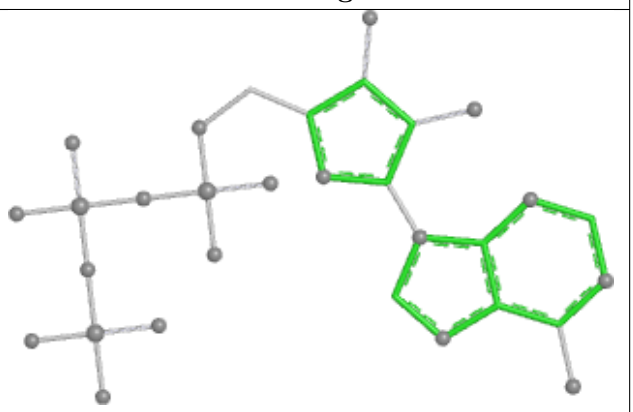
Bond lengths



Bond angles



Torsions



Rings

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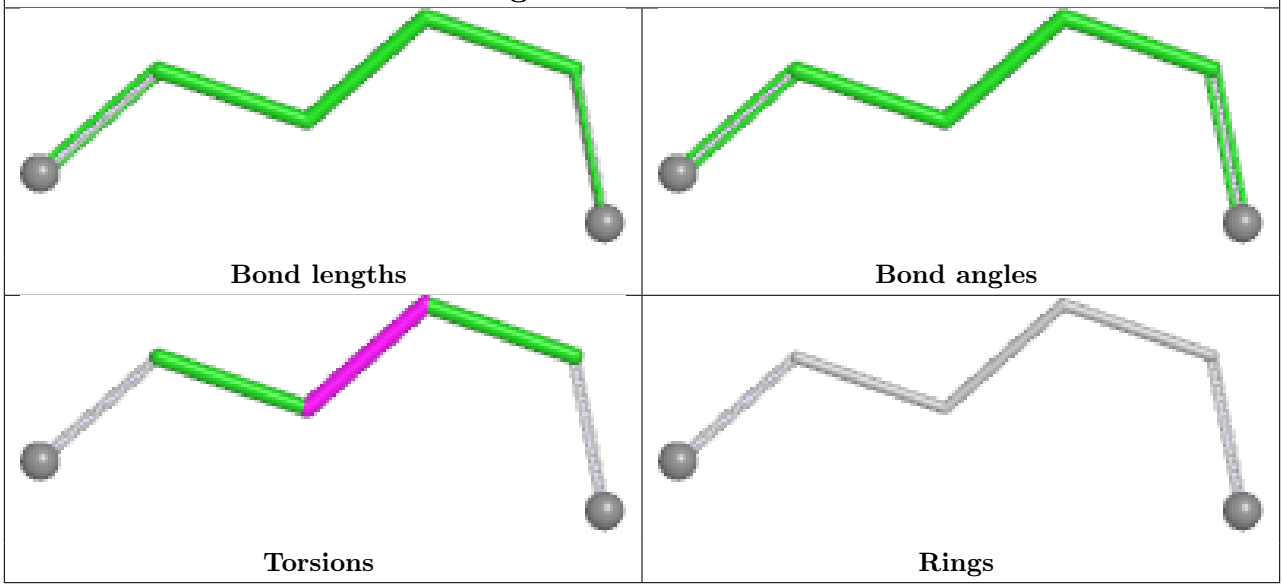
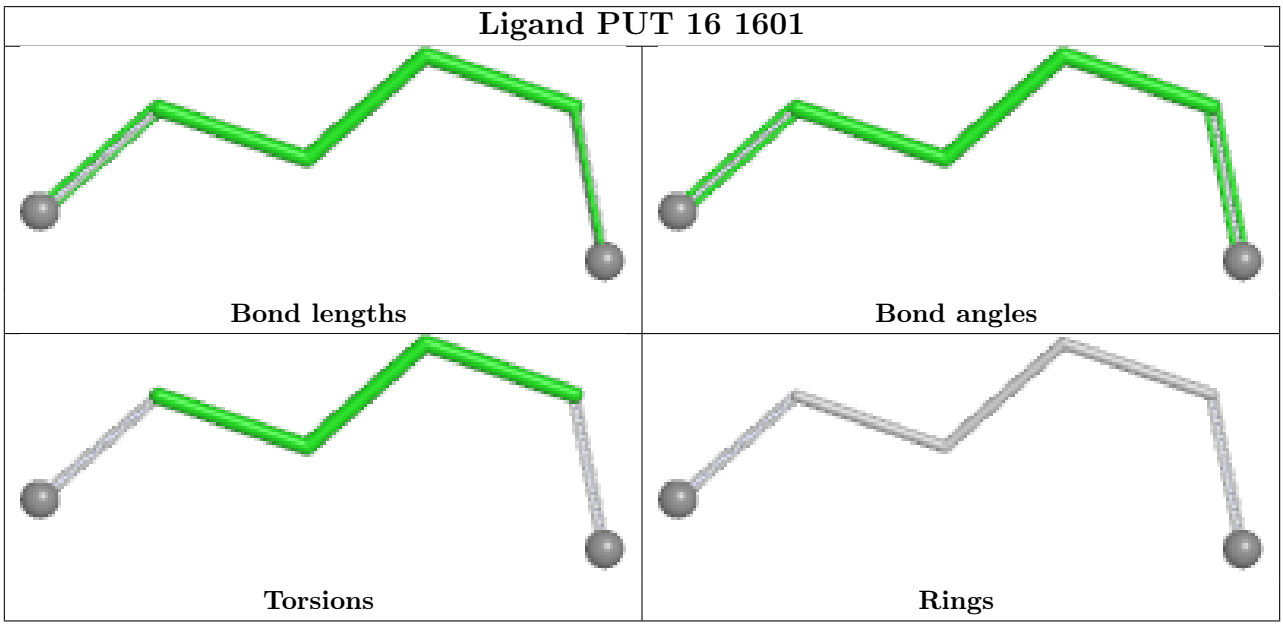


Ligand PUT 16 1601



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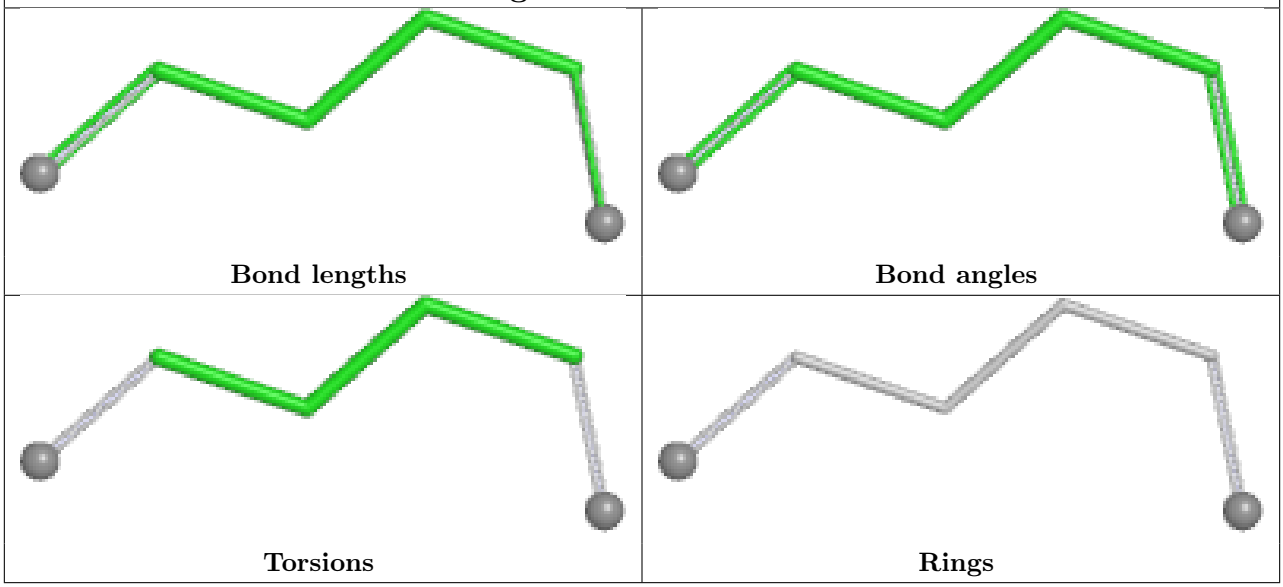

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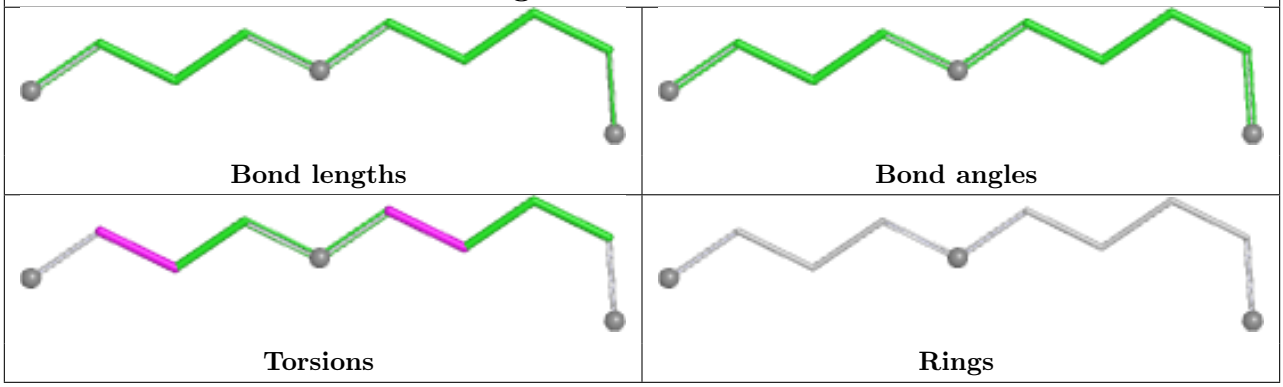

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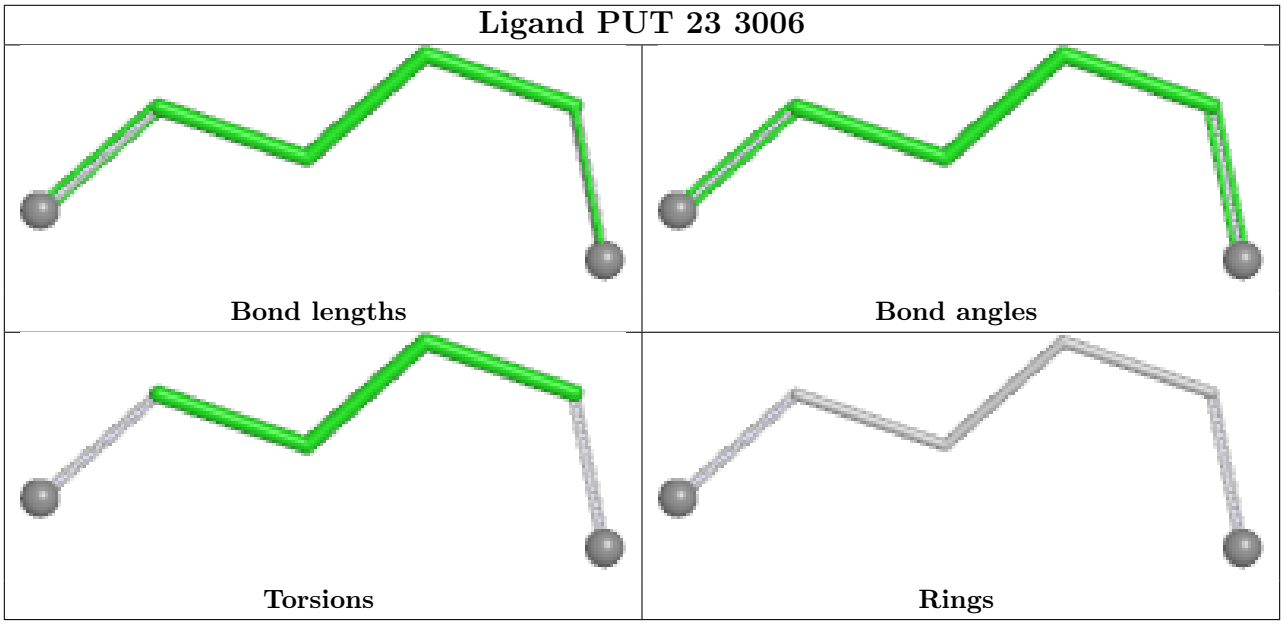

