Full wwPDB EM Validation Report ⓘ

Apr 20, 2024 – 03:37 pm BST

PDB ID	:	6ZTO
EMDB ID	:	EMD-11422
Title	:	E. coli 70S-RNAP expressome complex in uncoupled state 1
Authors	:	Webster, M.W.; Takacs, M.; Weixlbaumer, A.
Deposited on	:	2020-07-20
Resolution	:	3.00 Å(reported)
Based on initial models	:	6ALH, 4YBB

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:

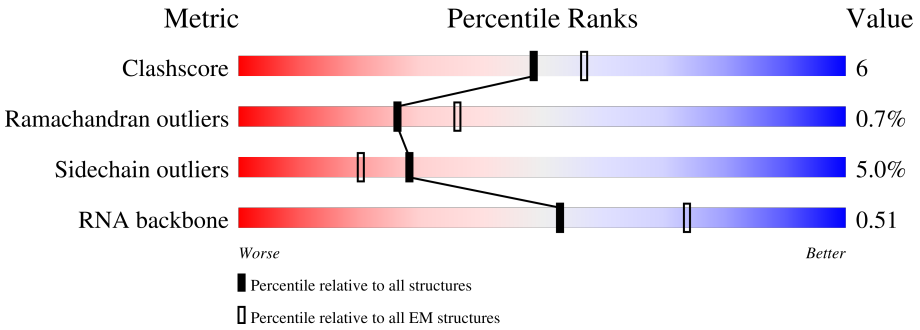
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	AA	1542	65% 27% 7%
2	AB	241	80% 71% 20% 6%
3	AC	233	6% 67% 22% 10%
4	AD	206	32% 72% 26%
5	AE	167	13% 74% 19% 7%
6	AF	131	40% 49% 27% 21%
7	AG	156	22% 78% 19%

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Mol	Chain	Length	Quality of chain
8	AH	130	14% 85% 12%
9	AI	130	68% 28%
10	AJ	103	30% 60% 29% 8%
11	AK	129	32% 65% 22% 9%
12	AL	124	12% 73% 22%
13	AM	118	9% 69% 27%
14	AN	101	77% 22%
15	AO	89	20% 76% 21%
16	AP	82	11% 82% 17%
17	AQ	84	18% 82% 11% 5%
18	AR	75	28% 75% 11% 12%
19	AS	92	74% 16% 10%
20	AT	87	8% 86% 8% 5%
21	AU	71	80% 76% 18%
22	AV	53	21% 19% 8% 17% 8% 49%
23	AW	77	42% 53% 34% 12%
24	AX	76	67% 42% 39% 16%
25	BA	2904	13% 66% 27% 6%
26	BB	120	9% 82% 16%
27	BC	273	9% 82% 17%
28	BD	209	12% 82% 15%
29	BE	201	34% 81% 16%
30	BF	179	82% 70% 27%
31	BG	177	58% 76% 21%
32	BH	149	97% 74% 22%

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Mol	Chain	Length	Quality of chain
33	BK	142	10% 84% 16%
34	BL	123	20% 84% 15%
35	BM	144	16% 83% 16%
36	BN	136	10% 82% 18%
37	BO	127	7% 80% 12% 6%
38	BP	117	27% 68% 29%
39	BQ	115	20% 81% 17%
40	BR	118	10% 81% 18%
41	BS	103	19% 80% 20%
42	BT	110	15% 70% 28%
43	BU	100	33% 79% 16%
44	BV	104	34% 75% 22%
45	BW	94	31% 81% 17%
46	BX	85	9% 81% 6% 11%
47	BY	78	17% 82% 17%
48	BZ	63	43% 76% 21%
49	B1	59	17% 76% 20%
50	B2	57	21% 79% 19%
51	B3	55	85% 67% 25%
52	B4	46	83% 13%
53	B5	65	11% 80% 14% 5%
54	B6	50	58% 16% 24%
55	B7	70	96% 74% 23%
56	CN	39	64% 23% 44% 10% 23%
57	CT	39	36% 13% 41% 23% 23%

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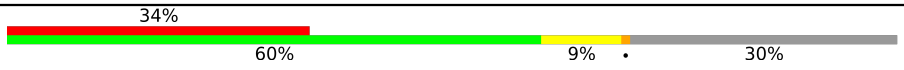
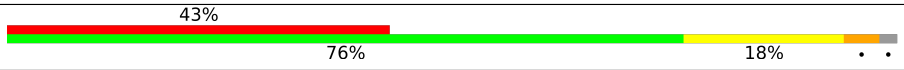
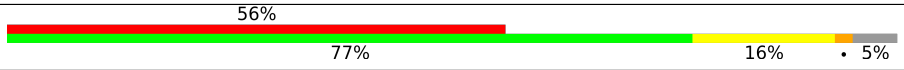
Mol	Chain	Length	Quality of chain
58	CA	329	
58	CB	329	
59	CC	1342	
60	CD	1407	
61	CE	91	

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 172846 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	AA	1533	32909	14684	6037	10655	1533	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AB	226	1765	1116	317	324	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	AC	209	1640	1038	308	291	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	AD	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	AE	156	1148	715	217	210	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	9	CYS	GLY	conflict	UNP A0A090BZW5

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	154	Total	C	N	O	S	0	0
			1214	756	235	219	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	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	AI	128	Total	C	N	O	S	0	0
			1031	639	207	182	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	100	Total	C	N	O	S	0	0
			800	500	153	146	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	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	AL	122	Total	C	N	O	S	0	0
			951	588	195	163	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	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	AN	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	AO	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	AP	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	AQ	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	AR	66	Total	C	N	O	S	0	0
			545	344	102	98	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	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	AU	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	27	Total	C	N	O	P	0	0
			572	256	102	187	27		

- Molecule 23 is a RNA chain called tRNA(fmet) P-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AW	77	Total	C	N	O	P	S	0	0
			1645	734	297	536	77	1		

- Molecule 24 is a RNA chain called Phe-NH-tRNA(Phe) A-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AX	76	Total	C	N	O	P	S	0	0
			1630	730	290	533	76	1		

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BA	2900	Total	C	N	O	P	0	0
			62270	27786	11456	20128	2900		

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BB	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BC	272	Total	C	N	O	S	0	0
			2092	1294	425	366	7		

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BD	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BF	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BG	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

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

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BM	144	Total	C	N	O	S	0	0
			1052	653	207	190	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BM	77	VAL	ILE	conflict	UNP P02413

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BP	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BU	96	Total 764	C 484	N 142	O 136	S 2	0	0

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	BV	103	Total 789	C 498	N 148	O 143	0	0

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BX	76	Total 582	C 360	N 117	O 104	S 1	0	0

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B1	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B2	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	B3	53	Total	C	N	O	0	0
			436	281	80	75		

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B4	46	Total	C	N	O	S	0	0
			376	228	89	57	2		

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B5	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B6	38	Total	C	N	O	S	0	0
			301	185	65	47	4		

- Molecule 55 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B7	70	Total	C	N	O	S	0	0
			549	339	104	100	6		

- Molecule 56 is a DNA chain called Non-template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	CN	30	Total	C	N	O	P	0	0
			618	294	114	180	30		

- Molecule 57 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	CT	30	Total	C	N	O	P	0	0
			606	288	105	183	30		

- Molecule 58 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	CA	229	Total	C	N	O	S	0	0
			1775	1106	313	350	6		
58	CB	219	Total	C	N	O	S	0	0
			1684	1051	295	332	6		

- Molecule 59 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	CC	1320	Total	C	N	O	S	0	0
			10415	6535	1815	2021	44		

- Molecule 60 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	CD	1333	Total	C	N	O	S	0	0
			10375	6518	1851	1956	50		

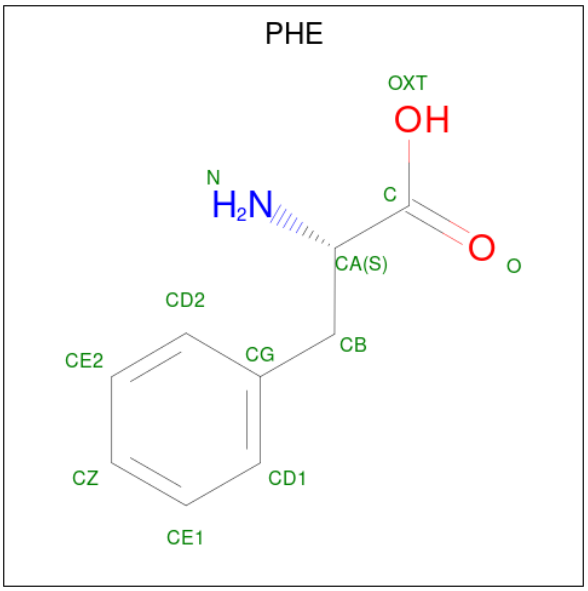
- Molecule 61 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	CE	61	Total	C	N	O	S	0	0
			478	295	90	92	1		

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
62	AA	143	Total	Mg	0
			143	143	
62	AI	1	Total	Mg	0
			1	1	
62	AL	1	Total	Mg	0
			1	1	
62	AM	1	Total	Mg	0
			1	1	
62	AW	5	Total	Mg	0
			5	5	
62	AX	1	Total	Mg	0
			1	1	
62	BA	317	Total	Mg	0
			317	317	
62	BB	9	Total	Mg	0
			9	9	
62	BC	3	Total	Mg	0
			3	3	
62	BN	1	Total	Mg	0
			1	1	
62	BO	1	Total	Mg	0
			1	1	
62	BQ	1	Total	Mg	0
			1	1	
62	BV	1	Total	Mg	0
			1	1	
62	BX	1	Total	Mg	0
			1	1	
62	CD	1	Total	Mg	0
			1	1	

- Molecule 63 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
63	AX	1	Total	C	N	O	0
			11	9	1	1	

- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn).

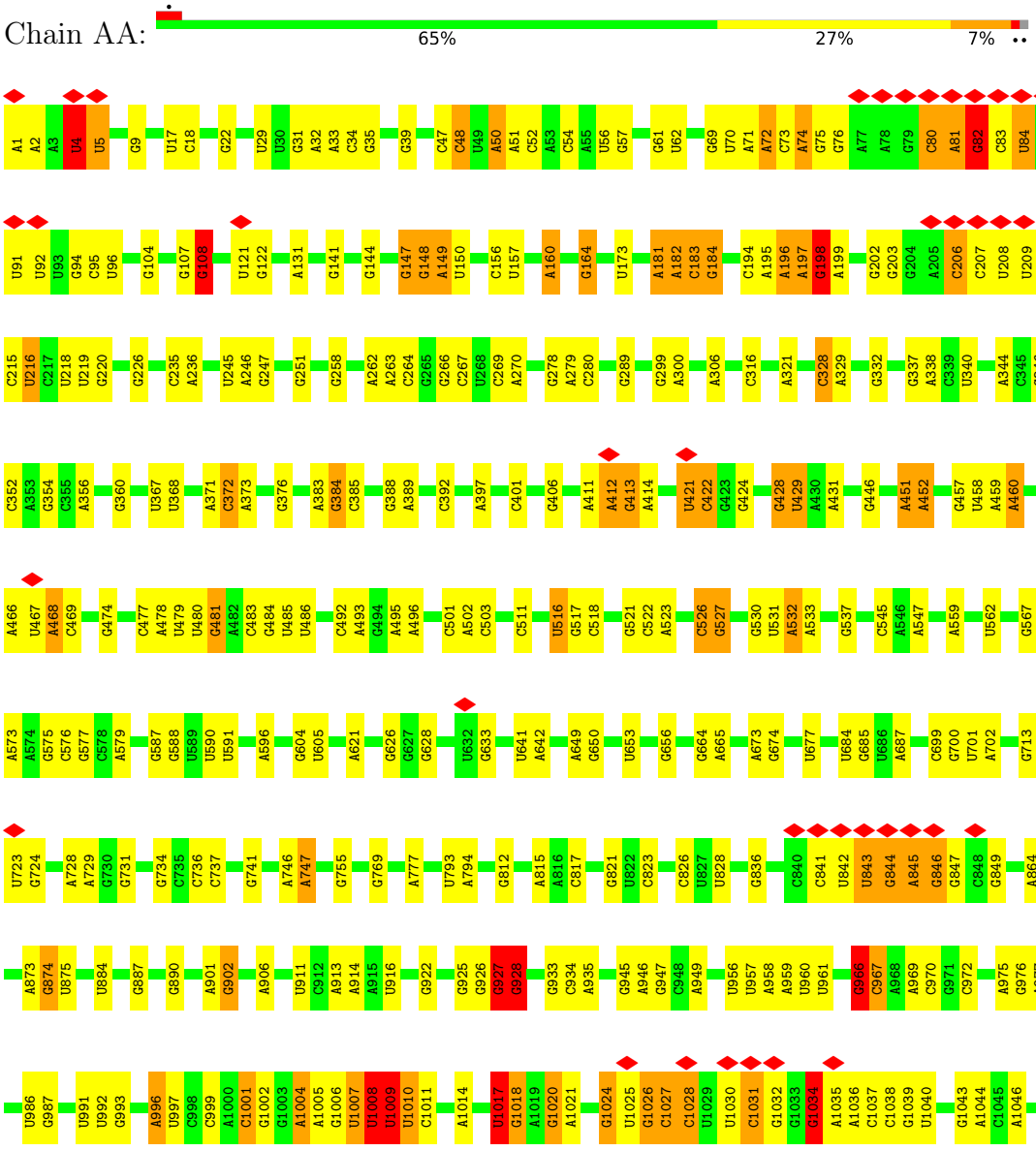
Mol	Chain	Residues	Atoms		AltConf
64	B6	1	Total	Zn	0
			1	1	
64	B7	1	Total	Zn	0
			1	1	
64	CD	2	Total	Zn	0
			2	2	

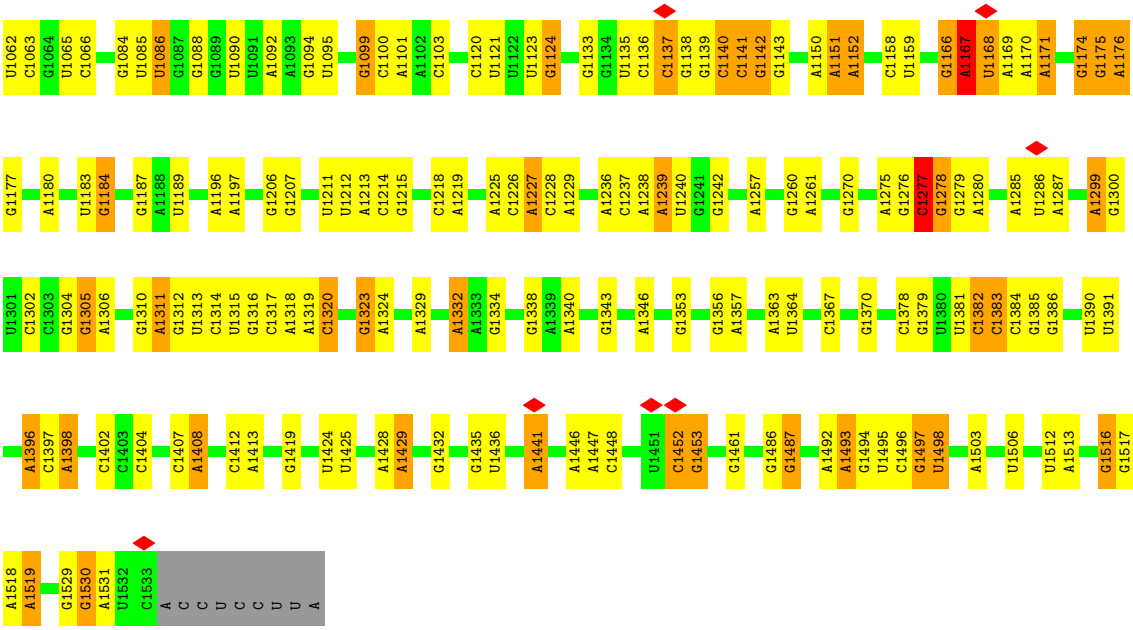
3 Residue-property plots (i)

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 ribosomal RNA

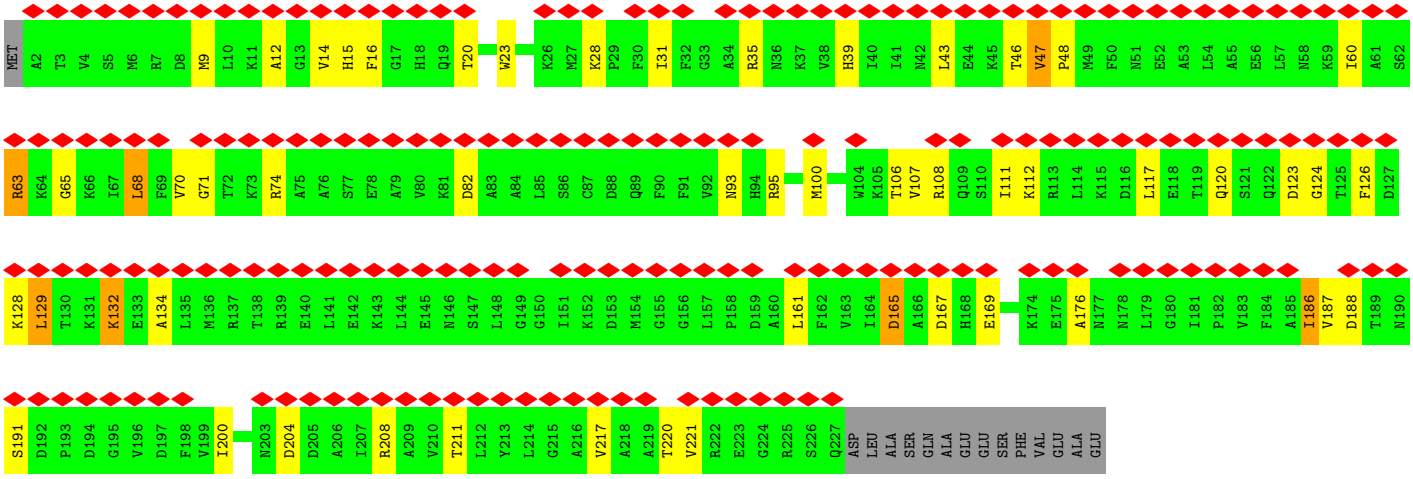
Chain AA:





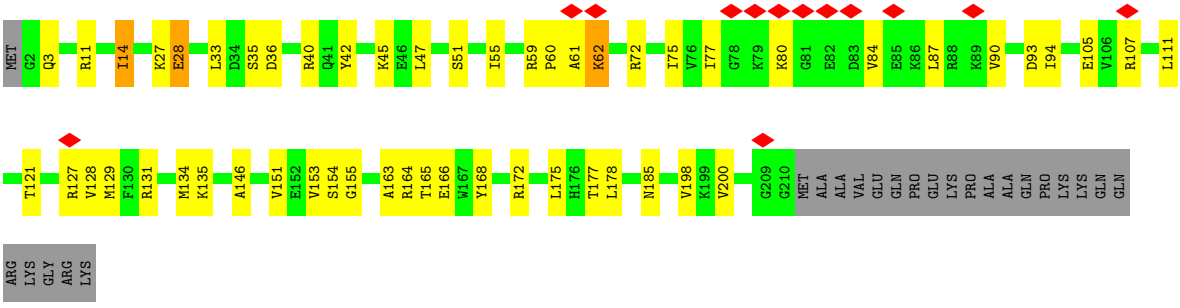
• Molecule 2: 30S ribosomal protein S2

Chain AB:



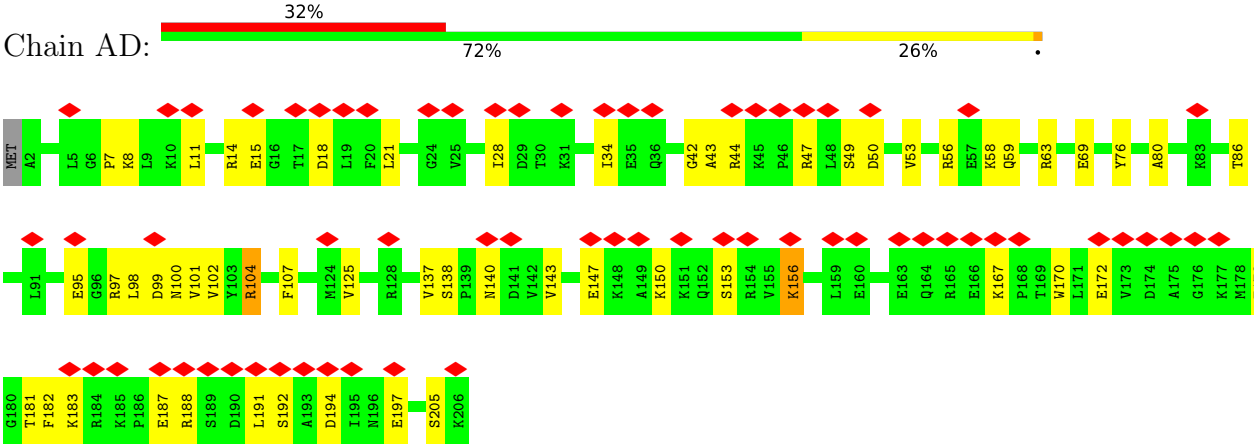
• Molecule 3: 30S ribosomal protein S3

Chain AC:



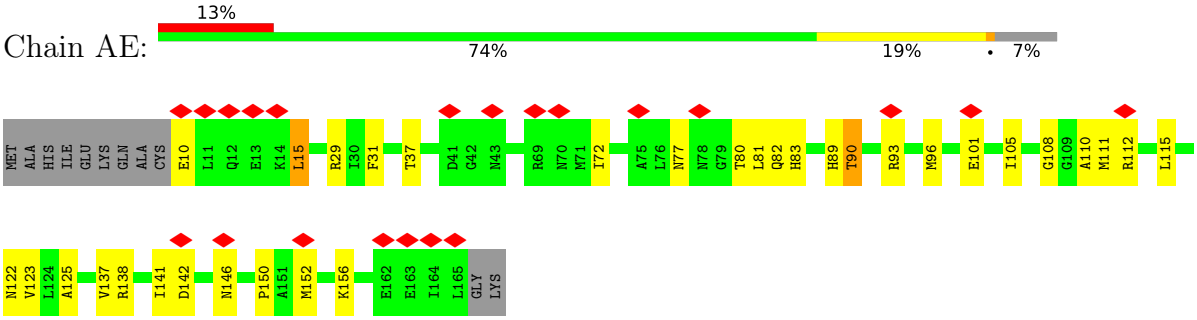
• Molecule 4: 30S ribosomal protein S4

Chain AD:



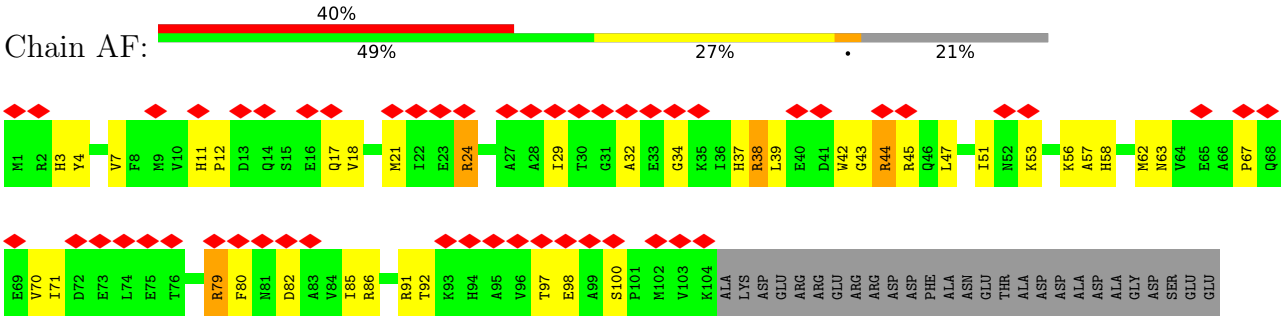
• Molecule 5: 30S ribosomal protein S5

Chain AE:



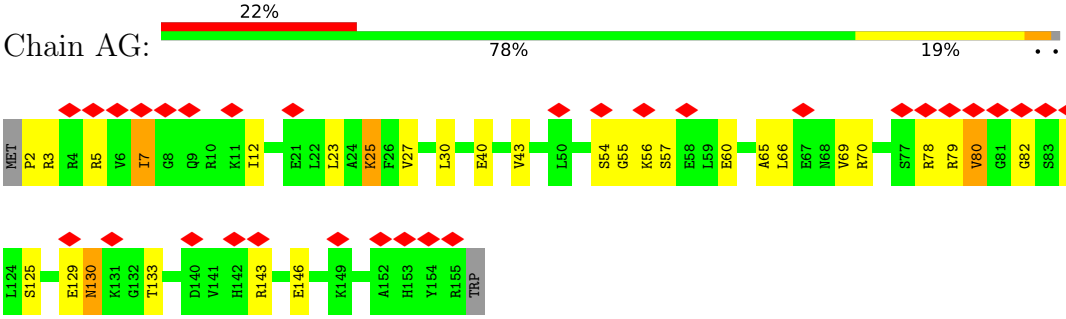
• Molecule 6: 30S ribosomal protein S6

Chain AF:



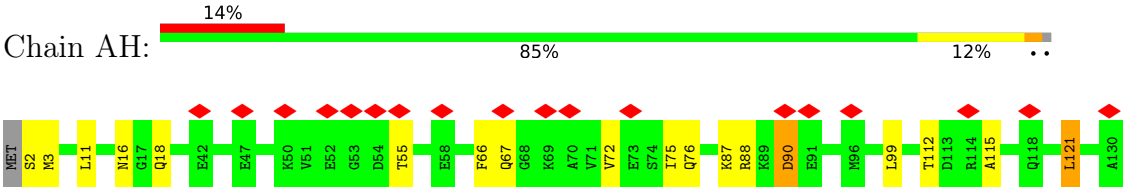
• Molecule 7: 30S ribosomal protein S7

Chain AG:



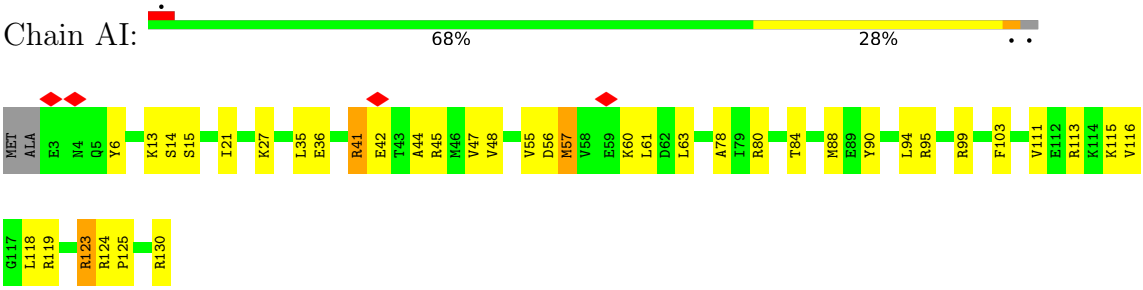
• Molecule 8: 30S ribosomal protein S8

Chain AH:



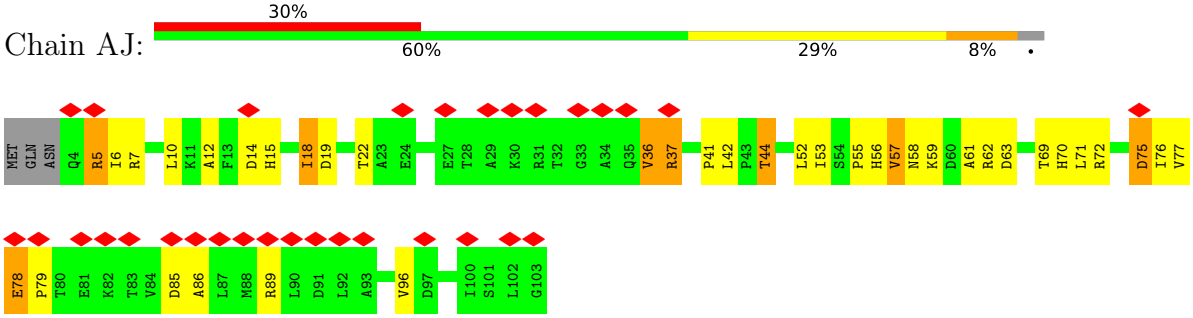
• Molecule 9: 30S ribosomal protein S9

Chain AI:



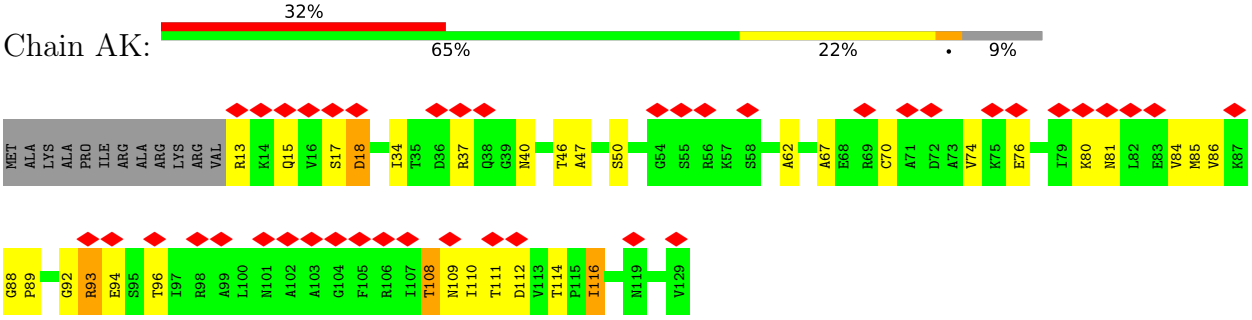
• Molecule 10: 30S ribosomal protein S10

Chain AJ:



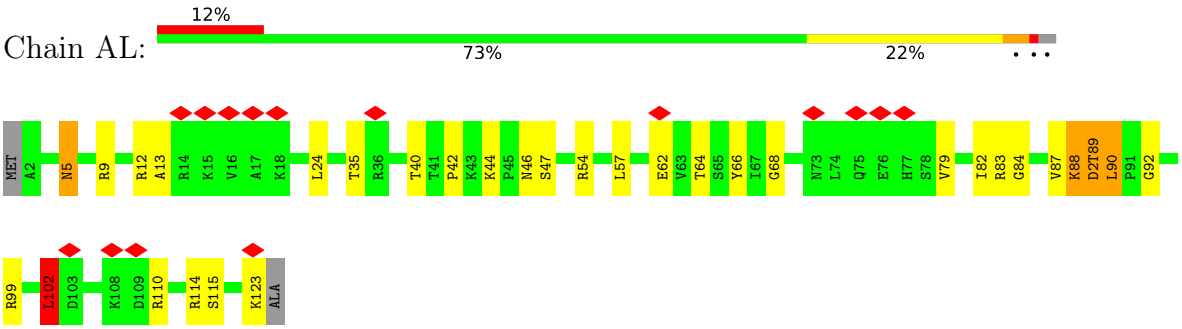
• Molecule 11: 30S ribosomal protein S11

Chain AK:



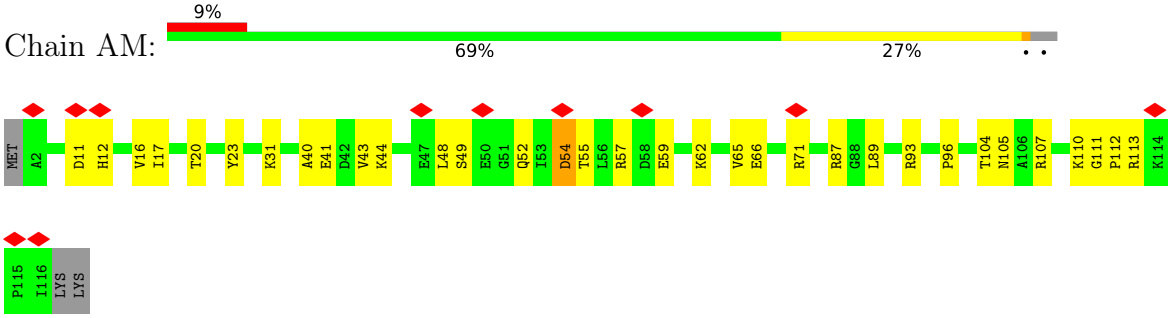
• Molecule 12: 30S ribosomal protein S12

Chain AL:



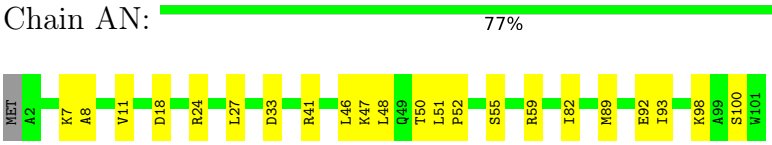
• Molecule 13: 30S ribosomal protein S13

Chain AM:



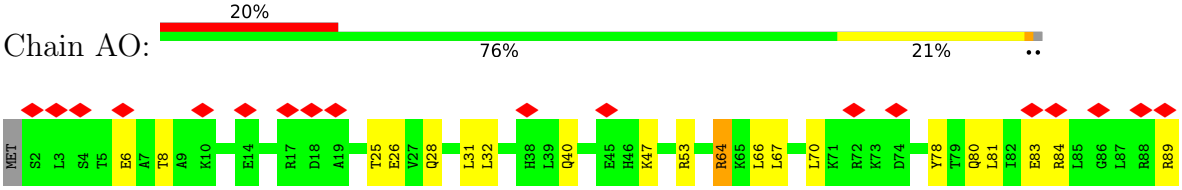
• Molecule 14: 30S ribosomal protein S14

Chain AN:



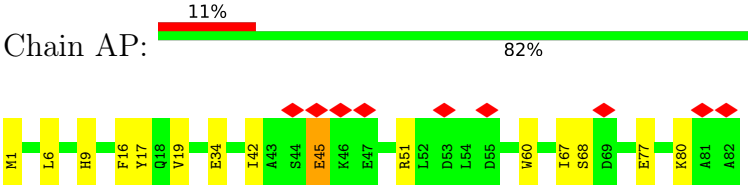
• Molecule 15: 30S ribosomal protein S15

Chain AO:



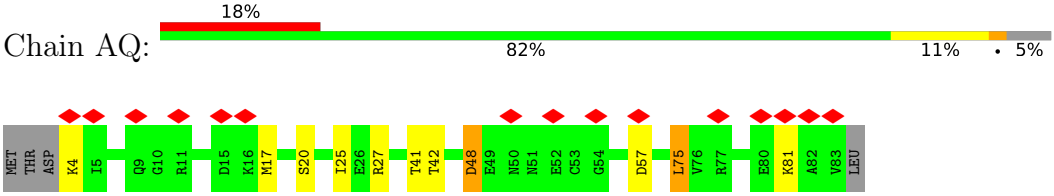
• Molecule 16: 30S ribosomal protein S16

Chain AP:



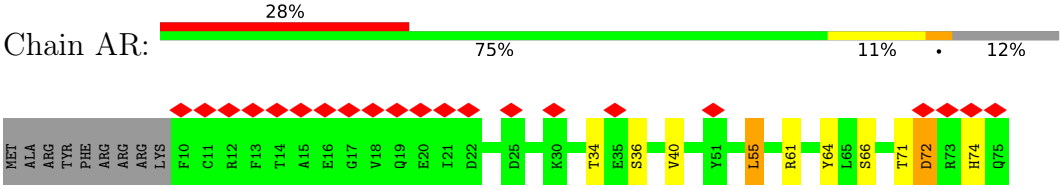
• Molecule 17: 30S ribosomal protein S17

Chain AQ:



• Molecule 18: 30S ribosomal protein S18

Chain AR:

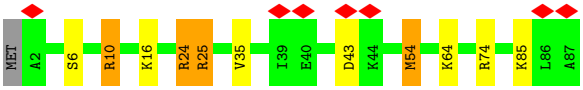


• Molecule 19: 30S ribosomal protein S19

Chain AS:

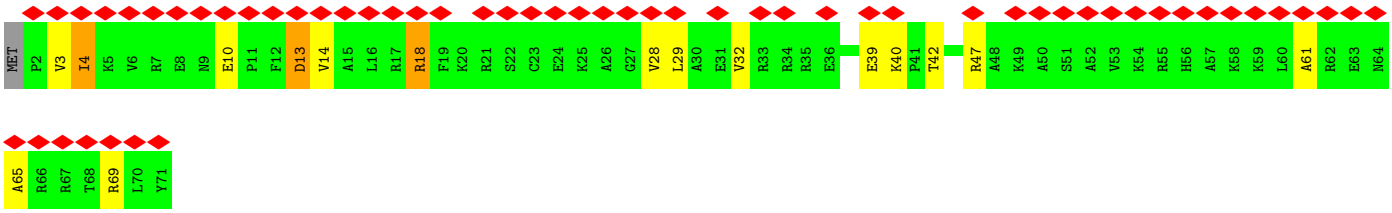
• Molecule 20: 30S ribosomal protein S20

Chain AT:



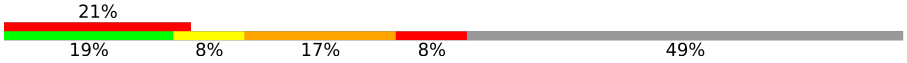
• Molecule 21: 30S ribosomal protein S21

Chain AU:



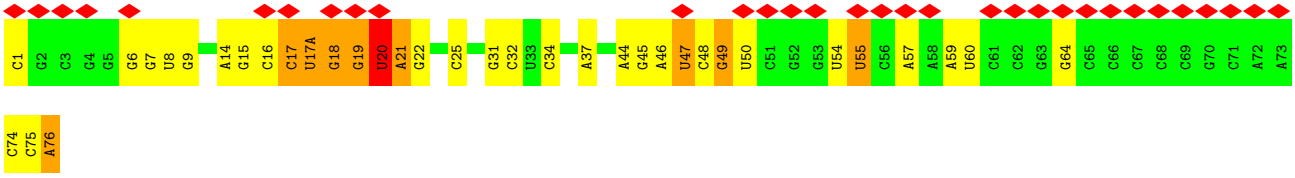
• Molecule 22: mRNA

Chain AV:



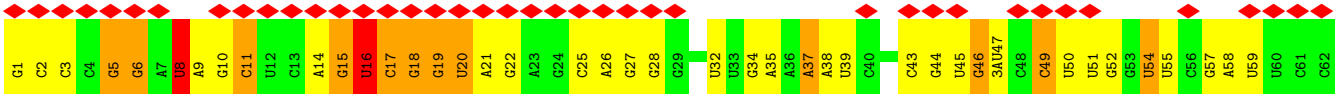
• Molecule 23: tRNA(fmet) P-site

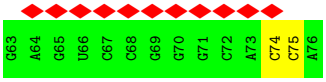
Chain AW:



• Molecule 24: Phe-NH-tRNA(Phe) A-site

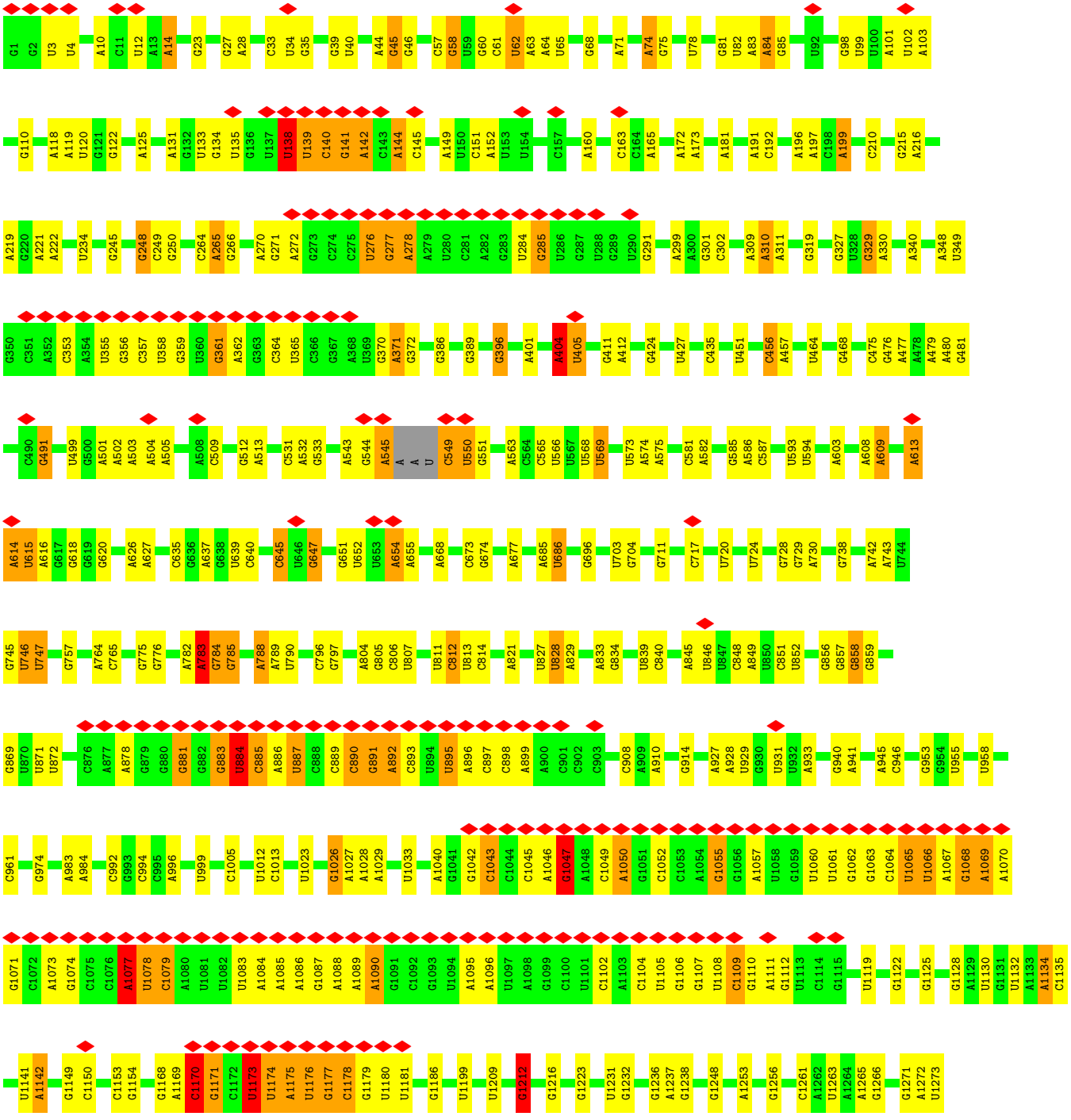
Chain AX:

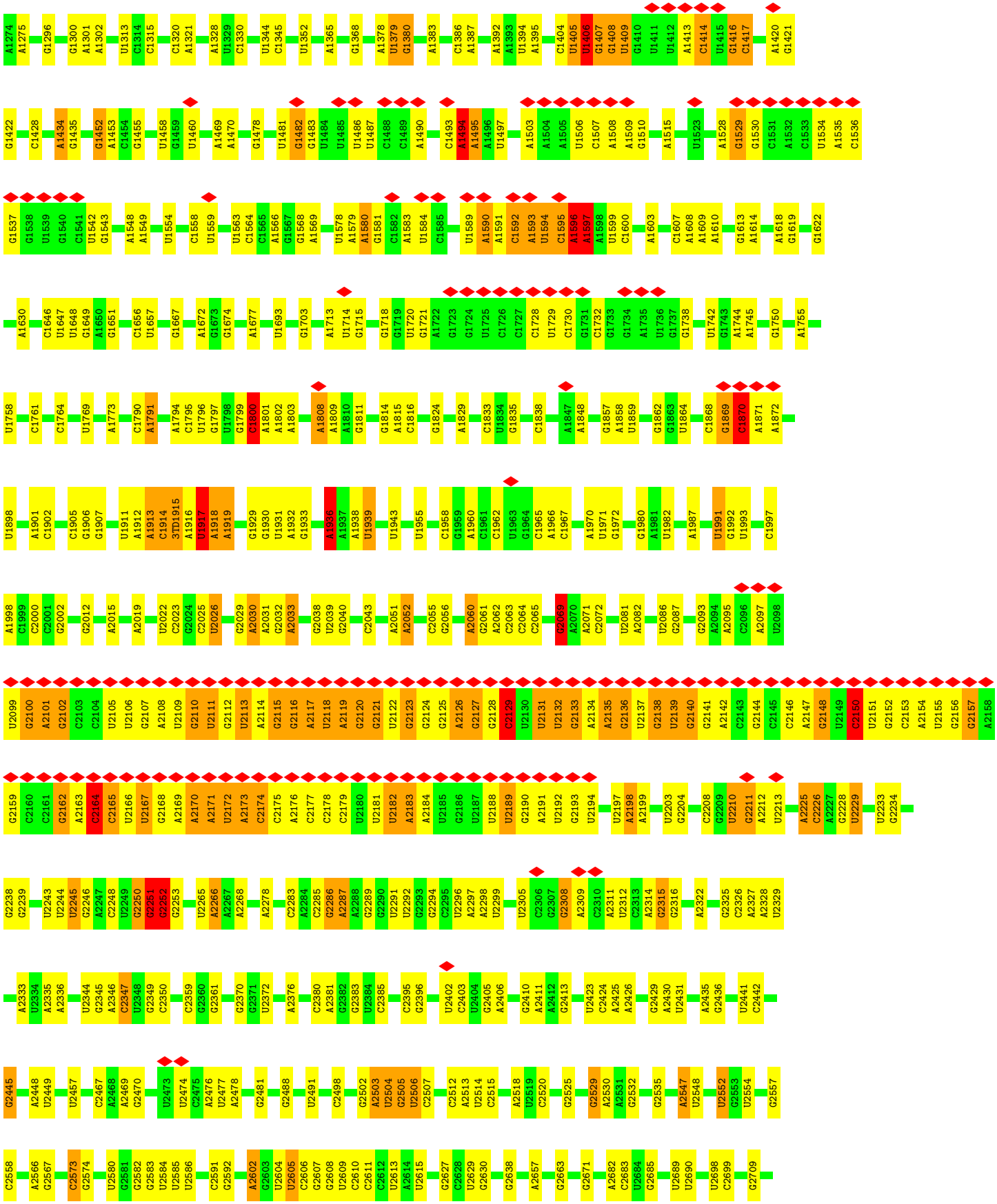




• Molecule 25: 23S ribosomal RNA

Chain BA:

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G1422 C1428 A1434 G1435 G1452 A1453 C1454 G1455 U1458 G1459 U1460 A1469 A1470 G1478 U1481 G1482 G1483 U1484 U1485 U1486 U1487 C1488 C1489 A1490 C1493 A1494 A1495 A1496 U1497 A1503 A1504 A1505 U1506 C1507 A1508 A1509 G1510 A1515 U1523 A1528 G1529 G1530 C1531 A1532 C1533 U1534 A1535 C1536
G1537 G1538 U1539 G1540 C1541 U1542 G1543 A1548 A1549 U1554 C1558 U1559 U1563 C1564 C1565 A1566 G1567 G1568 A1569 U1578 A1579 A1580 G1581 C1582 A1583 U1584 C1585 U1589 A1590 A1591 C1592 A1593 U1594 C1595 A1596 A1597 A1598 U1599 C1600 A1603 C1607 A1608 A1609 A1610 G1613 A1614 A1618 G1619 G1622
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U1758 C1761 C1764 U1769 A1773 C1790 A1791 A1794 C1795 U1796 G1797 U1798 G1799 C1800 A1801 A1802 A1803 A1808 A1809 A1810 G1811 G1814 A1815 C1816 G1824 A1829 C1833 U1834 G1835 C1838 A1847 A1848 G1857 A1858 U1859 G1862 G1863 U1864 C1868 G1869 C1870 A1871 A1872
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A1998 C1999 C2000 C2001 G2002 G2012 A2015 A2019 U2022 C2023 G2024 C2025 U2026 G2029 A2030 A2031 G2032 A2033 G2038 U2039 G2040 C2043 A2051 A2052 C2055 G2056 A2060 G2061 A2062 C2063 C2064 C2065 G2069 A2070 A2071 C2072 U2081 A2082 U2086 G2087 G2093 A2094 A2095 C2096 A2097 U2098
U2099 G2100 A2101 G2102 C2103 C2104 U2105 U2106 G2107 A2108 U2109 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 G2128 C2129 U2130 U2131 U2132 G2133 A2134 A2135 G2136 U2137 G2138 U2139 G2140 G2141 A2142 C2143 G2144 C2145 C2146 A2147 G2148 U2149 C2150 U2151 G2152 C2153 A2154 U2155 G2156 G2157 A2158
G2159 C2160 C2161 G2162 A2163 C2164 C2165 U2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 U2181 U2182 A2183 A2184 U2185 G2186 U2187 U2188 U2189 G2190 A2191 U2192 G2193 U2194 U2197 A2198 A2199 U2203 G2204 C2208 G2209 U2210 G2211 A2212 U2213 A2225 C2226 A2227 G2228 U2229 U2233 G2234
G2238 G2239 U2243 U2244 U2245 G2246 A2247 C2248 U2249 G2250 G2251 G2252 G2253 U2265 A2266 A2267 A2268 A2278 C2283 A2284 C2285 G2286 A2287 A2288 G2289 G2290 U2291 U2292 G2293 G2294 C2295 U2296 A2297 A2298 U2299 U2305 C2306 G2307 G2308 A2309 C2310 A2311 U2312 C2313 A2314 G2315 G2316 A2322 G2325 C2326 A2327 A2328 U2329
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G2445 A2448 U2449 U2457 C2467 A2468 A2469 G2470 U2473 U2474 C2475 A2476 U2477 A2478 G2481 G2488 U2491 C2498 G2502 A2503 U2504 G2505 U2506 C2507 C2512 A2513 U2514 C2515 A2518 U2519 C2520 G2525 G2529 A2530 A2531 G2532 G2535 A2547 U2548 U2552 G2553 U2554 G2557
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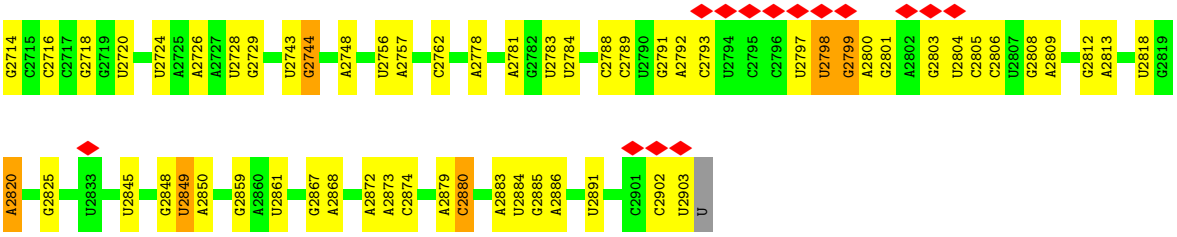
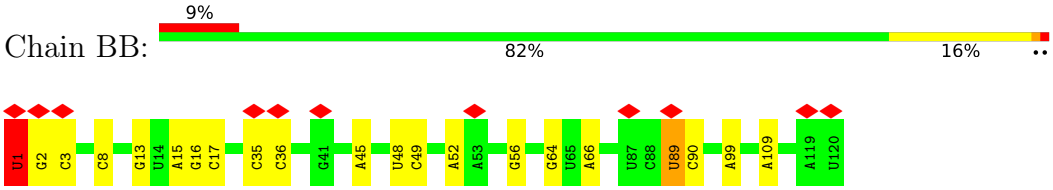
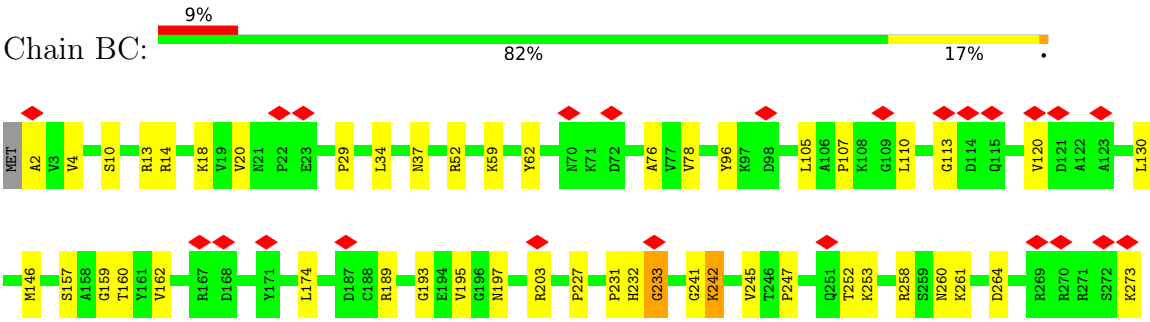


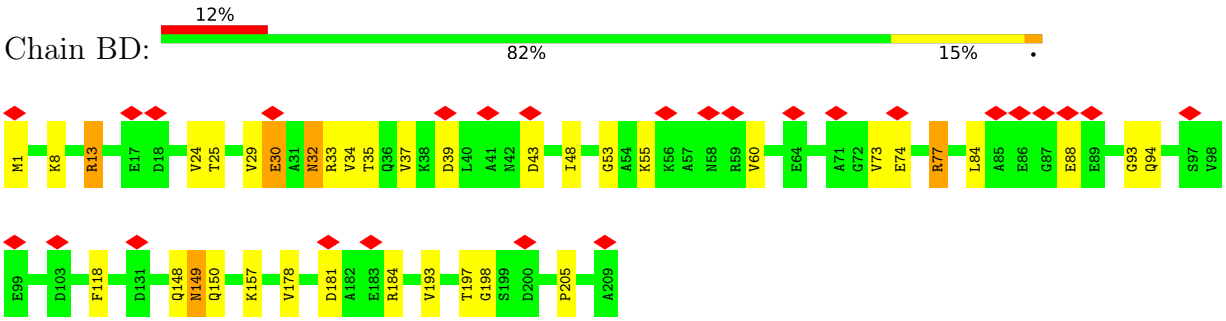
• Molecule 26: 5S ribosomal RNA



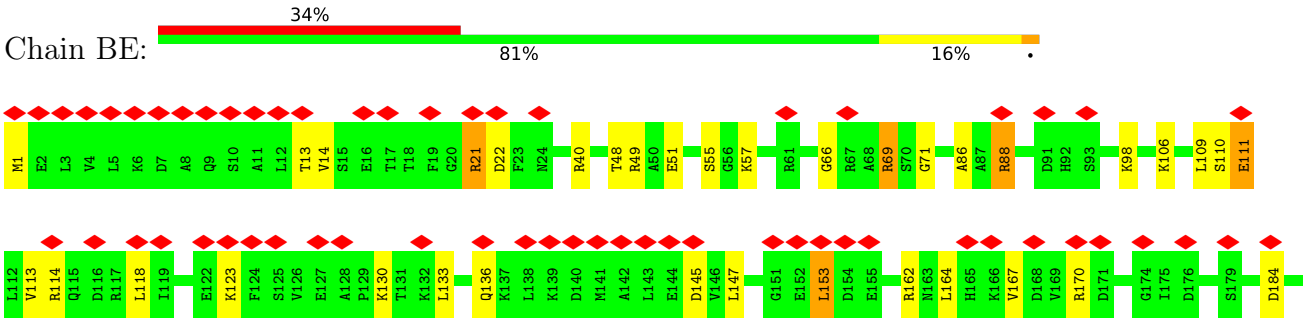
• Molecule 27: 50S ribosomal protein L2

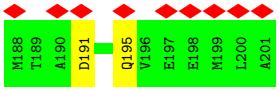


• Molecule 28: 50S ribosomal protein L3



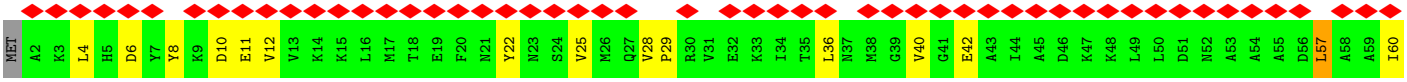
• Molecule 29: 50S ribosomal protein L4

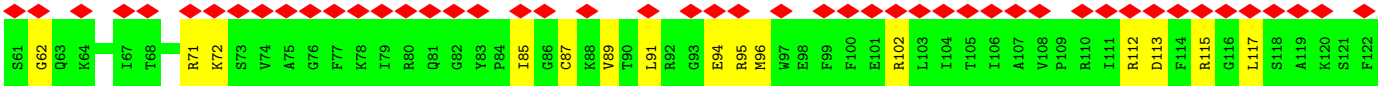




• Molecule 30: 50S ribosomal protein L5

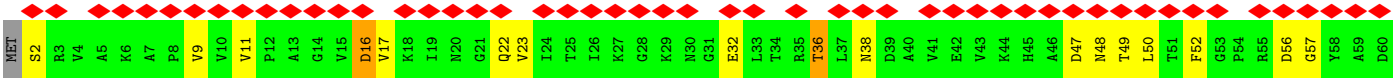
Chain BF:

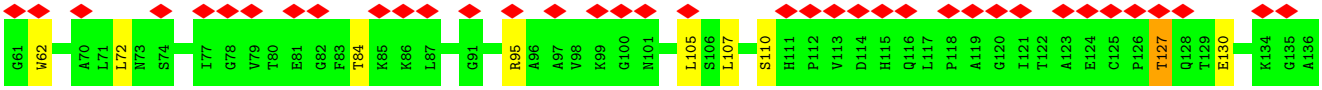


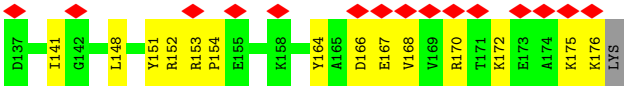


• Molecule 31: 50S ribosomal protein L6

Chain BG:

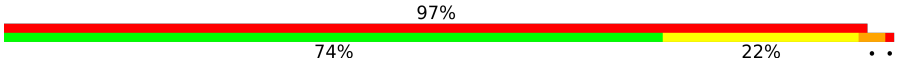


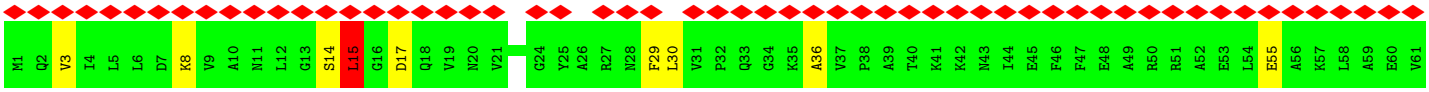


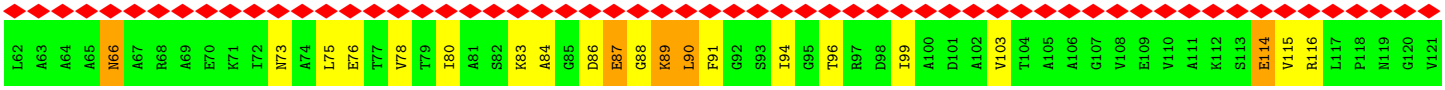


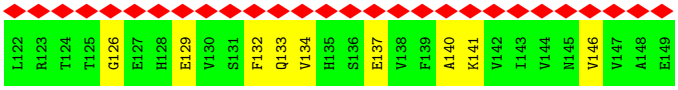
• Molecule 32: 50S ribosomal protein L9

Chain BH:



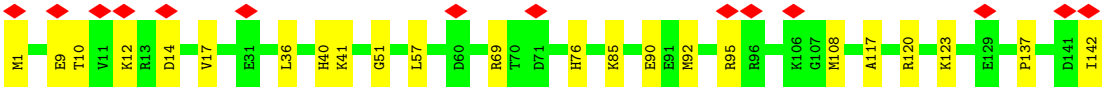






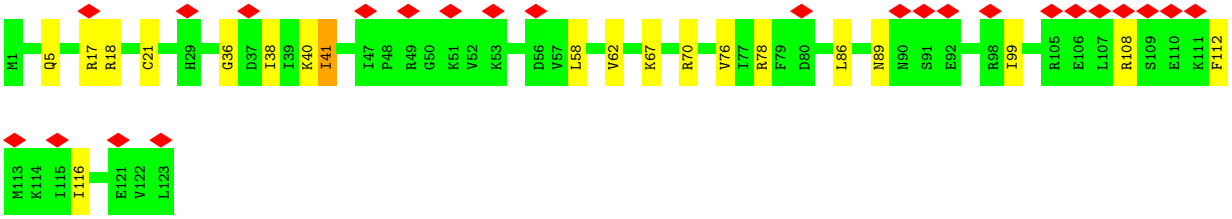
• Molecule 33: 50S ribosomal protein L13

Chain BK:



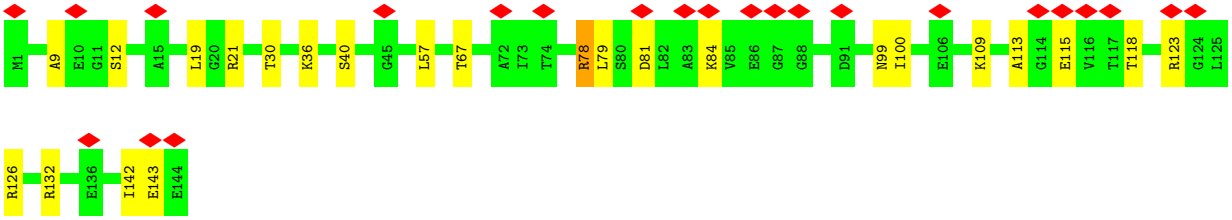
• Molecule 34: 50S ribosomal protein L14

Chain BL:



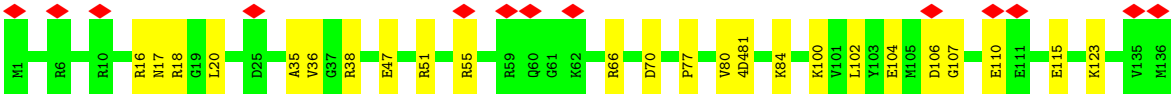
• Molecule 35: 50S ribosomal protein L15

Chain BM:



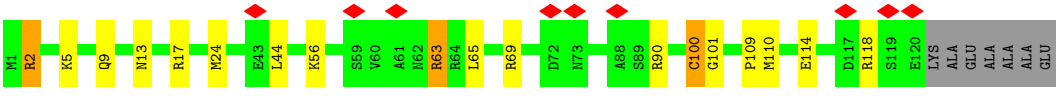
• Molecule 36: 50S ribosomal protein L16

Chain BN:



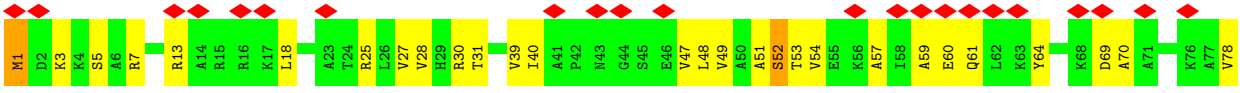
• Molecule 37: 50S ribosomal protein L17

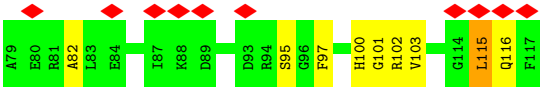
Chain BO:



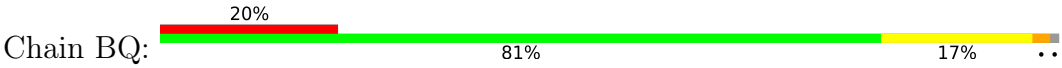
• Molecule 38: 50S ribosomal protein L18

Chain BP:

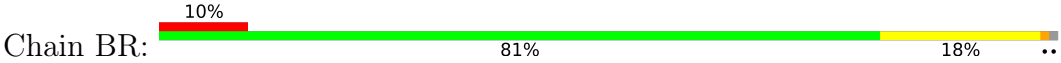


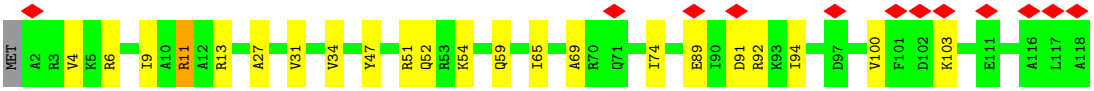


• Molecule 39: 50S ribosomal protein L19

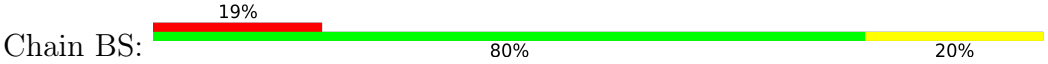


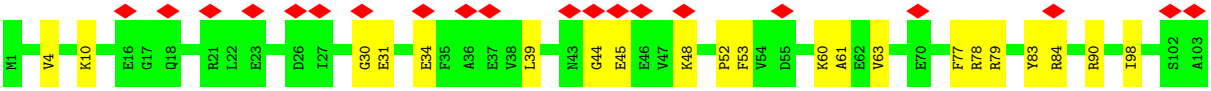
• Molecule 40: 50S ribosomal protein L20



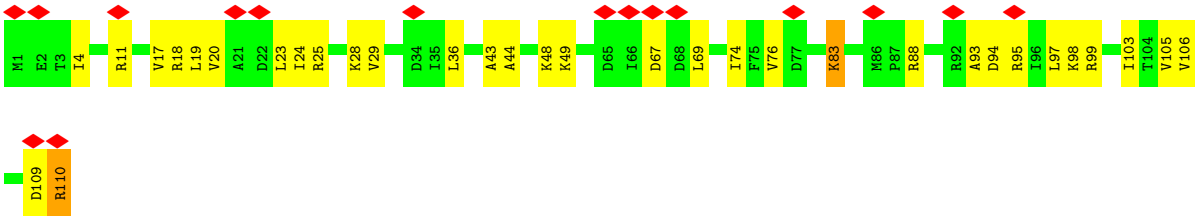


• Molecule 41: 50S ribosomal protein L21

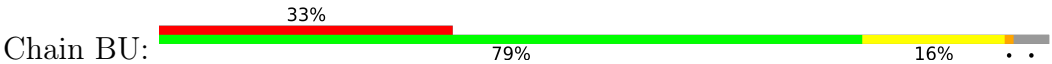


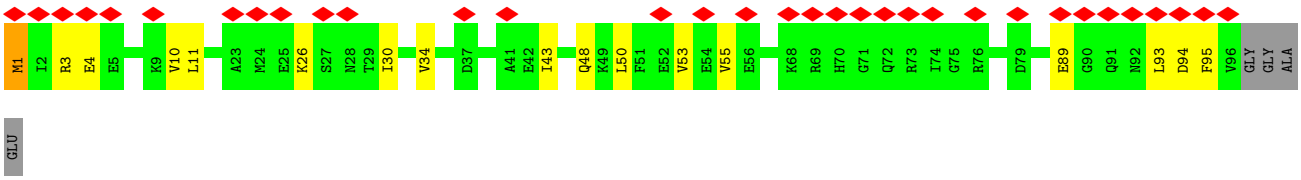


• Molecule 42: 50S ribosomal protein L22



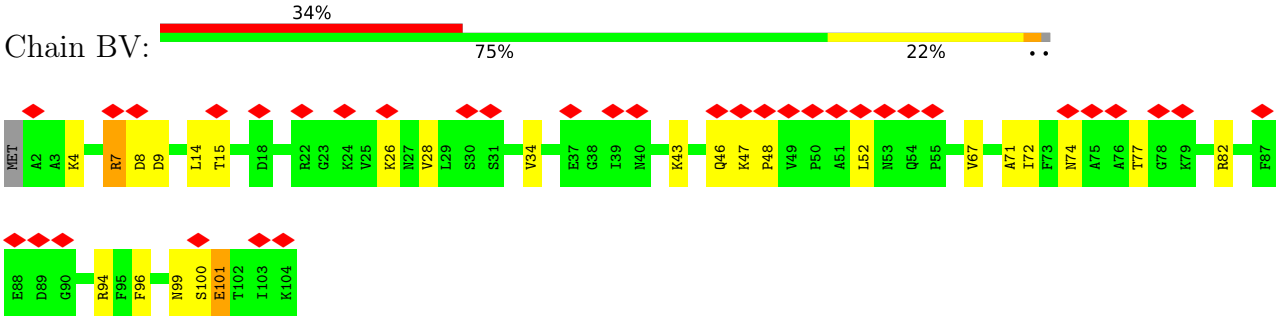
• Molecule 43: 50S ribosomal protein L23





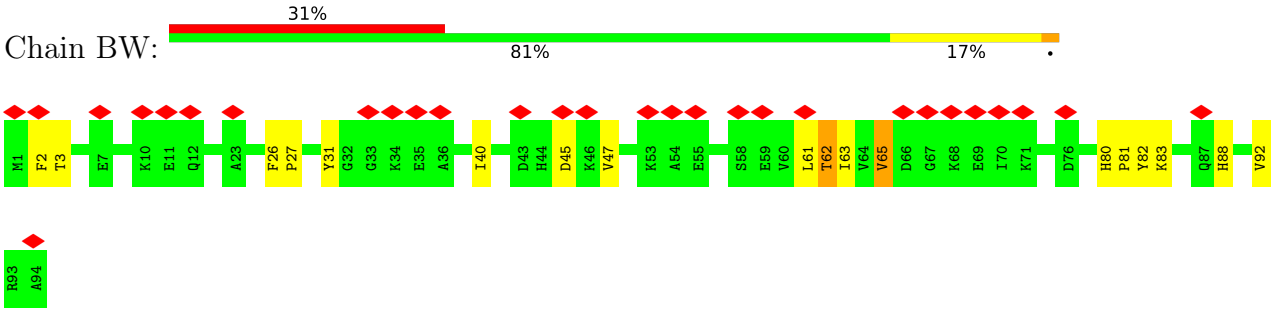
• Molecule 44: 50S ribosomal protein L24

Chain BV:



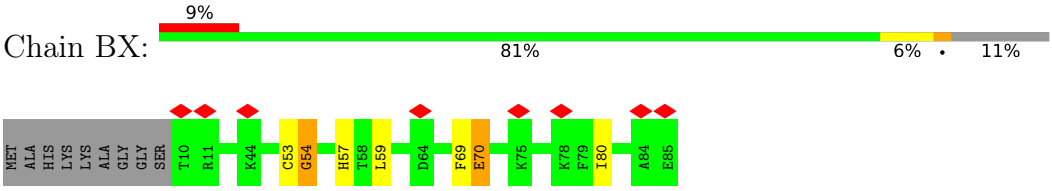
• Molecule 45: 50S ribosomal protein L25

Chain BW:



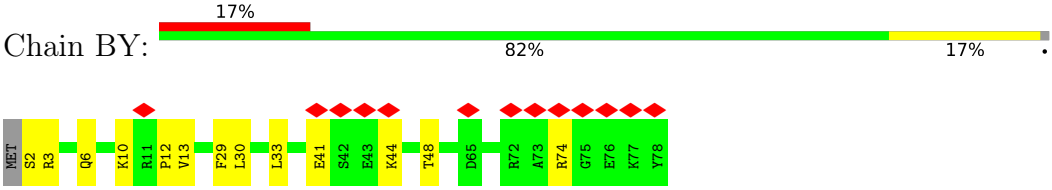
• Molecule 46: 50S ribosomal protein L27

Chain BX:



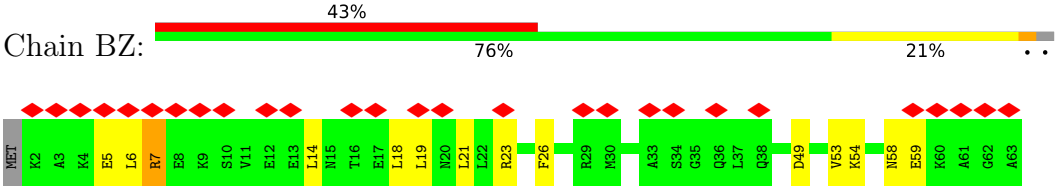
• Molecule 47: 50S ribosomal protein L28

Chain BY:



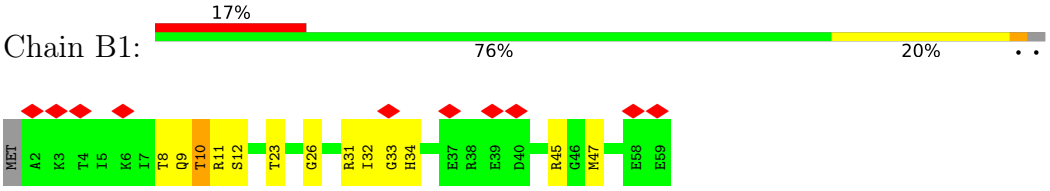
• Molecule 48: 50S ribosomal protein L29

Chain BZ:



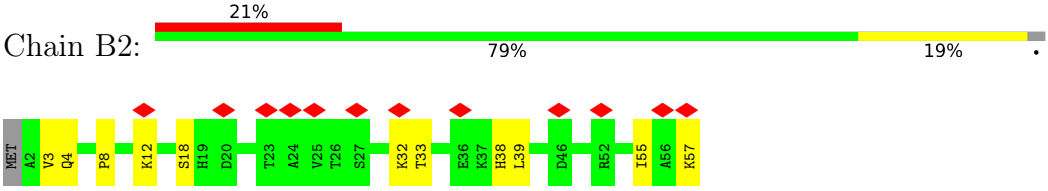
• Molecule 49: 50S ribosomal protein L30

Chain B1:



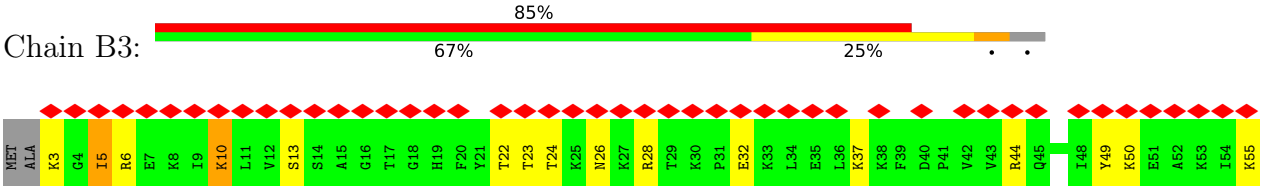
• Molecule 50: 50S ribosomal protein L32

Chain B2:



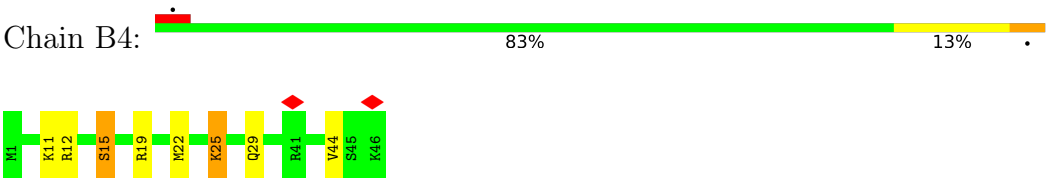
• Molecule 51: 50S ribosomal protein L33

Chain B3:



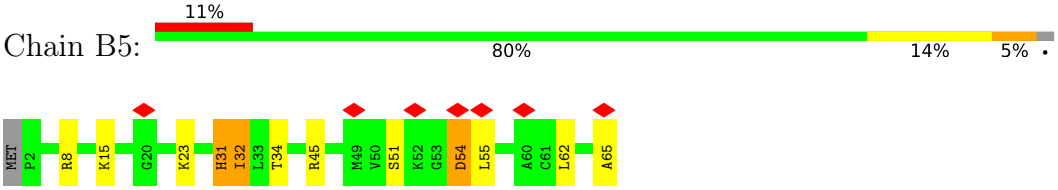
• Molecule 52: 50S ribosomal protein L34

Chain B4:



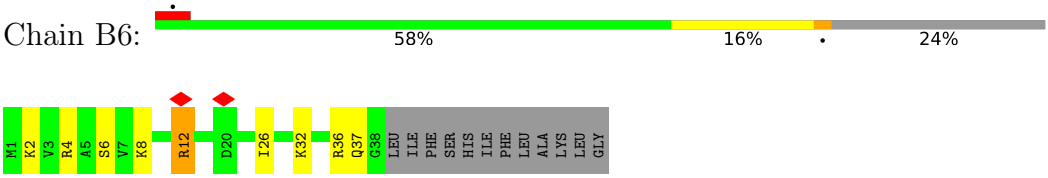
• Molecule 53: 50S ribosomal protein L35

Chain B5:



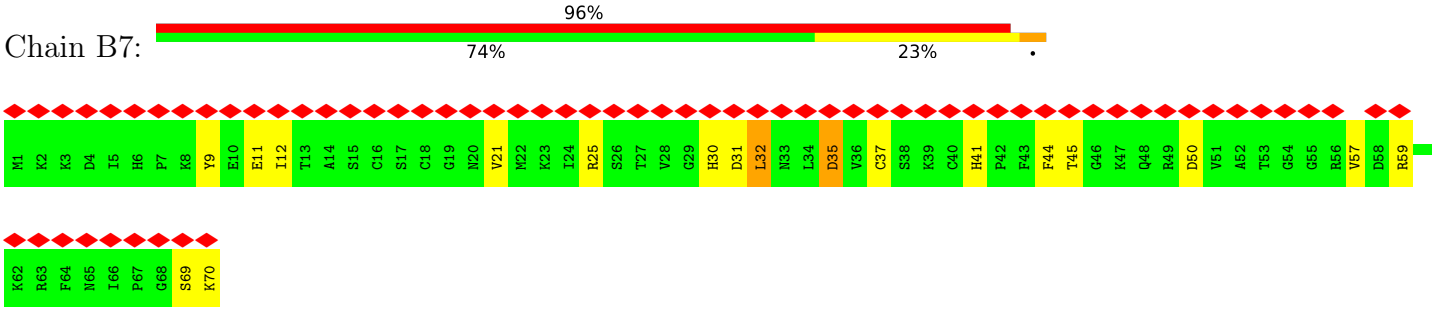
• Molecule 54: 50S ribosomal protein L36

Chain B6:



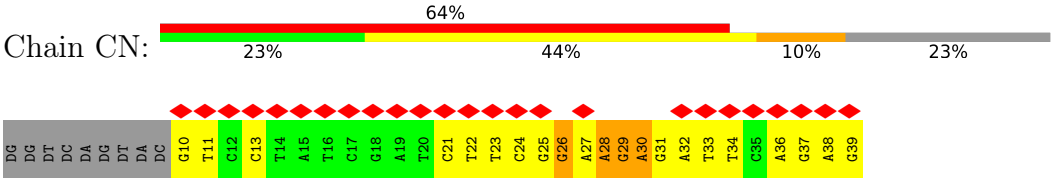
• Molecule 55: 50S ribosomal protein L31

Chain B7:



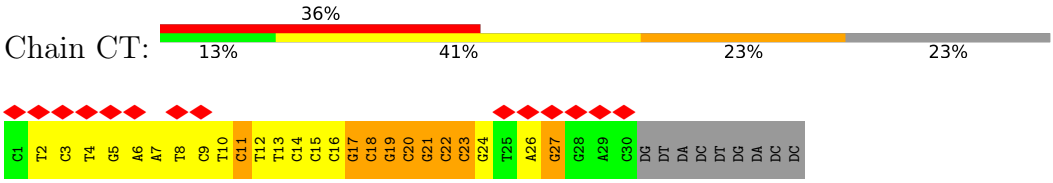
• Molecule 56: Non-template DNA strand

Chain CN:



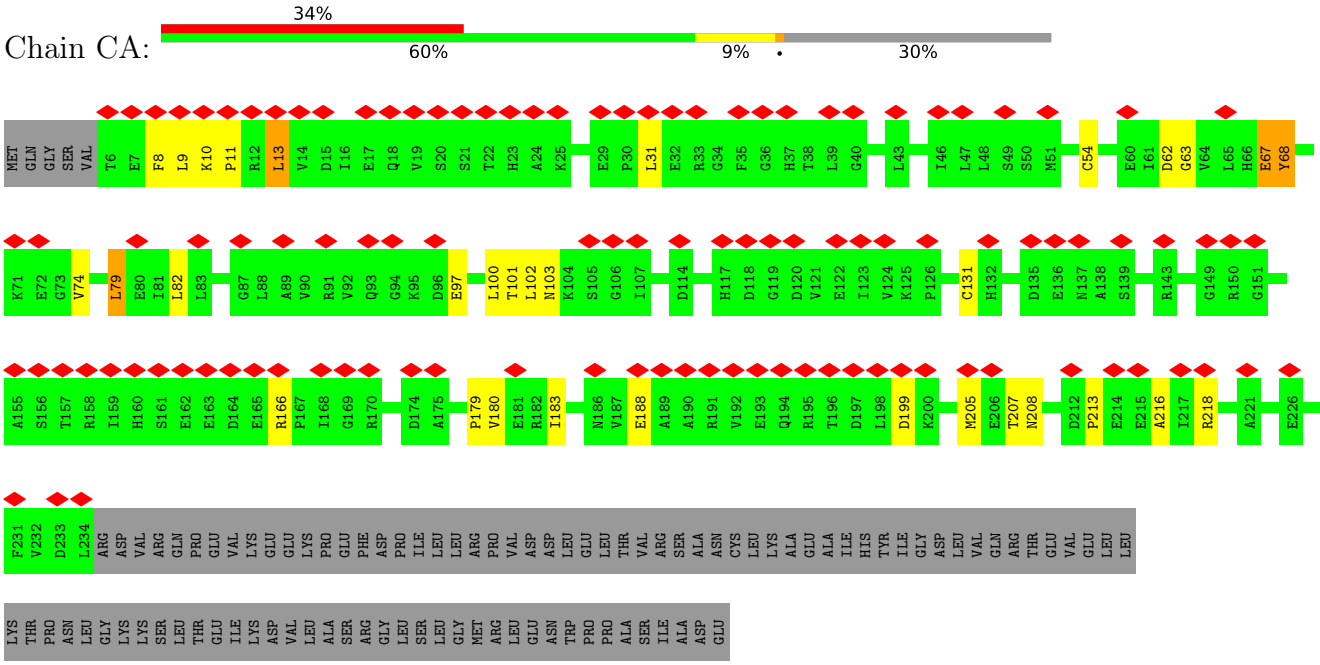
• Molecule 57: Template DNA strand

Chain CT:



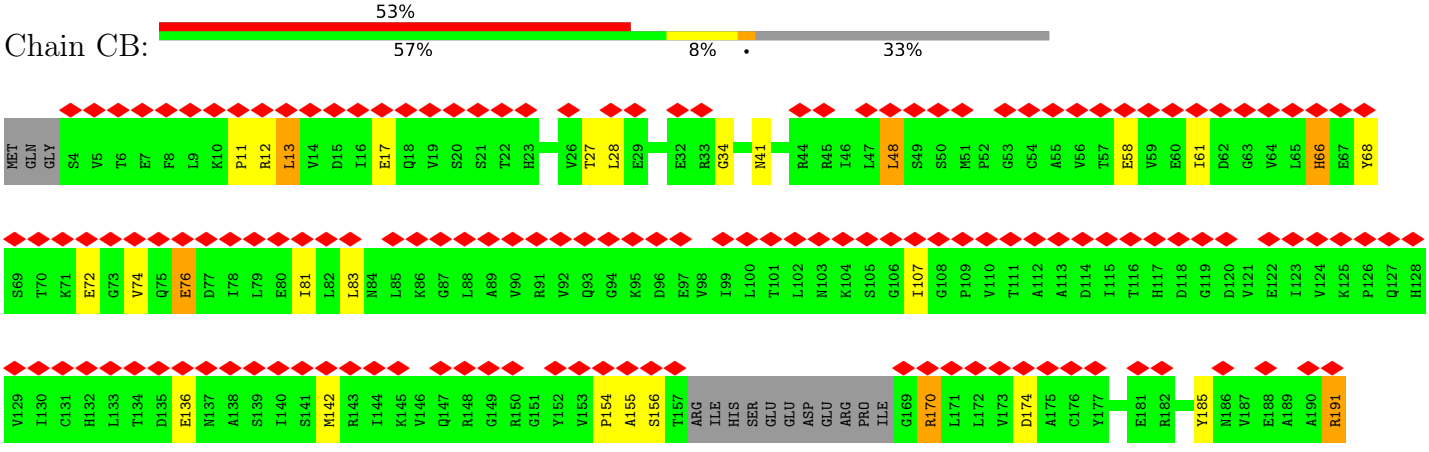
• Molecule 58: DNA-directed RNA polymerase subunit alpha

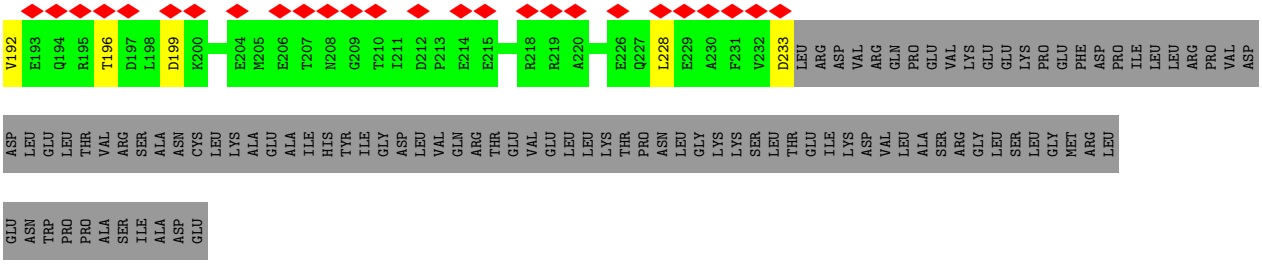
Chain CA:



• Molecule 58: DNA-directed RNA polymerase subunit alpha

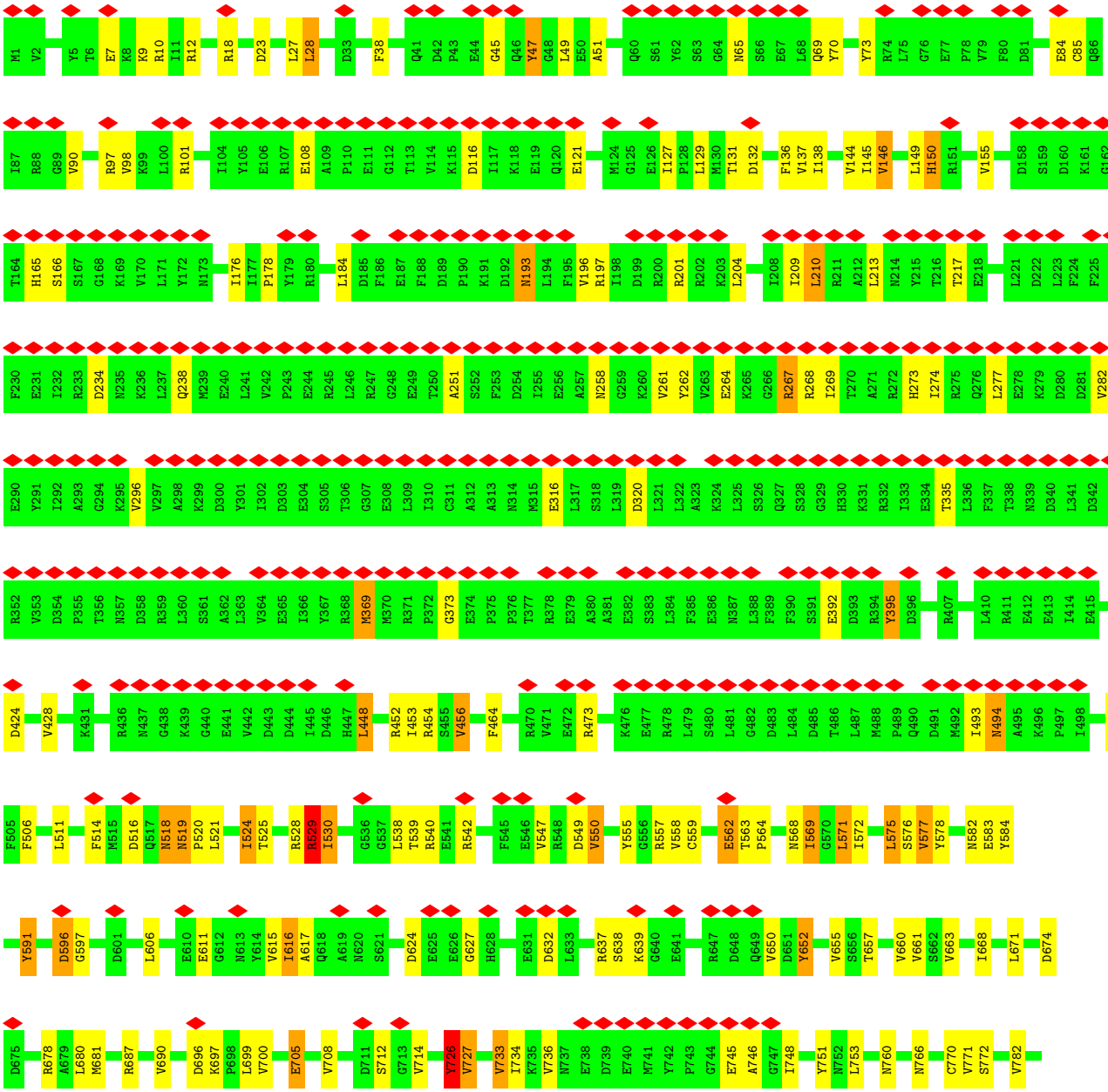
Chain CB:

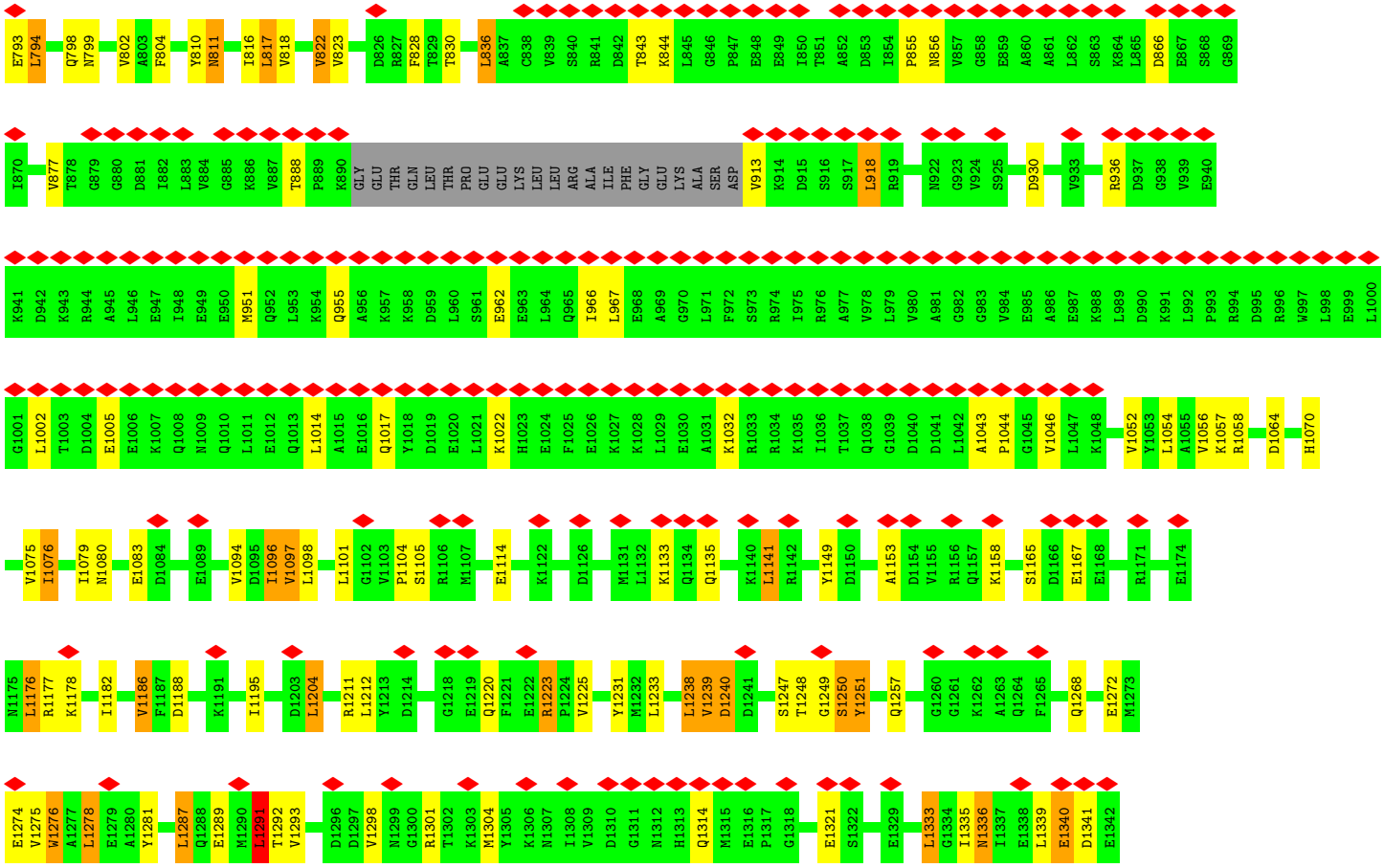




• Molecule 59: DNA-directed RNA polymerase subunit beta

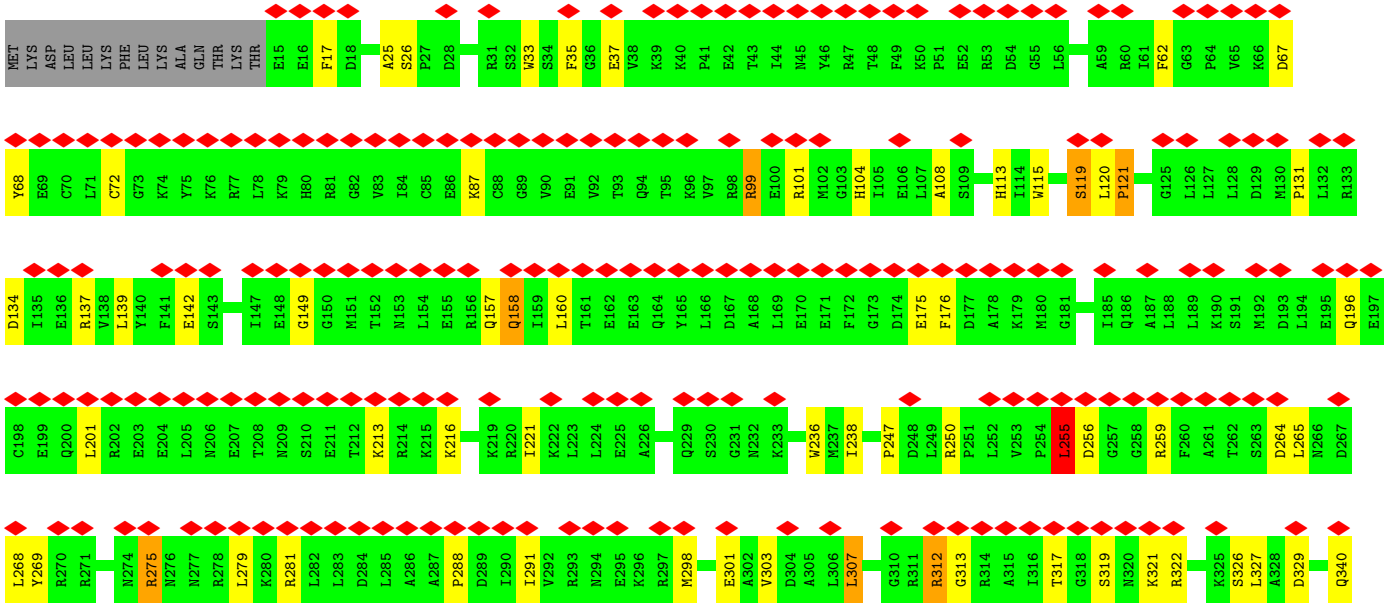
Chain CC:

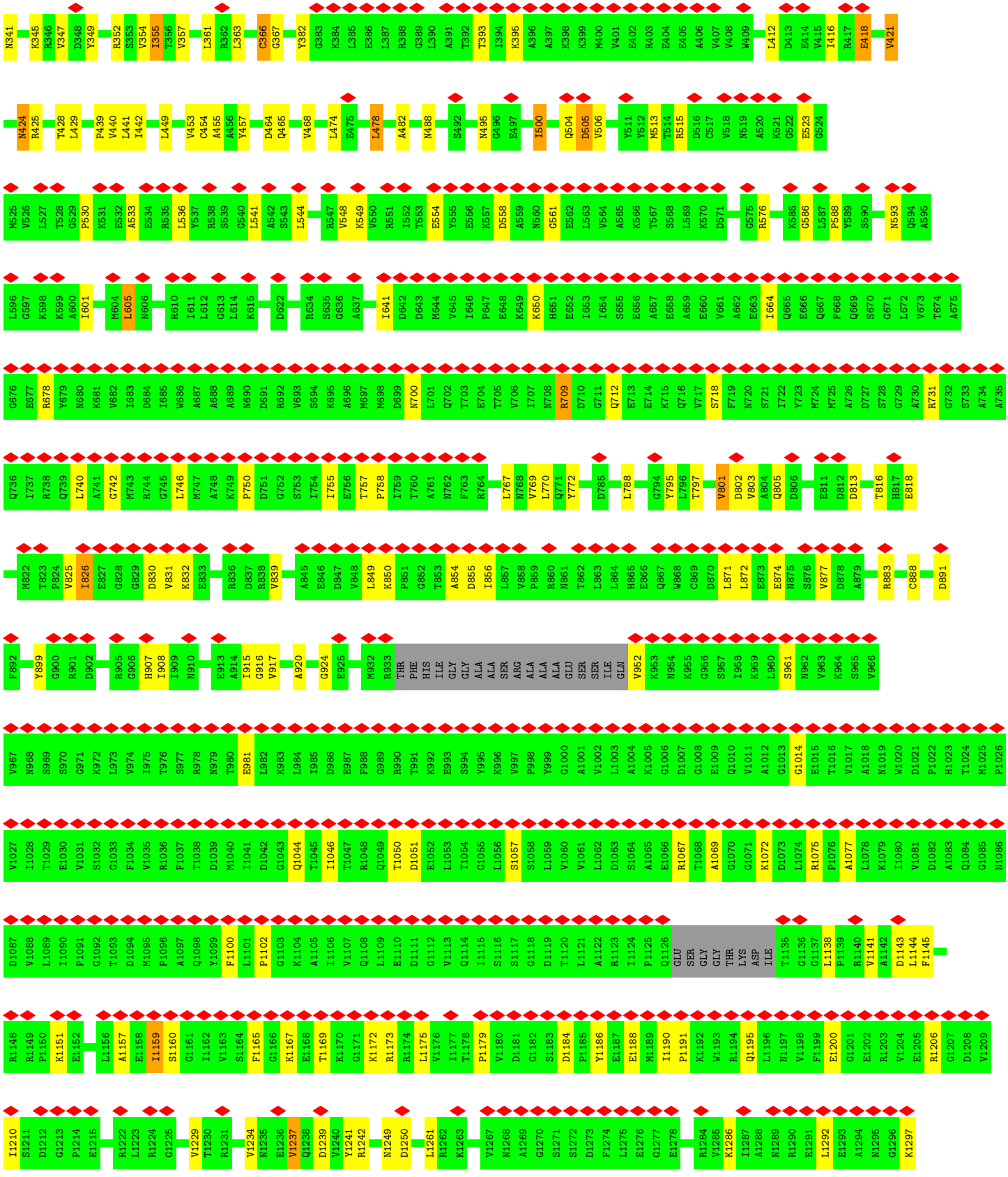


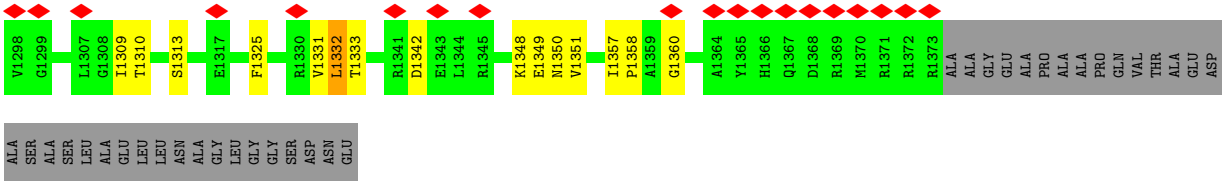


• Molecule 60: DNA-directed RNA polymerase subunit beta'

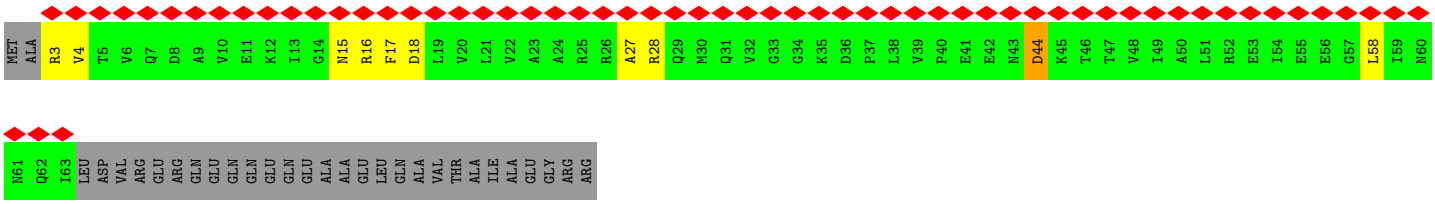
Chain CD:




N341 K345 R346 V347 D348 Y349 R352 S353 V354 I355 T356 V357 L361 R362 L363 C366 G367 Y382 G383 K384 L385 E386 L387 R388 G389 L390 A391 T392 T393 I394 K395 A396 A397 K398 K399 M400 V401 E402 R403 E404 E405 A406 V407 V408 W409 L412 D413 E414 V415 I416 R417 E418 V421
N424 R425 T428 L429 P439 V440 L441 I442 L449 V453 C454 A455 A456 Y457 D464 Q465 V468 L474 E475 L478 A482 N488 S492 N495 G496 E497 I500 Q504 D505 V506 Y511 Y512 M513 T514 R515 D516 C517 V518 N519 A520 K521 G522 E523 G524
M525 V526 L527 T528 G529 P530 K531 E532 A533 E534 R535 L536 Y537 R538 S539 G540 L541 A542 S543 L544 R547 V548 K549 V550 R551 I552 T553 E554 Y555 E556 K557 D558 A559 N560 G561 E562 L563 V564 A565 K566 T567 S568 L569 K570 D571 G575 R576 K585 G586 L587 P588 Y589 S590 N593 Q594 A595
L596 G597 K598 K599 A600 I601 M604 L605 N606 R610 I611 L612 G613 L614 K615 D622 R634 S635 G636 A637 I641 D642 D643 M644 V645 I646 P647 E648 K649 K650 H651 E652 I653 I654 S655 E656 A657 E658 A659 E660 V661 A662 E663 I664 Q665 E666 Q667 F668 Q669 S670 G671 L672 V673 T674 A675
G676 E677 R678 Y679 N680 K681 V682 I683 D684 I685 W686 A687 A688 A689 N690 D691 R692 V693 S694 K695 A696 M697 M698 D699 N700 L701 Q702 T703 E704 T705 V706 I707 N708 R709 D710 G711 Q712 E713 E714 K715 Q716 V717 S718 F719 N720 S721 I722 Y723 M724 M725 A726 D727 S728 G729 A730 R731 G732 S733 A734 A735
Q736 I737 R738 Q739 L740 A741 G742 M743 R744 G745 L746 M747 A748 K749 P750 D751 G752 S753 I754 I755 E756 T757 P758 I759 T760 A761 N762 F763 R764 L767 W768 V769 L770 Q771 Y772 D785 L788 G794 Y795 L796 T797 V801 D802 V803 A804 Q805 D806 E811 D812 D813 T816 H817 E818
M822 T823 P824 V825 I826 E827 G828 G829 D830 V831 K832 E833 R836 D837 R838 V839 A845 E846 D847 V848 L849 K850 P851 G852 T853 A854 D855 I856 L857 V858 P859 R860 N861 T862 L863 L864 H865 E866 Q867 W868 C869 D870 L871 L872 E873 E874 N875 S876 V877 D878 A879 R883 C888 D891
F892 Y899 G900 R901 D902 R905 G906 H907 I908 I909 N910 E913 A914 I915 G916 V917 A920 G924 E925 M932 R933 THR PHE HIS ILE GLY GLY ALA ALA SER ARG ALA ALA ALA GLU SER SER ILE GLN V952 K953 N954 K955 G956 S957 I958 K959 L960 S961 N962 V963 K964 S965 V966
V967 N968 S969 S970 G971 K972 L973 V974 I975 T976 S977 R978 N979 T980 E981 L982 K983 L984 I985 D986 E987 F988 G989 R990 T991 K992 E993 S994 Y995 K996 V997 P998 Y999 G1000 A1001 V1002 L1003 A1004 K1005 G1006 D1007 G1008 E1009 Q1010 V1011 A1012 G1013 G1014 E1015 T1016 V1017 A1018 N1019 W1020 D1021 P1022 H1023 T1024 M1025 P1026
V1027 I1028 T1029 E1030 V1031 S1032 G1033 F1034 V1035 R1036 F1037 T1038 D1039 M1040 I1041 D1042 G1043 Q1044 T1045 I1046 T1047 R1048 Q1049 T1050 D1051 E1052 L1053 T1054 G1055 L1056 S1057 S1058 L1059 V1060 V1061 L1062 D1063 S1064 A1065 E1066 R1067 T1068 A1069 G1070 G1071 K1072 D1073 L1074 R1075 P1076 A1077 L1078 K1079 I1080 V1081 D1082 A1083 Q1084 G1085 N1086
D1087 V1088 L1089 I1090 P1091 G1092 T1093 D1094 M1095 P1096 A1097 Q1098 Y1099 F1100 L1101 P1102 G1103 K1104 A1105 I1106 V1107 Q1108 L1109 E1110 D1111 G1112 V1113 Q1114 I1115 S1116 S1117 G1118 D1119 T1120 L1121 A1122 R1123 I1124 P1125 Q1126 GLU SER GLY GLY THR LYS ASP ILE T1135 G1136 G1137 L1138 P1139 R1140 V1141 A1142 D1143 L1144 F1145
R1148 R1149 P1150 K1151 E1152 L1156 A1157 E1158 I1159 S1160 G1161 I1162 V1163 S1164 F1165 G1166 K1167 E1168 T1169 K1170 G1171 K1172 R1173 R1174 L1175 V1176 I1177 T1178 P1179 V1180 D1181 G1182 S1183 D1184 P1185 Y1186 E1187 E1188 M1189 I1190 P1191 K1192 W1193 R1194 Q1195 L1196 N1197 V1198 F1199 E1200 G1201 E1202 R1203 V1204 E1205 R1206 G1207 D1208 V1209
I1210 S1211 D1212 G1213 P1214 E1215 R1222 L1223 R1224 G1225 V1229 T1230 R1231 V1234 N1235 E1236 V1237 Q1238 D1239 V1240 Y1241 R1242 N1249 D1250 L1261 R1262 K1263 V1267 N1268 A1269 G1270 S1271 S1272 D1273 F1274 L1275 E1276 G1277 E1278 R1284 V1285 K1286 I1287 A1288 N1289 R1290 E1291 L1292 E1293 A1294 N1295 G1296 K1297



• Molecule 61: DNA-directed RNA polymerase subunit omega



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32195	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.947	Depositor
Minimum map value	-0.436	Depositor
Average map value	0.029	Depositor
Map value standard deviation	0.076	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	547.04004, 547.04004, 547.04004	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, 1MG, G7M, H2U, MA6, OMG, 5MU, 3TD, 3AU, OMC, MIA, PSU, MEQ, 4OC, 7MG, 4SU, 4D4, UR3, D2T, 5MC, MG, ZN, 6MZ, 2MA, 2MG

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	AA	1.04	0/36569	0.95	44/57044 (0.1%)
2	AB	0.34	0/1796	0.53	0/2420
3	AC	0.52	0/1667	0.60	0/2246
4	AD	0.40	0/1665	0.54	0/2227
5	AE	0.45	0/1161	0.60	0/1563
6	AF	0.41	0/867	0.59	0/1171
7	AG	0.38	0/1230	0.59	2/1649 (0.1%)
8	AH	0.43	0/989	0.55	1/1326 (0.1%)
9	AI	0.56	0/1043	0.67	0/1387
10	AJ	0.50	0/810	0.69	0/1094
11	AK	0.39	0/893	0.56	0/1205
12	AL	0.48	0/954	0.68	0/1279
13	AM	0.43	0/900	0.62	1/1204 (0.1%)
14	AN	0.52	0/817	0.55	0/1088
15	AO	0.39	0/722	0.53	0/964
16	AP	0.48	0/659	0.54	0/884
17	AQ	0.45	0/657	0.59	0/881
18	AR	0.41	0/554	0.65	1/743 (0.1%)
19	AS	0.51	0/680	0.62	0/915
20	AT	0.41	0/676	0.53	0/895
21	AU	0.35	0/598	0.54	0/792
22	AV	1.98	28/637 (4.4%)	1.78	32/987 (3.2%)
23	AW	0.75	1/1725 (0.1%)	0.94	1/2687 (0.0%)
24	AX	0.58	1/1584 (0.1%)	0.84	1/2463 (0.0%)
25	BA	0.87	2/69165 (0.0%)	0.94	80/107893 (0.1%)
26	BB	0.74	0/2872	0.86	3/4478 (0.1%)
27	BC	0.46	0/2131	0.59	0/2863
28	BD	0.45	0/1576	0.57	0/2119
29	BE	0.40	0/1571	0.60	2/2113 (0.1%)
30	BF	0.35	0/1444	0.53	0/1937
31	BG	0.37	0/1333	0.57	0/1805

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	BH	0.29	0/1122	0.62	1/1515 (0.1%)
33	BK	0.43	0/1152	0.53	0/1551
34	BL	0.44	0/956	0.62	0/1279
35	BM	0.41	0/1061	0.62	0/1412
36	BN	0.41	0/1081	0.55	0/1443
37	BO	0.45	0/973	0.61	0/1301
38	BP	0.38	0/910	0.59	0/1219
39	BQ	0.43	0/929	0.56	0/1242
40	BR	0.51	0/960	0.56	0/1278
41	BS	0.44	0/829	0.62	0/1107
42	BT	0.41	0/864	0.60	0/1156
43	BU	0.38	0/771	0.53	0/1031
44	BV	0.38	0/797	0.53	0/1062
45	BW	0.40	0/766	0.56	0/1025
46	BX	0.43	0/589	0.52	0/779
47	BY	0.43	0/635	0.53	0/848
48	BZ	0.32	0/502	0.53	0/667
49	B1	0.37	0/453	0.56	0/605
50	B2	0.43	0/450	0.60	0/599
51	B3	0.34	0/443	0.61	0/587
52	B4	0.42	0/379	0.55	0/496
53	B5	0.40	0/513	0.62	0/676
54	B6	0.46	0/302	0.58	0/397
55	B7	0.31	0/559	0.67	0/745
56	CN	1.77	12/693 (1.7%)	1.24	3/1068 (0.3%)
57	CT	2.53	38/676 (5.6%)	1.33	9/1039 (0.9%)
58	CA	1.13	7/1797 (0.4%)	0.91	2/2436 (0.1%)
58	CB	0.80	1/1703 (0.1%)	0.86	3/2308 (0.1%)
59	CC	1.41	120/10581 (1.1%)	0.97	31/14275 (0.2%)
60	CD	1.12	58/10532 (0.6%)	0.91	15/14219 (0.1%)
61	CE	0.55	0/480	0.73	0/647
All	All	0.90	268/184403 (0.1%)	0.88	232/272334 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	1
5	AE	0	1
13	AM	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
22	AV	0	1
25	BA	0	1
37	BO	0	1
46	BX	0	1
53	B5	0	1
All	All	0	8

All (268) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	1	C	OP3-P	-10.67	1.48	1.61
24	AX	1	G	OP3-P	-10.59	1.48	1.61
57	CT	18	DC	C3'-O3'	-10.26	1.30	1.44
60	CD	1357	ILE	C-N	-9.72	1.15	1.34
57	CT	14	DC	C3'-O3'	-9.51	1.31	1.44
57	CT	12	DT	N1-C2	-9.32	1.30	1.38
22	AV	51	G	N3-C4	-9.12	1.29	1.35
59	CC	146	VAL	CB-CG1	-8.98	1.34	1.52
59	CC	144	VAL	CB-CG1	-8.84	1.34	1.52
22	AV	50	C	N1-C6	-8.77	1.31	1.37
57	CT	16	DC	N1-C6	-8.73	1.31	1.37
57	CT	15	DC	C3'-O3'	-8.70	1.32	1.44
59	CC	146	VAL	CB-CG2	-8.49	1.35	1.52
57	CT	16	DC	C3'-O3'	-8.41	1.33	1.44
60	CD	457	TYR	CD2-CE2	-8.39	1.26	1.39
57	CT	13	DT	N1-C2	-8.36	1.31	1.38
59	CC	712	SER	CA-C	-8.34	1.31	1.52
60	CD	457	TYR	CE2-CZ	-8.33	1.27	1.38
59	CC	802	VAL	CB-CG1	-8.30	1.35	1.52
22	AV	51	G	C6-N1	-8.20	1.33	1.39
57	CT	22	DC	N1-C6	-8.16	1.32	1.37
59	CC	663	VAL	CB-CG2	-7.85	1.36	1.52
60	CD	421	VAL	CB-CG2	-7.85	1.36	1.52
59	CC	655	VAL	CB-CG1	-7.84	1.36	1.52
56	CN	28	DA	C3'-O3'	-7.76	1.33	1.44
57	CT	18	DC	N1-C6	-7.70	1.32	1.37
59	CC	591	TYR	CD2-CE2	-7.65	1.27	1.39
60	CD	457	TYR	CD1-CE1	-7.65	1.27	1.39
22	AV	53	G	N7-C5	-7.63	1.34	1.39
56	CN	28	DA	N3-C4	-7.63	1.30	1.34
59	CC	136	PHE	CB-CG	-7.60	1.38	1.51
60	CD	1145	PHE	CB-CG	-7.58	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	CC	591	TYR	CG-CD1	-7.58	1.29	1.39
59	CC	818	VAL	CB-CG2	-7.51	1.37	1.52
56	CN	26	DG	C3'-O3'	-7.37	1.34	1.44
59	CC	1239	VAL	CB-CG2	-7.34	1.37	1.52
60	CD	1141	VAL	CB-CG1	-7.31	1.37	1.52
59	CC	708	VAL	CB-CG1	-7.24	1.37	1.52
57	CT	19	DG	N7-C5	-7.13	1.34	1.39
59	CC	591	TYR	CD1-CE1	-7.13	1.28	1.39
22	AV	50	C	N3-C4	-7.12	1.28	1.33
59	CC	708	VAL	CB-CG2	-7.11	1.38	1.52
59	CC	137	VAL	CB-CG2	-7.09	1.38	1.52
60	CD	453	VAL	CB-CG1	-7.08	1.38	1.52
59	CC	802	VAL	CB-CG2	-7.08	1.38	1.52
22	AV	51	G	N1-C2	-7.05	1.32	1.37
22	AV	52	C	N1-C6	-6.99	1.32	1.37
59	CC	578	TYR	CE2-CZ	-6.99	1.29	1.38
59	CC	591	TYR	CE1-CZ	-6.96	1.29	1.38
59	CC	663	VAL	CB-CG1	-6.94	1.38	1.52
60	CD	457	TYR	CE1-CZ	-6.91	1.29	1.38
22	AV	47	G	N7-C5	-6.90	1.35	1.39
57	CT	16	DC	N1-C2	-6.88	1.33	1.40
22	AV	50	C	N1-C2	-6.88	1.33	1.40
57	CT	14	DC	N1-C6	-6.87	1.33	1.37
59	CC	1289	GLU	CB-CG	-6.87	1.39	1.52
59	CC	577	VAL	CB-CG1	-6.79	1.38	1.52
22	AV	47	G	C6-N1	-6.77	1.34	1.39
59	CC	652	TYR	CD1-CE1	-6.77	1.29	1.39
59	CC	822	VAL	CB-CG1	-6.76	1.38	1.52
22	AV	51	G	C5-C4	-6.75	1.33	1.38
59	CC	448	LEU	CA-C	-6.75	1.35	1.52
60	CD	801	VAL	CB-CG2	-6.73	1.38	1.52
59	CC	1094	VAL	CB-CG1	-6.70	1.38	1.52
59	CC	530	ILE	CB-CG2	-6.66	1.32	1.52
59	CC	705	GLU	CG-CD	-6.61	1.42	1.51
59	CC	558	VAL	CB-CG1	-6.60	1.39	1.52
57	CT	13	DT	C4-C5	-6.58	1.39	1.45
59	CC	1251	TYR	CE1-CZ	-6.58	1.29	1.38
59	CC	144	VAL	CB-CG2	-6.58	1.39	1.52
59	CC	464	PHE	CB-CG	-6.54	1.40	1.51
59	CC	578	TYR	CD2-CE2	-6.54	1.29	1.39
60	CD	772	TYR	CD2-CE2	-6.52	1.29	1.39
59	CC	591	TYR	CE2-CZ	-6.42	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	CD	424	ASN	CB-CG	-6.42	1.36	1.51
60	CD	801	VAL	CB-CG1	-6.42	1.39	1.52
59	CC	799	ASN	CB-CG	-6.42	1.36	1.51
59	CC	727	VAL	CB-CG2	-6.41	1.39	1.52
59	CC	1097	VAL	CB-CG1	-6.40	1.39	1.52
59	CC	591	TYR	CB-CG	-6.39	1.42	1.51
22	AV	51	G	N7-C5	-6.36	1.35	1.39
60	CD	421	VAL	CB-CG1	-6.36	1.39	1.52
59	CC	652	TYR	CE1-CZ	-6.35	1.30	1.38
60	CD	803	VAL	CB-CG1	-6.34	1.39	1.52
22	AV	51	G	C5-C6	-6.32	1.36	1.42
59	CC	1225	VAL	CB-CG2	-6.31	1.39	1.52
59	CC	519	ASN	CB-CG	-6.31	1.36	1.51
59	CC	1281	TYR	CD2-CE2	-6.27	1.29	1.39
22	AV	51	G	C2-N3	-6.25	1.27	1.32
60	CD	33	TRP	CB-CG	-6.24	1.39	1.50
59	CC	1186	VAL	CB-CG2	-6.21	1.39	1.52
60	CD	917	VAL	CB-CG1	-6.21	1.39	1.52
60	CD	1237	VAL	CB-CG2	-6.20	1.39	1.52
22	AV	52	C	N1-C2	-6.19	1.33	1.40
59	CC	578	TYR	CD1-CE1	-6.18	1.30	1.39
22	AV	49	G	N3-C4	-6.18	1.31	1.35
57	CT	17	DG	N3-C4	-6.17	1.31	1.35
57	CT	20	DC	N1-C6	-6.16	1.33	1.37
59	CC	1094	VAL	CB-CG2	-6.13	1.40	1.52
59	CC	823	VAL	CB-CG2	-6.09	1.40	1.52
59	CC	1149	TYR	CD2-CE2	-6.09	1.30	1.39
60	CD	1145	PHE	CD2-CE2	-6.08	1.27	1.39
60	CD	303	VAL	CB-CG2	-6.08	1.40	1.52
59	CC	1075	VAL	CB-CG2	-6.06	1.40	1.52
59	CC	1231	TYR	CE2-CZ	-6.06	1.30	1.38
59	CC	1239	VAL	CB-CG1	-6.05	1.40	1.52
59	CC	726	TYR	CD1-CE1	-6.04	1.30	1.39
60	CD	468	VAL	CB-CG2	-6.04	1.40	1.52
59	CC	518	ASN	CB-CG	-6.03	1.37	1.51
22	AV	51	G	N9-C4	-6.01	1.33	1.38
57	CT	12	DT	C4-C5	-6.01	1.39	1.45
58	CA	68	TYR	CD1-CE1	-6.00	1.30	1.39
60	CD	1145	PHE	CD1-CE1	-5.98	1.27	1.39
59	CC	818	VAL	CB-CG1	-5.97	1.40	1.52
59	CC	1231	TYR	CD2-CE2	-5.95	1.30	1.39
60	CD	795	TYR	CE1-CZ	-5.95	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	CD	899	TYR	CE2-CZ	-5.94	1.30	1.38
58	CA	68	TYR	CE1-CZ	-5.92	1.30	1.38
56	CN	13	DC	C3'-O3'	-5.91	1.36	1.44
59	CC	661	VAL	CB-CG2	-5.90	1.40	1.52
59	CC	660	VAL	CB-CG1	-5.90	1.40	1.52
22	AV	50	C	C4-C5	-5.89	1.38	1.43
60	CD	1241	TYR	CE1-CZ	-5.88	1.30	1.38
22	AV	53	G	C5-C6	-5.88	1.36	1.42
60	CD	888	CYS	CB-SG	-5.87	1.72	1.81
60	CD	772	TYR	CD1-CE1	-5.86	1.30	1.39
57	CT	19	DG	C3'-O3'	-5.84	1.36	1.44
57	CT	21	DG	C3'-O3'	-5.83	1.36	1.44
56	CN	29	DG	N7-C5	-5.83	1.35	1.39
57	CT	22	DC	N3-C4	-5.83	1.29	1.33
56	CN	28	DA	C6-N1	-5.81	1.31	1.35
59	CC	700	VAL	CB-CG2	-5.79	1.40	1.52
22	AV	53	G	C6-N1	-5.78	1.35	1.39
59	CC	1281	TYR	CE2-CZ	-5.78	1.31	1.38
59	CC	453	ILE	CB-CG2	-5.77	1.34	1.52
60	CD	354	VAL	CB-CG1	-5.77	1.40	1.52
58	CA	97	GLU	CB-CG	-5.76	1.41	1.52
59	CC	1052	VAL	CB-CG1	-5.76	1.40	1.52
59	CC	751	TYR	CE1-CZ	-5.76	1.31	1.38
56	CN	30	DA	N9-C8	-5.75	1.33	1.37
57	CT	27	DG	C3'-O3'	-5.75	1.36	1.44
59	CC	877	VAL	CB-CG2	-5.75	1.40	1.52
57	CT	17	DG	N7-C5	-5.74	1.35	1.39
58	CA	54	CYS	CB-SG	-5.74	1.72	1.81
59	CC	816	ILE	CB-CG2	-5.73	1.35	1.52
60	CD	347	VAL	CB-CG2	-5.72	1.40	1.52
57	CT	11	DC	C3'-O3'	-5.72	1.36	1.44
59	CC	506	PHE	CG-CD1	-5.71	1.30	1.38
57	CT	17	DG	N9-C4	-5.66	1.33	1.38
59	CC	578	TYR	CG-CD1	-5.66	1.31	1.39
60	CD	899	TYR	CE1-CZ	-5.64	1.31	1.38
56	CN	28	DA	C5-C6	-5.64	1.35	1.41
22	AV	49	G	C6-N1	-5.63	1.35	1.39
59	CC	559	CYS	CB-SG	-5.63	1.72	1.81
59	CC	1251	TYR	CD1-CE1	-5.62	1.30	1.39
57	CT	15	DC	C4'-C3'	-5.61	1.47	1.52
57	CT	16	DC	N3-C4	-5.61	1.30	1.33
59	CC	73	TYR	CE1-CZ	-5.61	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	CC	577	VAL	CB-CG2	-5.61	1.41	1.52
60	CD	349	TYR	CE2-CZ	-5.60	1.31	1.38
59	CC	828	PHE	CE2-CZ	-5.60	1.26	1.37
60	CD	269	TYR	CE1-CZ	-5.60	1.31	1.38
58	CA	9	LEU	C-N	-5.60	1.21	1.34
59	CC	1096	ILE	CB-CG2	-5.60	1.35	1.52
59	CC	660	VAL	CB-CG2	-5.58	1.41	1.52
59	CC	1056	VAL	CB-CG2	-5.58	1.41	1.52
60	CD	772	TYR	CE2-CZ	-5.58	1.31	1.38
60	CD	1331	VAL	CB-CG2	-5.58	1.41	1.52
60	CD	899	TYR	CD2-CE2	-5.58	1.30	1.39
59	CC	690	VAL	CB-CG2	-5.55	1.41	1.52
60	CD	366	CYS	CB-SG	-5.54	1.72	1.81
59	CC	798	GLN	CA-CB	-5.54	1.41	1.53
60	CD	795	TYR	CD2-CE2	-5.52	1.31	1.39
59	CC	1275	VAL	CB-CG1	-5.51	1.41	1.52
59	CC	1276	TRP	CB-CG	-5.50	1.40	1.50
57	CT	13	DT	C3'-O3'	-5.50	1.36	1.44
59	CC	652	TYR	CD2-CE2	-5.50	1.31	1.39
59	CC	782	VAL	CB-CG1	-5.48	1.41	1.52
57	CT	20	DC	C4-C5	-5.46	1.38	1.43
57	CT	12	DT	C1'-N1	-5.46	1.39	1.47
59	CC	811	ASN	CB-CG	-5.46	1.38	1.51
59	CC	674	ASP	CB-CG	-5.45	1.40	1.51
59	CC	456	VAL	CB-CG1	-5.43	1.41	1.52
60	CD	468	VAL	CB-CG1	-5.43	1.41	1.52
22	AV	53	G	N3-C4	-5.42	1.31	1.35
59	CC	810	TYR	CE2-CZ	-5.42	1.31	1.38
59	CC	804	PHE	CD1-CE1	-5.42	1.28	1.39
59	CC	823	VAL	CB-CG1	-5.41	1.41	1.52
59	CC	98	VAL	CB-CG2	-5.40	1.41	1.52
58	CA	131	CYS	CB-SG	-5.39	1.73	1.81
59	CC	137	VAL	CB-CG1	-5.39	1.41	1.52
59	CC	456	VAL	CB-CG2	-5.38	1.41	1.52
57	CT	11	DC	N3-C4	-5.38	1.30	1.33
57	CT	17	DG	C3'-O3'	-5.38	1.36	1.44
60	CD	465	GLN	CB-CG	-5.37	1.38	1.52
60	CD	1237	VAL	CB-CG1	-5.37	1.41	1.52
59	CC	591	TYR	CG-CD2	-5.36	1.32	1.39
57	CT	19	DG	C5-C4	-5.35	1.34	1.38
59	CC	136	PHE	CG-CD1	-5.35	1.30	1.38
60	CD	355	ILE	CB-CG2	-5.35	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	CC	73	TYR	CE2-CZ	-5.35	1.31	1.38
59	CC	584	TYR	CD2-CE2	-5.33	1.31	1.39
57	CT	16	DC	C2-O2	-5.32	1.19	1.24
57	CT	12	DT	C2-N3	-5.31	1.33	1.37
58	CB	185	TYR	CB-CG	-5.31	1.43	1.51
59	CC	690	VAL	CB-CG1	-5.31	1.41	1.52
59	CC	770	CYS	CB-SG	-5.30	1.73	1.81
59	CC	1231	TYR	CE1-CZ	-5.30	1.31	1.38
60	CD	1333	THR	CB-CG2	-5.30	1.34	1.52
60	CD	803	VAL	CB-CG2	-5.30	1.41	1.52
22	AV	45	C	N1-C2	-5.30	1.34	1.40
56	CN	29	DG	N9-C8	-5.30	1.34	1.37
59	CC	395	TYR	CD2-CE2	-5.29	1.31	1.39
60	CD	453	VAL	CB-CG2	-5.29	1.41	1.52
22	AV	47	G	N3-C4	-5.27	1.31	1.35
22	AV	50	C	C2-N3	-5.27	1.31	1.35
59	CC	930	ASP	CB-CG	-5.27	1.40	1.51
60	CD	269	TYR	CD1-CE1	-5.27	1.31	1.39
60	CD	457	TYR	CG-CD1	-5.26	1.32	1.39
59	CC	428	VAL	CB-CG2	-5.26	1.41	1.52
59	CC	520	PRO	CB-CG	-5.25	1.23	1.50
57	CT	23	DC	N1-C6	-5.25	1.34	1.37
60	CD	347	VAL	CB-CG1	-5.25	1.41	1.52
59	CC	733	VAL	CB-CG1	-5.24	1.41	1.52
59	CC	616	ILE	CB-CG2	-5.23	1.36	1.52
59	CC	1149	TYR	CD1-CE1	-5.23	1.31	1.39
59	CC	1149	TYR	CE1-CZ	-5.23	1.31	1.38
56	CN	29	DG	N3-C4	-5.22	1.31	1.35
59	CC	155	VAL	CB-CG2	-5.22	1.41	1.52
60	CD	1145	PHE	CG-CD1	-5.22	1.30	1.38
59	CC	555	TYR	CD1-CE1	-5.22	1.31	1.39
56	CN	30	DA	N9-C4	-5.22	1.34	1.37
60	CD	769	VAL	CB-CG1	-5.22	1.41	1.52
60	CD	428	THR	CA-CB	-5.21	1.39	1.53
57	CT	17	DG	C5-C6	-5.19	1.37	1.42
59	CC	584	TYR	CD1-CE1	-5.19	1.31	1.39
59	CC	578	TYR	CG-CD2	-5.18	1.32	1.39
59	CC	502	VAL	CB-CG2	-5.17	1.42	1.52
59	CC	714	VAL	CB-CG1	-5.17	1.42	1.52
22	AV	49	G	C5-C4	-5.17	1.34	1.38
22	AV	52	C	C4-C5	-5.16	1.38	1.43
59	CC	550	VAL	CB-CG2	-5.14	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	CT	19	DG	C5-C6	-5.14	1.37	1.42
22	AV	47	G	C5-C6	-5.12	1.37	1.42
59	CC	70	TYR	CD2-CE2	-5.12	1.31	1.39
60	CD	795	TYR	CD1-CE1	-5.11	1.31	1.39
25	BA	543	A	C1'-N9	-5.11	1.39	1.46
59	CC	373	GLY	C-N	-5.11	1.22	1.34
59	CC	751	TYR	CE2-CZ	-5.11	1.31	1.38
59	CC	804	PHE	CD2-CE2	-5.11	1.29	1.39
60	CD	382	TYR	CD2-CE2	-5.10	1.31	1.39
59	CC	547	VAL	CB-CG2	-5.09	1.42	1.52
57	CT	12	DT	C2-O2	-5.09	1.18	1.22
60	CD	115	TRP	CG-CD1	-5.09	1.29	1.36
60	CD	506	VAL	CB-CG2	-5.09	1.42	1.52
57	CT	17	DG	C6-N1	-5.07	1.35	1.39
60	CD	1229	VAL	CB-CG1	-5.07	1.42	1.52
25	BA	545	A	C1'-N9	-5.07	1.39	1.46
60	CD	115	TRP	CB-CG	-5.07	1.41	1.50
56	CN	30	DA	C3'-O3'	-5.06	1.37	1.44
59	CC	572	ILE	CB-CG2	-5.06	1.37	1.52
59	CC	771	VAL	CB-CG2	-5.05	1.42	1.52
60	CD	1234	VAL	CB-CG1	-5.05	1.42	1.52
58	CA	67	GLU	CG-CD	5.05	1.59	1.51
59	CC	1149	TYR	CE2-CZ	-5.04	1.31	1.38
60	CD	269	TYR	CD2-CE2	-5.02	1.31	1.39
59	CC	136	PHE	CD2-CE2	-5.02	1.29	1.39
59	CC	1272	GLU	CB-CG	-5.00	1.42	1.52