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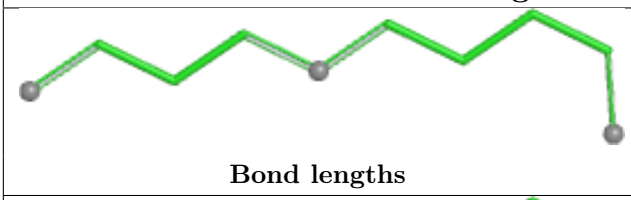
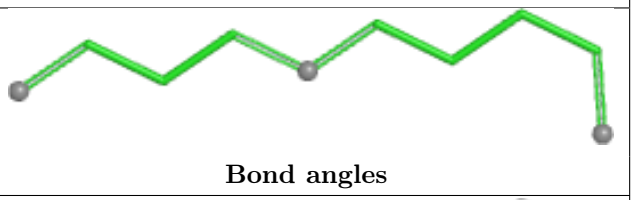
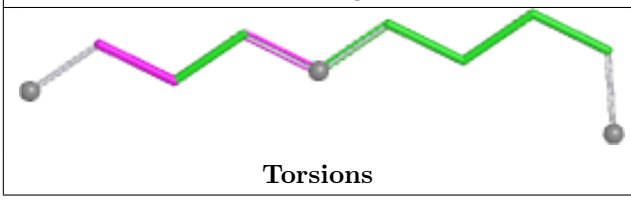


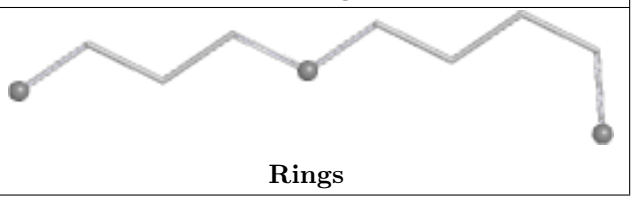
Bond lengths



Bond angles

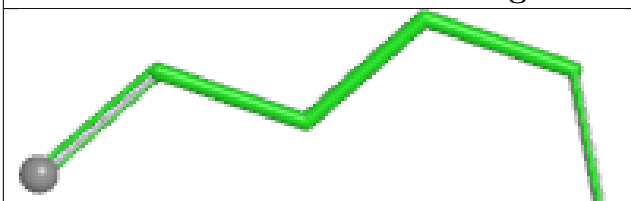


Torsions

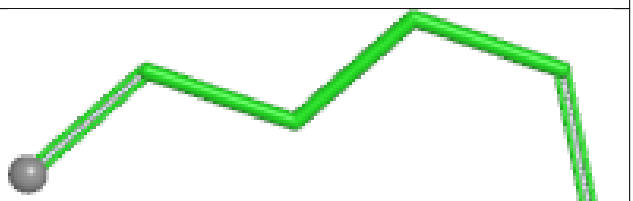


Rings

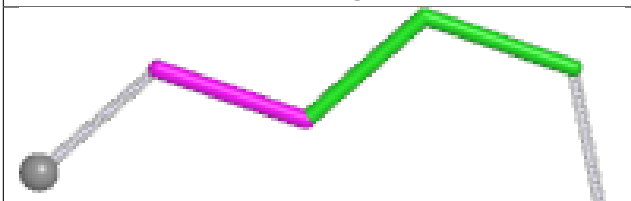
Ligand PUT 23 3007



Bond lengths



Bond angles



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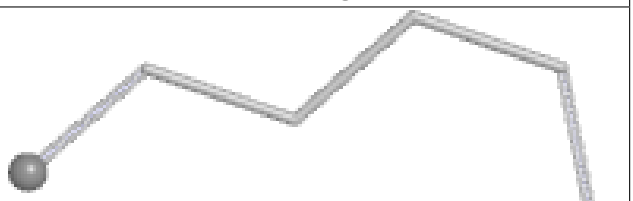
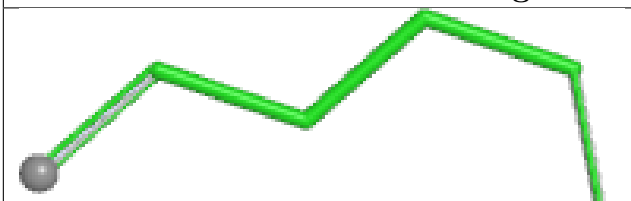


Rings

Ligand PUT LC 301



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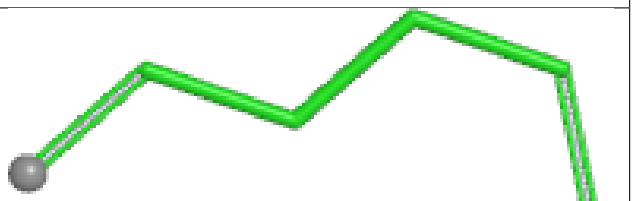
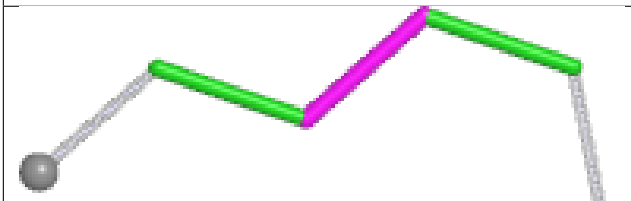
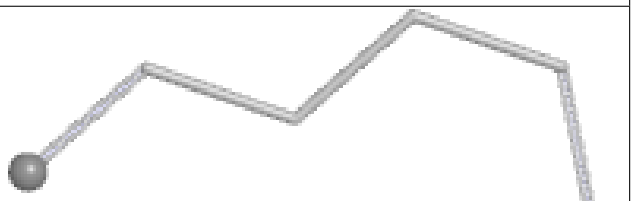