All (232) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1027	C	C2-N1-C1'	12.29	132.32	118.80
57	CT	19	DG	O4'-C1'-N9	10.11	115.07	108.00
1	AA	1027	C	C6-N1-C1'	-9.76	109.09	120.80
22	AV	52	C	C6-N1-C2	-9.48	116.51	120.30
1	AA	812	G	O4'-C1'-N9	9.05	115.44	108.20
1	AA	108	G	O4'-C1'-N9	-8.63	101.30	108.20
1	AA	206	C	C2-N1-C1'	8.59	128.24	118.80
25	BA	2164	C	C2-N1-C1'	8.55	128.20	118.80
1	AA	206	C	C6-N1-C2	-8.46	116.92	120.30
22	AV	45	C	O5'-P-OP2	-8.34	98.20	105.70
22	AV	52	C	N1-C2-O2	-8.19	113.99	118.90
1	AA	452	A	O4'-C1'-N9	8.12	114.70	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BA	2506	U	N1-C2-O2	8.00	128.40	122.80
22	AV	49	G	O5'-P-OP1	-7.99	98.51	105.70
29	BE	69	ARG	NE-CZ-NH1	7.93	124.27	120.30
22	AV	44	A	C8-N9-C4	7.91	108.97	105.80
25	BA	2175	C	C2-N1-C1'	7.85	127.43	118.80
25	BA	1047	G	O4'-C1'-N9	7.79	114.43	108.20
25	BA	2506	U	C2-N1-C1'	7.73	126.98	117.70
59	CC	210	LEU	CA-CB-CG	-7.67	97.66	115.30
59	CC	571	LEU	CB-CG-CD2	-7.66	97.99	111.00
25	BA	2175	C	N1-C2-O2	7.64	123.48	118.90
25	BA	884	U	C5-C6-N1	7.51	126.45	122.70
1	AA	1027	C	N1-C2-O2	7.43	123.36	118.90
22	AV	51	G	C2-N3-C4	-7.38	108.21	111.90
25	BA	1104	C	C6-N1-C2	-7.37	117.35	120.30
1	AA	1007	U	N3-C2-O2	-7.30	117.09	122.20
22	AV	51	G	N1-C2-N3	7.26	128.26	123.90
57	CT	18	DC	O5'-P-OP1	-7.25	99.18	105.70
59	CC	794	LEU	CB-CG-CD1	-7.19	98.78	111.00
25	BA	2506	U	N3-C2-O2	-7.18	117.17	122.20
25	BA	2573	C	N1-C1'-C2'	-7.17	104.11	112.00
25	BA	512	G	O4'-C1'-N9	7.17	113.94	108.20
22	AV	53	G	C6-C5-N7	-7.15	126.11	130.40
25	BA	1870	C	O5'-P-OP2	7.14	119.27	110.70
22	AV	50	C	N1-C2-O2	-7.13	114.62	118.90
59	CC	149	LEU	CB-CG-CD1	-7.13	98.88	111.00
25	BA	2286	G	O4'-C1'-N9	7.11	113.88	108.20
18	AR	55	LEU	CA-CB-CG	7.10	131.63	115.30
59	CC	1238	LEU	CB-CG-CD1	-7.09	98.95	111.00
25	BA	138	U	N1-C1'-C2'	-7.02	104.28	112.00
22	AV	53	G	C4-C5-N7	6.99	113.60	110.80
25	BA	2573	C	C2-N1-C1'	6.97	126.46	118.80
1	AA	4	U	P-O3'-C3'	6.95	128.03	119.70
25	BA	1173	U	C5'-C4'-O4'	-6.91	100.81	109.10
25	BA	1171	G	C8-N9-C1'	-6.83	118.12	127.00
22	AV	53	G	C8-N9-C4	-6.79	103.69	106.40
25	BA	885	C	C6-N1-C2	-6.78	117.59	120.30
25	BA	1728	C	C2-N1-C1'	-6.77	111.35	118.80
1	AA	206	C	C5-C6-N1	6.76	124.38	121.00
25	BA	1936	A	O4'-C1'-N9	-6.75	102.80	108.20
58	CB	48	LEU	CA-CB-CG	6.75	130.81	115.30
1	AA	928	G	N9-C1'-C2'	-6.73	104.59	112.00
25	BA	1434	A	O4'-C1'-N9	6.72	113.58	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1008	U	O4'-C1'-N1	6.71	113.57	108.20
22	AV	53	G	C5-N7-C8	-6.71	100.95	104.30
60	CD	307	LEU	CA-CB-CG	-6.69	99.91	115.30
59	CC	575	LEU	CB-CG-CD2	-6.65	99.69	111.00
1	AA	1124	G	C8-N9-C4	-6.62	103.75	106.40
25	BA	1052	C	N1-C2-O2	-6.61	114.94	118.90
22	AV	49	G	O3'-P-O5'	-6.56	91.53	104.00
25	BA	783	A	C2-N3-C4	6.56	113.88	110.60
25	BA	884	U	C2-N1-C1'	6.56	125.57	117.70
60	CD	478	LEU	CA-CB-CG	-6.55	100.24	115.30
1	AA	1027	C	C5-C6-N1	6.53	124.27	121.00
1	AA	1167	A	P-O3'-C3'	6.53	127.53	119.70
25	BA	2164	C	N1-C2-O2	6.53	122.82	118.90
26	BB	1	U	N1-C1'-C2'	-6.52	104.83	112.00
25	BA	1170	C	C2-N1-C1'	6.52	125.97	118.80
1	AA	206	C	C6-N1-C1'	-6.48	113.03	120.80
25	BA	138	U	C6-N1-C2	-6.46	117.12	121.00
57	CT	17	DG	O4'-C1'-N9	6.45	112.51	108.00
25	BA	2252	G	N9-C1'-C2'	-6.42	104.94	112.00
25	BA	1857	G	O4'-C1'-N9	6.41	113.33	108.20
59	CC	213	LEU	CA-CB-CG	-6.41	100.56	115.30
25	BA	138	U	O4'-C1'-N1	6.39	113.31	108.20
60	CD	449	LEU	CB-CG-CD1	-6.38	100.16	111.00
60	CD	1332	LEU	CB-CG-CD2	-6.36	100.19	111.00
59	CC	1287	LEU	CB-CG-CD1	-6.35	100.20	111.00
59	CC	511	LEU	CB-CG-CD1	-6.33	100.24	111.00
25	BA	404	A	O4'-C1'-N9	6.30	113.24	108.20
59	CC	521	LEU	CB-CG-CD1	-6.29	100.31	111.00
25	BA	1800	C	C6-N1-C2	-6.29	117.78	120.30
25	BA	2164	C	C6-N1-C1'	-6.29	113.25	120.80
57	CT	16	DC	O4'-C1'-N1	6.28	112.39	108.00
59	CC	1076	ILE	CG1-CB-CG2	-6.21	97.74	111.40
22	AV	46	G	C5-C6-N1	6.20	114.60	111.50
1	AA	108	G	C4-N9-C1'	6.18	134.53	126.50
59	CC	817	LEU	CB-CG-CD1	-6.18	100.50	111.00
22	AV	53	G	N7-C8-N9	6.15	116.18	113.10
1	AA	927	G	N9-C1'-C2'	-6.14	105.25	112.00
1	AA	1034	G	C8-N9-C1'	-6.13	119.03	127.00
26	BB	17	C	O4'-C1'-N1	6.12	113.09	108.20
25	BA	1313	U	C2-N1-C1'	6.10	125.02	117.70
1	AA	431	A	N1-C6-N6	-6.09	114.95	118.60
25	BA	1212	G	O4'-C1'-N9	6.08	113.06	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	AV	45	C	O4'-C1'-N1	6.03	113.02	108.20
25	BA	2573	C	C6-N1-C1'	-6.01	113.59	120.80
25	BA	2638	G	O4'-C1'-N9	6.01	113.01	108.20
60	CD	1144	LEU	CB-CG-CD1	-6.01	100.78	111.00
59	CC	529	ARG	CA-CB-CG	6.01	126.62	113.40
60	CD	255	LEU	CA-CB-CG	5.97	129.03	115.30
32	BH	90	LEU	CA-CB-CG	5.97	129.03	115.30
57	CT	18	DC	O4'-C1'-N1	5.97	112.18	108.00
1	AA	1001	C	O4'-C1'-N1	5.96	112.97	108.20
25	BA	1406	U	C5-C6-N1	5.96	125.68	122.70
22	AV	52	C	N1-C2-N3	5.95	123.36	119.20
26	BB	15	A	O4'-C1'-N9	-5.95	103.44	108.20
25	BA	2808	G	O4'-C1'-N9	5.94	112.95	108.20
60	CD	363	LEU	CB-CG-CD1	-5.94	100.91	111.00
56	CN	25	DG	C1'-O4'-C4'	-5.92	104.18	110.10
56	CN	26	DG	O4'-C4'-C3'	-5.92	102.13	104.50
60	CD	307	LEU	CB-CG-CD2	-5.92	100.94	111.00
25	BA	1313	U	N3-C2-O2	-5.92	118.06	122.20
25	BA	199	A	O4'-C1'-N9	5.90	112.92	108.20
25	BA	858	G	O4'-C1'-N9	5.90	112.92	108.20
1	AA	1009	U	N3-C2-O2	-5.90	118.07	122.20
25	BA	2848	G	O4'-C1'-N9	5.90	112.92	108.20
1	AA	1432	G	O4'-C1'-N9	5.89	112.92	108.20
58	CA	13	LEU	CA-CB-CG	5.89	128.84	115.30
59	CC	1204	LEU	CA-CB-CG	-5.88	101.78	115.30
25	BA	2175	C	C2-N3-C4	5.88	122.84	119.90
60	CD	605	LEU	CB-CG-CD2	-5.87	101.03	111.00
59	CC	1278	LEU	CB-CG-CD2	-5.86	101.03	111.00
22	AV	47	G	C6-C5-N7	-5.84	126.89	130.40
59	CC	1291	LEU	CB-CG-CD2	-5.83	101.09	111.00
25	BA	27	G	O4'-C1'-N9	5.83	112.86	108.20
1	AA	1009	U	N1-C2-O2	5.83	126.88	122.80
60	CD	327	LEU	CB-CG-CD2	-5.83	101.10	111.00
22	AV	48	C	C6-N1-C2	-5.82	117.97	120.30
25	BA	370	G	O4'-C1'-N9	-5.81	103.55	108.20
25	BA	1452	G	O4'-C1'-N9	5.80	112.84	108.20
59	CC	1141	LEU	CB-CG-CD1	-5.79	101.15	111.00
22	AV	46	G	N1-C6-O6	-5.79	116.43	119.90
25	BA	2174	C	N1-C2-O2	5.79	122.38	118.90
25	BA	2175	C	C6-N1-C1'	-5.79	113.86	120.80
57	CT	20	DC	O5'-P-OP2	-5.78	100.50	105.70
25	BA	1171	G	C4-N9-C1'	5.78	134.01	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1038	C	C6-N1-C2	-5.78	117.99	120.30
25	BA	1266	G	O4'-C1'-N9	5.78	112.82	108.20
1	AA	452	A	C4-N9-C1'	5.77	136.69	126.30
25	BA	1171	G	N9-C4-C5	-5.77	103.09	105.40
1	AA	884	U	C6-N1-C2	-5.75	117.55	121.00
22	AV	44	A	O4'-C1'-N9	5.75	112.80	108.20
59	CC	452	ARG	NE-CZ-NH1	-5.70	117.45	120.30
58	CB	228	LEU	CA-CB-CG	-5.70	102.19	115.30
25	BA	1313	U	N1-C2-O2	5.68	126.78	122.80
1	AA	198	G	N9-C1'-C2'	-5.67	105.76	112.00
60	CD	1332	LEU	CB-CG-CD1	-5.67	101.36	111.00
25	BA	2175	C	C5-C6-N1	5.66	123.83	121.00
25	BA	1170	C	C5-C6-N1	5.64	123.82	121.00
25	BA	1077	A	O4'-C1'-N9	5.63	112.71	108.20
25	BA	2150	C	N1-C2-O2	5.62	122.27	118.90
59	CC	802	VAL	CG1-CB-CG2	-5.61	101.92	110.90
25	BA	1936	A	N1-C2-N3	5.61	132.10	129.30
25	BA	12	U	N3-C2-O2	-5.60	118.28	122.20
1	AA	431	A	O4'-C1'-N9	5.60	112.68	108.20
22	AV	53	G	C4-N9-C1'	5.59	133.77	126.50
22	AV	41	C	C2-N1-C1'	5.58	124.94	118.80
58	CB	13	LEU	CA-CB-CG	5.56	128.09	115.30
22	AV	51	G	C8-N9-C4	-5.55	104.18	106.40
25	BA	1494	A	P-O3'-C3'	5.54	126.35	119.70
60	CD	412	LEU	CB-CG-CD1	-5.54	101.57	111.00
59	CC	836	LEU	CB-CG-CD2	-5.53	101.59	111.00
7	AG	54	SER	C-N-CA	-5.49	110.76	122.30
1	AA	1382	C	C6-N1-C2	-5.49	118.10	120.30
1	AA	108	G	N7-C8-N9	5.48	115.84	113.10
60	CD	449	LEU	CB-CG-CD2	-5.48	101.69	111.00
59	CC	28	LEU	CA-CB-CG	-5.47	102.71	115.30
60	CD	1138	LEU	CB-CG-CD2	-5.45	101.73	111.00
1	AA	1027	C	N3-C4-N4	5.43	121.80	118.00
59	CC	184	LEU	CB-CG-CD1	-5.43	101.78	111.00
1	AA	1408	A	N9-C1'-C2'	-5.42	106.04	112.00
22	AV	47	G	C4-N9-C1'	5.42	133.55	126.50
25	BA	2266	A	O4'-C1'-N9	-5.42	103.87	108.20
25	BA	1079	C	C2-N1-C1'	5.41	124.75	118.80
25	BA	1936	A	C2-N3-C4	-5.41	107.90	110.60
22	AV	51	G	C5-N7-C8	-5.40	101.60	104.30
59	CC	671	LEU	CB-CG-CD2	-5.37	101.88	111.00
1	AA	1277	C	O4'-C1'-N1	5.36	112.49	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	BE	69	ARG	NE-CZ-NH2	-5.36	117.62	120.30
25	BA	1728	C	C6-N1-C1'	5.36	127.23	120.80
7	AG	55	GLY	N-CA-C	5.35	126.48	113.10
25	BA	2506	U	C6-N1-C1'	-5.35	113.71	121.20
25	BA	2174	C	C2-N1-C1'	5.33	124.67	118.80
59	CC	1054	LEU	CB-CG-CD2	-5.33	101.93	111.00
25	BA	138	U	C6-N1-C1'	-5.33	113.74	121.20
8	AH	121	LEU	CA-CB-CG	5.32	127.55	115.30
22	AV	45	C	C6-N1-C1'	-5.31	114.42	120.80
25	BA	1597	A	N9-C1'-C2'	-5.31	106.16	112.00
22	AV	44	A	N7-C8-N9	-5.31	111.15	113.80
25	BA	1596	A	O4'-C1'-N9	5.29	112.43	108.20
59	CC	1064	ASP	CB-CG-OD2	5.28	123.05	118.30
24	AX	19	G	O4'-C1'-N9	-5.28	103.98	108.20
59	CC	210	LEU	CB-CG-CD2	-5.27	102.04	111.00
1	AA	1034	G	C8-N9-C4	-5.26	104.30	106.40
1	AA	1261	A	O4'-C1'-N9	-5.25	104.00	108.20
1	AA	328	C	C2-N1-C1'	5.25	124.58	118.80
25	BA	1170	C	C6-N1-C2	-5.25	118.20	120.30
57	CT	8	DT	N3-C4-O4	5.24	123.04	119.90
57	CT	12	DT	N3-C4-O4	5.24	123.04	119.90
22	AV	53	G	N9-C1'-C2'	5.23	120.80	114.00
25	BA	884	U	C6-N1-C2	-5.23	117.86	121.00
25	BA	142	A	O4'-C1'-N9	-5.23	104.02	108.20
23	AW	47	U	P-O3'-C3'	5.22	125.97	119.70
25	BA	2129	C	O5'-P-OP1	5.21	116.96	110.70
59	CC	1333	LEU	CB-CG-CD2	-5.21	102.14	111.00
57	CT	13	DT	N3-C4-O4	5.20	123.02	119.90
59	CC	1176	LEU	CB-CG-CD2	-5.19	102.17	111.00
1	AA	1017	U	O4'-C1'-N1	-5.17	104.06	108.20
1	AA	1066	C	C6-N1-C2	-5.16	118.23	120.30
1	AA	1010	U	N3-C2-O2	-5.15	118.59	122.20
59	CC	616	ILE	CG1-CB-CG2	-5.11	100.16	111.40
22	AV	51	G	N3-C4-N9	-5.10	122.94	126.00
25	BA	1503	A	O4'-C1'-N9	5.10	112.28	108.20
1	AA	1028	C	C2-N1-C1'	-5.09	113.20	118.80
1	AA	452	A	C8-N9-C1'	-5.09	118.54	127.70
22	AV	46	G	C6-N1-C2	-5.08	122.06	125.10
25	BA	884	U	N3-C4-O4	5.08	122.95	119.40
25	BA	2326	C	C5'-C4'-O4'	5.07	115.19	109.10
59	CC	1233	LEU	CA-CB-CG	5.07	126.96	115.30
58	CA	79	LEU	CB-CG-CD1	-5.06	102.39	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BA	1171	G	O4'-C1'-N9	-5.05	104.16	108.20
56	CN	21	DC	O4'-C1'-N1	5.04	111.53	108.00
59	CC	918	LEU	CA-CB-CG	-5.04	103.71	115.30
25	BA	783	A	C8-N9-C4	-5.03	103.79	105.80
1	AA	82	G	C8-N9-C4	-5.03	104.39	106.40
22	AV	52	C	C2-N3-C4	-5.03	117.39	119.90
60	CD	788	LEU	CB-CG-CD1	-5.03	102.46	111.00
25	BA	828	U	O4'-C1'-N1	-5.01	104.19	108.20
25	BA	1104	C	C2-N1-C1'	5.01	124.31	118.80
13	AM	54	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1034	G	Sidechain
5	AE	89	HIS	Peptide
13	AM	65	VAL	Peptide
22	AV	45	C	Sidechain
53	B5	31	HIS	Peptide
25	BA	138	U	Sidechain
37	BO	100	CYS	Mainchain
46	BX	54	GLY	Mainchain

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	AA	32909	0	16580	275	0
2	AB	1765	0	1792	36	0
3	AC	1640	0	1713	27	0
4	AD	1643	0	1707	31	0
5	AE	1148	0	1195	19	0
6	AF	848	0	846	29	0
7	AG	1214	0	1267	18	0
8	AH	979	0	1031	10	0
9	AI	1031	0	1076	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	800	0	839	28	0
11	AK	877	0	887	25	0
12	AL	951	0	1012	25	0
13	AM	891	0	952	21	0
14	AN	805	0	844	13	0
15	AO	714	0	734	11	0
16	AP	649	0	666	8	0
17	AQ	648	0	691	6	0
18	AR	545	0	560	5	0
19	AS	663	0	688	11	0
20	AT	670	0	719	11	0
21	AU	590	0	629	12	0
22	AV	572	0	294	20	0
23	AW	1645	0	842	13	0
24	AX	1630	0	838	30	0
25	BA	62270	0	31335	443	0
26	BB	2569	0	1301	9	0
27	BC	2092	0	2167	32	0
28	BD	1566	0	1618	24	0
29	BE	1552	0	1618	23	0
30	BF	1420	0	1457	32	0
31	BG	1313	0	1358	20	0
32	BH	1111	0	1148	31	0
33	BK	1129	0	1162	10	0
34	BL	947	0	1023	11	0
35	BM	1052	0	1127	11	0
36	BN	1075	0	1155	13	0
37	BO	960	0	1000	12	0
38	BP	900	0	935	22	0
39	BQ	917	0	962	13	0
40	BR	947	0	1019	16	0
41	BS	816	0	839	10	0
42	BT	857	0	922	26	0
43	BU	764	0	829	9	0
44	BV	789	0	843	14	0
45	BW	753	0	780	11	0
46	BX	582	0	598	4	0
47	BY	625	0	652	6	0
48	BZ	501	0	531	8	0
49	B1	449	0	488	6	0
50	B2	444	0	458	7	0
51	B3	436	0	477	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	B4	376	0	414	7	0
53	B5	504	0	572	9	0
54	B6	301	0	340	4	0
55	B7	549	0	551	14	0
56	CN	618	0	339	29	0
57	CT	606	0	338	37	0
58	CA	1775	0	1800	17	0
58	CB	1684	0	1713	19	0
59	CC	10415	0	10432	164	0
60	CD	10375	0	10597	147	0
61	CE	478	0	496	7	0
62	AA	143	0	0	0	0
62	AI	1	0	0	0	0
62	AL	1	0	0	0	0
62	AM	1	0	0	0	0
62	AW	5	0	0	0	0
62	AX	1	0	0	0	0
62	BA	317	0	0	0	0
62	BB	9	0	0	0	0
62	BC	3	0	0	0	0
62	BN	1	0	0	0	0
62	BO	1	0	0	0	0
62	BQ	1	0	0	0	0
62	BV	1	0	0	0	0
62	BX	1	0	0	0	0
62	CD	1	0	0	0	0
63	AX	11	0	8	1	0
64	B6	1	0	0	0	0
64	B7	1	0	0	0	0
64	CD	2	0	0	0	0
All	All	172846	0	123804	1795	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 6.