Bond angles

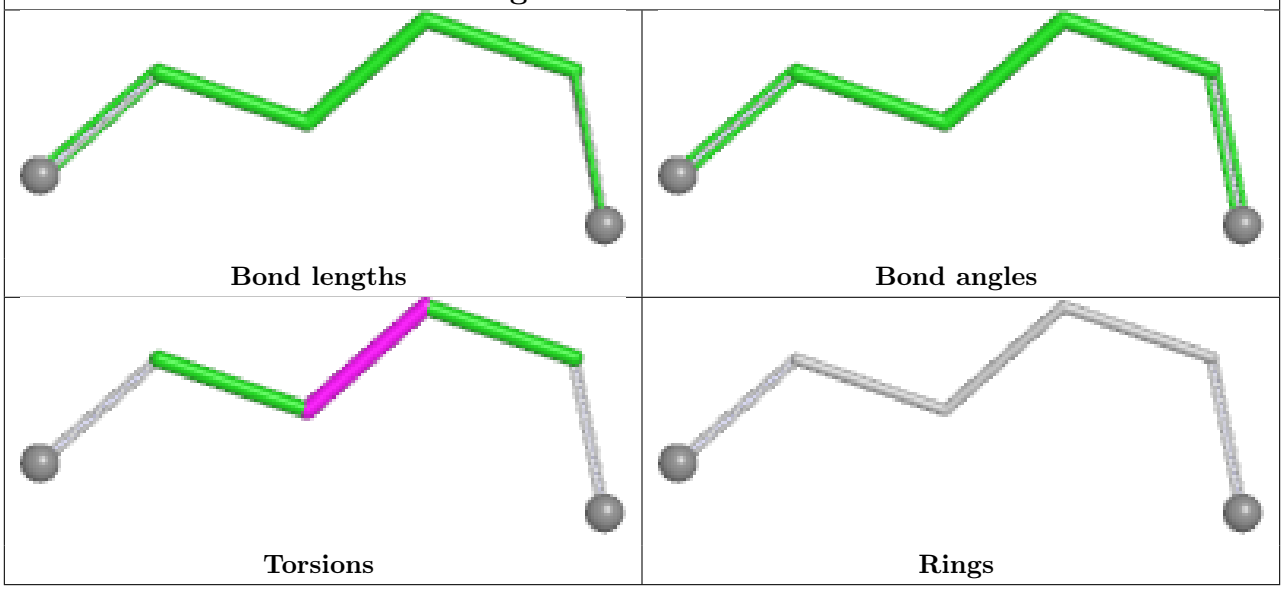


Torsions

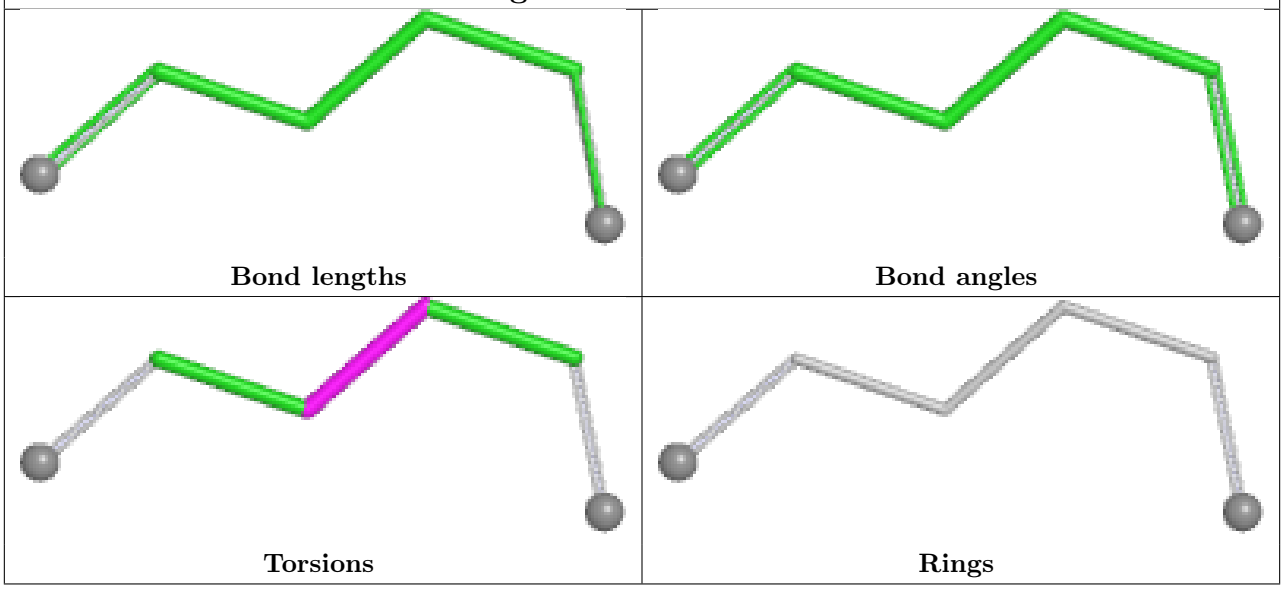


Rings

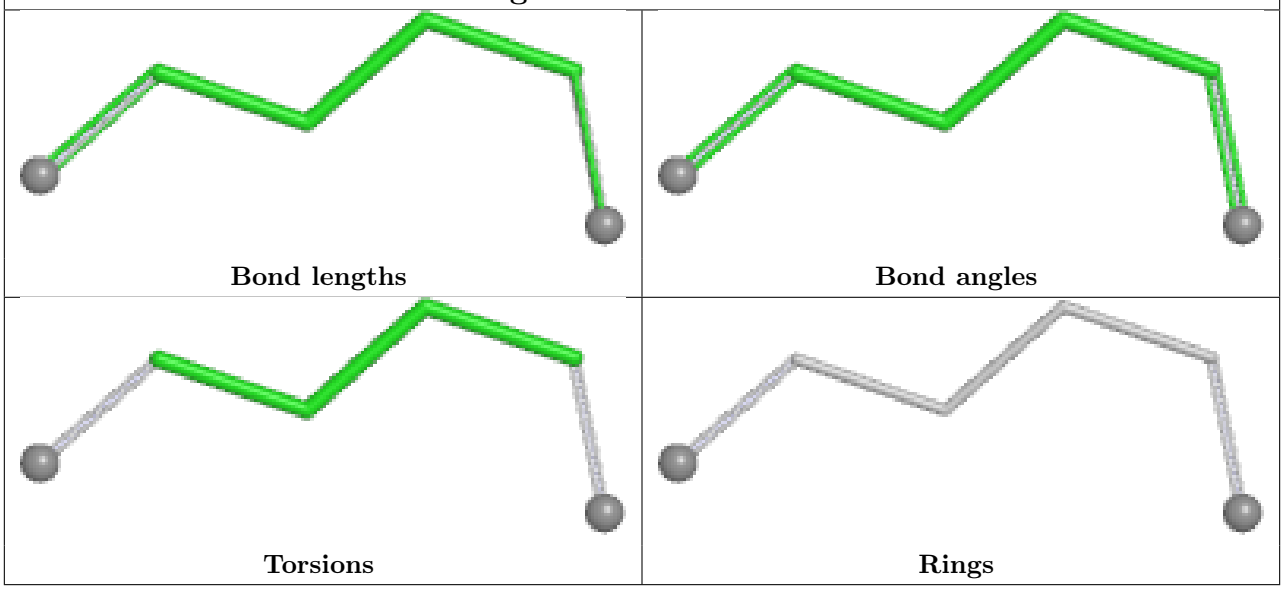
Ligand PUT 23 3014



Ligand PUT 23 3011



Ligand PUT 23 3020



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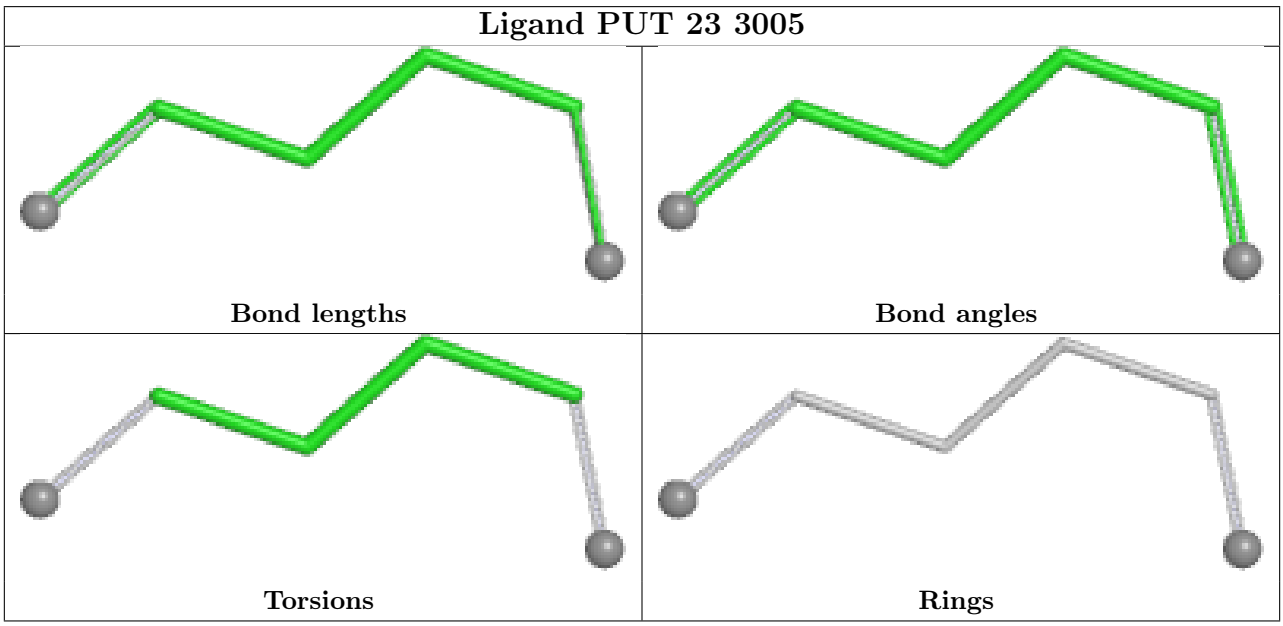
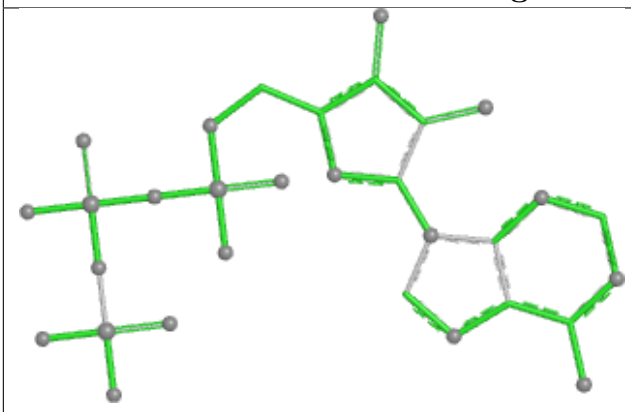
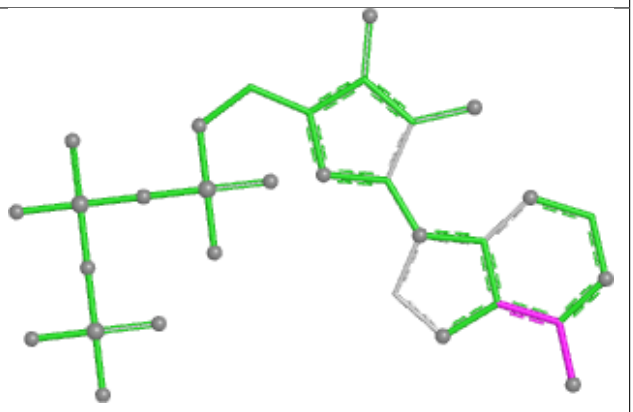