All (1795) 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)
25:BA:2285:C:OP2	51:B3:6:ARG:NH1	1.99	0.94
1:AA:481:G:O2'	1:AA:483:C:N4	2.01	0.93
25:BA:1936:A:H2	25:BA:1943:U:H3	1.16	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:411:A:H4'	1:AA:412:A:H5'	1.53	0.90
18:AR:36:SER:HA	18:AR:72:ASP:HB2	1.52	0.90
24:AX:18:G:O2'	24:AX:57:G:N2	2.07	0.88
13:AM:107:ARG:NH1	13:AM:111:GLY:O	2.07	0.88
6:AF:86:ARG:NH1	18:AR:64:TYR:O	2.08	0.87
25:BA:1216:G:OP1	40:BR:11:ARG:NH1	2.09	0.86
17:AQ:48:ASP:HB2	17:AQ:75:LEU:HD23	1.59	0.84
17:AQ:27:ARG:NH1	17:AQ:42:THR:OG1	2.10	0.84
6:AF:42:TRP:HB3	6:AF:45:ARG:HH11	1.40	0.84
1:AA:522:C:O2	1:AA:527:G7M:N2	2.10	0.83
22:AV:50:C:H2'	22:AV:51:G:H8	1.43	0.83
9:AI:119:ARG:HH11	9:AI:125:PRO:HB3	1.44	0.82
5:AE:115:LEU:HD13	5:AE:123:VAL:HG11	1.58	0.82
48:BZ:14:LEU:HD22	48:BZ:53:VAL:HG23	1.62	0.81
1:AA:864:A:H5"	5:AE:90:THR:HB	1.63	0.81
25:BA:2880:C:O2'	37:BO:90:ARG:NH1	2.14	0.81
22:AV:51:G:H2'	22:AV:52:C:H6	1.44	0.81
58:CB:191:ARG:HB3	58:CB:196:THR:HG23	1.63	0.80
3:AC:77:ILE:HA	3:AC:84:VAL:HG23	1.63	0.80
25:BA:1590:A:H2'	25:BA:1591:A:C8	2.16	0.80
25:BA:2164:C:OP2	25:BA:2170:A:N6	2.15	0.80
1:AA:1025:U:H5"	1:AA:1026:G:H5'	1.64	0.79
25:BA:475:C:O2	25:BA:479:A:N6	2.15	0.79
12:AL:83:ARG:NH1	12:AL:84:GLY:O	2.16	0.79
1:AA:537:G:OP1	12:AL:110:ARG:NH2	2.15	0.78
25:BA:783:A:H2'	25:BA:783:A:N3	1.99	0.78
25:BA:2718:G:O4'	25:BA:2718:G:O2'	1.90	0.78
29:BE:111:GLU:OE1	29:BE:114:ARG:NH1	2.16	0.78
1:AA:1239:A:H62	1:AA:1299:A:H62	1.30	0.78
25:BA:2685:G:OP1	34:BL:78:ARG:NH2	2.17	0.77
57:CT:18:DC:H2'	57:CT:19:DG:C8	2.19	0.77
60:CD:429:LEU:H	60:CD:429:LEU:HD22	1.46	0.77
24:AX:26:A:H61	24:AX:44:G:H1	1.29	0.77
25:BA:284:U:H3	25:BA:356:G:H1	1.32	0.77
11:AK:88:GLY:O	11:AK:93:ARG:NH1	2.18	0.77
60:CD:1186:TYR:OH	60:CD:1188:GLU:OE1	2.01	0.76
25:BA:2069:G7M:N2	25:BA:2442:C:O2	2.12	0.76
27:BC:78:VAL:O	27:BC:113:GLY:N	2.15	0.76
25:BA:1528:A:H2'	25:BA:1529:G:O4'	1.84	0.76
58:CB:74:VAL:HG21	58:CB:81:ILE:HD11	1.66	0.76
9:AI:84:THR:HG21	9:AI:103:PHE:HB3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AL:68:GLY:O	12:AL:99:ARG:NH1	2.19	0.76
28:BD:8:LYS:O	28:BD:198:GLY:N	2.18	0.76
58:CA:62:ASP:OD1	58:CA:63:GLY:N	2.19	0.76
25:BA:2135:A:H3'	25:BA:2136:G:H8	1.51	0.76
24:AX:26:A:N6	24:AX:44:G:H1	1.83	0.75
25:BA:2116:G:H1	25:BA:2164:C:H42	1.32	0.75
38:BP:7:ARG:NH1	38:BP:95:SER:O	2.19	0.75
25:BA:1918:A:O2'	25:BA:1919:A:N7	2.19	0.75
25:BA:1998:A:HO2'	25:BA:2724:U:HO2'	1.34	0.75
22:AV:50:C:H2'	22:AV:51:G:C8	2.21	0.75
25:BA:2467:C:O2	36:BN:123:LYS:NZ	2.20	0.75
43:BU:30:ILE:HG21	43:BU:93:LEU:HD13	1.69	0.75
60:CD:816:THR:OG1	60:CD:818:GLU:OE1	2.04	0.75
4:AD:147:GLU:HA	4:AD:150:LYS:HB2	1.67	0.75
33:BK:12:LYS:NZ	33:BK:14:ASP:OD1	2.20	0.74
47:BY:41:GLU:OE2	47:BY:44:LYS:NZ	2.19	0.74
59:CC:10:ARG:NH2	59:CC:793:GLU:OE1	2.21	0.74
1:AA:1305:G:H21	1:AA:1332:A:H2	1.33	0.74
25:BA:2308:G:O6	25:BA:2311:A:N7	2.21	0.74
1:AA:664:G:H22	1:AA:741:G:H1	1.36	0.74
25:BA:2312:U:H5'	30:BF:85:ILE:HD11	1.68	0.74
6:AF:21:MET:HG2	6:AF:24:ARG:HH21	1.53	0.74
13:AM:54:ASP:OD1	13:AM:55:THR:N	2.21	0.74
51:B3:6:ARG:HG2	51:B3:24:THR:HB	1.70	0.73
2:AB:129:LEU:HB2	2:AB:134:ALA:HB2	1.68	0.73
25:BA:2012:G:OP1	42:BT:11:ARG:NH2	2.21	0.73
25:BA:2243:U:H2'	25:BA:2244:U:C6	2.24	0.73
1:AA:4:U:O2'	1:AA:5:U:O5'	2.07	0.73
25:BA:276:U:O2'	25:BA:278:A:N7	2.22	0.73
4:AD:188:ARG:NH2	4:AD:192:SER:O	2.19	0.73
25:BA:881:G:H1	25:BA:895:U:H3	1.37	0.73
25:BA:1808:A:O2'	47:BY:3:ARG:NH1	2.21	0.73
1:AA:263:A:OP1	20:AT:74:ARG:NH1	2.22	0.72
6:AF:17:GLN:HG2	32:BH:87:GLU:HB3	1.71	0.72
25:BA:2298:A:OP1	30:BF:71:ARG:NH2	2.22	0.72
1:AA:1311:A:OP1	55:B7:59:ARG:NH2	2.19	0.72
6:AF:24:ARG:NH1	32:BH:86:ASP:OD2	2.22	0.72
10:AJ:53:ILE:HD11	10:AJ:63:ASP:HB2	1.72	0.72
25:BA:807:U:O2	29:BE:69:ARG:NH2	2.23	0.72
25:BA:1607:C:N4	25:BA:1622:G:OP2	2.23	0.72
60:CD:1179:PRO:HD2	60:CD:1184:ASP:HA	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AJ:10:LEU:HB3	10:AJ:18:ILE:HD11	1.72	0.72
19:AS:36:ARG:NH2	19:AS:75:ALA:O	2.22	0.72
22:AV:51:G:H2'	22:AV:52:C:C6	2.25	0.72
29:BE:1:MET:HB3	29:BE:14:VAL:HG23	1.72	0.72
3:AC:33:LEU:HD21	14:AN:93:ILE:HG12	1.71	0.71
59:CC:27:LEU:O	59:CC:528:ARG:NH1	2.24	0.71
1:AA:1086:U:O4	1:AA:1099:G:N1	2.15	0.71
60:CD:454:CYS:SG	60:CD:455:ALA:N	2.64	0.71
37:BO:63:ARG:HG2	37:BO:63:ARG:HH21	1.56	0.71
25:BA:1406:U:C2'	25:BA:1407:G:H5"	2.20	0.71
25:BA:1407:G:H2'	25:BA:1408:G:H8	1.54	0.71
25:BA:2683:C:OP1	39:BQ:51:ARG:NH1	2.24	0.71
34:BL:36:GLY:N	34:BL:62:VAL:O	2.22	0.71
23:AW:21:A:O2'	23:AW:46:A:N6	2.23	0.71
44:BV:28:VAL:HG22	44:BV:34:VAL:HG12	1.73	0.71
25:BA:2162:G:OP2	25:BA:2164:C:N4	2.23	0.70
1:AA:90:C:H2'	1:AA:91:U:H6	1.55	0.70
42:BT:4:ILE:HG12	42:BT:106:VAL:HG22	1.72	0.70
1:AA:736:C:OP1	18:AR:61:ARG:NH1	2.25	0.70
25:BA:545:A:C2	25:BA:549:C:C2	2.80	0.70
25:BA:550:U:H2'	25:BA:551:G:H8	1.56	0.70
37:BO:9:GLN:O	37:BO:17:ARG:NH2	2.24	0.70
25:BA:568:U:H1'	25:BA:2030:6MZ:H9C1	1.74	0.70
1:AA:1452:C:H4'	1:AA:1453:G:H5"	1.74	0.70
4:AD:95:GLU:OE1	4:AD:100:ASN:ND2	2.25	0.70
3:AC:93:ASP:OD1	3:AC:94:ILE:N	2.25	0.69
25:BA:2172:U:O2'	25:BA:2174:C:OP2	2.10	0.69
37:BO:24:MET:HG2	37:BO:44:LEU:HD22	1.75	0.69
25:BA:1108:U:H2'	25:BA:1109:C:C6	2.27	0.69
25:BA:2139:U:O2	25:BA:2152:G:O6	2.09	0.69
25:BA:2182:U:O2	25:BA:2183:A:N6	2.22	0.69
37:BO:101:GLY:O	37:BO:110:MET:N	2.23	0.69
38:BP:31:THR:O	38:BP:102:ARG:NH1	2.25	0.69
60:CD:1157:ALA:HB2	60:CD:1210:ILE:HD11	1.74	0.68
25:BA:2370:G:O2'	51:B3:44:ARG:NH1	2.25	0.68
25:BA:78:U:OP1	48:BZ:7:ARG:NH2	2.27	0.68
25:BA:1494:A:O2'	25:BA:1495:A:OP1	2.10	0.68
57:CT:19:DG:H2'	57:CT:20:DC:C6	2.29	0.68
6:AF:38:ARG:NH1	6:AF:98:GLU:O	2.24	0.68
25:BA:2118:U:O4	25:BA:2148:G:N2	2.27	0.68
25:BA:1177:G:O2'	25:BA:1178:C:O5'	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:B3:6:ARG:NH1	51:B3:26:ASN:HB2	2.09	0.68
19:AS:27:ASP:OD1	19:AS:29:LYS:N	2.27	0.67
12:AL:87:VAL:HG11	12:AL:90:LEU:HD22	1.76	0.67
27:BC:107:PRO:HD2	27:BC:110:LEU:HD22	1.75	0.67
25:BA:673:C:OP1	29:BE:49:ARG:NH2	2.27	0.67
60:CD:504:GLN:NE2	60:CD:505:ASP:OD1	2.18	0.67
25:BA:871:U:H2'	25:BA:872:U:C6	2.30	0.67
4:AD:28:ILE:HD12	4:AD:34:ILE:HG12	1.76	0.67
25:BA:389:G:C8	25:BA:2413:G:H4'	2.29	0.67
25:BA:1916:A:H2'	25:BA:1917:PSU:C6	2.30	0.67
1:AA:1017:U:O2'	1:AA:1018:G:O4'	2.13	0.67
1:AA:1343:G:H1'	9:AI:123:ARG:HH12	1.58	0.67
1:AA:1397:C:OP2	5:AE:29:ARG:NH2	2.27	0.66
11:AK:109:ASN:ND2	21:AU:4:ILE:O	2.28	0.66
24:AX:37:MIA:O2'	25:BA:1913:A:N1	2.26	0.66
59:CC:624:ASP:OD1	59:CC:627:GLY:N	2.25	0.66
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.77	0.66
2:AB:186:ILE:HA	2:AB:200:ILE:HG13	1.75	0.66
25:BA:2245:U:O2'	25:BA:2436:G:OP2	2.12	0.66
25:BA:2530:A:N7	31:BG:172:LYS:NZ	2.43	0.66
1:AA:1239:A:H62	1:AA:1299:A:N6	1.94	0.66
4:AD:172:GLU:HG3	4:AD:183:LYS:HE3	1.76	0.66
1:AA:523:A:N6	12:AL:89:D2T:OD2	2.24	0.66
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.76	0.66
25:BA:2720:U:OP1	39:BQ:53:ARG:NH2	2.28	0.66
25:BA:711:G:H1	25:BA:720:U:H3	1.44	0.66
25:BA:2162:G:O2'	25:BA:2163:A:N7	2.28	0.66
30:BF:112:ARG:NH1	30:BF:134:GLU:OE2	2.29	0.66
21:AU:13:ASP:OD1	21:AU:13:ASP:N	2.19	0.66
28:BD:33:ARG:HA	28:BD:94:GLN:O	1.96	0.66
60:CD:256:ASP:O	60:CD:259:ARG:NH2	2.21	0.66
25:BA:812:C:OP1	40:BR:13:ARG:NH1	2.29	0.66
1:AA:202:G:HO2'	1:AA:468:A:H8	1.44	0.66
25:BA:1592:C:H2'	25:BA:1593:A:H8	1.60	0.66
36:BN:66:ARG:NH1	36:BN:104:GLU:OE2	2.29	0.66
22:AV:49:G:H5"	59:CC:540:ARG:NH2	2.11	0.66
25:BA:550:U:H2'	25:BA:551:G:C8	2.31	0.66
25:BA:1084:A:H2'	25:BA:1085:A:C8	2.31	0.66
25:BA:2252:G:H2'	25:BA:2253:G:H8	1.60	0.66
28:BD:30:GLU:OE2	28:BD:30:GLU:N	2.29	0.66
31:BG:16:ASP:OD1	31:BG:16:ASP:N	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:501:C:OP1	12:AL:114:ARG:NH2	2.29	0.65
25:BA:284:U:O2	25:BA:356:G:N2	2.26	0.65
25:BA:652:U:OP2	25:BA:654:A:N6	2.30	0.65
25:BA:2134:A:N6	25:BA:2157:G:O2'	2.30	0.65
57:CT:17:DG:C5	57:CT:18:DC:C5	2.84	0.65
4:AD:18:ASP:HB2	4:AD:28:ILE:HD13	1.79	0.65
6:AF:45:ARG:O	6:AF:56:LYS:HA	1.95	0.65
10:AJ:42:LEU:HB2	10:AJ:71:LEU:HB3	1.78	0.65
1:AA:1010:U:H2'	1:AA:1011:C:C6	2.31	0.65
25:BA:2153:C:H2'	25:BA:2154:A:C8	2.31	0.65
25:BA:2683:C:O2	34:BL:70:ARG:NH2	2.30	0.65
60:CD:429:LEU:HD22	60:CD:429:LEU:N	2.12	0.65
1:AA:195:A:O2'	1:AA:196:A:H5'	1.97	0.65
11:AK:92:GLY:O	11:AK:94:GLU:N	2.28	0.65
56:CN:32:DA:H5'	56:CN:32:DA:C8	2.32	0.65
3:AC:40:ARG:NH1	3:AC:55:ILE:O	2.30	0.64
2:AB:15:HIS:HB3	2:AB:43:LEU:HD11	1.79	0.64
10:AJ:36:VAL:HA	10:AJ:76:ILE:HA	1.78	0.64
1:AA:1061:G:OP2	3:AC:3:GLN:NE2	2.29	0.64
2:AB:186:ILE:HD11	2:AB:204:ASP:HA	1.79	0.64
26:BB:8:C:O3'	38:BP:25:ARG:NH1	2.30	0.64
28:BD:48:ILE:HG23	28:BD:84:LEU:HD11	1.80	0.64
57:CT:19:DG:C6	57:CT:20:DC:C4	2.86	0.64
57:CT:19:DG:H2'	57:CT:20:DC:H6	1.63	0.64
59:CC:251:ALA:HB2	59:CC:269:ILE:HD11	1.80	0.64
59:CC:582:ASN:OD1	59:CC:583:GLU:N	2.31	0.64
5:AE:80:THR:HG23	5:AE:122:ASN:O	1.98	0.63
12:AL:79:VAL:HG12	12:AL:102:LEU:HD23	1.80	0.63
13:AM:23:TYR:HB3	13:AM:66:GLU:HG2	1.80	0.63
30:BF:102:ARG:NH1	55:B7:9:TYR:OH	2.32	0.63
10:AJ:75:ASP:OD1	10:AJ:75:ASP:N	2.32	0.63
25:BA:265:A:N1	25:BA:427:U:O2'	2.25	0.63
25:BA:2140:G:H2'	25:BA:2141:G:C8	2.33	0.63
25:BA:1592:C:H2'	25:BA:1593:A:C8	2.33	0.63
25:BA:2120:G:H5"	25:BA:2172:U:H5"	1.79	0.63
1:AA:823:C:HO2'	8:AH:2:SER:N	1.97	0.63
25:BA:210:C:OP1	52:B4:29:GLN:NE2	2.29	0.63
59:CC:638:SER:OG	59:CC:639:LYS:N	2.32	0.63
52:B4:11:LYS:O	52:B4:15:SER:OG	2.16	0.63
59:CC:18:ARG:NH1	59:CC:1188:ASP:OD1	2.31	0.63
25:BA:2071:A:H2'	25:BA:2072:C:C6	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BH:126:GLY:H	32:BH:146:VAL:HB	1.63	0.63
1:AA:337:G:H2'	1:AA:338:A:C8	2.34	0.62
25:BA:2349:G:OP1	53:B5:45:ARG:NH2	2.32	0.62
57:CT:19:DG:C5	57:CT:20:DC:C5	2.87	0.62
31:BG:17:VAL:HG11	31:BG:50:LEU:HD21	1.80	0.62
15:AO:64:ARG:NH1	15:AO:89:ARG:O	2.26	0.62
31:BG:164:TYR:HB2	31:BG:167:GLU:HB3	1.80	0.62
36:BN:106:ASP:OD1	36:BN:107:GLY:N	2.32	0.62
24:AX:17:C:H1'	24:AX:18:G:H5"	1.82	0.62
25:BA:1870:C:H4'	25:BA:1870:C:OP2	1.98	0.62
44:BV:7:ARG:NH1	44:BV:26:LYS:O	2.32	0.62
49:B1:9:GLN:O	49:B1:33:GLY:N	2.31	0.62
56:CN:38:DA:H2"	56:CN:39:DG:N7	2.14	0.62
58:CB:27:THR:C	58:CB:28:LEU:HD22	2.19	0.62
1:AA:1277:C:HO2'	1:AA:1278:G:P	2.22	0.62
14:AN:33:ASP:O	14:AN:41:ARG:NH2	2.33	0.62
42:BT:110:ARG:OXT	42:BT:110:ARG:NE	2.29	0.62
2:AB:16:PHE:HE1	2:AB:35:ARG:HH21	1.48	0.62
15:AO:80:GLN:O	15:AO:83:GLU:HG2	2.00	0.62
25:BA:1407:G:H2'	25:BA:1408:G:C8	2.34	0.62
29:BE:153:LEU:HD12	29:BE:153:LEU:H	1.64	0.62
1:AA:90:C:H2'	1:AA:91:U:C6	2.33	0.62
1:AA:197:A:O2'	1:AA:220:G:N2	2.32	0.62
25:BA:1178:C:H2'	25:BA:1179:G:C8	2.35	0.62
57:CT:9:DC:H2'	57:CT:10:DT:C6	2.34	0.62
60:CD:576:ARG:NH1	60:CD:593:ASN:O	2.32	0.62
6:AF:29:ILE:HG23	6:AF:34:GLY:HA3	1.82	0.62
25:BA:545:A:N1	25:BA:549:C:C4	2.67	0.62
25:BA:1871:A:O2'	25:BA:1872:A:O4'	2.16	0.62
1:AA:746:A:H2'	1:AA:747:A:C8	2.34	0.62
1:AA:1174:G:H2'	1:AA:1175:G:H5'	1.82	0.62
5:AE:31:PHE:HE1	22:AV:24:A:H62	1.48	0.62
21:AU:40:LYS:HE2	21:AU:42:THR:HG22	1.82	0.62
27:BC:252:THR:HG23	27:BC:253:LYS:HG3	1.81	0.62
35:BM:123:ARG:NH1	35:BM:143:GLU:OE2	2.34	0.61
38:BP:39:VAL:HB	38:BP:49:VAL:HG22	1.82	0.61
1:AA:35:G:N3	12:AL:115:SER:OG	2.34	0.61
11:AK:67:ALA:HB2	11:AK:96:THR:HG23	1.82	0.61
25:BA:340:A:O2'	29:BE:162:ARG:NH1	2.33	0.61
1:AA:421:U:O2	3:AC:127:ARG:NH2	2.33	0.61
25:BA:2126:A:O2'	25:BA:2162:G:N2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2792:A:H2'	25:BA:2793:C:C6	2.35	0.61
3:AC:134:MET:HG2	3:AC:168:TYR:HD2	1.66	0.61
25:BA:491:G:O6	42:BT:49:LYS:NZ	2.32	0.61
25:BA:620:G:O6	29:BE:98:LYS:NZ	2.33	0.61
2:AB:28:LYS:HA	2:AB:31:ILE:HD12	1.82	0.61
11:AK:92:GLY:C	11:AK:94:GLU:H	2.04	0.61
58:CA:8:PHE:O	58:CA:10:LYS:NZ	2.26	0.61
25:BA:2110:G:H5'	25:BA:2118:U:O2'	2.01	0.61
25:BA:2127:G:H2'	25:BA:2128:G:C8	2.36	0.61
1:AA:844:G:C2	1:AA:846:G:H1'	2.36	0.61
49:B1:12:SER:HB2	49:B1:32:ILE:HD11	1.82	0.61
3:AC:36:ASP:OD1	3:AC:59:ARG:NH1	2.33	0.61
9:AI:21:ILE:HD12	9:AI:61:LEU:HD23	1.83	0.61
9:AI:57:MET:HB3	9:AI:61:LEU:HD13	1.83	0.61
24:AX:26:A:N1	24:AX:44:G:N2	2.48	0.61
25:BA:1095:A:H2'	25:BA:1096:A:C8	2.36	0.61
25:BA:1386:C:H2'	25:BA:1387:A:C8	2.36	0.61
25:BA:1404:C:C2'	25:BA:1405:U:H5'	2.31	0.61
25:BA:1494:A:H2'	25:BA:1495:A:C8	2.36	0.61
25:BA:1579:A:H2'	25:BA:1580:A:C8	2.36	0.60
25:BA:2189:U:H2'	25:BA:2190:G:C8	2.35	0.60
25:BA:2250:G:OP1	36:BN:84:LYS:NZ	2.24	0.60
57:CT:18:DC:H2'	57:CT:19:DG:H8	1.65	0.60
25:BA:2128:G:H3'	25:BA:2129:C:C5'	2.31	0.60
35:BM:78:ARG:HG2	35:BM:113:ALA:HB3	1.84	0.60
60:CD:504:GLN:HG3	60:CD:505:ASP:H	1.65	0.60
1:AA:1004:A:C6	1:AA:1026:G:H1'	2.36	0.60
15:AO:47:LYS:O	15:AO:53:ARG:NH2	2.27	0.60
25:BA:1404:C:H2'	25:BA:1405:U:H5'	1.84	0.60
27:BC:232:HIS:HA	27:BC:242:LYS:HD3	1.83	0.60
1:AA:890:G:O2'	1:AA:906:A:N6	2.34	0.60
42:BT:17:VAL:HG11	42:BT:103:ILE:HG12	1.83	0.60
59:CC:705:GLU:HB3	59:CC:794:LEU:H	1.67	0.60
60:CD:797:THR:HG22	60:CD:924:GLY:HA3	1.83	0.60
13:AM:71:ARG:NH1	55:B7:50:ASP:OD2	2.33	0.60
42:BT:25:ARG:HG3	42:BT:74:ILE:HG22	1.84	0.60
60:CD:441:LEU:HD22	60:CD:441:LEU:N	2.16	0.60
2:AB:43:LEU:O	2:AB:47:VAL:HG22	2.01	0.60
7:AG:57:SER:HB3	7:AG:60:GLU:HG2	1.84	0.60
25:BA:1169:A:H2'	25:BA:1170:C:C6	2.35	0.60
25:BA:2286:G:OP2	51:B3:6:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BH:115:VAL:O	32:BH:116:ARG:NH1	2.33	0.60
56:CN:26:DG:OP2	59:CC:542:ARG:NH1	2.35	0.60
59:CC:525:THR:HG21	59:CC:687:ARG:HH11	1.67	0.60
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.36	0.60
1:AA:4:U:HO2'	1:AA:5:U:C5'	2.14	0.60
1:AA:927:G:O2'	1:AA:928:G:H5'	2.02	0.60
8:AH:18:GLN:HE21	8:AH:72:VAL:HG12	1.67	0.60
38:BP:69:ASP:OD1	38:BP:70:ALA:N	2.34	0.60
1:AA:73:C:C2'	1:AA:74:A:H5'	2.32	0.60
1:AA:81:A:N6	1:AA:89:G:O6	2.35	0.60
1:AA:108:G:C6	20:AT:10:ARG:HG2	2.37	0.60
4:AD:15:GLU:OE2	4:AD:56:ARG:NH2	2.35	0.59
23:AW:76:A:HO2'	63:AX:101:PHE:N	2.00	0.59
56:CN:27:DA:C4	56:CN:28:DA:C8	2.90	0.59
20:AT:35:VAL:HG21	20:AT:54:MET:HG2	1.84	0.59
25:BA:245:G:O6	53:B5:8:ARG:NH1	2.35	0.59
36:BN:77:PRO:HG2	36:BN:80:VAL:HG11	1.84	0.59
25:BA:2000:C:OP1	37:BO:5:LYS:NZ	2.35	0.59
1:AA:933:G:O6	7:AG:3:ARG:NH2	2.35	0.59
2:AB:108:ARG:O	2:AB:111:ILE:HG12	2.02	0.59
29:BE:191:ASP:OD2	29:BE:195:GLN:NE2	2.36	0.59
60:CD:650:LYS:HE3	60:CD:742:GLY:O	2.02	0.59
1:AA:1008:U:H2'	1:AA:1009:U:C6	2.37	0.59
39:BQ:7:GLN:O	39:BQ:11:GLU:HG3	2.03	0.59
1:AA:1035:A:H2'	1:AA:1036:A:H8	1.67	0.59
1:AA:1276:G:O2'	1:AA:1277:C:H5'	2.02	0.59
4:AD:11:LEU:HD13	4:AD:63:ARG:HG2	1.83	0.59
25:BA:1406:U:H2'	25:BA:1407:G:H5"	1.84	0.59
28:BD:35:THR:HG22	28:BD:73:VAL:HG21	1.84	0.59
1:AA:1137:C:O2	1:AA:1138:G:N1	2.36	0.59
47:BY:6:GLN:O	47:BY:74:ARG:NH2	2.35	0.59
57:CT:20:DC:H2'	57:CT:21:DG:H8	1.68	0.59
1:AA:198:G:H2'	1:AA:199:A:H8	1.67	0.58
10:AJ:86:ALA:N	10:AJ:89:ARG:HH11	2.00	0.58
1:AA:148:G:O2'	1:AA:149:A:O5'	2.21	0.58
23:AW:19:G:H5"	23:AW:20:H2U:H52	1.85	0.58
25:BA:1169:A:H2'	25:BA:1170:C:H6	1.67	0.58
25:BA:1868:C:H2'	25:BA:1869:G:H8	1.67	0.58
33:BK:9:GLU:HG2	33:BK:10:THR:N	2.18	0.58
1:AA:1390:U:H2'	1:AA:1391:U:C6	2.38	0.58
36:BN:20:LEU:HD13	45:BW:81:PRO:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:CA:67:GLU:OE1	59:CC:1057:LYS:NZ	2.33	0.58
4:AD:63:ARG:HH11	4:AD:63:ARG:HG3	1.68	0.58
9:AI:57:MET:HG3	9:AI:60:LYS:HD2	1.85	0.58
25:BA:2469:A:N6	25:BA:2481:G:O2'	2.36	0.58
43:BU:34:VAL:HG21	43:BU:43:ILE:HD11	1.85	0.58
59:CC:696:ASP:CG	59:CC:697:LYS:H	2.06	0.58
12:AL:57:LEU:HD11	12:AL:82:ILE:HD11	1.86	0.58
59:CC:23:ASP:OD1	59:CC:23:ASP:N	2.34	0.58
60:CD:515:ARG:NH2	60:CD:718:SER:O	2.37	0.58
60:CD:1169:THR:OG1	60:CD:1173:ARG:HB3	2.02	0.58
1:AA:1343:G:OP1	9:AI:124:ARG:NH1	2.36	0.58
25:BA:2129:C:OP1	25:BA:2129:C:H4'	2.04	0.58
27:BC:157:SER:O	27:BC:160:THR:OG1	2.14	0.58
45:BW:3:THR:HA	45:BW:62:THR:HG23	1.85	0.58
57:CT:17:DG:C6	57:CT:18:DC:C4	2.91	0.58
60:CD:1069:ALA:HA	60:CD:1072:LYS:HB2	1.85	0.58
4:AD:125:VAL:HG22	4:AD:143:VAL:HG22	1.86	0.58
6:AF:67:PRO:HG2	6:AF:70:VAL:HG23	1.86	0.58
22:AV:44:A:O2'	22:AV:45:C:OP2	2.21	0.58
33:BK:9:GLU:HG2	33:BK:10:THR:HG23	1.85	0.58
1:AA:1169:A:H2'	1:AA:1170:A:C8	2.39	0.58
21:AU:10:GLU:OE1	21:AU:18:ARG:NH1	2.36	0.58
22:AV:48:C:H2'	22:AV:49:G:O4'	2.04	0.58
24:AX:18:G:HO2'	24:AX:57:G:H22	1.45	0.58
25:BA:1177:G:O2'	25:BA:1178:C:H6	1.87	0.58
25:BA:2189:U:H2'	25:BA:2190:G:H8	1.69	0.58
33:BK:92:MET:SD	33:BK:95:ARG:NH2	2.77	0.58
54:B6:12:ARG:HB3	54:B6:12:ARG:HH11	1.69	0.58
59:CC:525:THR:HG21	59:CC:687:ARG:NH1	2.18	0.58
1:AA:182:A:O2'	1:AA:183:C:H3'	2.03	0.58
1:AA:198:G:H2'	1:AA:199:A:C8	2.39	0.58
8:AH:11:LEU:HD22	8:AH:75:ILE:HD11	1.85	0.58
25:BA:1028:A:H2'	25:BA:1029:A:C8	2.39	0.58
25:BA:1174:U:O2'	25:BA:1175:A:O4'	2.22	0.58
25:BA:1494:A:HO2'	25:BA:1495:A:P	2.27	0.58
59:CC:320:ASP:N	59:CC:320:ASP:OD1	2.37	0.57
60:CD:429:LEU:H	60:CD:429:LEU:CD2	2.13	0.57
61:CE:44:ASP:OD1	61:CE:44:ASP:N	2.29	0.57
53:B5:51:SER:OG	53:B5:54:ASP:OD1	2.20	0.57
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.40	0.57
6:AF:38:ARG:HG2	6:AF:63:ASN:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:CN:28:DA:H2"	56:CN:29:DG:H8	1.70	0.57
2:AB:217:VAL:O	2:AB:221:VAL:HG12	2.04	0.57
3:AC:105:GLU:OE1	3:AC:107:ARG:HD3	2.05	0.57
6:AF:12:PRO:O	6:AF:44:ARG:NH2	2.38	0.57
14:AN:47:LYS:O	14:AN:50:THR:OG1	2.12	0.57
25:BA:1105:U:H2'	25:BA:1106:G:H8	1.68	0.57
41:BS:30:GLY:N	41:BS:63:VAL:O	2.36	0.57
44:BV:4:LYS:O	44:BV:94:ARG:NH2	2.35	0.57
57:CT:19:DG:C4	57:CT:20:DC:C5	2.93	0.57
7:AG:27:VAL:HG11	7:AG:40:GLU:HG2	1.86	0.57
25:BA:1591:A:H2'	25:BA:1592:C:H6	1.69	0.57
25:BA:1808:A:H3'	25:BA:1809:A:C8	2.39	0.57
29:BE:145:ASP:HB3	29:BE:184:ASP:HB2	1.86	0.57
37:BO:100:CYS:O	37:BO:110:MET:HB2	2.05	0.57
1:AA:496:A:H2'	1:AA:496:A:N3	2.20	0.57
25:BA:2122:U:H3'	25:BA:2123:G:H8	1.68	0.57
25:BA:2315:G:O2'	25:BA:2316:G:O4'	2.23	0.57
42:BT:20:VAL:HG11	42:BT:44:ALA:HA	1.85	0.57
57:CT:26:DA:H2"	57:CT:27:DG:C8	2.39	0.57
59:CC:421:SER:H	59:CC:424:ASP:HB2	1.69	0.57
8:AH:66:PHE:CD2	8:AH:67:GLN:HG3	2.40	0.57
25:BA:1168:G:H1	25:BA:1181:U:H3	1.53	0.57
37:BO:2:ARG:NE	37:BO:2:ARG:O	2.38	0.57
2:AB:12:ALA:O	2:AB:208:ARG:NH1	2.36	0.57
25:BA:1408:G:H2'	25:BA:1409:U:C6	2.40	0.57
56:CN:34:DT:H6	56:CN:34:DT:H5'	1.70	0.57
60:CD:495:ASN:OD1	60:CD:495:ASN:N	2.38	0.57
1:AA:474:G:OP1	16:AP:80:LYS:NZ	2.30	0.56
2:AB:47:VAL:HG23	2:AB:48:PRO:HD3	1.87	0.56
59:CC:591:TYR:OH	59:CC:637:ARG:NH2	2.36	0.56
27:BC:29:PRO:HG2	27:BC:34:LEU:HD11	1.86	0.56
59:CC:726:TYR:HB3	59:CC:733:VAL:CG1	2.34	0.56
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.70	0.56
9:AI:44:ALA:O	9:AI:48:VAL:HG12	2.05	0.56
24:AX:37:MIA:H152	24:AX:38:A:N1	2.21	0.56
25:BA:994:C:OP2	40:BR:54:LYS:NZ	2.36	0.56
25:BA:2119:A:H2'	25:BA:2168:G:H22	1.69	0.56
25:BA:2328:A:H2'	25:BA:2329:U:C6	2.39	0.56
42:BT:11:ARG:NH1	42:BT:99:ARG:O	2.38	0.56
59:CC:12:ARG:HH21	59:CC:793:GLU:CD	2.07	0.56
25:BA:160:A:N3	25:BA:2208:C:O2'	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:187:GLU:O	4:AD:191:LEU:HD22	2.06	0.56
25:BA:2591:C:H2'	25:BA:2592:G:C8	2.41	0.56
28:BD:33:ARG:NH1	28:BD:53:GLY:O	2.37	0.56
60:CD:523:GLU:CD	60:CD:709:ARG:HH22	2.08	0.56
1:AA:157:U:O2	1:AA:164:G:O6	2.24	0.56
25:BA:639:U:H2'	25:BA:640:C:C6	2.40	0.56
25:BA:2116:G:O4'	25:BA:2165:C:N4	2.39	0.56
36:BN:35:ALA:HB2	36:BN:102:LEU:HD11	1.88	0.56
2:AB:108:ARG:O	2:AB:112:LYS:HG3	2.05	0.56
12:AL:35:THR:OG1	12:AL:54:ARG:O	2.21	0.56
25:BA:2506:U:O2	25:BA:2506:U:H2'	2.05	0.56
1:AA:842:U:H4'	1:AA:846:G:C6	2.41	0.56
20:AT:24:ARG:HH11	20:AT:24:ARG:HA	1.71	0.56
25:BA:1153:C:OP1	40:BR:92:ARG:NH1	2.39	0.56
59:CC:1340:GLU:OE1	59:CC:1341:ASP:N	2.34	0.56
25:BA:2547:A:H2'	25:BA:2548:U:C6	2.41	0.56
32:BH:89:LYS:HG3	32:BH:90:LEU:H	1.71	0.56
1:AA:844:G:N7	1:AA:845:A:N6	2.53	0.56
7:AG:7:ILE:HD13	7:AG:7:ILE:H	1.71	0.56
32:BH:73:ASN:HD21	32:BH:141:LYS:H	1.54	0.56
10:AJ:42:LEU:HB2	10:AJ:71:LEU:CB	2.35	0.55
9:AI:47:VAL:HG13	9:AI:80:ARG:HD3	1.87	0.55
25:BA:1794:A:H2'	25:BA:1795:C:C6	2.41	0.55
29:BE:21:ARG:NH2	29:BE:106:LYS:HD3	2.22	0.55
50:B2:32:LYS:HG3	50:B2:33:THR:HG23	1.86	0.55
1:AA:1311:A:H5"	55:B7:59:ARG:NH1	2.21	0.55
21:AU:14:VAL:O	21:AU:18:ARG:HG2	2.05	0.55
51:B3:6:ARG:HH12	51:B3:26:ASN:HB2	1.69	0.55
55:B7:30:HIS:CG	55:B7:31:ASP:H	2.24	0.55
25:BA:2252:G:H2'	25:BA:2253:G:C8	2.40	0.55
58:CB:13:LEU:HA	58:CB:28:LEU:HD13	1.89	0.55
60:CD:37:GLU:HB2	60:CD:104:HIS:CE1	2.42	0.55
25:BA:645:C:H2'	25:BA:647:G:C8	2.41	0.55
32:BH:83:LYS:O	32:BH:90:LEU:HD12	2.06	0.55
60:CD:160:LEU:HD23	60:CD:160:LEU:H	1.71	0.55
1:AA:1383:C:H2'	1:AA:1384:C:C6	2.42	0.55
25:BA:927:A:H2'	25:BA:928:A:C8	2.42	0.55
21:AU:61:ALA:O	21:AU:65:ALA:HB3	2.07	0.55
25:BA:686:U:H6	25:BA:788:A:N1	2.05	0.55
30:BF:57:LEU:HD12	30:BF:87:CYS:SG	2.47	0.55
42:BT:17:VAL:HG12	42:BT:76:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BX:59:LEU:HD12	46:BX:80:ILE:HD12	1.88	0.55
48:BZ:5:GLU:HG2	48:BZ:6:LEU:HD12	1.89	0.55
54:B6:6:SER:OG	54:B6:8:LYS:NZ	2.34	0.55
1:AA:202:G:H21	1:AA:466:A:H61	1.53	0.55
25:BA:464:U:O3'	52:B4:12:ARG:NH1	2.40	0.55
25:BA:2144:G:O2'	25:BA:2147:A:N6	2.40	0.55
11:AK:93:ARG:NH2	11:AK:112:ASP:OD2	2.39	0.55
25:BA:833:A:H2'	25:BA:834:G:C8	2.41	0.55
29:BE:113:VAL:HG12	29:BE:118:LEU:HD23	1.89	0.55
13:AM:16:VAL:HG13	13:AM:17:ILE:HD12	1.89	0.55
25:BA:1141:U:H4'	25:BA:1142:A:O4'	2.06	0.55
38:BP:1:MET:O	38:BP:5:SER:OG	2.25	0.55
44:BV:34:VAL:HG13	44:BV:67:VAL:HG22	1.88	0.55
28:BD:149:ASN:OD1	28:BD:150:MEQ:N	2.40	0.54
31:BG:52:PHE:CE1	31:BG:72:LEU:HD22	2.42	0.54
1:AA:842:U:O2'	1:AA:845:A:OP2	2.18	0.54
3:AC:11:ARG:NH2	3:AC:177:THR:O	2.38	0.54
58:CB:76:GLU:H	58:CB:76:GLU:CD	2.08	0.54
59:CC:1165:SER:O	59:CC:1167:GLU:N	2.37	0.54
2:AB:14:VAL:HG23	2:AB:43:LEU:HD21	1.90	0.54
25:BA:881:G:O6	25:BA:895:U:O4	2.26	0.54
25:BA:1108:U:H2'	25:BA:1109:C:H6	1.68	0.54
25:BA:1261:C:OP2	42:BT:83:LYS:NZ	2.40	0.54
25:BA:1405:U:O2'	25:BA:1406:U:O4'	2.25	0.54
1:AA:1020:G:OP1	1:AA:1020:G:H4'	2.06	0.54
4:AD:80:ALA:HA	4:AD:86:THR:HG22	1.89	0.54
4:AD:102:VAL:HG13	4:AD:107:PHE:HB2	1.90	0.54
25:BA:139:U:O4	43:BU:1:MET:N	2.39	0.54
25:BA:1595:C:O2'	25:BA:1596:A:H5'	2.08	0.54
25:BA:2153:C:H2'	25:BA:2154:A:H8	1.73	0.54
60:CD:301:GLU:OE1	60:CD:312:ARG:NH1	2.37	0.54
25:BA:2291:U:H2'	25:BA:2292:U:C6	2.42	0.54
59:CC:538:LEU:HD12	59:CC:539:THR:N	2.23	0.54
59:CC:1070:HIS:NE2	59:CC:1114:GLU:OE1	2.41	0.54
1:AA:104:G:OP1	20:AT:16:LYS:NZ	2.33	0.54
11:AK:86:VAL:HG11	11:AK:93:ARG:HG3	1.89	0.54
25:BA:1047:G:N2	25:BA:1110:G:O2'	2.40	0.54
25:BA:1594:U:H2'	25:BA:1595:C:C6	2.43	0.54
25:BA:2064:C:H2'	25:BA:2065:C:C6	2.42	0.54
25:BA:2136:G:O6	25:BA:2155:U:O2	2.26	0.54
59:CC:632:ASP:N	59:CC:632:ASP:OD1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:966:2MG:HM22	23:AW:34:C:H5'	1.90	0.54
9:AI:88:MET:SD	9:AI:95:ARG:HG2	2.47	0.54
25:BA:1796:U:H2'	25:BA:1797:G:H8	1.72	0.54
56:CN:31:DG:H2"	56:CN:32:DA:C8	2.42	0.54
1:AA:107:G:N7	20:AT:10:ARG:NH2	2.55	0.54
59:CC:1079:ILE:HG23	59:CC:1079:ILE:O	2.08	0.54
9:AI:21:ILE:HG23	9:AI:61:LEU:HD23	1.88	0.54
15:AO:6:GLU:CD	15:AO:6:GLU:H	2.11	0.54
19:AS:3:ARG:HE	19:AS:7:LYS:HB3	1.72	0.54
25:BA:1057:A:N7	25:BA:1086:A:H2'	2.21	0.54
48:BZ:18:LEU:HD21	48:BZ:54:LYS:HE3	1.90	0.54
56:CN:26:DG:C6	56:CN:27:DA:N6	2.76	0.54
59:CC:1176:LEU:O	59:CC:1178:LYS:N	2.39	0.54
1:AA:986:U:H2'	1:AA:987:G:C8	2.43	0.54
11:AK:34:ILE:HB	11:AK:74:VAL:HG11	1.89	0.54
30:BF:8:TYR:HA	30:BF:12:VAL:HB	1.90	0.54
59:CC:524:ILE:HG22	59:CC:525:THR:N	2.22	0.54
11:AK:89:PRO:HG3	21:AU:32:VAL:HG11	1.90	0.53
60:CD:367:GLY:HA2	60:CD:440:VAL:O	2.08	0.53
60:CD:825:VAL:HG13	60:CD:825:VAL:O	2.08	0.53
11:AK:47:ALA:HB1	11:AK:62:ALA:HB1	1.90	0.53
25:BA:1591:A:H2'	25:BA:1592:C:C6	2.43	0.53
25:BA:1800:C:H5'	27:BC:146:MET:HE3	1.90	0.53
31:BG:52:PHE:CZ	31:BG:72:LEU:HD22	2.43	0.53
1:AA:196:A:OP1	20:AT:64:LYS:NZ	2.42	0.53
1:AA:864:A:C5'	5:AE:90:THR:HB	2.36	0.53
1:AA:181:A:O2'	1:AA:194:C:N4	2.42	0.53
4:AD:8:LYS:HB3	4:AD:21:LEU:HB3	1.90	0.53
25:BA:84:A:N1	25:BA:98:G:O2'	2.37	0.53
25:BA:1090:A:C2	25:BA:1102:C:H1'	2.44	0.53
29:BE:21:ARG:O	29:BE:114:ARG:NH2	2.41	0.53
25:BA:2244:U:H2'	25:BA:2245:U:C6	2.44	0.53
41:BS:34:GLU:HG2	41:BS:60:LYS:HG2	1.89	0.53
59:CC:150:HIS:CE1	59:CC:454:ARG:HG3	2.43	0.53
39:BQ:14:LYS:HE3	39:BQ:77:HIS:HA	1.89	0.53
48:BZ:19:LEU:HD23	48:BZ:23:ARG:HH22	1.73	0.53
4:AD:49:SER:O	4:AD:53:VAL:HG13	2.09	0.53
25:BA:585:G:N7	40:BR:6:ARG:NH1	2.57	0.53
25:BA:1394:U:H4'	25:BA:1603:A:H4'	1.91	0.53
57:CT:21:DG:C6	57:CT:22:DC:N4	2.77	0.53
1:AA:1310:G:OP2	13:AM:87:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:674:G:H5"	29:BE:71:GLY:N	2.24	0.53
25:BA:1590:A:H2'	25:BA:1591:A:H8	1.72	0.53
25:BA:2127:G:H2'	25:BA:2128:G:H8	1.72	0.53
29:BE:48:THR:HG23	29:BE:86:ALA:HB3	1.91	0.53
60:CD:441:LEU:HD22	60:CD:441:LEU:H	1.73	0.53
24:AX:75:C:O2	25:BA:2507:C:O2'	2.26	0.53
60:CD:35:PHE:CD1	60:CD:101:ARG:HB3	2.44	0.53
1:AA:356:A:N3	1:AA:368:U:O2'	2.34	0.52
25:BA:992:C:OP1	40:BR:47:TYR:OH	2.23	0.52
32:BH:78:VAL:HG21	32:BH:103:VAL:HG22	1.91	0.52
59:CC:696:ASP:OD1	59:CC:697:LYS:N	2.39	0.52
1:AA:299:G:H2'	1:AA:300:A:C8	2.44	0.52
25:BA:285:G:O6	25:BA:355:U:O2	2.27	0.52
25:BA:301:G:OP2	44:BV:82:ARG:NH1	2.42	0.52
25:BA:2144:G:H1'	25:BA:2147:A:H61	1.73	0.52
30:BF:36:LEU:HB2	30:BF:89:VAL:CG1	2.39	0.52
49:B1:23:THR:HG23	49:B1:47:MET:HG2	1.90	0.52
1:AA:206:C:H2'	1:AA:207:C:O4'	2.09	0.52
1:AA:945:G:C2	1:AA:946:A:C8	2.98	0.52
1:AA:946:A:H2'	1:AA:947:G:C8	2.45	0.52
1:AA:966:2MG:H5"	1:AA:967:5MC:OP2	2.08	0.52
25:BA:2178:C:H2'	25:BA:2179:C:C6	2.44	0.52
25:BA:2244:U:O2'	25:BA:2245:U:H5'	2.09	0.52
25:BA:2685:G:P	34:BL:78:ARG:HH22	2.33	0.52
30:BF:22:TYR:OH	30:BF:165:GLU:OE2	2.14	0.52
38:BP:82:ALA:HB3	38:BP:115:LEU:HD11	1.91	0.52
59:CC:392:GLU:CD	59:CC:392:GLU:H	2.12	0.52
59:CC:423:ASP:N	59:CC:423:ASP:OD1	2.33	0.52
1:AA:913:A:OP1	12:AL:88:LYS:NZ	2.42	0.52
1:AA:1383:C:O2'	1:AA:1384:C:H5'	2.09	0.52
3:AC:131:ARG:NH2	3:AC:166:GLU:OE1	2.42	0.52
25:BA:1379:U:O3'	25:BA:1380:G:H8	1.93	0.52
51:B3:3:LYS:HG2	51:B3:5:ILE:HG12	1.91	0.52
58:CB:191:ARG:NH2	58:CB:192:VAL:O	2.42	0.52
59:CC:85:CYS:SG	59:CC:90:VAL:HG23	2.50	0.52
25:BA:1084:A:O2'	25:BA:1105:U:O2'	2.27	0.52
25:BA:1469:A:H2'	25:BA:1470:A:C8	2.45	0.52
29:BE:130:LYS:HB2	29:BE:133:LEU:HD12	1.89	0.52
59:CC:193:ASN:HD22	59:CC:193:ASN:N	2.08	0.52
60:CD:907:HIS:ND1	60:CD:908:ILE:O	2.36	0.52
6:AF:11:HIS:ND1	6:AF:12:PRO:HD2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:43:GLY:HA2	6:AF:58:HIS:CE1	2.45	0.52
14:AN:48:LEU:HD12	14:AN:51:LEU:HD12	1.91	0.52
60:CD:801:VAL:HG12	60:CD:920:ALA:HB3	1.91	0.52
1:AA:1277:C:O2'	1:AA:1278:G:O5'	2.24	0.52
18:AR:34:THR:HG22	18:AR:40:VAL:HG22	1.92	0.52
27:BC:159:GLY:HA2	27:BC:195:VAL:O	2.10	0.52
1:AA:1495:U:O2'	25:BA:1919:A:N1	2.34	0.52
25:BA:645:C:H2'	25:BA:647:G:N7	2.25	0.52
25:BA:2128:G:H3'	25:BA:2129:C:H5"	1.92	0.52
45:BW:2:PHE:HB2	45:BW:61:LEU:HD23	1.92	0.52
58:CA:218:ARG:NH1	58:CB:233:ASP:OD1	2.42	0.52
59:CC:178:PRO:HB3	59:CC:395:TYR:CZ	2.44	0.52
60:CD:312:ARG:HG2	60:CD:313:GLY:N	2.24	0.52
25:BA:2150:C:H2'	25:BA:2151:U:C6	2.45	0.52
59:CC:267:ARG:NE	59:CC:268:ARG:O	2.37	0.52
8:AH:18:GLN:HG3	8:AH:72:VAL:HG13	1.92	0.52
9:AI:113:ARG:HG3	9:AI:115:LYS:HZ3	1.75	0.52
60:CD:1075:ARG:HH21	60:CD:1102:PRO:HA	1.75	0.52
1:AA:1167:A:H1'	1:AA:1168:U:OP1	2.10	0.51
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	1.91	0.51
39:BQ:33:VAL:O	39:BQ:33:VAL:HG12	2.10	0.51
59:CC:12:ARG:NE	59:CC:793:GLU:OE2	2.36	0.51
59:CC:726:TYR:CD1	59:CC:727:VAL:N	2.78	0.51
60:CD:67:ASP:N	60:CD:67:ASP:OD1	2.43	0.51
1:AA:401:C:O2'	1:AA:621:A:N3	2.36	0.51
1:AA:1311:A:H5"	55:B7:59:ARG:HH12	1.76	0.51
10:AJ:53:ILE:HD11	10:AJ:63:ASP:CB	2.39	0.51
25:BA:1529:G:H2'	25:BA:1530:G:H8	1.74	0.51
25:BA:2171:A:O2'	25:BA:2173:A:OP1	2.29	0.51
25:BA:2728:U:HO2'	25:BA:2729:G:H8	1.57	0.51
26:BB:1:U:HO2'	26:BB:2:G:H8	1.57	0.51
28:BD:13:ARG:O	39:BQ:12:GLN:NE2	2.41	0.51
57:CT:18:DC:O2	57:CT:19:DG:C8	2.64	0.51
1:AA:1166:G:O2'	1:AA:1167:A:OP1	2.24	0.51
1:AA:1183:U:H3'	1:AA:1184:G:C5'	2.41	0.51
9:AI:84:THR:HG21	9:AI:103:PHE:CB	2.39	0.51
25:BA:856:G:H2'	25:BA:857:G:C8	2.46	0.51
25:BA:1296:G:OP1	25:BA:2709:G:O2'	2.21	0.51
25:BA:1596:A:O2'	25:BA:1597:A:H5'	2.10	0.51
41:BS:61:ALA:HB2	41:BS:98:ILE:HD13	1.92	0.51
47:BY:12:PRO:HB3	47:BY:30:LEU:HD23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:CC:705:GLU:CD	59:CC:705:GLU:H	2.14	0.51
1:AA:673:A:H2'	1:AA:674:G:C8	2.45	0.51
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.46	0.51
25:BA:614:A:O2'	25:BA:615:U:OP2	2.25	0.51
25:BA:2503:2MA:O2'	25:BA:2505:G:OP2	2.29	0.51
59:CC:296:VAL:O	59:CC:335:THR:HB	2.10	0.51
1:AA:714:G:H2'	1:AA:715:A:C8	2.46	0.51
10:AJ:55:PRO:HA	14:AN:82:ILE:HD11	1.91	0.51
22:AV:43:A:OP2	59:CC:1250:SER:OG	2.22	0.51
23:AW:50:U:H3	23:AW:64:G:H1	1.57	0.51
59:CC:519:ASN:C	59:CC:519:ASN:OD1	2.46	0.51
1:AA:56:U:H2'	1:AA:57:G:C8	2.46	0.51
1:AA:1175:G:O2'	1:AA:1176:A:H8	1.92	0.51
1:AA:1270:G:HO2'	1:AA:1313:U:HO2'	1.57	0.51
1:AA:1383:C:H2'	1:AA:1384:C:H6	1.75	0.51
3:AC:61:ALA:O	3:AC:62:LYS:HD3	2.10	0.51
4:AD:140:ASN:N	4:AD:182:PHE:O	2.44	0.51
29:BE:110:SER:O	29:BE:113:VAL:HG22	2.10	0.51
60:CD:1159:ILE:O	60:CD:1206:ARG:N	2.42	0.51
1:AA:31:G:O2'	1:AA:48:C:N4	2.43	0.51
24:AX:15:G:H3'	24:AX:16:H2U:H62	1.93	0.51
44:BV:74:ASN:HB3	44:BV:96:PHE:CE1	2.46	0.51
1:AA:413:G:N2	1:AA:428:G:H1'	2.25	0.51
3:AC:47:LEU:HD21	3:AC:87:LEU:HD11	1.92	0.51
11:AK:109:ASN:HD21	11:AK:111:THR:HG23	1.76	0.51
25:BA:172:A:H2'	25:BA:173:A:C8	2.46	0.51
25:BA:396:G:OP2	47:BY:10:LYS:NZ	2.44	0.51
25:BA:2119:A:C8	25:BA:2168:G:N1	2.79	0.51
25:BA:2165:C:H2'	25:BA:2166:U:O4'	2.10	0.51
25:BA:2788:C:H2'	25:BA:2789:C:C6	2.46	0.51
30:BF:171:ALA:O	30:BF:174:ASP:N	2.42	0.51
44:BV:99:ASN:OD1	44:BV:101:GLU:HB2	2.11	0.51
1:AA:91:U:H2'	1:AA:92:U:C6	2.46	0.51
7:AG:79:ARG:NH1	7:AG:82:GLY:O	2.44	0.51
24:AX:14:A:H2'	24:AX:15:G:O4'	2.10	0.51
31:BG:56:ASP:OD1	31:BG:57:GLY:N	2.44	0.51
45:BW:27:PRO:O	45:BW:88:HIS:HA	2.10	0.51
1:AA:371:A:H2'	1:AA:372:C:O4'	2.11	0.50
25:BA:889:C:H2'	25:BA:890:C:C6	2.46	0.50
25:BA:1049:C:C2'	25:BA:1050:A:H5'	2.41	0.50
25:BA:1796:U:H2'	25:BA:1797:G:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BH:73:ASN:ND2	32:BH:141:LYS:H	2.09	0.50
38:BP:51:ALA:HB3	38:BP:78:VAL:HB	1.92	0.50
58:CA:68:TYR:CD1	58:CA:68:TYR:N	2.79	0.50
59:CC:1321:GLU:OE2	60:CD:99:ARG:NH1	2.41	0.50
24:AX:54:5MU:H4'	36:BN:51:ARG:HE	1.76	0.50
25:BA:2025:C:H2'	25:BA:2026:U:C6	2.46	0.50
25:BA:2615:U:C2	50:B2:4:GLN:HA	2.46	0.50
59:CC:855:PRO:HG3	59:CC:913:VAL:HG23	1.92	0.50
1:AA:147:G:O2'	1:AA:148:G:O4'	2.29	0.50
25:BA:929:U:H1'	49:B1:26:GLY:O	2.10	0.50
25:BA:2133:G:H2'	25:BA:2157:G:H22	1.75	0.50
25:BA:2799:G:O2'	25:BA:2800:A:H5"	2.11	0.50
56:CN:28:DA:H2"	56:CN:29:DG:C8	2.45	0.50
6:AF:3:HIS:HB2	6:AF:92:THR:O	2.12	0.50
10:AJ:56:HIS:ND1	10:AJ:57:VAL:HG22	2.27	0.50
22:AV:51:G:C4	22:AV:52:C:C5	3.00	0.50
25:BA:2127:G:H21	25:BA:2173:A:C4'	2.25	0.50
25:BA:2155:U:H2'	25:BA:2156:G:C8	2.47	0.50
32:BH:86:ASP:O	32:BH:88:GLY:N	2.42	0.50
58:CB:28:LEU:HD22	58:CB:28:LEU:N	2.27	0.50
60:CD:504:GLN:HG3	60:CD:505:ASP:N	2.25	0.50
1:AA:1229:A:OP2	13:AM:113:ARG:NH1	2.40	0.50
22:AV:52:C:H2'	22:AV:53:G:C1'	2.41	0.50
25:BA:219:A:N3	25:BA:234:U:O2'	2.37	0.50
25:BA:2154:A:H2'	25:BA:2155:U:O4'	2.12	0.50
2:AB:100:MET:HA	2:AB:107:VAL:HG21	1.94	0.50
13:AM:52:GLN:OE1	13:AM:52:GLN:N	2.45	0.50
25:BA:499:U:H5"	44:BV:43:LYS:HE2	1.93	0.50
25:BA:784:G:H5'	25:BA:785:G:OP1	2.12	0.50
25:BA:1814:G:OP2	25:BA:1815:A:O2'	2.24	0.50
31:BG:105:LEU:HD11	31:BG:148:LEU:HD22	1.94	0.50
56:CN:23:DT:H1'	56:CN:24:DC:C4	2.47	0.50
42:BT:24:ILE:HD13	42:BT:36:LEU:HD11	1.94	0.50
44:BV:14:LEU:HD11	44:BV:71:ALA:HB2	1.93	0.50
56:CN:27:DA:C6	56:CN:28:DA:C6	3.00	0.50
60:CD:175:GLU:CD	60:CD:175:GLU:H	2.15	0.50
10:AJ:5:ARG:HH21	10:AJ:7:ARG:CZ	2.24	0.50
12:AL:5:ASN:O	12:AL:9:ARG:HG3	2.12	0.50
25:BA:1916:A:H2'	25:BA:1917:PSU:H6	1.77	0.50
30:BF:141:ILE:C	30:BF:141:ILE:HD12	2.32	0.50
31:BG:22:GLN:NE2	31:BG:38:ASN:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:BR:27:ALA:HB1	40:BR:31:VAL:HB	1.93	0.50
59:CC:726:TYR:CD1	59:CC:726:TYR:C	2.84	0.50
25:BA:1506:U:H2'	25:BA:1507:C:C6	2.47	0.50
25:BA:1744:A:H3'	25:BA:1745:A:H8	1.76	0.50
25:BA:1901:A:OP2	27:BC:253:LYS:NZ	2.29	0.50
58:CB:11:PRO:O	58:CB:12:ARG:HD2	2.12	0.50
60:CD:137:ARG:HG3	60:CD:142:GLU:HB2	1.94	0.50
5:AE:80:THR:HG22	5:AE:81:LEU:H	1.77	0.49
25:BA:890:C:OP2	25:BA:890:C:H6	1.95	0.49
25:BA:1868:C:H2'	25:BA:1869:G:C8	2.45	0.49
27:BC:4:VAL:HG23	27:BC:18:LYS:HB2	1.94	0.49
38:BP:52:SER:HB2	38:BP:54:VAL:HG22	1.94	0.49
57:CT:17:DG:C6	57:CT:18:DC:C5	3.00	0.49
59:CC:1083:GLU:CD	59:CC:1083:GLU:H	2.13	0.49
60:CD:288:PRO:HD2	60:CD:291:ILE:HD12	1.93	0.49
60:CD:366:CYS:O	60:CD:439:PRO:HA	2.11	0.49
1:AA:684:U:H2'	1:AA:685:G:O4'	2.12	0.49
1:AA:1530:G:H2'	1:AA:1531:A:C8	2.47	0.49
3:AC:105:GLU:OE1	3:AC:107:ARG:NH1	2.33	0.49
28:BD:30:GLU:OE1	28:BD:77:ARG:NH1	2.45	0.49
57:CT:9:DC:H2'	57:CT:10:DT:H71	1.93	0.49
58:CA:102:LEU:HD23	58:CA:103:ASN:N	2.27	0.49
59:CC:516:ASP:O	59:CC:518:ASN:N	2.41	0.49
60:CD:1360:GLY:HA2	61:CE:17:PHE:CZ	2.47	0.49
1:AA:477:C:H2'	1:AA:478:A:C8	2.47	0.49
1:AA:713:G:H2'	1:AA:714:G:C8	2.47	0.49
2:AB:167:ASP:OD2	2:AB:191:SER:OG	2.26	0.49
25:BA:1579:A:H2'	25:BA:1580:A:H8	1.76	0.49
25:BA:2345:G:N3	25:BA:2381:A:H2'	2.28	0.49
25:BA:2477:U:O2	54:B6:4:ARG:NH2	2.46	0.49
42:BT:36:LEU:HD13	42:BT:48:LYS:HA	1.93	0.49
1:AA:677:U:H3	1:AA:713:G:H22	1.58	0.49
1:AA:1240:U:O4	7:AG:109:ARG:NH1	2.45	0.49
9:AI:55:VAL:HG11	9:AI:94:LEU:HD13	1.94	0.49
22:AV:51:G:C2	22:AV:52:C:C4	3.00	0.49
41:BS:78:ARG:HB3	41:BS:83:TYR:HB3	1.94	0.49
59:CC:274:ILE:HA	59:CC:277:LEU:HD12	1.93	0.49
60:CD:275:ARG:HH11	60:CD:298:MET:HB3	1.76	0.49
60:CD:813:ASP:OD1	60:CD:883:ARG:NH2	2.35	0.49
1:AA:346:G:OP1	39:BQ:39:ARG:NH2	2.45	0.49
1:AA:1001:C:H2'	1:AA:1002:G:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:65:ALA:O	7:AG:69:VAL:HG23	2.13	0.49
25:BA:1055:G:HO2'	25:BA:1085:A:H2	1.59	0.49
42:BT:74:ILE:HD12	42:BT:105:VAL:HG22	1.94	0.49
46:BX:69:PHE:C	46:BX:70:GLU:HG3	2.33	0.49
56:CN:28:DA:C6	56:CN:29:DG:C6	3.01	0.49
57:CT:20:DC:H2'	57:CT:21:DG:C8	2.47	0.49
59:CC:617:ALA:HB2	59:CC:650:VAL:HG21	1.93	0.49
60:CD:961:SER:HB2	60:CD:981:GLU:HB2	1.94	0.49
24:AX:5:G:O2'	24:AX:6:G:H5'	2.12	0.49
25:BA:1047:G:O2'	25:BA:1110:G:N1	2.40	0.49
25:BA:1794:A:H2'	25:BA:1795:C:H6	1.77	0.49
30:BF:127:ASN:HD22	30:BF:158:THR:H	1.60	0.49
31:BG:127:THR:HG23	31:BG:130:GLU:HB2	1.93	0.49
42:BT:11:ARG:HH21	42:BT:98:LYS:HE3	1.77	0.49
2:AB:68:LEU:HD22	2:AB:70:VAL:HG22	1.94	0.49
4:AD:76:TYR:HH	4:AD:205:SER:HG	1.60	0.49
16:AP:6:LEU:HD22	16:AP:17:TYR:HB3	1.95	0.49
25:BA:2147:A:C4	25:BA:2148:G:H1'	2.48	0.49
34:BL:76:VAL:HG12	39:BQ:73:VAL:HB	1.95	0.49
59:CC:811:ASN:ND2	59:CC:1097:VAL:O	2.43	0.49
60:CD:326:SER:O	60:CD:329:ASP:N	2.43	0.49
1:AA:949:A:N7	13:AM:105:ASN:ND2	2.61	0.49
7:AG:125:SER:O	7:AG:129:GLU:HG2	2.13	0.49
9:AI:119:ARG:HB3	9:AI:123:ARG:HG2	1.95	0.49
13:AM:71:ARG:NH2	30:BF:113:ASP:OD1	2.45	0.49
25:BA:2060:A:OP2	29:BE:66:GLY:HA2	2.13	0.49
28:BD:25:THR:HG21	28:BD:193:VAL:HG22	1.95	0.49
30:BF:117:LEU:O	30:BF:178:ARG:HB2	2.13	0.49
31:BG:23:VAL:HG22	31:BG:36:THR:HB	1.95	0.49
60:CD:850:LYS:N	60:CD:855:ASP:O	2.33	0.49
1:AA:1006:G:C6	1:AA:1024:G:C2	3.00	0.49
1:AA:1305:G:HO2'	1:AA:1306:A:H8	1.60	0.49
1:AA:1382:C:C2'	1:AA:1383:C:H5'	2.42	0.49
11:AK:114:THR:HG21	21:AU:32:VAL:HG21	1.94	0.49
25:BA:1672:A:C2	25:BA:2582:G:H5'	2.48	0.49
59:CC:261:VAL:HG21	59:CC:264:GLU:HG2	1.94	0.49
60:CD:1292:LEU:HD11	60:CD:1297:LYS:HB2	1.95	0.49
1:AA:72:A:H2'	1:AA:73:C:O4'	2.13	0.49
1:AA:1025:U:H5"	1:AA:1026:G:C5'	2.40	0.49
2:AB:107:VAL:O	2:AB:111:ILE:HG23	2.12	0.49
24:AX:49:C:H2'	24:AX:50:U:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:886:A:N6	25:BA:887:U:O2	2.45	0.49
51:B3:5:ILE:HG21	51:B3:28:ARG:HD2	1.94	0.49
59:CC:1239:VAL:HG13	59:CC:1240:ASP:N	2.27	0.49
13:AM:57:ARG:NE	55:B7:35:ASP:OD2	2.46	0.48
19:AS:27:ASP:OD1	19:AS:28:LYS:N	2.46	0.48
25:BA:1175:A:H62	25:BA:1177:G:H1'	1.78	0.48
25:BA:2112:G:H3'	25:BA:2113:U:C6	2.48	0.48
57:CT:9:DC:H2'	57:CT:10:DT:C5	2.48	0.48
60:CD:530:PRO:O	60:CD:533:ALA:HB3	2.12	0.48
60:CD:1313:SER:HG	60:CD:1325:PHE:HE2	1.60	0.48
1:AA:87:C:H2'	1:AA:88:U:C6	2.48	0.48
1:AA:841:C:H2'	1:AA:843:U:H5'	1.95	0.48
1:AA:874:G:C6	1:AA:875:U:C4	3.01	0.48
1:AA:1516:2MG:N2	1:AA:1519:MA6:OP2	2.46	0.48
25:BA:728:G:H4'	27:BC:13:ARG:HD3	1.96	0.48
25:BA:1065:U:O2'	25:BA:1066:U:O5'	2.31	0.48
25:BA:1231:U:H2'	25:BA:1232:G:H8	1.78	0.48
25:BA:2166:U:H5	25:BA:2170:A:H61	1.60	0.48
25:BA:2210:U:H4'	25:BA:2211:G:H5'	1.95	0.48
26:BB:1:U:O2'	26:BB:2:G:H8	1.96	0.48
32:BH:115:VAL:HG22	32:BH:132:PHE:CZ	2.48	0.48
45:BW:31:TYR:O	45:BW:92:VAL:HA	2.12	0.48
57:CT:19:DG:C4	57:CT:20:DC:C6	3.01	0.48
59:CC:7:GLU:O	59:CC:9:LYS:N	2.35	0.48
60:CD:767:LEU:HD12	60:CD:767:LEU:N	2.28	0.48
60:CD:805:GLN:OE1	60:CD:1348:LYS:HB2	2.13	0.48
8:AH:90:ASP:OD1	8:AH:90:ASP:N	2.43	0.48
10:AJ:77:VAL:HG12	10:AJ:78:GLU:OE1	2.14	0.48
25:BA:1914:C:H2'	25:BA:1915:3TD:O4	2.14	0.48
45:BW:63:ILE:HG22	45:BW:65:VAL:HG22	1.95	0.48
2:AB:47:VAL:HG23	2:AB:48:PRO:CD	2.43	0.48
15:AO:25:THR:HG21	15:AO:70:LEU:HD13	1.95	0.48
23:AW:44:A:H2'	23:AW:45:G:O4'	2.14	0.48
25:BA:1175:A:H8	25:BA:1176:U:H4'	1.78	0.48
58:CB:34:GLY:N	58:CB:199:ASP:OD2	2.46	0.48
60:CD:158:GLN:NE2	60:CD:158:GLN:O	2.46	0.48
1:AA:4:U:HO2'	1:AA:5:U:P	2.35	0.48
1:AA:1493:A:H2'	25:BA:1913:A:N1	2.28	0.48
22:AV:44:A:O2'	22:AV:44:A:N3	2.33	0.48
25:BA:581:C:H2'	25:BA:582:A:C8	2.49	0.48
25:BA:2182:U:H1'	25:BA:2183:A:N7	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2344:U:H3'	51:B3:37:LYS:O	2.13	0.48
28:BD:30:GLU:H	28:BD:30:GLU:CD	2.15	0.48
59:CC:1238:LEU:N	59:CC:1238:LEU:HD23	2.29	0.48
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.49	0.48
1:AA:1498:UR3:OP2	22:AV:16:A:O2'	2.31	0.48
38:BP:1:MET:O	38:BP:5:SER:CB	2.62	0.48
55:B7:30:HIS:CG	55:B7:31:ASP:N	2.81	0.48
59:CC:234:ASP:HB3	59:CC:238:GLN:NE2	2.29	0.48
1:AA:246:A:N1	1:AA:278:G:O2'	2.40	0.48
1:AA:1014:A:C2	1:AA:1219:A:H1'	2.49	0.48
8:AH:18:GLN:HG3	8:AH:72:VAL:CG1	2.42	0.48
25:BA:1568:G:H4'	27:BC:59:LYS:HG2	1.95	0.48
25:BA:2038:G:H2'	25:BA:2039:U:O4'	2.14	0.48
37:BO:56:LYS:NZ	37:BO:90:ARG:O	2.46	0.48
42:BT:17:VAL:HA	42:BT:43:ALA:HB1	1.95	0.48
42:BT:88:ARG:NH2	42:BT:94:ASP:OD2	2.46	0.48
56:CN:32:DA:H1'	56:CN:33:DT:O4'	2.14	0.48
57:CT:22:DC:C2	57:CT:23:DC:C5	3.01	0.48
59:CC:529:ARG:NH2	59:CC:562:GLU:OE2	2.46	0.48
59:CC:1292:THR:OG1	59:CC:1293:VAL:N	2.47	0.48
1:AA:866:C:C4	1:AA:867:G:H1'	2.49	0.48
25:BA:1057:A:C8	25:BA:1086:A:H2'	2.49	0.48
25:BA:1068:G:O6	25:BA:1069:A:N6	2.47	0.48
25:BA:2698:U:H2'	25:BA:2699:C:C6	2.49	0.48
27:BC:142:HIS:HD2	27:BC:193:GLY:O	1.96	0.48
29:BE:147:LEU:HD11	29:BE:170:ARG:HD2	1.95	0.48
56:CN:27:DA:C2	56:CN:28:DA:C4	3.02	0.48
58:CB:61:ILE:HD12	58:CB:142:MET:HB3	1.96	0.48
1:AA:50:A:O2'	1:AA:360:G:N2	2.47	0.48
1:AA:1318:A:H5"	19:AS:3:ARG:NH2	2.29	0.48
6:AF:85:ILE:HG13	6:AF:86:ARG:N	2.29	0.48
11:AK:34:ILE:HG12	11:AK:70:CYS:SG	2.54	0.48
25:BA:2114:A:N6	25:BA:2168:G:O6	2.47	0.48
26:BB:2:G:H2'	26:BB:3:C:C6	2.49	0.48
43:BU:48:GLN:HE21	43:BU:55:VAL:H	1.62	0.48
59:CC:267:ARG:HH22	59:CC:273:HIS:CE1	2.31	0.48
59:CC:696:ASP:OD1	59:CC:696:ASP:N	2.45	0.48
59:CC:794:LEU:HA	59:CC:794:LEU:HD12	1.71	0.48
1:AA:218:U:H2'	1:AA:219:U:O4'	2.14	0.48
1:AA:1090:U:HO2'	1:AA:1171:A:HO2'	1.60	0.48
1:AA:1316:G:N1	1:AA:1319:A:OP2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1042:G:O2'	25:BA:1043:C:H6	1.97	0.48
25:BA:2532:G:O2'	25:BA:2657:A:N1	2.43	0.48
59:CC:1278:LEU:HD23	59:CC:1278:LEU:HA	1.49	0.48
1:AA:269:C:H2'	1:AA:270:A:C8	2.48	0.47
1:AA:562:U:H1'	12:AL:12:ARG:HB3	1.95	0.47
4:AD:101:VAL:HG21	4:AD:137:VAL:HG21	1.96	0.47
30:BF:4:LEU:HD23	30:BF:4:LEU:HA	1.73	0.47
59:CC:766:ASN:CG	59:CC:766:ASN:O	2.53	0.47
1:AA:56:U:H2'	1:AA:57:G:H8	1.79	0.47
1:AA:844:G:H2'	1:AA:845:A:C8	2.49	0.47
1:AA:1039:G:H2'	1:AA:1040:U:C6	2.49	0.47
1:AA:1152:A:OP1	10:AJ:70:HIS:ND1	2.47	0.47
7:AG:79:ARG:HG3	7:AG:84:THR:HG22	1.95	0.47
13:AM:16:VAL:O	13:AM:20:THR:HG23	2.14	0.47
25:BA:581:C:H2'	25:BA:582:A:H8	1.79	0.47
55:B7:12:ILE:HD12	55:B7:32:LEU:HB2	1.96	0.47
59:CC:269:ILE:HD12	59:CC:269:ILE:N	2.29	0.47
59:CC:576:SER:OG	59:CC:577:VAL:N	2.47	0.47
1:AA:1034:G:H2'	1:AA:1035:A:C8	2.50	0.47
6:AF:79:ARG:HG3	6:AF:80:PHE:N	2.28	0.47
13:AM:59:GLU:OE2	13:AM:62:LYS:NZ	2.42	0.47
28:BD:55:LYS:HD3	28:BD:60:VAL:HG22	1.95	0.47
32:BH:8:LYS:NZ	32:BH:137:GLU:OE2	2.46	0.47
47:BY:13:VAL:HG22	47:BY:29:PHE:HB2	1.95	0.47
59:CC:1133:LYS:O	59:CC:1135:GLN:NE2	2.47	0.47
1:AA:73:C:O2'	1:AA:74:A:H5'	2.15	0.47
1:AA:481:G:HO2'	1:AA:483:C:H41	1.57	0.47
6:AF:67:PRO:HG2	6:AF:70:VAL:CG2	2.43	0.47
9:AI:41:ARG:HH21	9:AI:41:ARG:HG3	1.79	0.47
25:BA:1407:G:O2'	25:BA:1408:G:H5'	2.15	0.47
25:BA:2131:U:H5'	25:BA:2132:U:OP1	2.15	0.47
25:BA:2135:A:H3'	25:BA:2136:G:C8	2.41	0.47
25:BA:2138:G:H2'	25:BA:2139:U:O4'	2.14	0.47
25:BA:2141:G:H2'	25:BA:2142:A:O4'	2.15	0.47
25:BA:2233:U:H2'	25:BA:2234:G:C8	2.50	0.47
57:CT:21:DG:H2'	57:CT:22:DC:C6	2.49	0.47
2:AB:120:GLN:OE1	2:AB:124:GLY:HA3	2.14	0.47
3:AC:72:ARG:HD3	3:AC:75:ILE:HD12	1.97	0.47
3:AC:153:VAL:HG13	3:AC:198:VAL:HG22	1.96	0.47
25:BA:134:G:H2'	25:BA:135:U:C6	2.50	0.47
59:CC:696:ASP:CG	59:CC:697:LYS:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:66:LEU:O	7:AG:70:ARG:HG3	2.15	0.47
9:AI:55:VAL:HG12	9:AI:57:MET:SD	2.55	0.47
25:BA:2243:U:H2'	25:BA:2244:U:H6	1.77	0.47
25:BA:2327:A:H2'	25:BA:2328:A:C8	2.49	0.47
46:BX:53:CYS:SG	46:BX:57:HIS:HA	2.54	0.47
1:AA:160:A:H1'	1:AA:344:A:C5	2.49	0.47
1:AA:1054:C:N4	24:AX:34:G:C8	2.83	0.47
1:AA:1088:G:H21	1:AA:1167:A:N6	2.13	0.47
3:AC:135:LYS:NZ	3:AC:168:TYR:OH	2.47	0.47
5:AE:111:MET:HE2	5:AE:125:ALA:HB1	1.97	0.47
8:AH:112:THR:HG23	8:AH:115:ALA:H	1.78	0.47
15:AO:8:THR:HG23	15:AO:31:LEU:HD21	1.95	0.47
22:AV:49:G:H5"	59:CC:540:ARG:HH22	1.79	0.47
24:AX:27:G:H2'	24:AX:28:G:C8	2.49	0.47
25:BA:141:G:H4'	25:BA:1596:A:H5"	1.95	0.47
25:BA:613:A:H5"	25:BA:613:A:H8	1.80	0.47
25:BA:811:U:H2'	35:BM:21:ARG:HA	1.96	0.47
25:BA:1614:A:C2	42:BT:93:ALA:HB2	2.50	0.47
25:BA:2743:U:H2'	25:BA:2744:G:O4'	2.15	0.47
28:BD:32:ASN:HD22	28:BD:32:ASN:N	2.11	0.47
29:BE:51:GLU:OE1	29:BE:88:ARG:NH1	2.48	0.47
45:BW:80:HIS:CE1	45:BW:83:LYS:HD2	2.50	0.47
59:CC:69:GLN:OE1	59:CC:101:ARG:NE	2.44	0.47
60:CD:746:LEU:HD23	60:CD:758:PRO:HB3	1.96	0.47
1:AA:451:A:H1'	1:AA:452:A:C2	2.49	0.47
1:AA:901:A:C5	1:AA:902:G:H1'	2.50	0.47