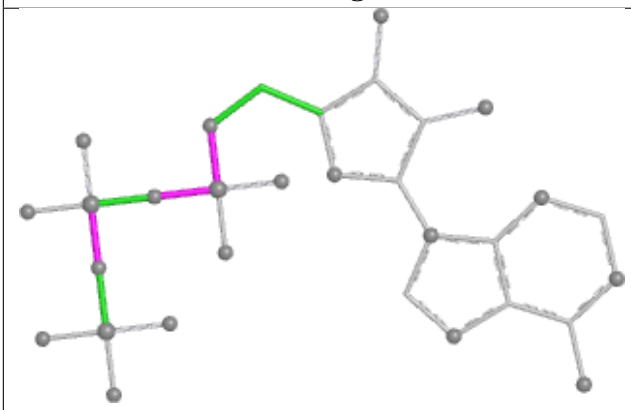
Ligand ATP 23 3001



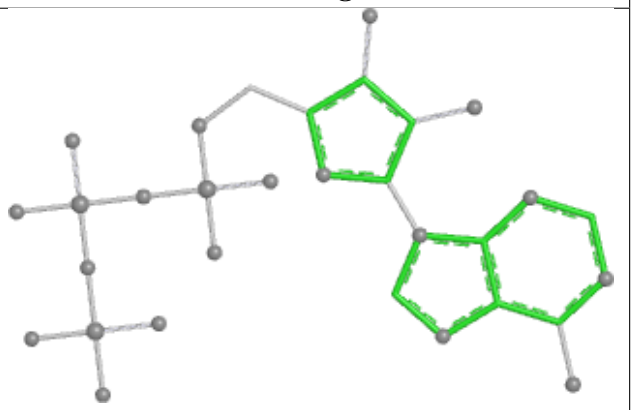
Bond lengths



Bond angles

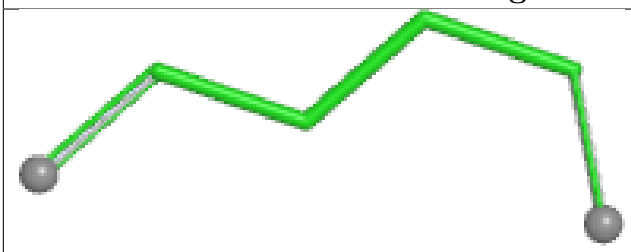


Torsions

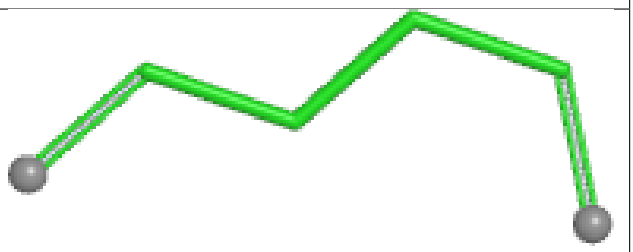


Rings

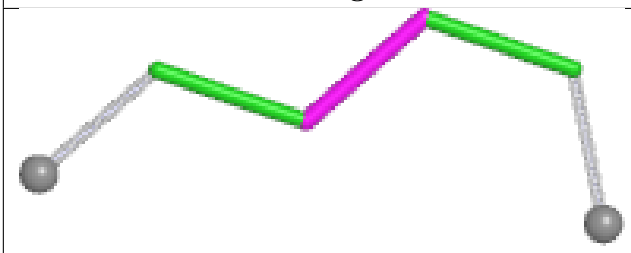
Ligand PUT 23 3017



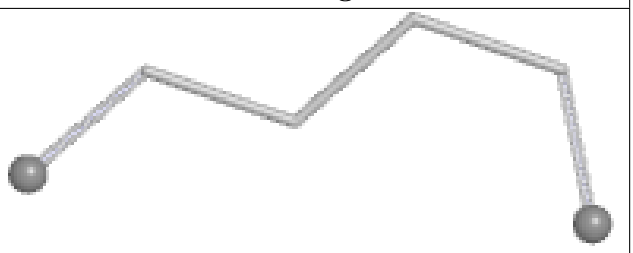
Bond lengths



Bond angles

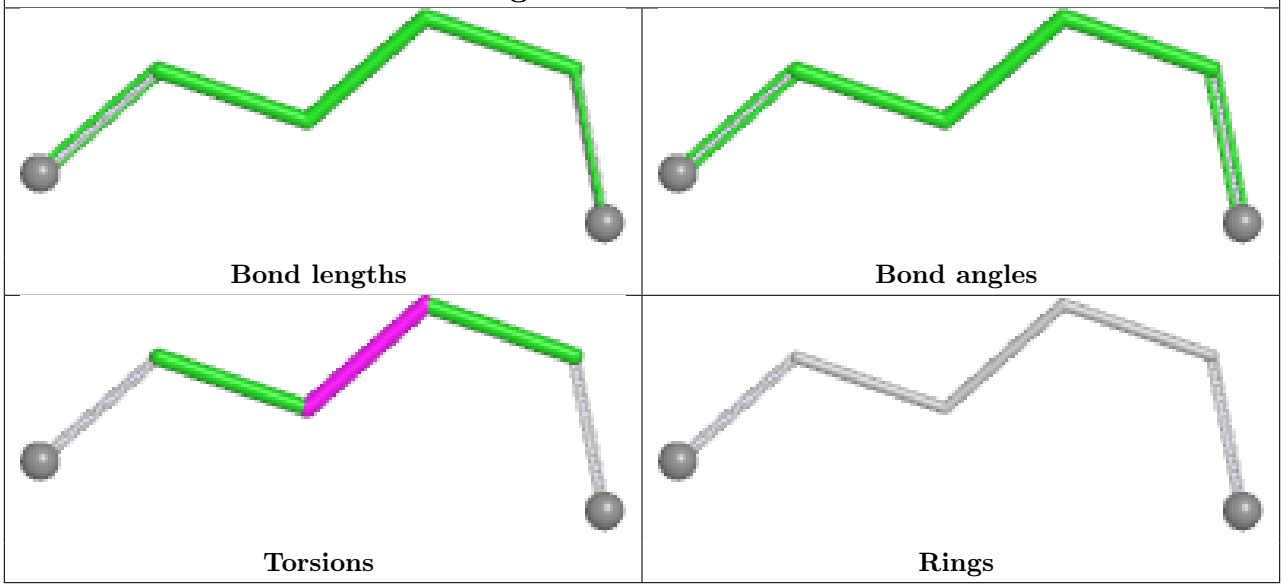


Torsions

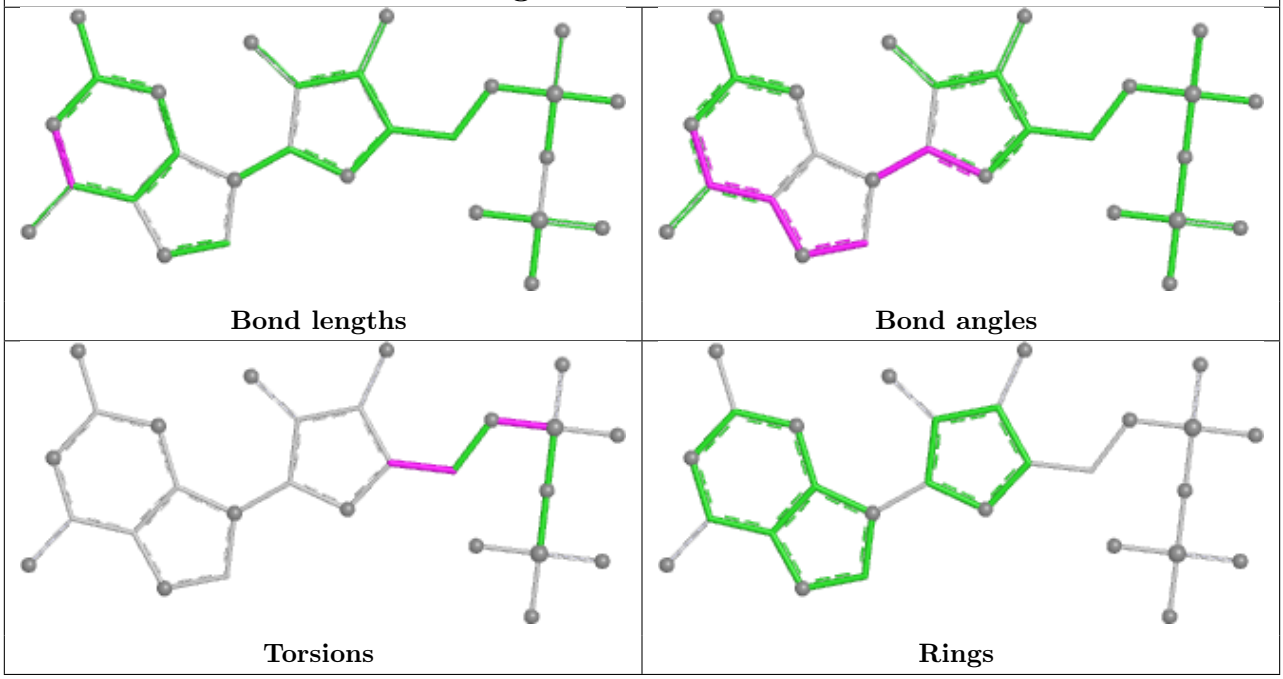


Rings

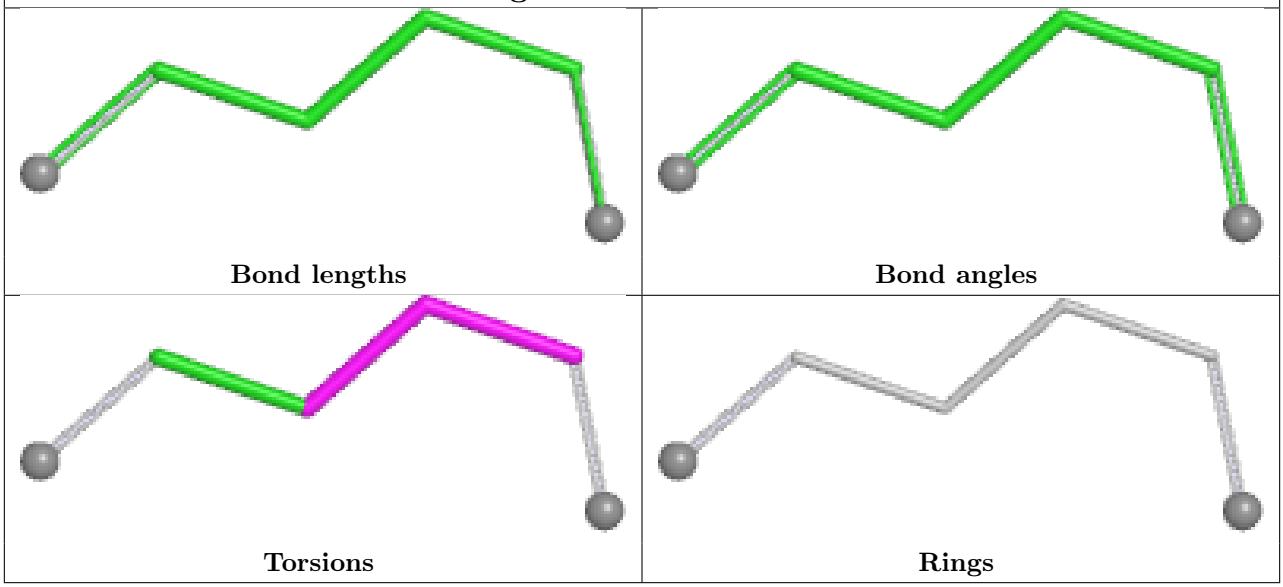
Ligand PUT 23 3015



Ligand GDP EF 803



Ligand PUT 16 1602



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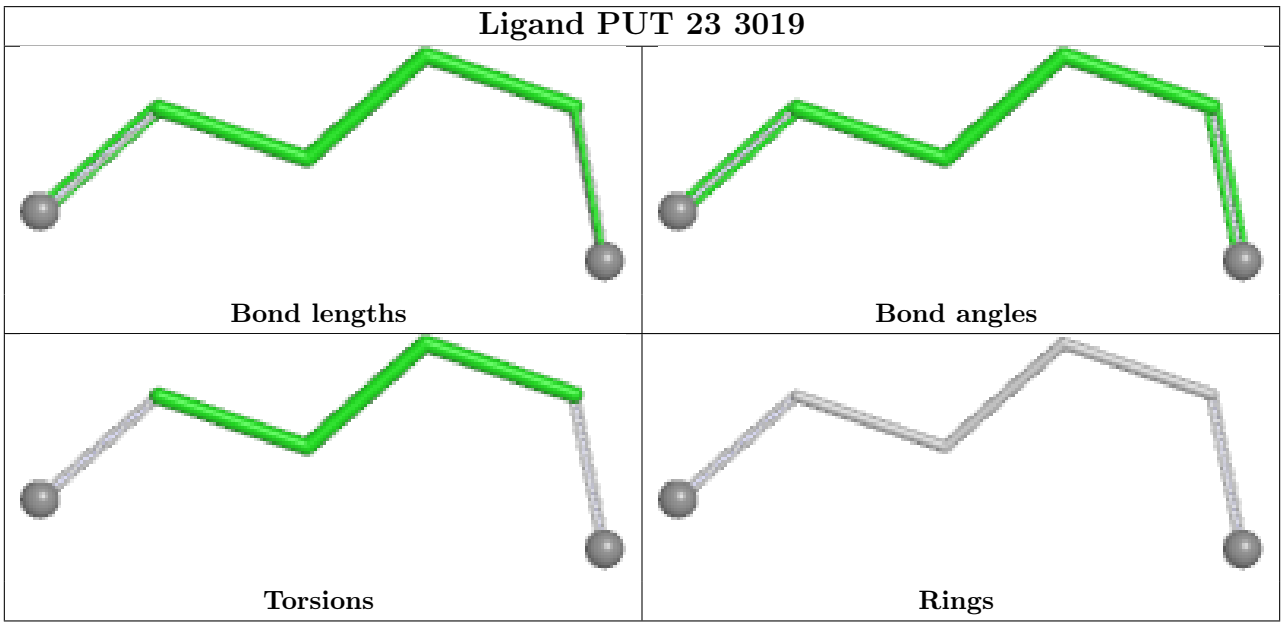
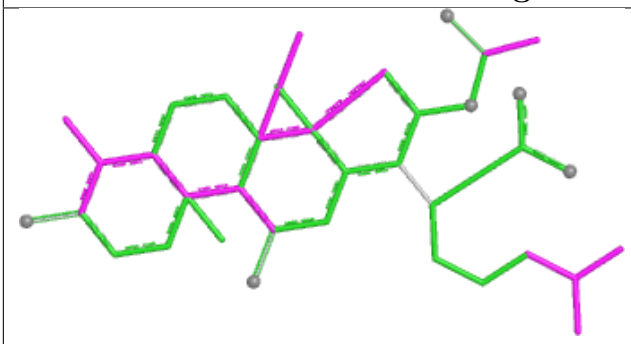
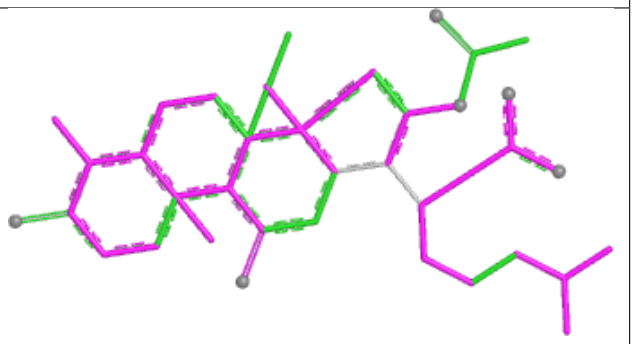


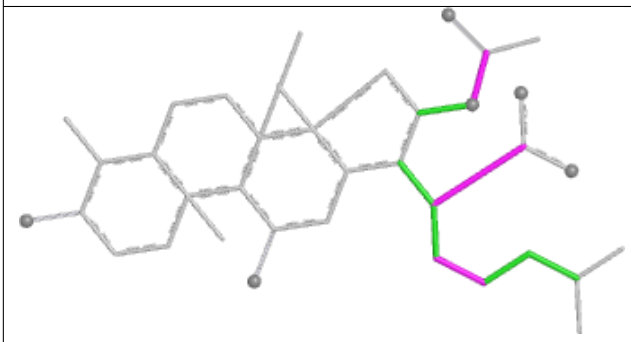
Ligand FUA EF 802



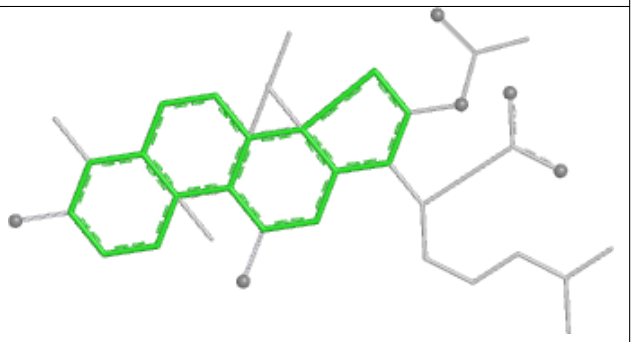
Bond lengths



Bond angles

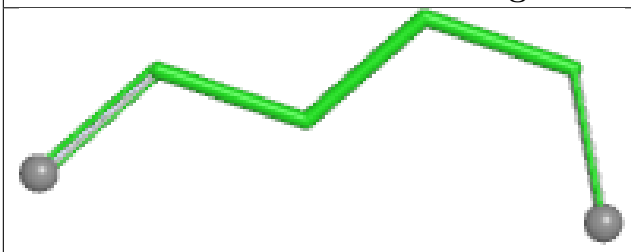


Torsions

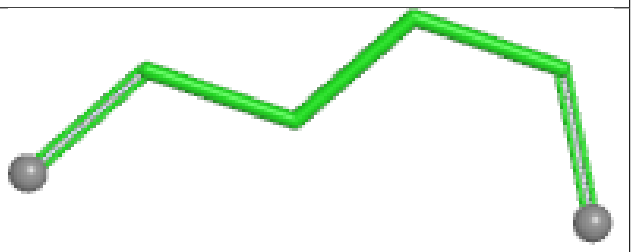


Rings

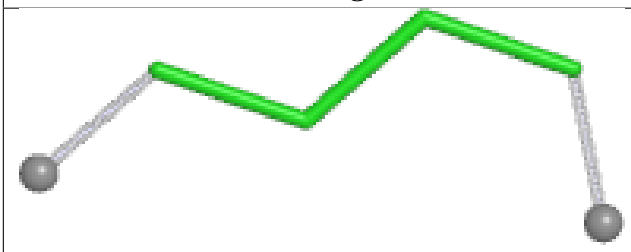
Ligand PUT 23 3004



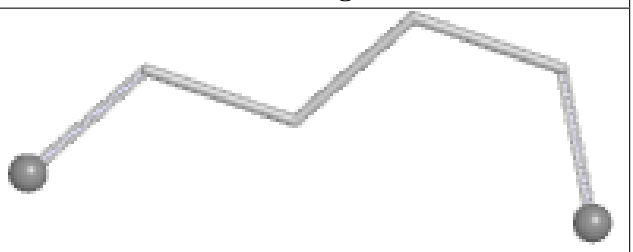
Bond lengths



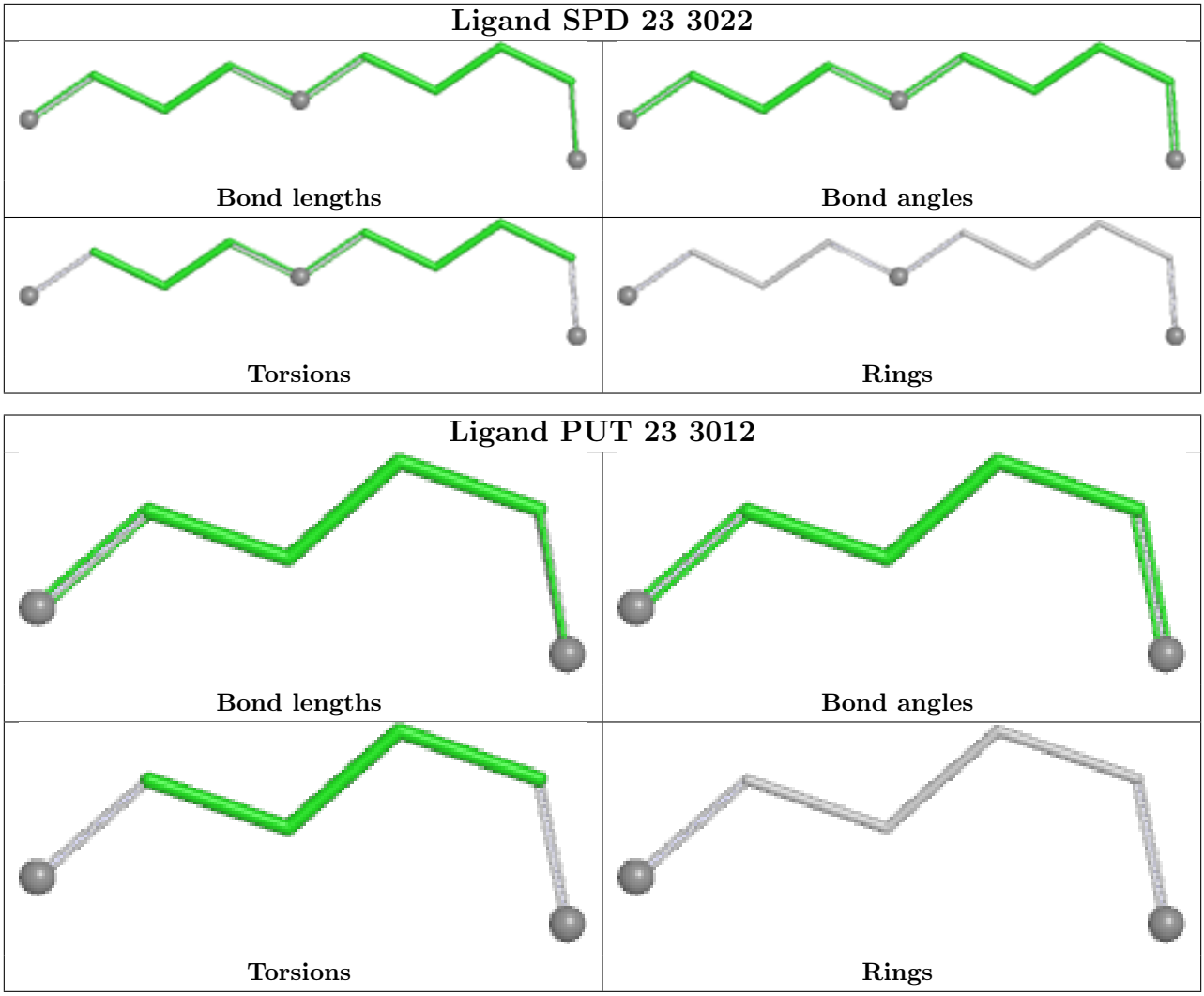
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

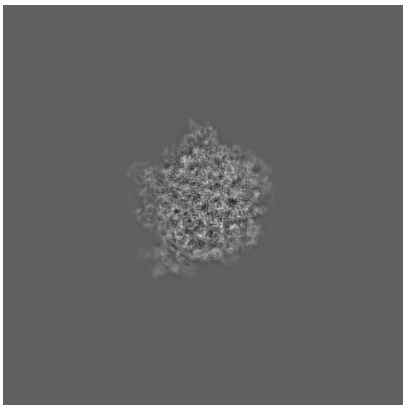
6 Map visualisation

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.

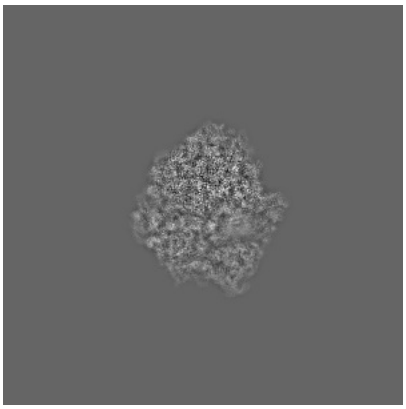
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

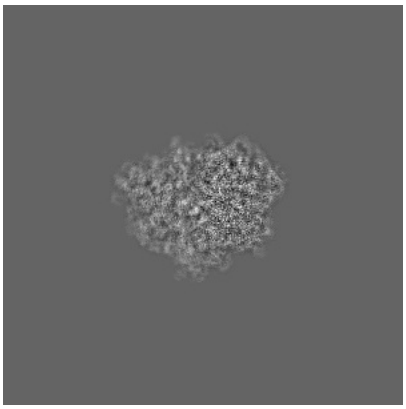
6.1.1 Primary map



X

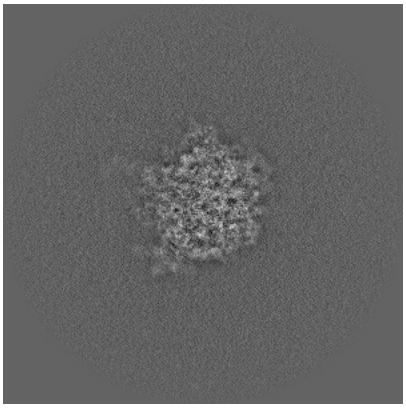


Y

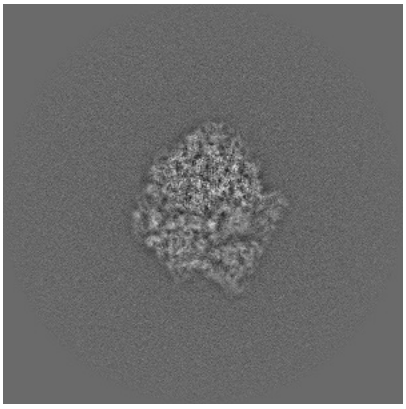


Z

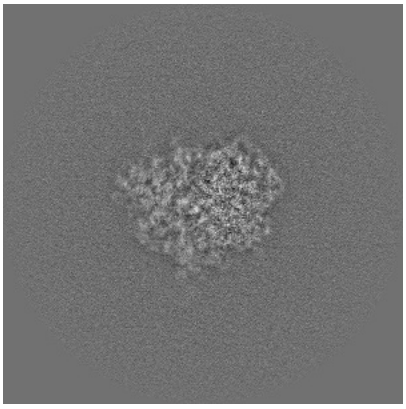
6.1.2 Raw map



X



Y

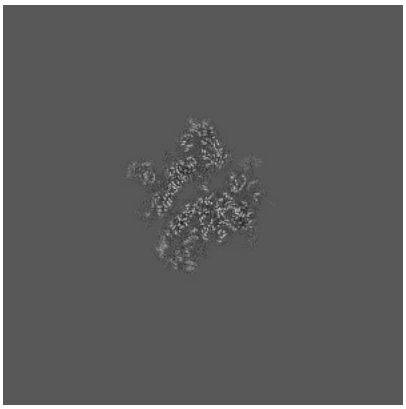


Z

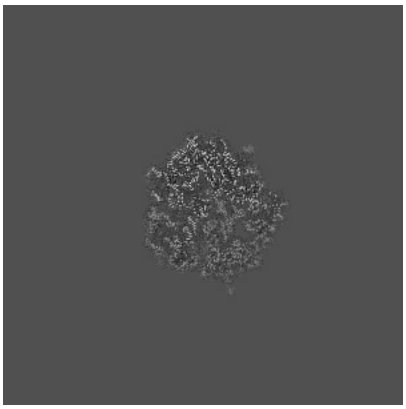
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