10:AJ:52:LEU:HD21	10:AJ:59:LYS:HD2	1.96	0.47
25:BA:626:A:H2'	35:BM:78:ARG:NH2	2.30	0.47
25:BA:1315:C:O2'	25:BA:1392:A:N3	2.41	0.47
25:BA:2119:A:H62	25:BA:2167:U:H1'	1.80	0.47
27:BC:227:PRO:HA	27:BC:233:GLY:HA2	1.95	0.47
33:BK:69:ARG:HG2	33:BK:90:GLU:HG3	1.95	0.47
59:CC:705:GLU:OE1	59:CC:705:GLU:N	2.41	0.47
60:CD:1159:ILE:HB	60:CD:1160:SER:H	1.59	0.47
1:AA:91:U:H2'	1:AA:92:U:H6	1.80	0.47
1:AA:1026:G:C4	1:AA:1027:C:C5	3.02	0.47
4:AD:59:GLN:OE1	4:AD:63:ARG:NH1	2.42	0.47
6:AF:85:ILE:HG13	6:AF:86:ARG:H	1.80	0.47
32:BH:17:ASP:OD1	32:BH:17:ASP:N	2.46	0.47
59:CC:530:ILE:HA	59:CC:530:ILE:HD13	1.64	0.47
2:AB:187:VAL:HG13	2:AB:191:SER:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AX:15:G:C3’	24:AX:16:H2U:H62	2.45	0.47
25:BA:1386:C:H2’	25:BA:1387:A:H8	1.79	0.47
25:BA:1405:U:H2’	25:BA:1406:U:C6	2.50	0.47
34:BL:38:ILE:HD11	34:BL:112:PHE:CZ	2.50	0.47
51:B3:13:SER:HB3	51:B3:49:TYR:CZ	2.49	0.47
60:CD:393:THR:HG23	60:CD:395:LYS:H	1.80	0.47
1:AA:842:U:H4’	1:AA:846:G:N1	2.29	0.46
25:BA:813:U:H2’	25:BA:814:C:C6	2.51	0.46
25:BA:2114:A:H2’	25:BA:2114:A:N3	2.29	0.46
27:BC:105:LEU:O	27:BC:107:PRO:HD3	2.16	0.46
32:BH:8:LYS:HA	32:BH:14:SER:HA	1.97	0.46
60:CD:255:LEU:HG	60:CD:256:ASP:H	1.80	0.46
1:AA:81:A:N6	1:AA:89:G:C6	2.84	0.46
1:AA:203:G:O2’	1:AA:465:A:N1	2.47	0.46
1:AA:464:U:O2’	1:AA:466:A:N7	2.31	0.46
1:AA:922:G:N3	1:AA:1398:A:H2	2.13	0.46
1:AA:1277:C:O2’	1:AA:1278:G:P	2.72	0.46
7:AG:2:PRO:HG2	7:AG:5:ARG:HB2	1.98	0.46
25:BA:1178:C:H2’	25:BA:1179:G:H8	1.77	0.46
53:B5:62:LEU:HB3	53:B5:65:ALA:HB2	1.98	0.46
56:CN:32:DA:H5’	56:CN:32:DA:H8	1.76	0.46
57:CT:19:DG:C5	57:CT:20:DC:C4	3.02	0.46
59:CC:1314:GLN:HG3	61:CE:28:ARG:HH22	1.81	0.46
59:CC:1333:LEU:O	59:CC:1335:ILE:N	2.48	0.46
60:CD:416:ILE:O	60:CD:416:ILE:HG23	2.15	0.46
1:AA:459:A:H2’	1:AA:460:A:C8	2.50	0.46
1:AA:1189:U:OP1	14:AN:98:LYS:NZ	2.48	0.46
2:AB:71:GLY:O	2:AB:93:ASN:HA	2.15	0.46
6:AF:39:LEU:HD13	6:AF:62:MET:HG2	1.97	0.46
40:BR:89:GLU:HG3	41:BS:52:PRO:HB3	1.98	0.46
60:CD:26:SER:HB3	60:CD:236:TRP:CZ2	2.49	0.46
1:AA:567:G:H2’	1:AA:568:G:O4’	2.16	0.46
1:AA:826:C:O2	8:AH:16:ASN:ND2	2.49	0.46
5:AE:80:THR:HG22	5:AE:81:LEU:N	2.30	0.46
13:AM:49:SER:HB2	13:AM:52:GLN:OE1	2.15	0.46
25:BA:1932:A:H2’	25:BA:1933:G:O4’	2.15	0.46
25:BA:2265:U:OP2	25:BA:2266:A:O2’	2.28	0.46
25:BA:2812:G:H2’	25:BA:2813:A:O4’	2.16	0.46
50:B2:38:HIS:ND1	50:B2:39:LEU:O	2.48	0.46
51:B3:22:THR:HG23	53:B5:34:THR:HG23	1.98	0.46
56:CN:10:DG:H2”	56:CN:11:DT:H72	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:CD:478:LEU:HD23	60:CD:478:LEU:HA	1.63	0.46
60:CD:664:ILE:HG22	60:CD:678:ARG:HG2	1.97	0.46
1:AA:195:A:C2'	1:AA:196:A:H5'	2.45	0.46
1:AA:280:C:N4	17:AQ:41:THR:HG1	2.13	0.46
3:AC:61:ALA:C	3:AC:62:LYS:HD3	2.36	0.46
4:AD:98:LEU:O	4:AD:101:VAL:HG22	2.15	0.46
13:AM:40:ALA:O	13:AM:43:VAL:HG22	2.14	0.46
16:AP:9:HIS:O	16:AP:16:PHE:N	2.44	0.46
25:BA:686:U:O4	52:B4:12:ARG:HB2	2.16	0.46
25:BA:851:C:H2'	25:BA:852:U:C6	2.50	0.46
58:CA:79:LEU:HD23	58:CA:79:LEU:O	2.15	0.46
1:AA:1006:G:C5	1:AA:1007:U:C5	3.04	0.46
2:AB:188:ASP:HB2	2:AB:204:ASP:OD2	2.16	0.46
4:AD:95:GLU:HG3	4:AD:191:LEU:HD11	1.98	0.46
25:BA:1790:C:H2'	25:BA:1791:A:C5	2.51	0.46
3:AC:27:LYS:HB3	3:AC:28:GLU:OE1	2.16	0.46
5:AE:101:GLU:OE1	5:AE:122:ASN:ND2	2.49	0.46
24:AX:2:C:H2'	24:AX:3:C:H6	1.80	0.46
25:BA:829:A:N7	25:BA:2248:C:H5'	2.31	0.46
30:BF:25:VAL:O	30:BF:28:VAL:HG22	2.16	0.46
60:CD:488:ASN:N	60:CD:488:ASN:OD1	2.48	0.46
60:CD:849:LEU:HA	60:CD:856:ILE:HA	1.96	0.46
14:AN:7:LYS:O	14:AN:11:VAL:HG13	2.15	0.46
23:AW:7:G:O2'	23:AW:49:G:O5'	2.30	0.46
25:BA:248:G:H5'	25:BA:250:G:N7	2.30	0.46
25:BA:348:A:H2'	25:BA:349:U:O4'	2.16	0.46
42:BT:69:LEU:HD23	42:BT:69:LEU:HA	1.77	0.46
58:CA:179:PRO:HA	58:CA:208:ASN:ND2	2.30	0.46
59:CC:1333:LEU:C	59:CC:1335:ILE:H	2.18	0.46
60:CD:247:PRO:HA	60:CD:250:ARG:CZ	2.45	0.46
60:CD:1249:ASN:OD1	60:CD:1250:ASP:N	2.49	0.46
1:AA:1175:G:N3	1:AA:1176:A:C8	2.84	0.46
24:AX:27:G:H2'	24:AX:28:G:H8	1.81	0.46
24:AX:51:U:H2'	24:AX:52:G:H8	1.80	0.46
42:BT:95:ARG:NH1	42:BT:95:ARG:HG2	2.30	0.46
59:CC:1291:LEU:HD21	60:CD:1351:VAL:HG13	1.97	0.46
60:CD:62:PHE:O	60:CD:101:ARG:NH2	2.46	0.46
60:CD:830:ASP:OD1	60:CD:832:LYS:NZ	2.43	0.46
1:AA:183:C:H4'	1:AA:184:G:OP2	2.15	0.46
11:AK:116:ILE:HD13	11:AK:116:ILE:H	1.80	0.46
17:AQ:25:ILE:O	17:AQ:25:ILE:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AV:52:C:H2'	22:AV:53:G:O4'	2.16	0.46
25:BA:133:U:H2'	25:BA:134:G:O4'	2.16	0.46
25:BA:144:A:H2'	25:BA:145:C:C6	2.51	0.46
25:BA:191:A:H2'	25:BA:192:C:C6	2.51	0.46
25:BA:355:U:H2'	25:BA:356:G:H8	1.81	0.46
25:BA:2086:U:H2'	25:BA:2087:G:C8	2.50	0.46
25:BA:2114:A:C6	25:BA:2115:G:H1'	2.50	0.46
30:BF:137:ILE:HG13	30:BF:138:PHE:N	2.31	0.46
39:BQ:66:ASN:OD1	39:BQ:66:ASN:N	2.49	0.46
40:BR:100:VAL:O	40:BR:103:LYS:NZ	2.48	0.46
60:CD:319:SER:O	60:CD:321:LYS:N	2.46	0.46
1:AA:337:G:H2'	1:AA:338:A:H8	1.78	0.45
1:AA:1176:A:H2'	1:AA:1177:G:C8	2.51	0.45
2:AB:129:LEU:CB	2:AB:134:ALA:HB2	2.41	0.45
24:AX:8:4SU:O2'	24:AX:21:A:N1	2.37	0.45
25:BA:1028:A:N6	25:BA:1125:G:H2'	2.31	0.45
25:BA:1838:C:N4	25:BA:1898:U:H2'	2.30	0.45
25:BA:2128:G:H4'	25:BA:2174:C:H4'	1.98	0.45
59:CC:514:PHE:CE1	59:CC:760:ASN:HB3	2.51	0.45
59:CC:563:THR:OG1	59:CC:564:PRO:HD2	2.16	0.45
59:CC:1204:LEU:HD23	59:CC:1204:LEU:HA	1.69	0.45
60:CD:1309:ILE:HG13	60:CD:1310:THR:N	2.31	0.45
1:AA:4:U:O2'	1:AA:5:U:P	2.75	0.45
1:AA:17:U:H2'	1:AA:18:C:C6	2.50	0.45
1:AA:1180:A:P	9:AI:99:ARG:HH22	2.39	0.45
1:AA:1305:G:O2'	1:AA:1306:A:H8	1.99	0.45
11:AK:110:ILE:HB	21:AU:4:ILE:HD13	1.98	0.45
25:BA:1667:G:O2'	25:BA:1991:U:O4	2.22	0.45
25:BA:1799:G:OP1	27:BC:258:ARG:HD2	2.16	0.45
25:BA:2123:G:H2'	25:BA:2123:G:N3	2.31	0.45
41:BS:60:LYS:HE2	41:BS:60:LYS:HB3	1.68	0.45
57:CT:4:DT:H2"	57:CT:5:DG:H8	1.82	0.45
1:AA:1356:G:H2'	1:AA:1357:A:H8	1.78	0.45
14:AN:8:ALA:O	14:AN:11:VAL:HG22	2.16	0.45
24:AX:43:C:H2'	24:AX:44:G:H8	1.80	0.45
25:BA:639:U:H2'	25:BA:640:C:H6	1.81	0.45
25:BA:1077:A:HO2'	25:BA:1078:U:P	2.40	0.45
25:BA:1486:U:H2'	25:BA:1487:U:C6	2.52	0.45
42:BT:18:ARG:HG3	42:BT:76:VAL:HB	1.98	0.45
54:B6:2:LYS:HE3	54:B6:32:LYS:O	2.15	0.45
59:CC:138:ILE:HA	59:CC:138:ILE:HD13	1.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:CC:145:ILE:CG2	59:CC:456:VAL:HG22	2.47	0.45
59:CC:1314:GLN:CG	61:CE:28:ARG:HH22	2.30	0.45
60:CD:317:THR:HG21	60:CD:321:LYS:HA	1.99	0.45
25:BA:2015:A:C6	50:B2:3:VAL:HG23	2.52	0.45
29:BE:109:LEU:O	29:BE:113:VAL:HG13	2.16	0.45
30:BF:8:TYR:HB2	30:BF:173:PHE:CZ	2.52	0.45
51:B3:10:LYS:HD2	51:B3:55:LYS:HG2	1.98	0.45
60:CD:1075:ARG:NH2	60:CD:1102:PRO:HA	2.31	0.45
25:BA:310:A:H5"	44:BV:15:THR:HG23	1.98	0.45
25:BA:545:A:C2	25:BA:549:C:N3	2.84	0.45
25:BA:1209:U:O2'	25:BA:1237:A:N1	2.46	0.45
25:BA:2039:U:H2'	25:BA:2040:G:C8	2.52	0.45
32:BH:88:GLY:O	32:BH:89:LYS:O	2.35	0.45
53:B5:15:LYS:HB2	53:B5:23:LYS:HZ3	1.81	0.45
60:CD:119:SER:OG	60:CD:120:LEU:N	2.50	0.45
60:CD:474:LEU:HD21	61:CE:27:ALA:HB3	1.97	0.45
1:AA:1060:U:H2'	1:AA:1061:G:H8	1.81	0.45
4:AD:104:ARG:HG2	4:AD:170:TRP:CZ2	2.52	0.45
7:AG:78:ARG:HG3	7:AG:80:VAL:HG22	1.99	0.45
9:AI:6:TYR:CE2	9:AI:90:TYR:HD1	2.34	0.45
23:AW:18:G:H8	23:AW:18:G:OP1	2.00	0.45
25:BA:2172:U:OP2	25:BA:2172:U:H4'	2.16	0.45
56:CN:26:DG:C4	56:CN:27:DA:N7	2.85	0.45
58:CB:66:HIS:CG	58:CB:68:TYR:HB3	2.52	0.45
59:CC:146:VAL:H	59:CC:146:VAL:HG22	1.59	0.45
1:AA:925:G:C6	1:AA:927:G:N7	2.84	0.45
1:AA:958:A:OP1	19:AS:55:ARG:NH1	2.41	0.45
1:AA:1061:G:H5'	10:AJ:61:ALA:HB2	1.98	0.45
1:AA:1435:G:H2'	1:AA:1436:U:C6	2.52	0.45
5:AE:111:MET:CE	5:AE:125:ALA:HB1	2.47	0.45
25:BA:1149:G:H2'	25:BA:1150:C:C6	2.51	0.45
25:BA:2228:G:H2'	25:BA:2229:U:H6	1.82	0.45
25:BA:2605:PSU:H2'	25:BA:2606:C:C6	2.52	0.45
35:BM:109:LYS:HG2	35:BM:126:ARG:HB2	1.98	0.45
36:BN:17:ASN:O	36:BN:38:ARG:NH1	2.49	0.45
59:CC:1043:ALA:O	59:CC:1046:VAL:HG22	2.17	0.45
59:CC:1212:LEU:HA	59:CC:1212:LEU:HD23	1.66	0.45
1:AA:927:G:C2'	1:AA:928:G:H5'	2.47	0.45
1:AA:1151:A:OP1	10:AJ:44:THR:HG22	2.16	0.45
1:AA:1367:C:H5"	9:AI:116:VAL:HG22	1.98	0.45
10:AJ:37:ARG:HH11	10:AJ:37:ARG:CA	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AV:24:A:H2'	22:AV:25:U:O4'	2.16	0.45
22:AV:51:G:C2	22:AV:52:C:C5	3.04	0.45
25:BA:404:A:H4'	25:BA:405:U:H5"	1.99	0.45
25:BA:677:A:O2'	25:BA:2071:A:H5'	2.17	0.45
26:BB:2:G:H2'	26:BB:3:C:H6	1.80	0.45
34:BL:5:GLN:N	34:BL:21:CYS:O	2.46	0.45
34:BL:38:ILE:HD11	34:BL:112:PHE:HZ	1.81	0.45
42:BT:20:VAL:O	42:BT:23:LEU:HB2	2.17	0.45
59:CC:1058:ARG:HH21	59:CC:1240:ASP:CG	2.20	0.45
9:AI:36:GLU:HA	9:AI:45:ARG:HE	1.82	0.45
25:BA:125:A:OP2	52:B4:19:ARG:NH2	2.41	0.45
25:BA:357:C:H2'	25:BA:358:U:H6	1.82	0.45
25:BA:1406:U:O2'	25:BA:1407:G:H5"	2.17	0.45
25:BA:2299:U:OP1	30:BF:72:LYS:NZ	2.50	0.45
27:BC:76:ALA:HB2	27:BC:96:TYR:CD2	2.51	0.45
35:BM:57:LEU:HD22	53:B5:54:ASP:HB2	1.99	0.45
1:AA:35:G:N2	12:AL:115:SER:OG	2.49	0.45
1:AA:522:C:N3	1:AA:527:G7M:N1	2.53	0.45
2:AB:60:ILE:CG2	2:AB:65:GLY:HA3	2.46	0.45
21:AU:39:GLU:OE2	21:AU:47:ARG:NE	2.33	0.45
27:BC:2:ALA:N	27:BC:20:VAL:O	2.50	0.45
27:BC:120:VAL:HG21	32:BH:91:PHE:CD2	2.52	0.45
30:BF:40:VAL:O	30:BF:42:GLU:N	2.43	0.45
30:BF:40:VAL:C	30:BF:42:GLU:H	2.19	0.45
32:BH:132:PHE:HB2	32:BH:140:ALA:HB3	1.99	0.45
42:BT:95:ARG:HH12	42:BT:97:LEU:HD21	1.81	0.45
43:BU:93:LEU:HD23	43:BU:94:ASP:O	2.15	0.45
44:BV:74:ASN:HB3	44:BV:96:PHE:CD1	2.52	0.45
59:CC:936:ARG:HH22	59:CC:1044:PRO:HA	1.82	0.45
60:CD:213:LYS:O	60:CD:213:LYS:HD3	2.17	0.45
11:AK:110:ILE:O	21:AU:4:ILE:HG23	2.17	0.44
12:AL:54:ARG:NH1	12:AL:64:THR:OG1	2.50	0.44
23:AW:17:C:H2'	23:AW:17(A):U:C6	2.52	0.44
25:BA:151:C:H2'	25:BA:152:A:H8	1.82	0.44
25:BA:1593:A:H2'	25:BA:1594:U:C6	2.52	0.44
35:BM:132:ARG:HG3	35:BM:142:ILE:HD12	1.99	0.44
59:CC:1098:LEU:N	59:CC:1098:LEU:HD12	2.30	0.44
59:CC:1276:TRP:CE2	60:CD:801:VAL:HG21	2.52	0.44
60:CD:265:LEU:O	60:CD:268:LEU:N	2.45	0.44
60:CD:307:LEU:HD23	60:CD:307:LEU:HA	1.77	0.44
60:CD:424:ASN:O	60:CD:424:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:105:ILE:O	5:AE:112:ARG:NH2	2.50	0.44
5:AE:110:ALA:HB1	5:AE:137:VAL:HG23	1.98	0.44
10:AJ:6:ILE:HG12	10:AJ:79:PRO:HG3	2.00	0.44
25:BA:197:A:H4'	25:BA:2069:G7M:OP2	2.17	0.44
25:BA:2081:U:H2'	25:BA:2082:A:C8	2.52	0.44
25:BA:2529:G:H4'	31:BG:175:LYS:HE2	1.99	0.44
28:BD:34:VAL:O	28:BD:93:GLY:HA2	2.17	0.44
52:B4:12:ARG:NH2	52:B4:44:VAL:HG21	2.31	0.44
59:CC:129:LEU:HD23	59:CC:129:LEU:HA	1.68	0.44
59:CC:1257:GLN:NE2	60:CD:345:LYS:HD3	2.32	0.44
60:CD:301:GLU:OE1	60:CD:312:ARG:NE	2.46	0.44
1:AA:459:A:H2'	1:AA:460:A:H8	1.82	0.44
1:AA:575:G:O2'	1:AA:821:G:OP2	2.23	0.44
1:AA:1496:C:H2'	1:AA:1497:G:O4'	2.17	0.44
4:AD:42:GLY:O	4:AD:44:ARG:N	2.45	0.44
14:AN:46:LEU:O	14:AN:50:THR:HG23	2.17	0.44
25:BA:2122:U:H5'	25:BA:2123:G:OP2	2.17	0.44
28:BD:84:LEU:HD22	28:BD:88:GLU:O	2.16	0.44
30:BF:10:ASP:HB2	30:BF:11:GLU:OE1	2.18	0.44
34:BL:108:ARG:HA	34:BL:116:ILE:HG13	1.98	0.44
59:CC:1314:GLN:CB	61:CE:28:ARG:HH22	2.31	0.44
60:CD:120:LEU:HB3	60:CD:121:PRO:CD	2.47	0.44
1:AA:81:A:H2'	1:AA:82:G:H5'	2.00	0.44
25:BA:371:A:H61	25:BA:401:A:H3'	1.82	0.44
25:BA:587:C:C2	35:BM:19:LEU:HD12	2.52	0.44
25:BA:593:U:H2'	25:BA:594:U:C6	2.52	0.44
25:BA:908:C:O2'	36:BN:70:ASP:OD2	2.31	0.44
30:BF:136:ILE:HA	30:BF:141:ILE:HD11	1.99	0.44
36:BN:36:VAL:HG22	45:BW:82:TYR:HB2	1.98	0.44
44:BV:47:LYS:HD2	44:BV:48:PRO:HD2	2.00	0.44
59:CC:38:PHE:CZ	59:CC:49:LEU:HD21	2.52	0.44
60:CD:317:THR:OG1	60:CD:322:ARG:O	2.20	0.44
60:CD:891:ASP:OD1	60:CD:1286:LYS:NZ	2.49	0.44
1:AA:1137:C:H1'	1:AA:1138:G:N2	2.33	0.44
1:AA:1228:C:OP2	13:AM:110:LYS:NZ	2.44	0.44
10:AJ:44:THR:HA	10:AJ:69:THR:O	2.17	0.44
14:AN:46:LEU:HD22	19:AS:13:LEU:HB2	1.98	0.44
15:AO:26:GLU:HG2	15:AO:81:LEU:HD22	1.98	0.44
25:BA:57:C:H2'	25:BA:58:G:O4'	2.18	0.44
25:BA:711:G:N2	25:BA:720:U:O2	2.38	0.44
25:BA:839:U:H2'	25:BA:840:C:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1027:A:C2	25:BA:2488:G:H5'	2.52	0.44
25:BA:2314:A:H1'	30:BF:155:THR:HG21	1.98	0.44
48:BZ:21:LEU:HD11	48:BZ:49:ASP:HB3	1.99	0.44
57:CT:4:DT:C2	57:CT:5:DG:N7	2.86	0.44
1:AA:90:C:C2	1:AA:91:U:C5	3.06	0.44
1:AA:413:G:H21	1:AA:428:G:H1'	1.81	0.44
9:AI:27:LYS:HB2	9:AI:27:LYS:HE3	1.60	0.44
17:AQ:17:MET:HG3	17:AQ:20:SER:HB2	2.00	0.44
25:BA:68:G:N2	25:BA:74:A:OP2	2.51	0.44
25:BA:615:U:H6	25:BA:615:U:H5'	1.82	0.44
25:BA:635:C:OP2	35:BM:126:ARG:NH2	2.50	0.44
25:BA:1596:A:O2'	25:BA:1597:A:C5'	2.65	0.44
25:BA:2121:G:H8	25:BA:2121:G:O5'	2.00	0.44
31:BG:2:SER:HA	31:BG:62:TRP:CE3	2.53	0.44
31:BG:148:LEU:HA	31:BG:151:TYR:HD2	1.82	0.44
39:BQ:34:GLU:OE2	39:BQ:39:ARG:NE	2.36	0.44
56:CN:28:DA:C4	56:CN:29:DG:C5	3.06	0.44
59:CC:1076:ILE:O	59:CC:1076:ILE:HG13	2.15	0.44
9:AI:21:ILE:HD13	9:AI:63:LEU:HG	1.99	0.44
12:AL:42:PRO:HB2	12:AL:46:ASN:HB2	1.99	0.44
25:BA:2052:A:H4'	28:BD:148:GLN:O	2.18	0.44
25:BA:2228:G:H2'	25:BA:2229:U:C6	2.52	0.44
58:CB:107:ILE:HD11	58:CB:136:GLU:HA	1.99	0.44
59:CC:210:LEU:HD23	59:CC:210:LEU:HA	1.60	0.44
59:CC:680:LEU:HD23	59:CC:680:LEU:C	2.38	0.44
60:CD:264:ASP:OD1	60:CD:264:ASP:N	2.51	0.44
60:CD:952:VAL:HG13	60:CD:1014:GLY:H	1.81	0.44
1:AA:383:A:C5	1:AA:384:G:H1'	2.53	0.44
5:AE:72:ILE:HD12	5:AE:72:ILE:O	2.18	0.44
25:BA:1744:A:H3'	25:BA:1745:A:C8	2.53	0.44
25:BA:2627:G:O2'	25:BA:2781:A:N1	2.36	0.44
27:BC:231:PRO:HB2	27:BC:245:VAL:HG21	1.99	0.44
55:B7:11:GLU:HA	55:B7:25:ARG:HA	2.00	0.44
59:CC:493:ILE:C	59:CC:493:ILE:HD12	2.39	0.44
1:AA:212:G:C2	1:AA:213:G:C8	3.05	0.44
3:AC:45:LYS:HB2	3:AC:45:LYS:HE3	1.75	0.44
25:BA:796:C:H2'	25:BA:797:G:C8	2.53	0.44
25:BA:2314:A:O2'	25:BA:2315:G:H5'	2.18	0.44
28:BD:33:ARG:NH2	28:BD:74:GLU:O	2.51	0.44
37:BO:63:ARG:HH21	37:BO:63:ARG:CG	2.27	0.44
58:CB:58:GLU:OE2	58:CB:170:ARG:NE	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:CC:28:LEU:HA	59:CC:28:LEU:HD23	1.54	0.44
59:CC:494:ASN:HD22	59:CC:494:ASN:C	2.08	0.44
1:AA:684:U:O2'	11:AK:40:ASN:HB3	2.16	0.43
14:AN:24:ARG:NH1	14:AN:55:SER:OG	2.51	0.43
25:BA:1212:G:H1'	25:BA:1237:A:N6	2.32	0.43
25:BA:1542:U:H2'	25:BA:1543:G:O4'	2.18	0.43
25:BA:2146:C:H4'	25:BA:2147:A:C8	2.53	0.43
25:BA:2820:A:N1	28:BD:197:THR:OG1	2.50	0.43
31:BG:9:VAL:O	31:BG:49:THR:HA	2.18	0.43
55:B7:69:SER:O	55:B7:70:LYS:O	2.35	0.43
58:CA:213:PRO:HA	58:CA:216:ALA:HB3	2.00	0.43
60:CD:149:GLY:HA2	60:CD:176:PHE:HB2	1.98	0.43
60:CD:576:ARG:HD3	60:CD:593:ASN:HA	2.00	0.43
1:AA:428:G:OP2	4:AD:7:PRO:HG2	2.17	0.43
1:AA:1031:C:H4'	1:AA:1032:G:C2	2.53	0.43
5:AE:15:LEU:HB2	5:AE:37:THR:HG22	1.99	0.43
6:AF:4:TYR:CE1	6:AF:91:ARG:HG2	2.54	0.43
6:AF:38:ARG:O	6:AF:38:ARG:HG3	2.17	0.43
9:AI:55:VAL:O	9:AI:57:MET:N	2.52	0.43
25:BA:138:U:H6	25:BA:140:C:N3	2.16	0.43
25:BA:1328:A:H2'	25:BA:1330:C:C5	2.53	0.43
27:BC:273:LYS:HB3	27:BC:273:LYS:HE2	1.89	0.43
31:BG:107:LEU:HD13	31:BG:152:ARG:HB2	2.00	0.43
44:BV:74:ASN:OD1	44:BV:77:THR:OG1	2.35	0.43
45:BW:26:PHE:HZ	45:BW:47:VAL:HG11	1.83	0.43
56:CN:30:DA:C6	56:CN:31:DG:C6	3.07	0.43
60:CD:357:VAL:O	60:CD:357:VAL:HG13	2.18	0.43
1:AA:699:C:C2'	1:AA:700:G:H5'	2.48	0.43
4:AD:50:ASP:O	4:AD:53:VAL:HG22	2.18	0.43
7:AG:30:LEU:HD22	7:AG:43:VAL:HG23	1.99	0.43
25:BA:2120:G:O2'	25:BA:2121:G:O5'	2.27	0.43
33:BK:40:HIS:CE1	33:BK:41:LYS:HG2	2.53	0.43
38:BP:53:THR:O	38:BP:59:ALA:HB2	2.18	0.43
59:CC:127:ILE:HG13	59:CC:127:ILE:O	2.18	0.43
60:CD:513:MET:HG3	60:CD:544:LEU:HD21	1.98	0.43
1:AA:604:G:H2'	1:AA:605:U:O4'	2.19	0.43
1:AA:978:A:C5	1:AA:1319:A:C2	3.06	0.43
11:AK:85:MET:HG2	11:AK:111:THR:OG1	2.18	0.43
25:BA:892:A:H2'	25:BA:893:C:C6	2.53	0.43
25:BA:1413:A:H2'	25:BA:1414:C:O4'	2.17	0.43
25:BA:1802:A:H2'	25:BA:1803:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2783:U:H2'	25:BA:2784:U:C6	2.54	0.43
25:BA:2803:G:H2'	25:BA:2804:U:C6	2.52	0.43
25:BA:2845:U:H5"	39:BQ:52:ASN:O	2.18	0.43
57:CT:10:DT:H2"	57:CT:11:DC:C6	2.53	0.43
57:CT:19:DG:C6	57:CT:20:DC:N4	2.87	0.43
59:CC:569:ILE:O	59:CC:571:LEU:N	2.51	0.43
59:CC:1238:LEU:N	59:CC:1238:LEU:CD2	2.81	0.43
60:CD:601:ILE:HG21	60:CD:601:ILE:HD13	1.72	0.43
1:AA:197:A:H4'	1:AA:198:G:O5'	2.17	0.43
6:AF:4:TYR:CD2	6:AF:71:ILE:HG12	2.54	0.43
10:AJ:41:PRO:HA	10:AJ:72:ARG:HD3	2.01	0.43
23:AW:76:A:H2'	25:BA:2602:A:N6	2.33	0.43
25:BA:65:U:O2'	25:BA:456:C:N3	2.45	0.43
25:BA:1077:A:H2'	25:BA:1078:U:O4'	2.19	0.43
33:BK:36:LEU:O	33:BK:51:GLY:HA3	2.18	0.43
37:BO:114:GLU:OE2	37:BO:118:ARG:NH2	2.51	0.43
57:CT:5:DG:H2'	57:CT:6:DA:C8	2.53	0.43
59:CC:699:LEU:HD23	59:CC:699:LEU:HA	1.61	0.43
59:CC:1096:ILE:HD13	59:CC:1096:ILE:HG21	1.65	0.43
60:CD:108:ALA:HB3	60:CD:279:LEU:HD23	2.00	0.43
60:CD:355:ILE:HG21	60:CD:355:ILE:HD13	1.78	0.43
60:CD:1143:ASP:C	60:CD:1143:ASP:OD1	2.57	0.43
1:AA:213:G:C8	1:AA:214:C:C5	3.06	0.43
1:AA:562:U:O2	12:AL:13:ALA:N	2.51	0.43
1:AA:957:U:O2	1:AA:959:A:H8	2.02	0.43
1:AA:1226:C:H4'	1:AA:1227:A:OP1	2.18	0.43
1:AA:1396:A:H4'	1:AA:1397:C:H5"	1.99	0.43
1:AA:1486:G:H2'	1:AA:1487:G:O4'	2.19	0.43
5:AE:152:MET:O	5:AE:156:LYS:HG3	2.19	0.43
6:AF:53:LYS:HB3	6:AF:53:LYS:HE2	1.71	0.43
9:AI:118:LEU:CD2	9:AI:124:ARG:HG2	2.49	0.43
11:AK:111:THR:HG22	21:AU:3:VAL:HG13	2.00	0.43
23:AW:55:PSU:O5'	23:AW:55:PSU:H6	2.00	0.43
24:AX:25:C:H2'	24:AX:26:A:O4'	2.18	0.43
25:BA:742:A:H2'	25:BA:743:A:C8	2.53	0.43
25:BA:1078:U:H5"	25:BA:1079:C:OP1	2.18	0.43
25:BA:1824:G:O3'	27:BC:247:PRO:HD3	2.19	0.43
25:BA:2108:A:H8	25:BA:2108:A:O5'	2.01	0.43
25:BA:2591:C:H2'	25:BA:2592:G:H8	1.83	0.43
32:BH:86:ASP:C	32:BH:88:GLY:H	2.21	0.43
39:BQ:22:PRO:HD3	39:BQ:50:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BT:95:ARG:HG2	42:BT:95:ARG:HH11	1.84	0.43
45:BW:80:HIS:ND1	45:BW:83:LYS:HB2	2.33	0.43
56:CN:26:DG:C4	56:CN:27:DA:C5	3.07	0.43
56:CN:36:DA:H2"	56:CN:37:DG:C8	2.54	0.43
59:CC:596:ASP:OD1	59:CC:597:GLY:N	2.38	0.43
60:CD:160:LEU:HD23	60:CD:160:LEU:N	2.34	0.43
1:AA:1236:A:H2'	1:AA:1237:C:C6	2.54	0.43
6:AF:32:ALA:HB1	6:AF:70:VAL:HG21	2.00	0.43
15:AO:70:LEU:HD12	15:AO:70:LEU:HA	1.71	0.43
25:BA:813:U:H2'	25:BA:814:C:H6	1.82	0.43
25:BA:1177:G:O2'	25:BA:1178:C:C6	2.71	0.43
25:BA:2798:U:H1'	25:BA:2799:G:C6	2.54	0.43
25:BA:2849:U:H4'	25:BA:2868:A:C2	2.54	0.43
27:BC:261:LYS:HA	27:BC:264:ASP:OD2	2.19	0.43
40:BR:9:ILE:HD13	40:BR:9:ILE:HA	1.87	0.43
56:CN:29:DG:H2"	56:CN:30:DA:O5'	2.18	0.43
59:CC:616:ILE:HA	59:CC:652:TYR:O	2.17	0.43
1:AA:843:U:O4	1:AA:844:G:N1	2.51	0.43
1:AA:970:C:N4	9:AI:130:ARG:O	2.51	0.43
1:AA:1225:A:H2'	1:AA:1226:C:C5	2.54	0.43
1:AA:1385:G:H2'	1:AA:1386:G:O4'	2.19	0.43
3:AC:111:LEU:HD22	3:AC:146:ALA:HB2	2.00	0.43
6:AF:18:VAL:HG21	6:AF:58:HIS:CD2	2.54	0.43
9:AI:41:ARG:HH21	9:AI:41:ARG:CG	2.31	0.43
25:BA:729:G:OP1	27:BC:10:SER:OG	2.25	0.43
33:BK:17:VAL:HG23	33:BK:137:PRO:HB2	2.00	0.43
33:BK:76:HIS:CE1	33:BK:85:LYS:HB2	2.53	0.43
36:BN:16:ARG:HD3	36:BN:16:ARG:HA	1.74	0.43
59:CC:549:ASP:OD1	59:CC:550:VAL:N	2.52	0.43
59:CC:1182:ILE:HD13	59:CC:1182:ILE:HG21	1.70	0.43
59:CC:1340:GLU:CD	59:CC:1341:ASP:H	2.21	0.43
60:CD:139:LEU:HD23	60:CD:139:LEU:HA	1.68	0.43
60:CD:265:LEU:HD23	60:CD:265:LEU:HA	1.67	0.43
60:CD:340:GLN:HG3	60:CD:341:ASN:OD1	2.18	0.43
60:CD:500:ILE:O	60:CD:500:ILE:HG22	2.18	0.43
1:AA:80:C:N4	1:AA:81:A:H62	2.16	0.43
1:AA:728:A:H2'	1:AA:729:A:C8	2.54	0.43
1:AA:1035:A:N3	1:AA:1036:A:C8	2.87	0.43
4:AD:8:LYS:HB3	4:AD:21:LEU:CB	2.49	0.43
7:AG:78:ARG:HE	7:AG:78:ARG:HB2	1.59	0.43
13:AM:44:LYS:O	13:AM:48:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:468:G:H5"	29:BE:55:SER:HB3	2.01	0.43
25:BA:1105:U:H2'	25:BA:1106:G:C8	2.52	0.43
25:BA:1263:U:O2'	50:B2:8:PRO:HD2	2.18	0.43
25:BA:1917:PSU:H2'	25:BA:1918:A:O4'	2.19	0.43
25:BA:2117:A:O2'	25:BA:2118:U:H4'	2.19	0.43
25:BA:2346:A:H4'	25:BA:2347:C:OP2	2.18	0.43
27:BC:105:LEU:HD23	27:BC:105:LEU:HA	1.89	0.43
30:BF:72:LYS:HE2	30:BF:72:LYS:HB3	1.75	0.43
38:BP:57:ALA:O	38:BP:61:GLN:HG2	2.19	0.43
43:BU:26:LYS:HB3	43:BU:26:LYS:HE2	1.73	0.43
56:CN:37:DG:H2"	56:CN:38:DA:OP2	2.19	0.43
58:CB:66:HIS:O	58:CB:66:HIS:ND1	2.44	0.43
59:CC:204:LEU:HD21	59:CC:369:MET:SD	2.59	0.43
59:CC:528:ARG:HH11	59:CC:528:ARG:HD2	1.63	0.43
59:CC:1336:ASN:HD22	59:CC:1336:ASN:C	2.22	0.43
1:AA:156:C:H2'	1:AA:157:U:O4'	2.19	0.43
1:AA:590:U:H2'	1:AA:591:U:C6	2.53	0.43
1:AA:1314:C:H2'	1:AA:1315:U:C6	2.54	0.43
1:AA:1424:U:H2'	1:AA:1425:U:O4'	2.19	0.43
2:AB:126:PHE:HE2	2:AB:129:LEU:HB3	1.84	0.43
5:AE:81:LEU:HD11	5:AE:96:MET:HG3	2.01	0.43
6:AF:37:HIS:O	6:AF:97:THR:HG23	2.19	0.43
10:AJ:56:HIS:O	10:AJ:57:VAL:O	2.37	0.43
25:BA:2081:U:H2'	25:BA:2082:A:H8	1.84	0.43
28:BD:37:VAL:HG22	28:BD:48:ILE:HG22	2.00	0.43
38:BP:3:LYS:HB3	38:BP:3:LYS:HE3	1.78	0.43
58:CB:28:LEU:HD13	58:CB:28:LEU:HA	1.75	0.43
59:CC:316:GLU:H	59:CC:316:GLU:CD	2.22	0.43
59:CC:836:LEU:HA	59:CC:836:LEU:HD23	1.83	0.43
1:AA:84:U:H2'	1:AA:86:G:N2	2.34	0.42
1:AA:147:G:H2'	1:AA:148:G:C8	2.54	0.42
2:AB:60:ILE:O	2:AB:63:ARG:HG3	2.19	0.42
25:BA:2019:A:H4'	40:BR:34:VAL:HG21	2.00	0.42
28:BD:1:MET:SD	28:BD:205:PRO:HG2	2.59	0.42
30:BF:8:TYR:OH	30:BF:29:PRO:O	2.25	0.42
32:BH:114:GLU:HG2	32:BH:134:VAL:HG12	2.00	0.42
52:B4:25:LYS:HE3	52:B4:25:LYS:HB3	1.85	0.42
57:CT:6:DA:C2	57:CT:7:DA:C5	3.07	0.42
59:CC:196:VAL:HG21	59:CC:209:ILE:HD11	2.00	0.42
1:AA:202:G:O2'	1:AA:468:A:H8	2.01	0.42
1:AA:1175:G:HO2'	1:AA:1176:A:P	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1492:A:OP1	12:AL:44:LYS:HB2	2.19	0.42
14:AN:27:LEU:HD23	14:AN:27:LEU:HA	1.91	0.42
25:BA:1026:G:OP1	25:BA:1134:A:O2'	2.28	0.42
25:BA:2312:U:H5'	30:BF:85:ILE:CD1	2.44	0.42
31:BG:11:VAL:N	31:BG:48:ASN:O	2.45	0.42
40:BR:69:ALA:HB1	40:BR:74:ILE:HG23	2.02	0.42
42:BT:28:LYS:HB3	42:BT:28:LYS:HE3	1.81	0.42
43:BU:10:VAL:HG12	43:BU:11:LEU:HD23	2.01	0.42
59:CC:1211:ARG:NH1	59:CC:1220:GLN:OE1	2.52	0.42
60:CD:425:ARG:HE	60:CD:464:ASP:CG	2.20	0.42
60:CD:442:ILE:HD12	60:CD:442:ILE:HG23	1.64	0.42
60:CD:541:LEU:HD23	60:CD:541:LEU:HA	1.84	0.42
1:AA:384:G:H2'	1:AA:385:C:C6	2.54	0.42
10:AJ:5:ARG:HB2	10:AJ:77:VAL:HA	2.01	0.42
13:AM:40:ALA:HB3	13:AM:43:VAL:HG13	2.01	0.42
15:AO:67:LEU:HD22	15:AO:78:TYR:CE1	2.55	0.42
24:AX:34:G:H2'	24:AX:35:A:C8	2.54	0.42
26:BB:48:U:P	38:BP:30:ARG:HH22	2.42	0.42
32:BH:66:ASN:C	32:BH:66:ASN:HD22	2.21	0.42
38:BP:57:ALA:O	38:BP:60:GLU:HG2	2.19	0.42
58:CA:82:LEU:HA	58:CA:82:LEU:HD23	1.65	0.42
60:CD:175:GLU:CD	60:CD:175:GLU:N	2.72	0.42
60:CD:1332:LEU:HA	60:CD:1332:LEU:HD12	1.74	0.42
6:AF:47:LEU:HD21	6:AF:57:ALA:HB3	2.00	0.42
25:BA:1494:A:H2'	25:BA:1495:A:H8	1.81	0.42
25:BA:2315:G:HO2'	25:BA:2316:G:H8	1.64	0.42
30:BF:148:ARG:HD2	30:BF:150:ARG:NH1	2.34	0.42
32:BH:84:ALA:HB2	32:BH:90:LEU:CD1	2.49	0.42
35:BM:81:ASP:HB3	35:BM:100:ILE:HD13	2.00	0.42
38:BP:18:LEU:HD23	38:BP:18:LEU:HA	1.70	0.42
56:CN:27:DA:C5	56:CN:28:DA:N7	2.88	0.42
57:CT:20:DC:O2	57:CT:21:DG:C8	2.73	0.42
59:CC:473:ARG:HH11	59:CC:473:ARG:HG3	1.83	0.42
59:CC:962:GLU:O	59:CC:966:ILE:HD13	2.20	0.42
60:CD:72:CYS:HB2	60:CD:87:LYS:HD3	2.02	0.42
60:CD:482:ALA:O	60:CD:488:ASN:ND2	2.50	0.42
60:CD:1350:ASN:ND2	60:CD:1358:PRO:HD3	2.34	0.42
1:AA:868:C:H2'	1:AA:869:G:O4'	2.19	0.42
1:AA:1320:C:O2	19:AS:36:ARG:NH1	2.51	0.42
23:AW:20:H2U:H61	23:AW:20:H2U:H5'	2.02	0.42
25:BA:565:C:H2'	25:BA:566:U:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:703:U:H2'	25:BA:704:G:O4'	2.20	0.42
57:CT:2:DT:H2"	57:CT:3:DC:H5	1.85	0.42
59:CC:1014:LEU:HD12	59:CC:1017:GLN:HB3	2.00	0.42
59:CC:1141:LEU:HD12	59:CC:1141:LEU:HA	1.84	0.42
60:CD:361:LEU:HA	60:CD:361:LEU:HD23	1.79	0.42
60:CD:755:ILE:HG22	60:CD:757:THR:H	1.85	0.42
60:CD:826:ILE:HG23	60:CD:831:VAL:HG12	2.02	0.42
1:AA:979:C:O2	14:AN:59:ARG:HD3	2.19	0.42
1:AA:1006:G:H2'	1:AA:1007:U:H6	1.85	0.42
9:AI:80:ARG:O	9:AI:84:THR:HG23	2.20	0.42
10:AJ:19:ASP:O	10:AJ:22:THR:HG22	2.19	0.42
13:AM:107:ARG:HH12	13:AM:112:PRO:C	2.23	0.42
24:AX:49:C:H2'	24:AX:50:U:H6	1.84	0.42
25:BA:848:C:H2'	25:BA:849:A:H8	1.85	0.42
25:BA:1980:G:O2'	25:BA:1982:U:OP2	2.32	0.42
27:BC:142:HIS:CG	27:BC:195:VAL:HG23	2.55	0.42
28:BD:24:VAL:HG12	28:BD:178:VAL:HG21	2.02	0.42
30:BF:141:ILE:HD12	30:BF:141:ILE:O	2.20	0.42
31:BG:23:VAL:HA	31:BG:36:THR:HA	2.02	0.42
40:BR:11:ARG:HG2	40:BR:11:ARG:HH11	1.84	0.42
57:CT:17:DG:C4	57:CT:18:DC:C6	3.07	0.42
59:CC:84:GLU:OE2	59:CC:1032:LYS:NZ	2.48	0.42
59:CC:1105:SER:HB2	60:CD:731:ARG:HB3	2.00	0.42
60:CD:213:LYS:HZ3	60:CD:216:LYS:HG3	1.84	0.42
60:CD:1342:ASP:OD1	60:CD:1342:ASP:C	2.58	0.42
1:AA:526:C:P	12:AL:88:LYS:HE2	2.60	0.42
1:AA:1123:U:C2'	1:AA:1124:G:H5'	2.49	0.42
2:AB:9:MET:O	2:AB:14:VAL:HG22	2.20	0.42
2:AB:161:LEU:HD22	2:AB:176:ALA:HB2	2.02	0.42
11:AK:18:ASP:HA	11:AK:81:ASN:O	2.19	0.42
25:BA:476:G:H4'	25:BA:502:A:N1	2.34	0.42
25:BA:1199:U:H1'	40:BR:4:VAL:HG22	2.02	0.42
25:BA:1548:A:H2'	25:BA:1549:A:C8	2.54	0.42
25:BA:1769:U:O2'	25:BA:1958:C:OP1	2.37	0.42
25:BA:2123:G:N1	25:BA:2176:A:N6	2.68	0.42
25:BA:2225:A:H4'	25:BA:2226:C:O5'	2.19	0.42
25:BA:2359:C:O2'	53:B5:54:ASP:OD2	2.34	0.42
37:BO:101:GLY:O	37:BO:109:PRO:HA	2.20	0.42
59:CC:196:VAL:HG22	59:CC:197:ARG:N	2.34	0.42
59:CC:571:LEU:HD23	59:CC:571:LEU:HA	1.47	0.42
59:CC:817:LEU:HA	59:CC:817:LEU:HD12	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:263:A:P	20:AT:74:ARG:HH12	2.43	0.42
1:AA:1441:A:H62	1:AA:1461:G:H21	1.68	0.42
7:AG:2:PRO:CG	7:AG:5:ARG:HB2	2.50	0.42
7:AG:12:ILE:O	7:AG:12:ILE:HG13	2.20	0.42
19:AS:51:VAL:HG21	19:AS:71:LEU:HB3	2.01	0.42
22:AV:51:G:N2	57:CT:18:DC:O2	2.52	0.42
25:BA:64:A:H2'	25:BA:65:U:C6	2.55	0.42
25:BA:1563:U:H2'	25:BA:1564:C:C6	2.55	0.42
25:BA:1599:U:H2'	25:BA:1600:C:C6	2.55	0.42
30:BF:148:ARG:HD2	30:BF:150:ARG:HH12	1.85	0.42
41:BS:44:GLY:O	41:BS:45:GLU:HG3	2.20	0.42
41:BS:77:PHE:HD1	41:BS:84:ARG:HB3	1.83	0.42
42:BT:36:LEU:HB3	42:BT:48:LYS:HB2	2.02	0.42
43:BU:50:LEU:HD23	48:BZ:26:PHE:CZ	2.55	0.42
58:CA:180:VAL:HG12	58:CA:207:THR:HG22	2.02	0.42
59:CC:45:GLY:O	59:CC:51:ALA:HB2	2.19	0.42
59:CC:131:THR:HG22	59:CC:132:ASP:N	2.34	0.42
60:CD:425:ARG:NH2	60:CD:464:ASP:OD2	2.41	0.42
60:CD:1175:LEU:HB2	60:CD:1190:ILE:HD12	2.02	0.42
61:CE:15:ASN:O	61:CE:17:PHE:N	2.48	0.42
1:AA:235:C:H2'	1:AA:236:A:C8	2.55	0.42
1:AA:502:A:H2'	1:AA:503:C:O4'	2.20	0.42
1:AA:532:A:N6	1:AA:1206:G:O2'	2.51	0.42
2:AB:43:LEU:HA	2:AB:46:THR:HB	2.02	0.42
7:AG:23:LEU:O	7:AG:27:VAL:HG23	2.20	0.42
11:AK:46:THR:O	11:AK:50:SER:OG	2.32	0.42
25:BA:277:G:H2'	25:BA:277:G:N3	2.35	0.42
25:BA:608:A:H2'	25:BA:609:A:C8	2.55	0.42
25:BA:1693:U:O2'	27:BC:14:ARG:NH2	2.53	0.42
25:BA:2805:C:H2'	25:BA:2806:C:O4'	2.20	0.42
57:CT:10:DT:H2"	57:CT:11:DC:C5	2.54	0.42
59:CC:1339:LEU:HD22	60:CD:17:PHE:CG	2.55	0.42
60:CD:424:ASN:ND2	60:CD:424:ASN:C	2.73	0.42
60:CD:548:VAL:HG22	60:CD:549:LYS:N	2.34	0.42
1:AA:1103:C:O2	2:AB:106:THR:HG21	2.20	0.42
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.60	0.42
3:AC:42:TYR:CZ	3:AC:90:VAL:HG11	2.54	0.42
6:AF:51:ILE:HD11	18:AR:66:SER:OG	2.20	0.42
7:AG:12:ILE:HD13	7:AG:25:LYS:HE3	2.02	0.42
12:AL:87:VAL:HG12	12:AL:89:D2T:OD2	2.20	0.42
13:AM:31:LYS:NZ	13:AM:41:GLU:OE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AO:28:GLN:OE1	15:AO:66:LEU:HD11	2.20	0.42
16:AP:67:ILE:HG22	16:AP:68:SER:O	2.20	0.42
22:AV:47:G:C6	22:AV:48:C:C4	3.07	0.42
24:AX:37:MIA:H163	24:AX:37:MIA:H122	1.72	0.42
25:BA:3:U:H2'	25:BA:4:U:C6	2.54	0.42
25:BA:39:G:H2'	25:BA:40:U:C6	2.55	0.42
25:BA:1529:G:H2'	25:BA:1530:G:C8	2.55	0.42
26:BB:49:C:OP1	38:BP:101:GLY:HA3	2.19	0.42
31:BG:105:LEU:HD13	31:BG:107:LEU:HD11	2.01	0.42
32:BH:73:ASN:ND2	32:BH:141:LYS:O	2.47	0.42
35:BM:9:ALA:O	35:BM:12:SER:OG	2.29	0.42
36:BN:36:VAL:HG13	45:BW:82:TYR:CD2	2.55	0.42
40:BR:65:ILE:CD1	40:BR:92:ARG:HB2	2.49	0.42
43:BU:4:GLU:CD	48:BZ:19:LEU:HD11	2.40	0.42
57:CT:20:DC:C2	57:CT:21:DG:N7	2.88	0.42
58:CB:154:PRO:C	58:CB:156:SER:H	2.23	0.42
59:CC:1251:TYR:CE1	59:CC:1301:ARG:NH1	2.88	0.42
60:CD:641:ILE:HA	60:CD:641:ILE:HD12	1.70	0.42
1:AA:1:A:H2'	1:AA:2:A:C8	2.55	0.41
1:AA:522:C:OP2	12:AL:66:TYR:OH	2.31	0.41
1:AA:911:U:OP1	12:AL:92:GLY:HA2	2.20	0.41
3:AC:178:LEU:HD23	3:AC:178:LEU:HA	1.73	0.41
20:AT:10:ARG:HD3	20:AT:10:ARG:HA	1.86	0.41
25:BA:1175:A:N7	25:BA:1176:U:O2'	2.47	0.41
25:BA:2012:G:P	42:BT:11:ARG:HH22	2.40	0.41
25:BA:2151:U:H2'	25:BA:2152:G:H8	1.85	0.41
58:CA:205:MET:SD	58:CA:213:PRO:HG3	2.60	0.41
60:CD:1172:LYS:HE3	60:CD:1191:PRO:HA	2.01	0.41
1:AA:33:A:H2'	1:AA:34:C:C6	2.55	0.41
1:AA:1100:C:OP2	2:AB:95:ARG:HD3	2.21	0.41
1:AA:1140:C:HO2'	1:AA:1141:C:C5'	2.33	0.41
3:AC:175:LEU:HA	3:AC:175:LEU:HD23	1.61	0.41
9:AI:15:SER:HB2	9:AI:78:ALA:HB2	2.02	0.41
25:BA:14:A:H2'	50:B2:18:SER:OG	2.20	0.41
25:BA:891:G:C2	25:BA:892:A:C8	3.08	0.41
25:BA:1656:C:H2'	25:BA:1657:U:H6	1.86	0.41
25:BA:2395:C:H2'	25:BA:2396:G:O4'	2.20	0.41
32:BH:30:LEU:HB3	32:BH:36:ALA:HB3	2.02	0.41
1:AA:845:A:H5"	1:AA:846:G:H8	1.85	0.41
1:AA:956:U:H2'	1:AA:957:U:O4'	2.20	0.41
3:AC:151:VAL:HG22	3:AC:200:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:99:ASP:OD1	4:AD:100:ASN:N	2.53	0.41
15:AO:32:LEU:HD23	15:AO:32:LEU:HA	1.93	0.41
16:AP:34:GLU:OE1	16:AP:60:TRP:NE1	2.29	0.41
29:BE:147:LEU:HD11	29:BE:170:ARG:HG3	2.01	0.41
30:BF:91:LEU:C	30:BF:96:MET:HB2	2.40	0.41
53:B5:15:LYS:HB2	53:B5:23:LYS:NZ	2.36	0.41
55:B7:37:CYS:O	55:B7:41:HIS:HB2	2.20	0.41
58:CA:11:PRO:HB3	58:CA:31:LEU:HD21	2.02	0.41
60:CD:871:LEU:O	60:CD:874:GLU:HB3	2.21	0.41
60:CD:1310:THR:O	60:CD:1310:THR:HG22	2.20	0.41
1:AA:61:G:H2'	1:AA:62:U:O4'	2.21	0.41
1:AA:1384:C:H2'	1:AA:1385:G:C8	2.56	0.41
12:AL:102:LEU:HD13	12:AL:102:LEU:H	1.86	0.41
25:BA:61:C:C4	25:BA:62:U:H5	2.38	0.41
25:BA:364:C:H2'	25:BA:365:U:C6	2.56	0.41
25:BA:1223:G:OP2	41:BS:90:ARG:NH1	2.45	0.41
25:BA:2032:G:C8	28:BD:150:MEQ:HE3	2.56	0.41
25:BA:2171:A:H4'	25:BA:2172:U:OP1	2.20	0.41
25:BA:2183:A:H2'	25:BA:2184:A:O4'	2.20	0.41
27:BC:260:ASN:HD22	27:BC:260:ASN:HA	1.73	0.41
33:BK:117:ALA:O	33:BK:120:ARG:HB2	2.21	0.41
38:BP:27:VAL:HG21	38:BP:40:ILE:HD12	2.03	0.41
40:BR:94:ILE:HG21	41:BS:4:VAL:HG11	2.01	0.41
51:B3:6:ARG:CG	51:B3:24:THR:HB	2.47	0.41
56:CN:27:DA:H1'	56:CN:28:DA:H5'	2.01	0.41
59:CC:668:ILE:HD13	59:CC:668:ILE:HG21	1.69	0.41
60:CD:558:ASP:OD1	60:CD:561:GLY:N	2.48	0.41
1:AA:492:C:H2'	1:AA:493:A:C8	2.56	0.41
1:AA:1086:U:H5	1:AA:1099:G:H22	1.67	0.41
1:AA:1141:C:HO2'	1:AA:1142:G:P	2.44	0.41
9:AI:35:LEU:HD11	9:AI:48:VAL:HG11	2.02	0.41
12:AL:123:LYS:HB2	12:AL:123:LYS:HE2	1.76	0.41
20:AT:85:LYS:HE3	20:AT:85:LYS:HB2	1.88	0.41
25:BA:358:U:H2'	25:BA:359:G:C8	2.55	0.41
25:BA:2251:OMG:HM23	25:BA:2251:OMG:H1'	1.69	0.41
25:BA:2405:G:O2'	25:BA:2411:A:N6	2.54	0.41
25:BA:2850:A:N7	25:BA:2868:A:O2'	2.43	0.41
30:BF:94:GLU:HG3	30:BF:95:ARG:N	2.36	0.41
32:BH:115:VAL:HG22	32:BH:132:PHE:CE2	2.55	0.41
55:B7:44:PHE:CD1	55:B7:45:THR:HG23	2.55	0.41
57:CT:4:DT:H2"	57:CT:5:DG:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:CA:102:LEU:HD23	58:CA:102:LEU:C	2.41	0.41
58:CB:66:HIS:CE1	58:CB:68:TYR:HD1	2.39	0.41
59:CC:753:LEU:HA	59:CC:753:LEU:HD23	1.75	0.41
59:CC:1251:TYR:CE1	59:CC:1301:ARG:CZ	3.03	0.41
59:CC:1268:GLN:OE1	60:CD:352:ARG:NH1	2.53	0.41
60:CD:416:ILE:O	60:CD:418:GLU:N	2.53	0.41
60:CD:770:LEU:HD13	60:CD:770:LEU:HA	1.70	0.41
1:AA:90:C:O2'	1:AA:91:U:H5'	2.20	0.41
1:AA:626:G:O3'	16:AP:51:ARG:NH2	2.53	0.41
1:AA:1006:G:C4	1:AA:1007:U:C6	3.09	0.41
1:AA:1140:C:O2'	1:AA:1141:C:O5'	2.36	0.41
1:AA:1512:U:H2'	1:AA:1513:A:C8	2.56	0.41
4:AD:14:ARG:HG3	4:AD:56:ARG:NH2	2.36	0.41
4:AD:97:ARG:O	4:AD:101:VAL:HG13	2.20	0.41
4:AD:153:SER:HA	4:AD:156:LYS:HG2	2.02	0.41
10:AJ:53:ILE:HG12	10:AJ:62:ARG:HA	2.02	0.41
23:AW:17:C:H2'	23:AW:17(A):U:H6	1.85	0.41
25:BA:2557:G:H2'	25:BA:2558:C:C6	2.56	0.41
25:BA:2607:G:H2'	25:BA:2608:G:O4'	2.21	0.41
29:BE:164:LEU:HB2	29:BE:167:VAL:HB	2.02	0.41
34:BL:40:LYS:NZ	34:BL:89:ASN:OD1	2.33	0.41
49:B1:31:ARG:HG2	49:B1:34:HIS:HB2	2.02	0.41
56:CN:28:DA:C4	56:CN:29:DG:N7	2.89	0.41
1:AA:421:U:H5'	1:AA:422:C:C6	2.55	0.41
5:AE:77:ASN:HB2	5:AE:82:GLN:NE2	2.36	0.41
11:AK:109:ASN:OD1	11:AK:111:THR:HG23	2.21	0.41
25:BA:833:A:H2'	25:BA:834:G:H8	1.84	0.41
25:BA:1902:C:H4'	27:BC:242:LYS:O	2.20	0.41
25:BA:2287:A:C8	25:BA:2289:G:C8	3.08	0.41
27:BC:162:VAL:HG11	27:BC:174:LEU:HD13	2.02	0.41
32:BH:80:ILE:HG12	32:BH:94:ILE:HG21	2.02	0.41
38:BP:7:ARG:HD2	38:BP:97:PHE:CZ	2.56	0.41
58:CA:183:ILE:HD12	58:CA:183:ILE:HG23	1.69	0.41
59:CC:166:SER:HB2	60:CD:1151:LYS:HE3	2.03	0.41
59:CC:176:ILE:HG21	59:CC:176:ILE:HD13	1.67	0.41
60:CD:35:PHE:CZ	60:CD:101:ARG:HD2	2.55	0.41
60:CD:201:LEU:HD23	60:CD:221:ILE:HG22	2.03	0.41
60:CD:554:GLU:OE1	60:CD:588:PRO:HA	2.20	0.41
60:CD:605:LEU:HD12	60:CD:605:LEU:HA	1.84	0.41
1:AA:149:A:H2'	1:AA:150:U:O4'	2.20	0.41
1:AA:545:C:H5'	4:AD:69:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1120:C:H2'	1:AA:1121:U:H6	1.85	0.41
1:AA:1175:G:O2'	1:AA:1176:A:P	2.78	0.41
10:AJ:10:LEU:HD23	10:AJ:10:LEU:HA	1.95	0.41
24:AX:5:G:C2	24:AX:6:G:C5	3.08	0.41
25:BA:569:U:H5"	25:BA:821:A:C2	2.55	0.41
25:BA:1153:C:H2'	25:BA:1154:G:O4'	2.20	0.41
25:BA:1416:G:HO2'	25:BA:1417:C:P	2.43	0.41
28:BD:39:ASP:N	28:BD:39:ASP:OD1	2.54	0.41
58:CA:100:LEU:HD13	58:CA:100:LEU:HA	1.82	0.41
59:CC:392:GLU:OE2	59:CC:392:GLU:N	2.38	0.41
59:CC:549:ASP:OD2	60:CD:750:PRO:HB3	2.21	0.41
59:CC:678:ARG:NH1	59:CC:681:MET:SD	2.94	0.41
59:CC:734:ILE:HG23	59:CC:734:ILE:HD12	1.77	0.41
59:CC:746:ALA:HB2	59:CC:967:LEU:HD21	2.02	0.41
59:CC:918:LEU:HD12	59:CC:918:LEU:HA	1.84	0.41
59:CC:1336:ASN:HB2	60:CD:25:ALA:HB2	2.01	0.41
1:AA:81:A:C6	1:AA:89:G:C6	3.08	0.41
1:AA:215:C:H2'	1:AA:216:U:O4'	2.19	0.41
1:AA:263:A:H2'	1:AA:264:C:C6	2.55	0.41
1:AA:428:G:H4'	1:AA:429:U:O5'	2.21	0.41
1:AA:1367:C:H5'	10:AJ:62:ARG:NH1	2.36	0.41
2:AB:20:THR:HA	2:AB:39:HIS:CE1	2.55	0.41
2:AB:60:ILE:HG23	2:AB:65:GLY:HA3	2.03	0.41
2:AB:208:ARG:O	2:AB:211:THR:OG1	2.30	0.41
5:AE:150:PRO:HG3	8:AH:99:LEU:HD21	2.03	0.41
10:AJ:15:HIS:O	10:AJ:18:ILE:HG22	2.21	0.41
11:AK:116:ILE:H	11:AK:116:ILE:CD1	2.34	0.41
16:AP:45:GLU:N	16:AP:45:GLU:OE1	2.54	0.41
24:AX:10:G:H2'	24:AX:11:C:C6	2.55	0.41
25:BA:28:A:H1'	25:BA:513:A:C2	2.56	0.41
25:BA:804:A:H2'	25:BA:806:C:C4	2.56	0.41
25:BA:1062:G:C2	25:BA:1077:A:N6	2.83	0.41
25:BA:1481:U:H2'	25:BA:1482:G:H4'	2.03	0.41
25:BA:2100:G:H1	25:BA:2189:U:H3	1.69	0.41
25:BA:2105:U:H2'	25:BA:2106:U:C6	2.56	0.41
25:BA:2210:U:H4'	25:BA:2211:G:C5'	2.51	0.41
25:BA:2291:U:H2'	25:BA:2292:U:H6	1.86	0.41
25:BA:2291:U:OP1	25:BA:2380:C:O2'	2.33	0.41
25:BA:2583:G:H2'	25:BA:2584:U:O4'	2.21	0.41
25:BA:2788:C:O2'	25:BA:2809:A:N3	2.41	0.41
28:BD:181:ASP:OD2	28:BD:184:ARG:NH1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BG:153:ARG:HG3	31:BG:154:PRO:HD2	2.03	0.41
32:BH:80:ILE:HG12	32:BH:94:ILE:CG2	2.50	0.41
32:BH:84:ALA:HB2	32:BH:90:LEU:HD12	2.02	0.41
32:BH:94:ILE:HG22	32:BH:99:ILE:HG13	2.02	0.41
32:BH:96:THR:HG22	32:BH:115:VAL:HB	2.02	0.41
46:BX:54:GLY:O	46:BX:57:HIS:N	2.54	0.41
50:B2:55:ILE:HG13	50:B2:57:LYS:H	1.85	0.41
56:CN:22:DT:C2	56:CN:22:DT:O5'	2.74	0.41
57:CT:5:DG:H2'	57:CT:6:DA:O4'	2.21	0.41
58:CB:66:HIS:ND1	58:CB:68:TYR:HB3	2.36	0.41
59:CC:736:VAL:H	59:CC:736:VAL:HG12	1.65	0.41
59:CC:951:MET:O	59:CC:955:GLN:HG2	2.21	0.41
59:CC:1104:PRO:HA	60:CD:740:LEU:HD11	2.03	0.41
60:CD:421:VAL:O	60:CD:421:VAL:HG23	2.21	0.41
60:CD:536:LEU:HD23	60:CD:536:LEU:HA	1.90	0.41
60:CD:872:LEU:HD22	60:CD:877:VAL:HG21	2.02	0.41
1:AA:996:A:C4	1:AA:997:U:C5	3.08	0.41
1:AA:1428:A:H2'	1:AA:1429:A:O4'	2.21	0.41
11:AK:108:THR:OG1	11:AK:109:ASN:N	2.54	0.41
24:AX:16:H2U:HN3	24:AX:59:U:H3	1.69	0.41
25:BA:309:A:N3	25:BA:329:G:O2'	2.43	0.41
25:BA:1071:G:N2	25:BA:1089:A:O2'	2.54	0.41
25:BA:2514:U:H2'	25:BA:2515:C:C6	2.56	0.41
27:BC:37:ASN:HB2	27:BC:62:TYR:HB2	2.02	0.41
30:BF:126:GLY:O	30:BF:127:ASN:ND2	2.54	0.41
38:BP:48:LEU:HD23	38:BP:48:LEU:HA	1.89	0.41
56:CN:26:DG:H5"	56:CN:26:DG:C8	2.56	0.41
59:CC:150:HIS:ND1	59:CC:150:HIS:O	2.54	0.41
59:CC:217:THR:HG23	59:CC:351:LEU:HD21	2.02	0.41
59:CC:557:ARG:NH2	59:CC:611:GLU:OE1	2.44	0.41
59:CC:615:VAL:O	59:CC:615:VAL:HG13	2.20	0.41
60:CD:238:ILE:HG23	60:CD:238:ILE:HD12	1.71	0.41
1:AA:1315:U:H2'	1:AA:1316:G:O4'	2.21	0.40
2:AB:132:LYS:HA	2:AB:132:LYS:HE3	2.03	0.40
2:AB:165:ASP:O	2:AB:169:GLU:HG2	2.21	0.40
6:AF:82:ASP:OD1	6:AF:82:ASP:N	2.54	0.40
13:AM:12:HIS:O	13:AM:44:LYS:HD2	2.21	0.40
25:BA:278:A:N1	25:BA:361:G:O2'	2.35	0.40
25:BA:958:U:H2'	26:BB:89:U:C2	2.56	0.40
25:BA:2112:G:H3'	25:BA:2113:U:C5	2.56	0.40
34:BL:41:ILE:HD11	34:BL:86:LEU:HD22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:CA:188:GLU:O	58:CA:199:ASP:HA	2.20	0.40
59:CC:1105:SER:OG	60:CD:731:ARG:NE	2.51	0.40
59:CC:1195:ILE:HD13	59:CC:1195:ILE:HG21	1.77	0.40
60:CD:544:LEU:HA	60:CD:544:LEU:HD12	1.74	0.40
1:AA:1014:A:N3	1:AA:1219:A:H1'	2.37	0.40
1:AA:1150:A:N6	1:AA:1151:A:N6	2.69	0.40
1:AA:1236:A:H4'	1:AA:1304:G:H4'	2.03	0.40
10:AJ:12:ALA:HB2	10:AJ:18:ILE:HD13	2.03	0.40
25:BA:2029:G:N1	25:BA:2033:A:OP2	2.31	0.40
25:BA:2111:U:O2'	25:BA:2112:G:H5'	2.21	0.40
25:BA:2114:A:N1	25:BA:2115:G:O2'	2.43	0.40
44:BV:96:PHE:O	44:BV:100:SER:HA	2.21	0.40
56:CN:27:DA:C4	56:CN:28:DA:N7	2.89	0.40
59:CC:97:ARG:HB3	59:CC:121:GLU:HB2	2.03	0.40
59:CC:138:ILE:HD12	59:CC:138:ILE:HG23	1.78	0.40
59:CC:197:ARG:NH1	59:CC:201:ARG:O	2.53	0.40
59:CC:524:ILE:HD13	59:CC:524:ILE:HG21	1.76	0.40
60:CD:157:GLN:CG	60:CD:158:GLN:H	2.34	0.40
60:CD:1044:GLN:O	60:CD:1067:ARG:HG2	2.21	0.40
60:CD:1239:ASP:OD1	60:CD:1242:ARG:NH2	2.40	0.40
1:AA:1492:A:OP1	12:AL:44:LYS:N	2.54	0.40
3:AC:128:VAL:HG12	3:AC:129:MET:N	2.36	0.40
11:AK:17:SER:O	11:AK:80:LYS:N	2.41	0.40
16:AP:6:LEU:HD23	16:AP:19:VAL:HG22	2.02	0.40
25:BA:1173:U:C4	25:BA:1176:U:O2	2.75	0.40
25:BA:1486:U:H2'	25:BA:1487:U:H6	1.86	0.40
25:BA:2198:A:N3	32:BH:29:PHE:HB2	2.36	0.40
38:BP:28:VAL:HG11	38:BP:103:VAL:HG22	2.02	0.40
59:CC:456:VAL:H	59:CC:456:VAL:HG23	1.53	0.40
59:CC:550:VAL:H	59:CC:550:VAL:HG12	1.69	0.40
59:CC:748:ILE:HG23	59:CC:748:ILE:O	2.22	0.40
59:CC:866:ASP:OD1	59:CC:866:ASP:C	2.60	0.40
60:CD:131:PRO:O	60:CD:134:ASP:N	2.55	0.40
60:CD:915:ILE:HG13	60:CD:916:GLY:N	2.37	0.40
60:CD:1050:THR:C	60:CD:1057:SER:HB3	2.41	0.40
60:CD:1077:ALA:HA	60:CD:1100:PHE:HA	2.04	0.40
60:CD:1349:GLU:H	60:CD:1349:GLU:CD	2.24	0.40
1:AA:501:C:H2'	1:AA:502:A:H8	1.86	0.40
17:AQ:81:LYS:HB2	17:AQ:81:LYS:HE2	1.63	0.40
19:AS:67:VAL:HG21	55:B7:57:VAL:HG22	2.03	0.40
24:AX:2:C:H2'	24:AX:3:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:81:G:H2'	25:BA:82:U:O4'	2.21	0.40
25:BA:1275:A:OP2	25:BA:1646:C:N4	2.35	0.40
25:BA:1421:G:C2	25:BA:1422:G:C8	3.10	0.40
25:BA:1596:A:O2'	25:BA:1597:A:O4'	2.39	0.40
25:BA:1720:U:H2'	25:BA:1721:G:O4'	2.22	0.40
32:BH:15:LEU:HD21	32:BH:55:GLU:HB3	2.04	0.40
57:CT:23:DC:H2"	57:CT:24:DG:H5'	2.04	0.40
59:CC:606:LEU:N	59:CC:606:LEU:HD12	2.36	0.40
59:CC:1101:LEU:HA	59:CC:1101:LEU:HD23	1.77	0.40
60:CD:441:LEU:N	60:CD:441:LEU:CD2	2.84	0.40
1:AA:736:C:H2'	1:AA:737:C:C6	2.57	0.40
1:AA:1412:C:H2'	1:AA:1413:A:C8	2.57	0.40
20:AT:25:ARG:HH11	20:AT:25:ARG:HG2	1.87	0.40
25:BA:44:A:H2'	25:BA:45:G:O4'	2.22	0.40
25:BA:299:A:N3	25:BA:319:G:O2'	2.43	0.40
25:BA:848:C:H2'	25:BA:849:A:C8	2.56	0.40
25:BA:883:G:H2'	25:BA:884:U:C6	2.57	0.40
25:BA:1599:U:H2'	25:BA:1600:C:H6	1.86	0.40
25:BA:2101:A:N6	25:BA:2102:G:O6	2.55	0.40
25:BA:2119:A:N7	25:BA:2170:A:H2	2.19	0.40
26:BB:52:A:N7	38:BP:64:TYR:OH	2.44	0.40
27:BC:78:VAL:HG21	27:BC:110:LEU:HD21	2.04	0.40
39:BQ:40:LEU:HD23	39:BQ:40:LEU:HA	1.91	0.40
49:B1:10:THR:HG22	49:B1:11:ARG:N	2.36	0.40
59:CC:261:VAL:HG21	59:CC:264:GLU:CD	2.42	0.40
59:CC:448:LEU:HD23	59:CC:448:LEU:HA	1.82	0.40
59:CC:473:ARG:HG3	59:CC:473:ARG:NH1	2.36	0.40
59:CC:705:GLU:HB3	59:CC:794:LEU:N	2.36	0.40
59:CC:1248:THR:HG22	59:CC:1249:GLY:N	2.35	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	AB	224/241 (93%)	210 (94%)	13 (6%)	1 (0%)	34 72
3	AC	207/233 (89%)	197 (95%)	6 (3%)	4 (2%)	8 36
4	AD	203/206 (98%)	192 (95%)	10 (5%)	1 (0%)	29 68
5	AE	154/167 (92%)	145 (94%)	7 (4%)	2 (1%)	12 45
6	AF	102/131 (78%)	97 (95%)	5 (5%)	0	100 100
7	AG	152/156 (97%)	144 (95%)	6 (4%)	2 (1%)	12 45
8	AH	127/130 (98%)	119 (94%)	8 (6%)	0	100 100
9	AI	126/130 (97%)	111 (88%)	12 (10%)	3 (2%)	6 29
10	AJ	98/103 (95%)	90 (92%)	5 (5%)	3 (3%)	4 23
11	AK	115/129 (89%)	100 (87%)	14 (12%)	1 (1%)	17 55
12	AL	119/124 (96%)	109 (92%)	8 (7%)	2 (2%)	9 39
13	AM	113/118 (96%)	108 (96%)	5 (4%)	0	100 100
14	AN	98/101 (97%)	96 (98%)	2 (2%)	0	100 100
15	AO	86/89 (97%)	84 (98%)	2 (2%)	0	100 100
16	AP	80/82 (98%)	78 (98%)	2 (2%)	0	100 100
17	AQ	78/84 (93%)	73 (94%)	5 (6%)	0	100 100
18	AR	64/75 (85%)	61 (95%)	2 (3%)	1 (2%)	9 40
19	AS	81/92 (88%)	80 (99%)	1 (1%)	0	100 100
20	AT	84/87 (97%)	83 (99%)	1 (1%)	0	100 100
21	AU	68/71 (96%)	68 (100%)	0	0	100 100
27	BC	270/273 (99%)	249 (92%)	18 (7%)	3 (1%)	14 50
28	BD	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	29 68
29	BE	199/201 (99%)	191 (96%)	8 (4%)	0	100 100
30	BF	176/179 (98%)	163 (93%)	10 (6%)	3 (2%)	9 39
31	BG	173/177 (98%)	159 (92%)	13 (8%)	1 (1%)	25 64
32	BH	147/149 (99%)	134 (91%)	10 (7%)	3 (2%)	7 34
33	BK	140/142 (99%)	136 (97%)	4 (3%)	0	100 100
34	BL	121/123 (98%)	115 (95%)	6 (5%)	0	100 100
35	BM	142/144 (99%)	132 (93%)	8 (6%)	2 (1%)	11 43
36	BN	133/136 (98%)	128 (96%)	5 (4%)	0	100 100
37	BO	118/127 (93%)	108 (92%)	10 (8%)	0	100 100
38	BP	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	17 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	BQ	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
40	BR	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
41	BS	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	15	53
42	BT	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
43	BU	94/100 (94%)	88 (94%)	5 (5%)	1 (1%)	14	50
44	BV	101/104 (97%)	97 (96%)	3 (3%)	1 (1%)	15	53
45	BW	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
46	BX	74/85 (87%)	70 (95%)	4 (5%)	0	100	100
47	BY	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
48	BZ	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
49	B1	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
50	B2	54/57 (95%)	54 (100%)	0	0	100	100
51	B3	51/55 (93%)	47 (92%)	4 (8%)	0	100	100
52	B4	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
53	B5	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	9	40
54	B6	36/50 (72%)	35 (97%)	1 (3%)	0	100	100
55	B7	68/70 (97%)	61 (90%)	7 (10%)	0	100	100
58	CA	227/329 (69%)	217 (96%)	10 (4%)	0	100	100
58	CB	215/329 (65%)	204 (95%)	10 (5%)	1 (0%)	29	68
59	CC	1316/1342 (98%)	1196 (91%)	111 (8%)	9 (1%)	22	60
60	CD	1327/1407 (94%)	1222 (92%)	95 (7%)	10 (1%)	19	57
61	CE	59/91 (65%)	53 (90%)	4 (7%)	2 (3%)	3	20
All	All	8766/9396 (93%)	8198 (94%)	508 (6%)	60 (1%)	26	60