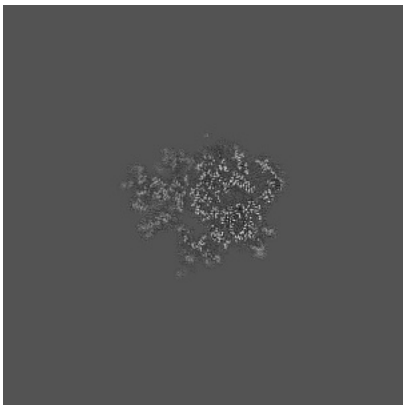
6.2.1 Primary map



X Index: 288

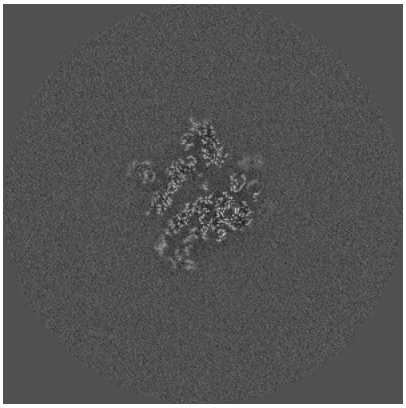


Y Index: 288

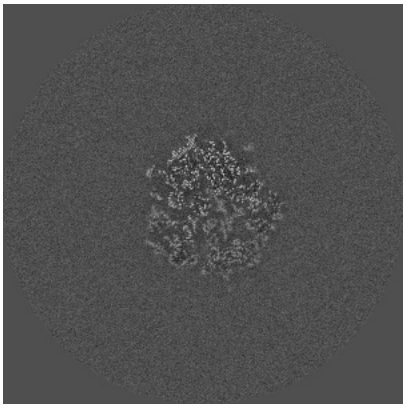


Z Index: 288

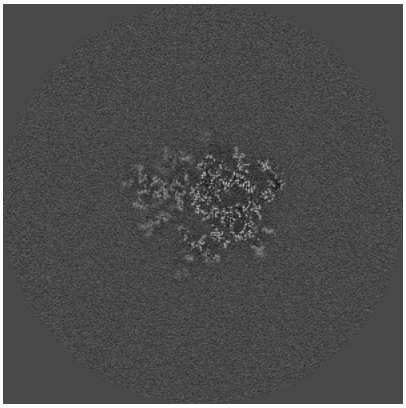
6.2.2 Raw map



X Index: 288



Y Index: 288

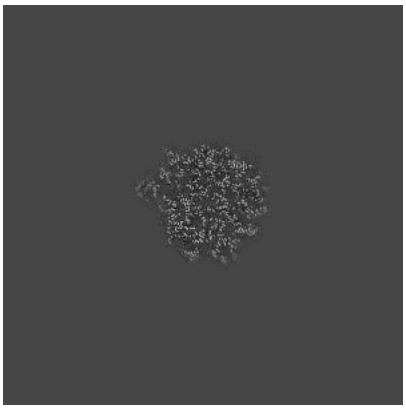


Z Index: 288

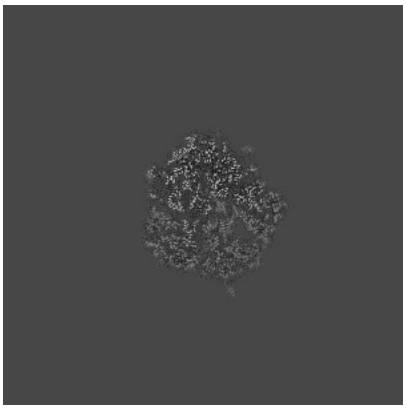
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

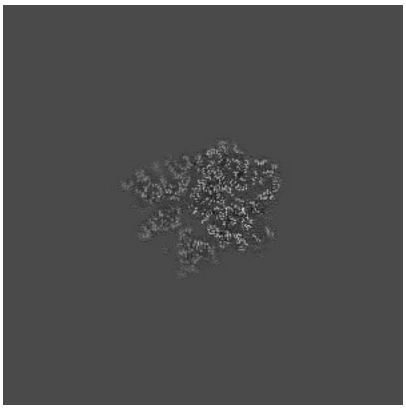
6.3.1 Primary map



X Index: 315

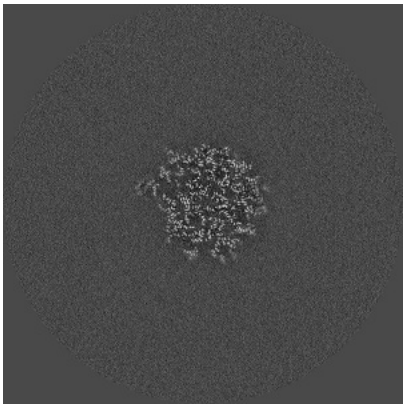


Y Index: 290

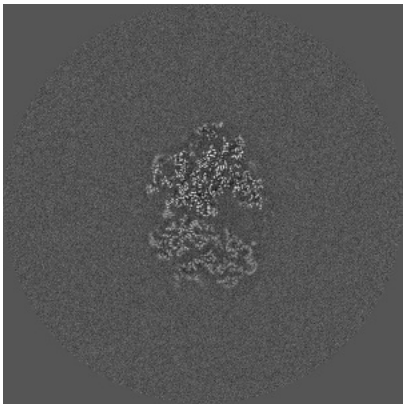


Z Index: 282

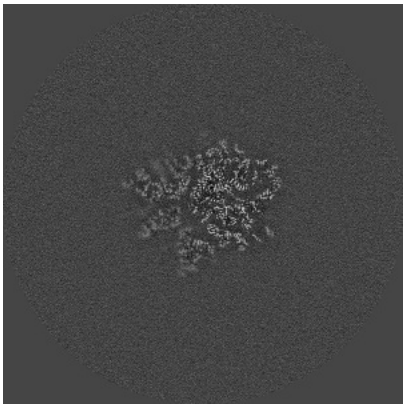
6.3.2 Raw map



X Index: 315



Y Index: 312

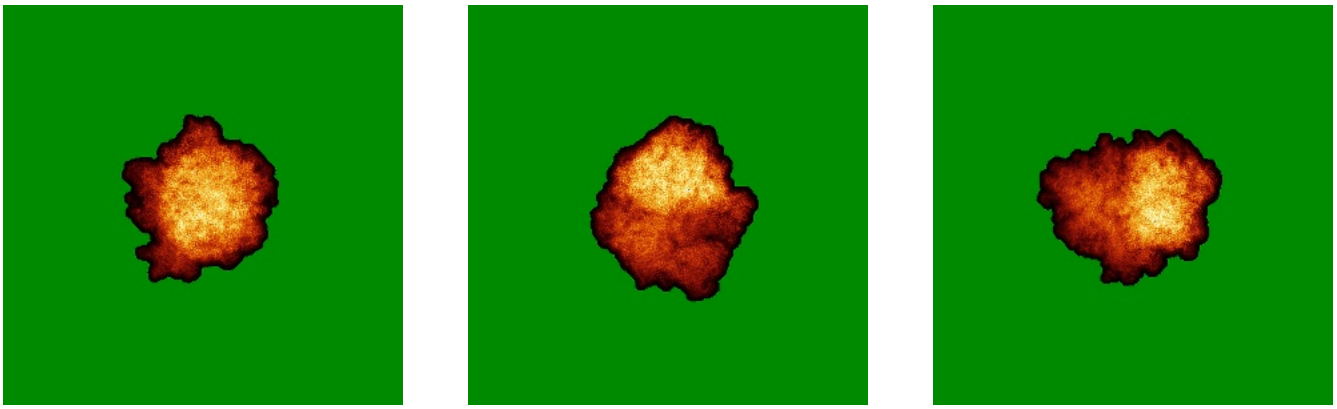


Z Index: 282

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

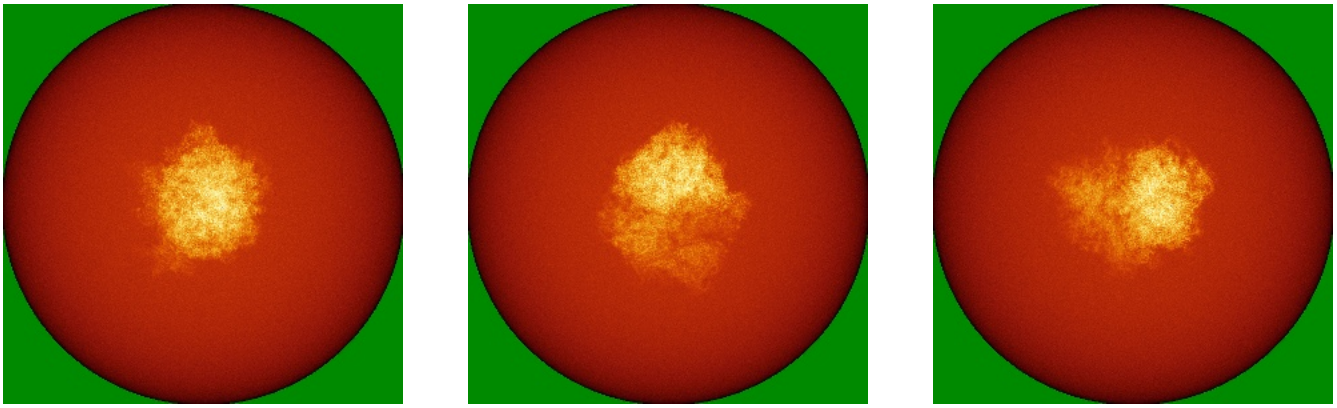
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

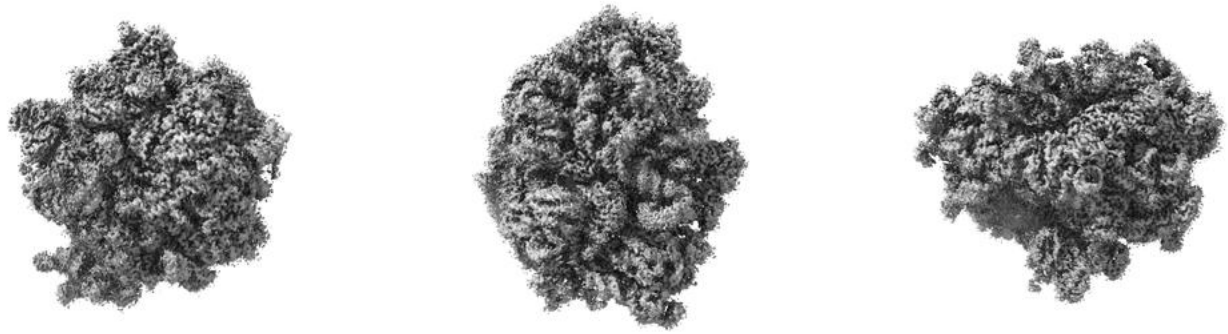


X Y Z

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)

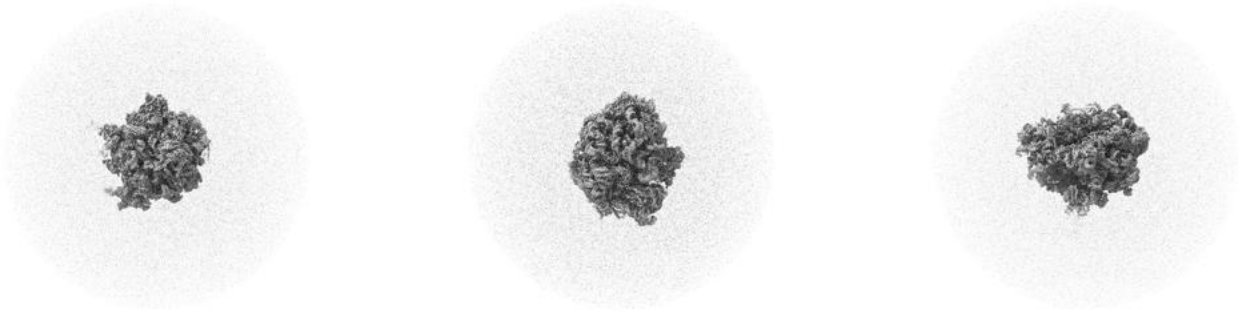
6.5.1 Primary map



X Y Z

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



X Y Z

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.