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	AG	56	LYS
9	AI	56	ASP
10	AJ	57	VAL
11	AK	93	ARG
12	AL	88	LYS
12	AL	102	LEU
31	BG	47	ASP

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Mol	Chain	Res	Type
32	BH	89	LYS
53	B5	32	ILE
59	CC	165	HIS
60	CD	1159	ILE
3	AC	51	SER
3	AC	80	LYS
9	AI	13	LYS
27	BC	241	GLY
30	BF	62	GLY
32	BH	15	LEU
35	BM	36	LYS
58	CB	155	ALA
59	CC	47	TYR
60	CD	1051	ASP
28	BD	149	ASN
38	BP	100	HIS
41	BS	53	PHE
59	CC	258	ASN
59	CC	1177	ARG
60	CD	119	SER
60	CD	121	PRO
60	CD	712	GLN
60	CD	854	ALA
60	CD	1200	GLU
2	AB	165	ASP
3	AC	14	ILE
5	AE	90	THR
7	AG	130	ASN
9	AI	14	SER
10	AJ	58	ASN
18	AR	72	ASP
30	BF	177	PHE
32	BH	76	GLU
59	CC	282	VAL
59	CC	596	ASP
59	CC	1153	ALA
60	CD	586	GLY
4	AD	43	ALA
35	BM	99	ASN
43	BU	3	ARG
44	BV	8	ASP
61	CE	16	ARG