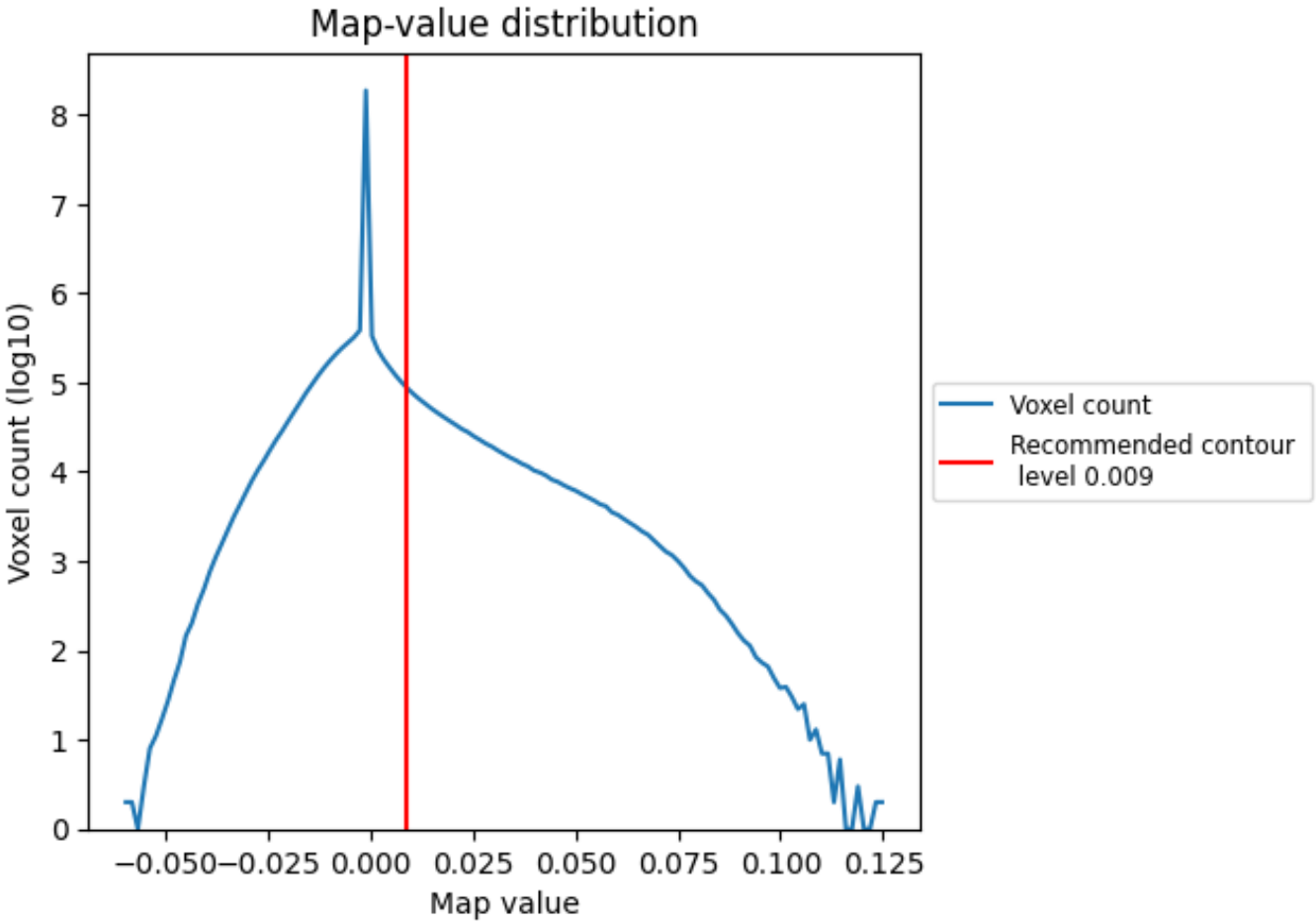
6.6 Mask visualisation (i)

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

7 Map analysis

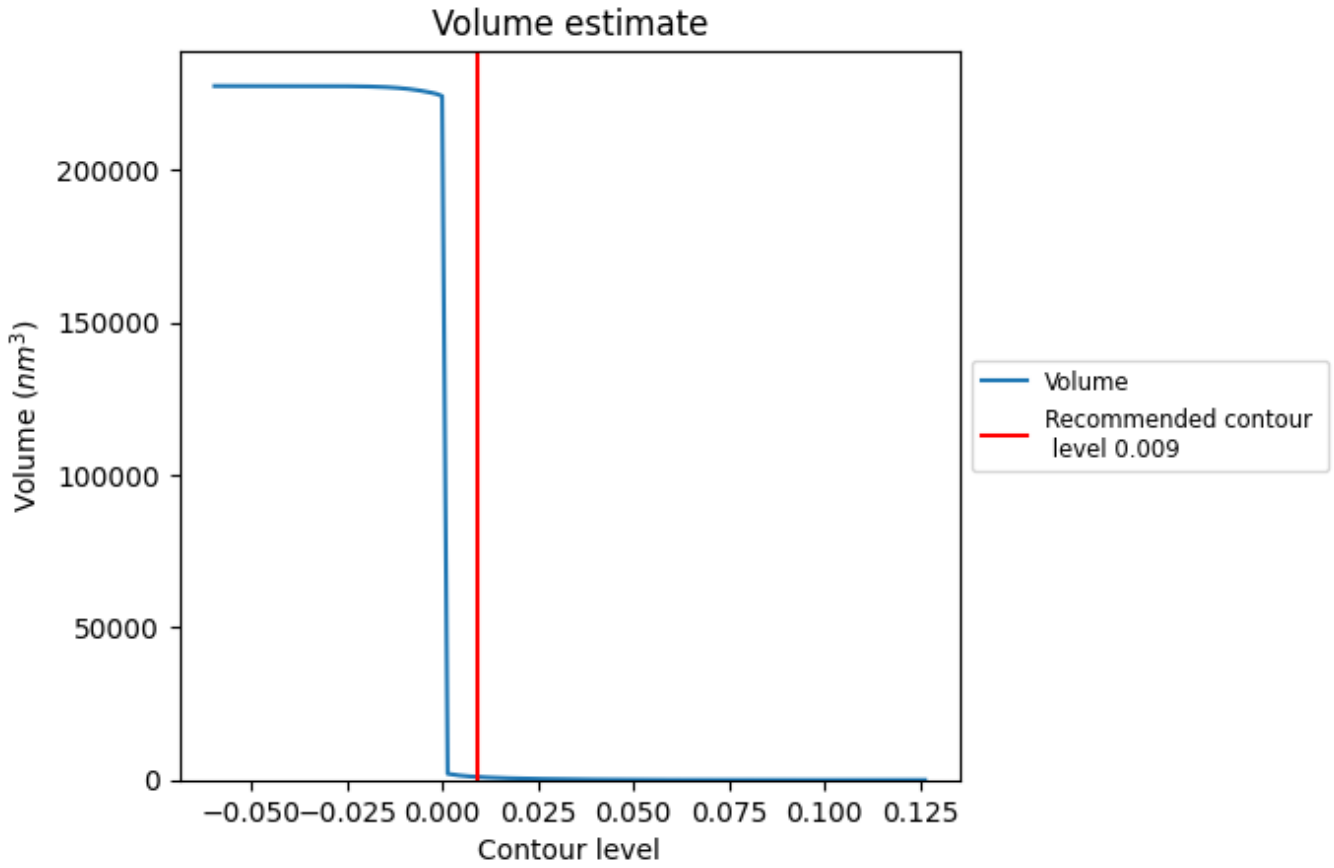
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

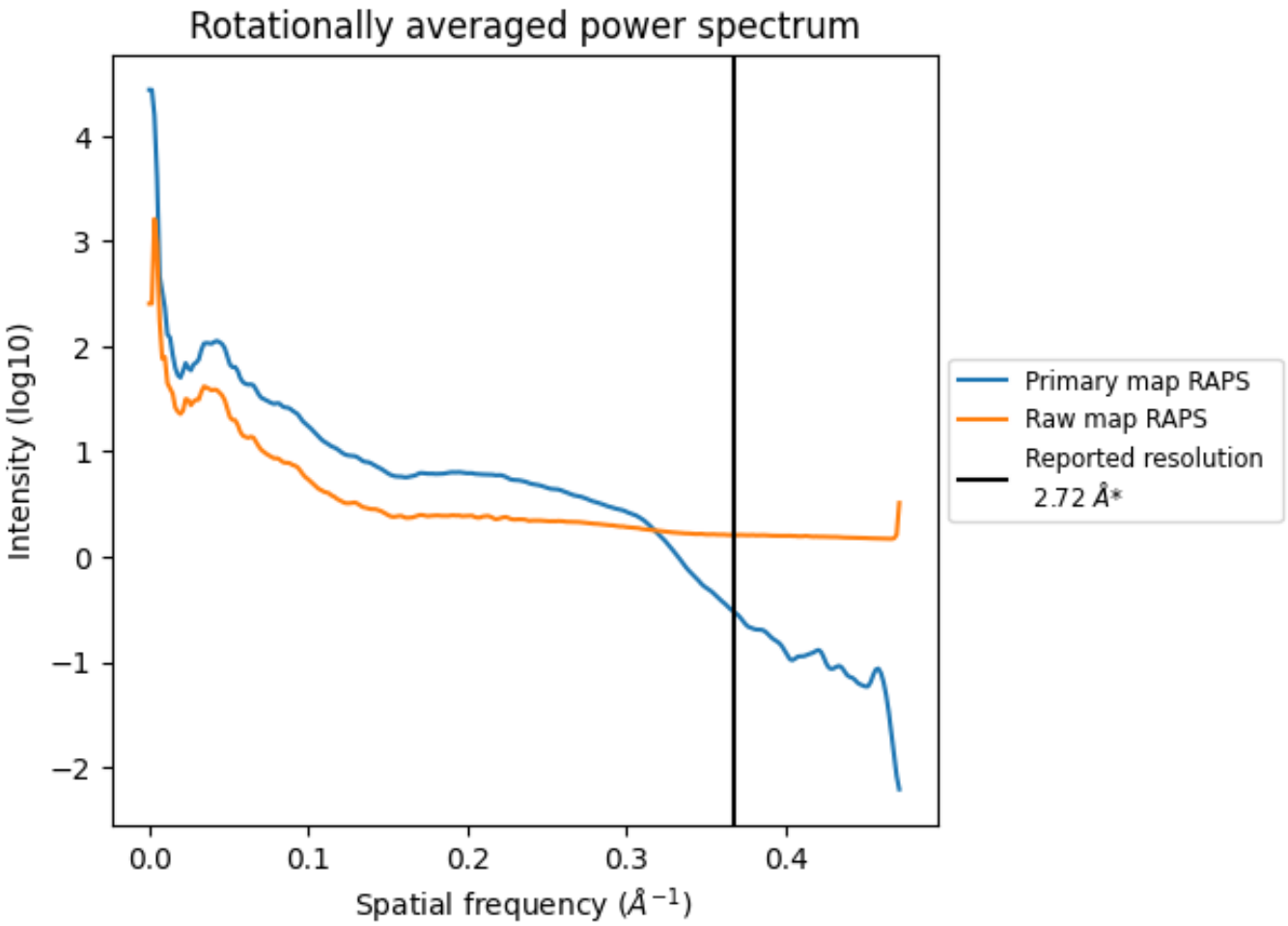
7.2 Volume estimate



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 (i)

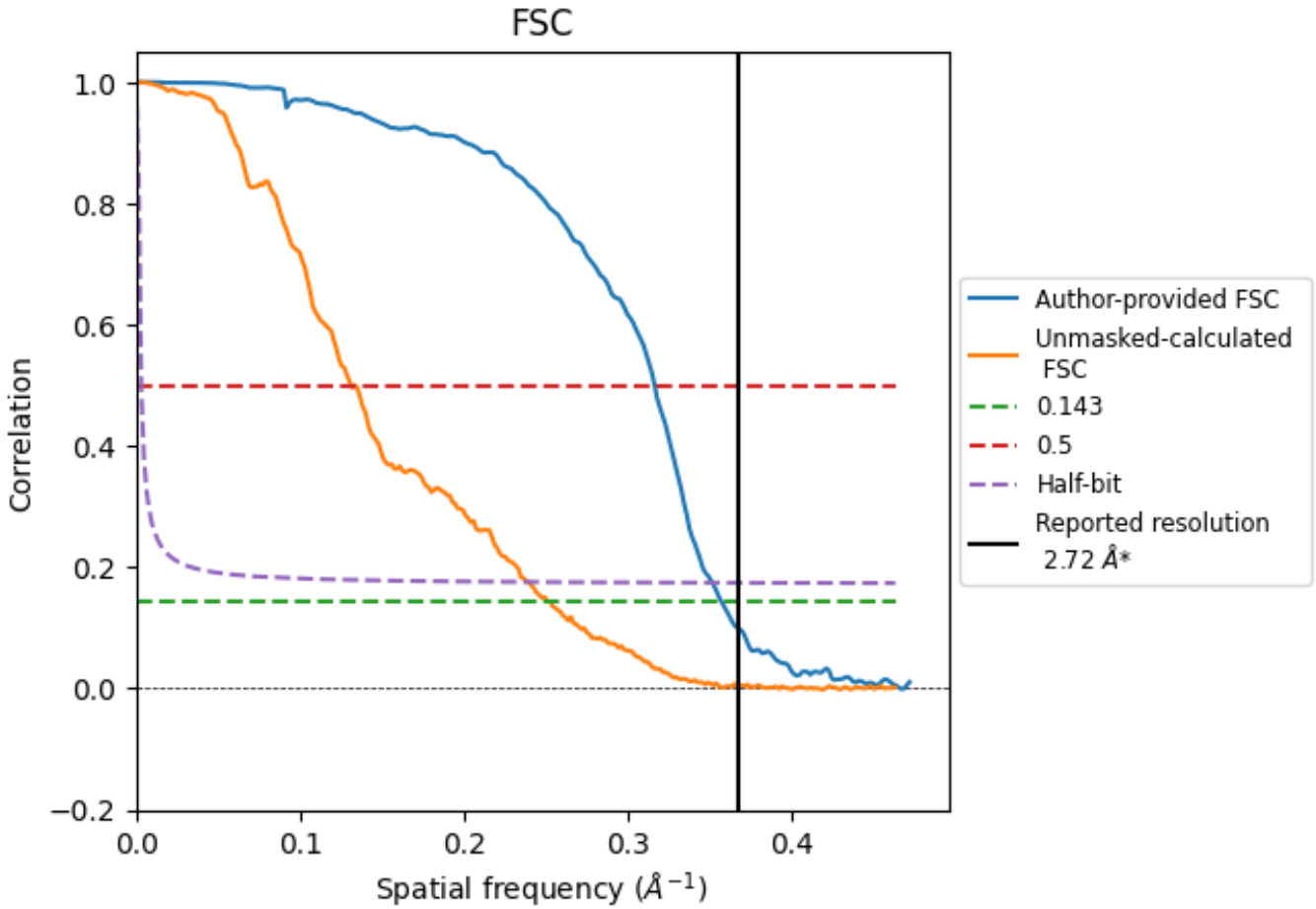


*Reported resolution corresponds to spatial frequency of 0.368 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.368 Å^{-1}

8.2 Resolution estimates (i)

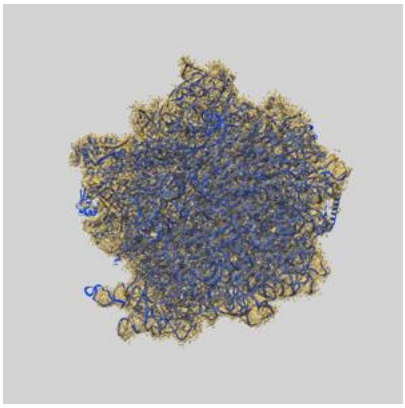
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	2.80	3.16	2.85
Unmasked-calculated*	3.96	7.63	4.18

*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 %

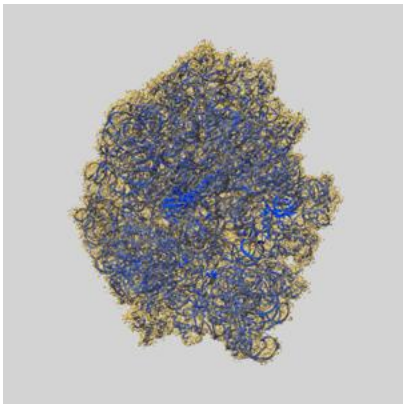
9 Map-model fit

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.

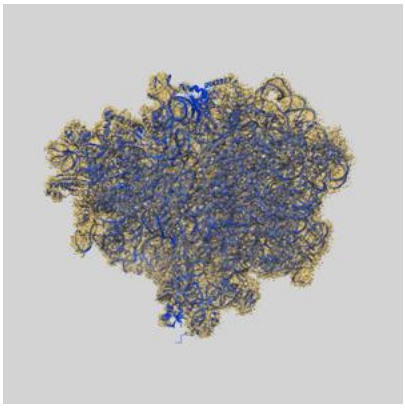
9.1 Map-model overlay



X



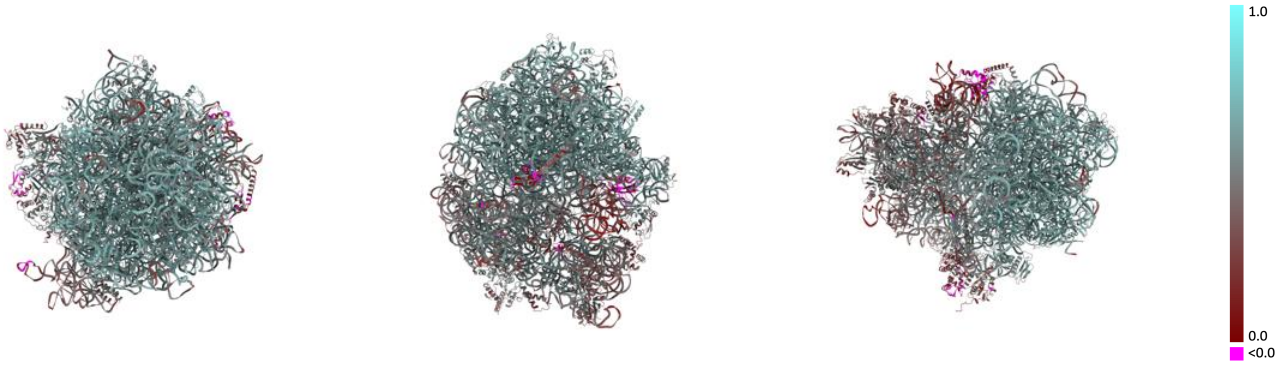
Y



Z

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.

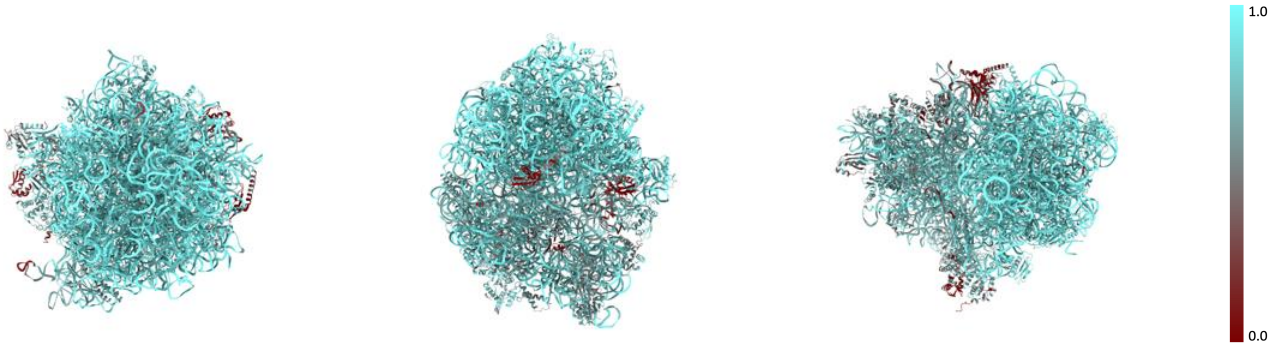
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

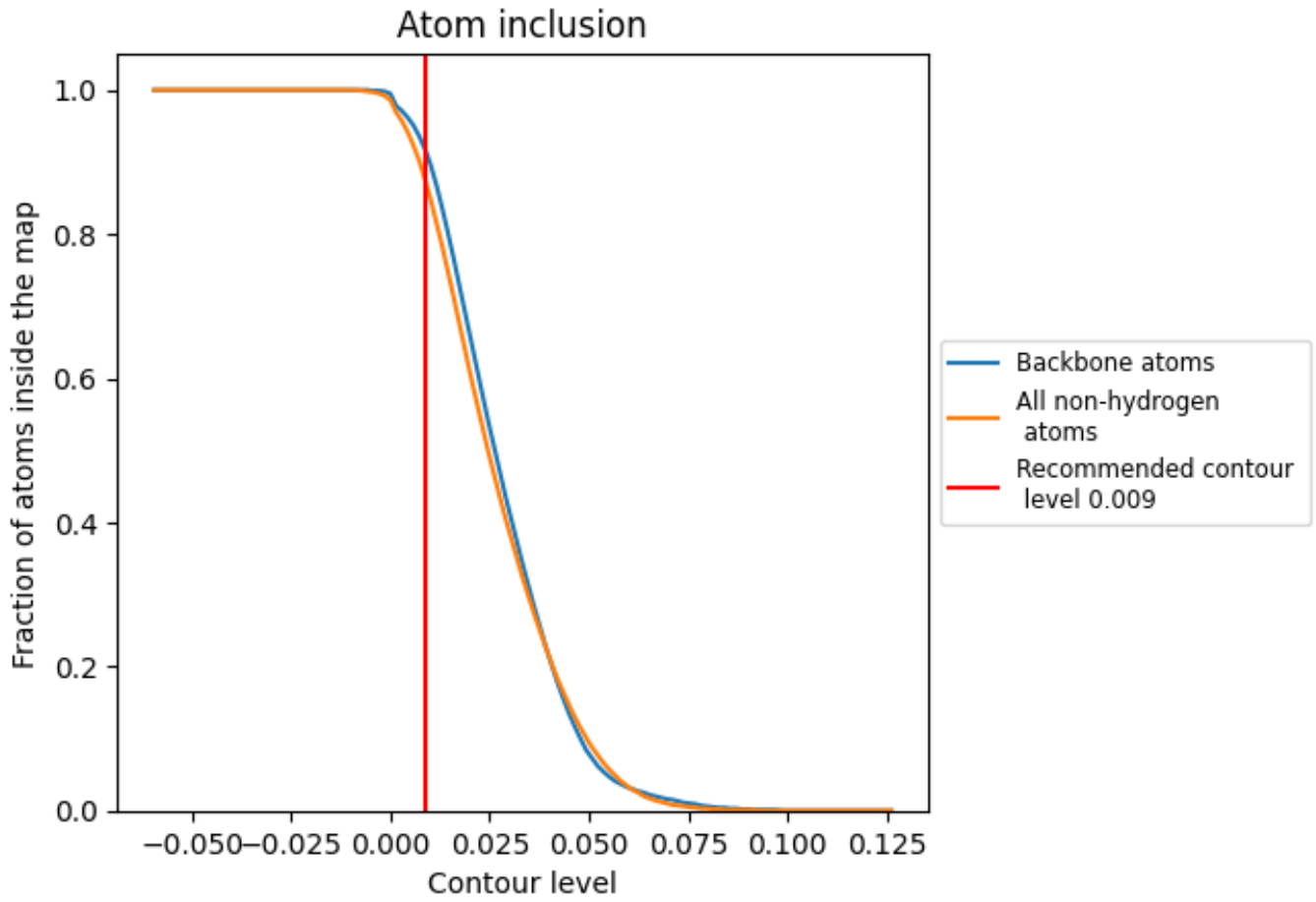
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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

Continued on next page...

Continued from previous page...

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