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Mol	Chain	Res	Type
3	AC	60	PRO
10	AJ	78	GLU
27	BC	197	ASN
27	BC	233	GLY
59	CC	1223	ARG
60	CD	312	ARG
61	CE	4	VAL
5	AE	108	GLY
30	BF	176	PRO
59	CC	1186	VAL
60	CD	500	ILE

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	AB	187/199 (94%)	174 (93%)	13 (7%)	15	47
3	AC	171/190 (90%)	161 (94%)	10 (6%)	20	55
4	AD	172/173 (99%)	162 (94%)	10 (6%)	20	55
5	AE	118/126 (94%)	110 (93%)	8 (7%)	16	48
6	AF	91/112 (81%)	85 (93%)	6 (7%)	16	49
7	AG	127/129 (98%)	119 (94%)	8 (6%)	18	51
8	AH	104/105 (99%)	97 (93%)	7 (7%)	16	49
9	AI	106/107 (99%)	101 (95%)	5 (5%)	26	63
10	AJ	87/90 (97%)	78 (90%)	9 (10%)	7	28
11	AK	90/99 (91%)	82 (91%)	8 (9%)	9	35
12	AL	102/103 (99%)	95 (93%)	7 (7%)	15	48
13	AM	93/96 (97%)	88 (95%)	5 (5%)	22	57
14	AN	83/84 (99%)	78 (94%)	5 (6%)	19	53
15	AO	76/77 (99%)	73 (96%)	3 (4%)	32	69
16	AP	65/65 (100%)	61 (94%)	4 (6%)	18	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	AQ	74/78 (95%)	70 (95%)	4 (5%)	22 57
18	AR	57/65 (88%)	54 (95%)	3 (5%)	22 58
19	AS	72/79 (91%)	71 (99%)	1 (1%)	67 88
20	AT	65/66 (98%)	59 (91%)	6 (9%)	9 34
21	AU	60/61 (98%)	54 (90%)	6 (10%)	7 29
27	BC	217/218 (100%)	212 (98%)	5 (2%)	50 80
28	BD	163/163 (100%)	155 (95%)	8 (5%)	25 61
29	BE	165/165 (100%)	155 (94%)	10 (6%)	18 53
30	BF	149/150 (99%)	139 (93%)	10 (7%)	16 49
31	BG	136/138 (99%)	124 (91%)	12 (9%)	10 36
32	BH	114/114 (100%)	106 (93%)	8 (7%)	15 47
33	BK	116/116 (100%)	111 (96%)	5 (4%)	29 66
34	BL	104/104 (100%)	98 (94%)	6 (6%)	20 55
35	BM	103/103 (100%)	95 (92%)	8 (8%)	12 42
36	BN	108/108 (100%)	102 (94%)	6 (6%)	21 56
37	BO	100/103 (97%)	95 (95%)	5 (5%)	24 60
38	BP	87/87 (100%)	81 (93%)	6 (7%)	15 48
39	BQ	99/100 (99%)	92 (93%)	7 (7%)	14 46
40	BR	89/90 (99%)	84 (94%)	5 (6%)	21 56
41	BS	84/84 (100%)	79 (94%)	5 (6%)	19 53
42	BT	93/93 (100%)	87 (94%)	6 (6%)	17 50
43	BU	83/84 (99%)	79 (95%)	4 (5%)	25 62
44	BV	84/85 (99%)	78 (93%)	6 (7%)	14 46
45	BW	78/78 (100%)	74 (95%)	4 (5%)	24 60
46	BX	58/63 (92%)	57 (98%)	1 (2%)	60 85
47	BY	67/68 (98%)	64 (96%)	3 (4%)	27 64
48	BZ	54/55 (98%)	51 (94%)	3 (6%)	21 56
49	B1	48/49 (98%)	45 (94%)	3 (6%)	18 51
50	B2	47/48 (98%)	46 (98%)	1 (2%)	53 82
51	B3	48/49 (98%)	43 (90%)	5 (10%)	7 27
52	B4	37/38 (97%)	34 (92%)	3 (8%)	11 40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
53	B5	51/52 (98%)	47 (92%)	4 (8%)	12 42
54	B6	34/44 (77%)	30 (88%)	4 (12%)	5 22
55	B7	62/62 (100%)	59 (95%)	3 (5%)	25 62
58	CA	197/286 (69%)	193 (98%)	4 (2%)	55 83
58	CB	187/286 (65%)	177 (95%)	10 (5%)	22 58
59	CC	1139/1157 (98%)	1097 (96%)	42 (4%)	34 70
60	CD	1118/1168 (96%)	1097 (98%)	21 (2%)	57 84
61	CE	52/75 (69%)	48 (92%)	4 (8%)	13 42
All	All	7371/7787 (95%)	7006 (95%)	365 (5%)	28 60

All (365) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	23	TRP
2	AB	47	VAL
2	AB	63	ARG
2	AB	68	LEU
2	AB	74	ARG
2	AB	82	ASP
2	AB	117	LEU
2	AB	123	ASP
2	AB	128	LYS
2	AB	129	LEU
2	AB	132	LYS
2	AB	186	ILE
2	AB	220	THR
3	AC	14	ILE
3	AC	28	GLU
3	AC	35	SER
3	AC	62	LYS
3	AC	121	THR
3	AC	154	SER
3	AC	164	ARG
3	AC	165	THR
3	AC	172	ARG
3	AC	185	ASN
4	AD	47	ARG
4	AD	58	LYS
4	AD	104	ARG

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Mol	Chain	Res	Type
4	AD	138	SER
4	AD	156	LYS
4	AD	167	LYS
4	AD	179	GLU
4	AD	181	THR
4	AD	194	ASP
4	AD	197	GLU
5	AE	10	GLU
5	AE	15	LEU
5	AE	83	HIS
5	AE	93	ARG
5	AE	138	ARG
5	AE	141	ILE
5	AE	142	ASP
5	AE	146	ASN
6	AF	7	VAL
6	AF	24	ARG
6	AF	38	ARG
6	AF	44	ARG
6	AF	79	ARG
6	AF	100	SER
7	AG	7	ILE
7	AG	25	LYS
7	AG	80	VAL
7	AG	123	GLU
7	AG	130	ASN
7	AG	133	THR
7	AG	143	ARG
7	AG	146	GLU
8	AH	3	MET
8	AH	55	THR
8	AH	76	GLN
8	AH	87	LYS
8	AH	88	ARG
8	AH	90	ASP
8	AH	121	LEU
9	AI	41	ARG
9	AI	42	GLU
9	AI	57	MET
9	AI	111	VAL
9	AI	123	ARG
10	AJ	5	ARG

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Mol	Chain	Res	Type
10	AJ	14	ASP
10	AJ	18	ILE
10	AJ	36	VAL
10	AJ	37	ARG
10	AJ	44	THR
10	AJ	75	ASP
10	AJ	85	ASP
10	AJ	96	VAL
11	AK	13	ARG
11	AK	15	GLN
11	AK	18	ASP
11	AK	37	ARG
11	AK	76	GLU
11	AK	84	VAL
11	AK	108	THR
11	AK	116	ILE
12	AL	5	ASN
12	AL	24	LEU
12	AL	40	THR
12	AL	47	SER
12	AL	62	GLU
12	AL	90	LEU
12	AL	102	LEU
13	AM	11	ASP
13	AM	89	LEU
13	AM	93	ARG
13	AM	96	PRO
13	AM	104	THR
14	AN	18	ASP
14	AN	52	PRO
14	AN	89	MET
14	AN	92	GLU
14	AN	100	SER
15	AO	40	GLN
15	AO	64	ARG
15	AO	84	ARG
16	AP	1	MET
16	AP	42	ILE
16	AP	45	GLU
16	AP	77	GLU
17	AQ	4	LYS
17	AQ	48	ASP

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Mol	Chain	Res	Type
17	AQ	57	ASP
17	AQ	75	LEU
18	AR	55	LEU
18	AR	71	THR
18	AR	74	HIS
19	AS	79	THR
20	AT	6	SER
20	AT	10	ARG
20	AT	24	ARG
20	AT	25	ARG
20	AT	43	ASP
20	AT	54	MET
21	AU	4	ILE
21	AU	13	ASP
21	AU	18	ARG
21	AU	28	VAL
21	AU	29	LEU
21	AU	69	ARG
27	BC	52	ARG
27	BC	130	LEU
27	BC	189	ARG
27	BC	203	ARG
27	BC	242	LYS
28	BD	13	ARG
28	BD	29	VAL
28	BD	30	GLU
28	BD	32	ASN
28	BD	43	ASP
28	BD	77	ARG
28	BD	118	PHE
28	BD	157	LYS
29	BE	13	THR
29	BE	21	ARG
29	BE	22	ASP
29	BE	40	ARG
29	BE	57	LYS
29	BE	88	ARG
29	BE	111	GLU
29	BE	123	LYS
29	BE	136	GLN
29	BE	153	LEU
30	BF	6	ASP

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Mol	Chain	Res	Type
30	BF	57	LEU
30	BF	60	ILE
30	BF	115	ARG
30	BF	123	ASP
30	BF	133	ARG
30	BF	140	GLU
30	BF	141	ILE
30	BF	152	LEU
30	BF	158	THR
31	BG	16	ASP
31	BG	32	GLU
31	BG	36	THR
31	BG	84	THR
31	BG	95	ARG
31	BG	110	SER
31	BG	127	THR
31	BG	141	ILE
31	BG	166	ASP
31	BG	168	VAL
31	BG	170	ARG
31	BG	176	LYS
32	BH	3	VAL
32	BH	15	LEU
32	BH	66	ASN
32	BH	75	LEU
32	BH	87	GLU
32	BH	114	GLU
32	BH	129	GLU
32	BH	133	GLN
33	BK	1	MET
33	BK	57	LEU
33	BK	108	MET
33	BK	123	LYS
33	BK	142	ILE
34	BL	17	ARG
34	BL	18	ARG
34	BL	41	ILE
34	BL	58	LEU
34	BL	67	LYS
34	BL	99	ILE
35	BM	30	THR
35	BM	40	SER

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Mol	Chain	Res	Type
35	BM	67	THR
35	BM	78	ARG
35	BM	79	LEU
35	BM	84	LYS
35	BM	115	GLU
35	BM	118	THR
36	BN	18	ARG
36	BN	47	GLU
36	BN	55	ARG
36	BN	100	LYS
36	BN	110	GLU
36	BN	115	GLU
37	BO	2	ARG
37	BO	13	ASN
37	BO	63	ARG
37	BO	65	LEU
37	BO	69	ARG
38	BP	1	MET
38	BP	13	ARG
38	BP	47	VAL
38	BP	52	SER
38	BP	115	LEU
38	BP	116	GLN
39	BQ	40	LEU
39	BQ	66	ASN
39	BQ	80	VAL
39	BQ	88	ARG
39	BQ	89	ARG
39	BQ	111	LYS
39	BQ	113	ARG
40	BR	11	ARG
40	BR	51	ARG
40	BR	52	GLN
40	BR	59	GLN
40	BR	91	ASP
41	BS	10	LYS
41	BS	31	GLU
41	BS	39	LEU
41	BS	48	LYS
41	BS	79	ARG
42	BT	19	LEU
42	BT	29	VAL

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Mol	Chain	Res	Type
42	BT	67	ASP
42	BT	83	LYS
42	BT	109	ASP
42	BT	110	ARG
43	BU	1	MET
43	BU	53	VAL
43	BU	89	GLU
43	BU	95	PHE
44	BV	7	ARG
44	BV	9	ASP
44	BV	46	GLN
44	BV	52	LEU
44	BV	72	ILE
44	BV	101	GLU
45	BW	40	ILE
45	BW	45	ASP
45	BW	62	THR
45	BW	65	VAL
46	BX	70	GLU
47	BY	2	SER
47	BY	33	LEU
47	BY	48	THR
48	BZ	7	ARG
48	BZ	58	ASN
48	BZ	59	GLU
49	B1	8	THR
49	B1	10	THR
49	B1	45	ARG
50	B2	12	LYS
51	B3	5	ILE
51	B3	10	LYS
51	B3	23	THR
51	B3	32	GLU
51	B3	50	LYS
52	B4	15	SER
52	B4	22	MET
52	B4	25	LYS
53	B5	31	HIS
53	B5	32	ILE
53	B5	54	ASP
53	B5	55	LEU
54	B6	12	ARG

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Mol	Chain	Res	Type
54	B6	26	ILE
54	B6	36	ARG
54	B6	37	GLN
55	B7	21	VAL
55	B7	32	LEU
55	B7	35	ASP
58	CA	13	LEU
58	CA	74	VAL
58	CA	101	THR
58	CA	166	ARG
58	CB	17	GLU
58	CB	41	ASN
58	CB	48	LEU
58	CB	66	HIS
58	CB	72	GLU
58	CB	76	GLU
58	CB	83	LEU
58	CB	170	ARG
58	CB	174	ASP
58	CB	191	ARG
59	CC	47	TYR
59	CC	65	ASN
59	CC	108	GLU
59	CC	116	ASP
59	CC	150	HIS
59	CC	193	ASN
59	CC	262	TYR
59	CC	267	ARG
59	CC	369	MET
59	CC	494	ASN
59	CC	524	ILE
59	CC	529	ARG
59	CC	562	GLU
59	CC	568	ASN
59	CC	569	ILE
59	CC	575	LEU
59	CC	657	THR
59	CC	726	TYR
59	CC	745	GLU
59	CC	772	SER
59	CC	822	VAL
59	CC	830	THR

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Mol	Chain	Res	Type
59	CC	843	THR
59	CC	844	LYS
59	CC	856	ASN
59	CC	888	THR
59	CC	1002	LEU
59	CC	1005	GLU
59	CC	1022	LYS
59	CC	1080	ASN
59	CC	1158	LYS
59	CC	1223	ARG
59	CC	1240	ASP
59	CC	1247	SER
59	CC	1250	SER
59	CC	1274	GLU
59	CC	1287	LEU
59	CC	1291	LEU
59	CC	1298	VAL
59	CC	1304	MET
59	CC	1336	ASN
59	CC	1340	GLU
60	CD	68	TYR
60	CD	99	ARG
60	CD	113	HIS
60	CD	158	GLN
60	CD	196	GLN
60	CD	255	LEU
60	CD	275	ARG
60	CD	281	ARG
60	CD	418	GLU
60	CD	505	ASP
60	CD	700	ASN
60	CD	709	ARG
60	CD	802	ASP
60	CD	826	ILE
60	CD	839	VAL
60	CD	1046	ILE
60	CD	1165	PHE
60	CD	1167	LYS
60	CD	1195	GLN
60	CD	1237	VAL
60	CD	1261	LEU
61	CE	3	ARG

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Mol	Chain	Res	Type
61	CE	18	ASP
61	CE	44	ASP
61	CE	58	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
6	AF	58	HIS
27	BC	128	ASN
30	BF	127	ASN
32	BH	73	ASN
41	BS	43	ASN
43	BU	48	GLN
44	BV	46	GLN
44	BV	54	GLN
44	BV	74	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	292 (19%)	28 (1%)
22	AV	25/53 (47%)	9 (36%)	1 (4%)
23	AW	76/77 (98%)	22 (28%)	8 (10%)
24	AX	73/76 (96%)	16 (21%)	1 (1%)
25	BA	2895/2904 (99%)	557 (19%)	65 (2%)
26	BB	120/120 (100%)	12 (10%)	1 (0%)
All	All	4718/4772 (98%)	908 (19%)	104 (2%)

All (908) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G
1	AA	22	G
1	AA	29	U
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C

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Mol	Chain	Res	Type
1	AA	50	A
1	AA	51	A
1	AA	52	C
1	AA	54	C
1	AA	69	G
1	AA	70	U
1	AA	71	A
1	AA	72	A
1	AA	74	A
1	AA	75	G
1	AA	76	G
1	AA	80	C
1	AA	81	A
1	AA	82	G
1	AA	83	C
1	AA	84	U
1	AA	87	C
1	AA	89	G
1	AA	90	C
1	AA	94	G
1	AA	95	C
1	AA	96	U
1	AA	108	G
1	AA	121	U
1	AA	122	G
1	AA	131	A
1	AA	141	G
1	AA	144	G
1	AA	148	G
1	AA	149	A
1	AA	160	A
1	AA	164	G
1	AA	173	U
1	AA	181	A
1	AA	182	A
1	AA	183	C
1	AA	184	G
1	AA	196	A
1	AA	198	G
1	AA	208	U
1	AA	209	U
1	AA	210	C

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Mol	Chain	Res	Type
1	AA	211	G
1	AA	212	G
1	AA	216	U
1	AA	226	G
1	AA	245	U
1	AA	247	G
1	AA	251	G
1	AA	258	G
1	AA	262	A
1	AA	266	G
1	AA	267	C
1	AA	279	A
1	AA	289	G
1	AA	306	A
1	AA	316	C
1	AA	321	A
1	AA	328	C
1	AA	329	A
1	AA	332	G
1	AA	340	U
1	AA	347	G
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	376	G
1	AA	384	G
1	AA	388	G
1	AA	389	A
1	AA	392	C
1	AA	397	A
1	AA	406	G
1	AA	412	A
1	AA	413	G
1	AA	414	A
1	AA	421	U
1	AA	422	C
1	AA	424	G
1	AA	429	U
1	AA	446	G
1	AA	451	A

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Mol	Chain	Res	Type
1	AA	457	G
1	AA	458	U
1	AA	460	A
1	AA	463	U
1	AA	464	U
1	AA	467	U
1	AA	468	A
1	AA	469	C
1	AA	479	U
1	AA	480	U
1	AA	481	G
1	AA	484	G
1	AA	485	U
1	AA	486	U
1	AA	495	A
1	AA	511	C
1	AA	516	PSU
1	AA	517	G
1	AA	518	C
1	AA	521	G
1	AA	526	C
1	AA	530	G
1	AA	531	U
1	AA	532	A
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	568	G
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	579	A
1	AA	588	G
1	AA	596	A
1	AA	628	G
1	AA	633	G
1	AA	642	A
1	AA	649	A
1	AA	650	G
1	AA	653	U
1	AA	656	G

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Mol	Chain	Res	Type
1	AA	665	A
1	AA	687	A
1	AA	702	A
1	AA	723	U
1	AA	724	G
1	AA	731	G
1	AA	734	G
1	AA	747	A
1	AA	755	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	815	A
1	AA	817	C
1	AA	828	U
1	AA	836	G
1	AA	843	U
1	AA	844	G
1	AA	845	A
1	AA	846	G
1	AA	847	G
1	AA	849	G
1	AA	874	G
1	AA	887	G
1	AA	902	G
1	AA	914	A
1	AA	916	U
1	AA	926	G
1	AA	927	G
1	AA	928	G
1	AA	934	C
1	AA	935	A
1	AA	960	U
1	AA	961	U
1	AA	966	2MG
1	AA	969	A
1	AA	972	C
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	991	U
1	AA	992	U

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Mol	Chain	Res	Type
1	AA	993	G
1	AA	996	A
1	AA	999	C
1	AA	1004	A
1	AA	1005	A
1	AA	1008	U
1	AA	1009	U
1	AA	1017	U
1	AA	1018	G
1	AA	1020	G
1	AA	1021	A
1	AA	1024	G
1	AA	1026	G
1	AA	1028	C
1	AA	1030	U
1	AA	1031	C
1	AA	1037	C
1	AA	1043	G
1	AA	1044	A
1	AA	1046	A
1	AA	1065	U
1	AA	1084	G
1	AA	1085	U
1	AA	1086	U
1	AA	1092	A
1	AA	1094	G
1	AA	1095	U
1	AA	1099	G
1	AA	1101	A
1	AA	1133	G
1	AA	1135	U
1	AA	1136	C
1	AA	1137	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1142	G
1	AA	1143	G
1	AA	1151	A
1	AA	1152	A
1	AA	1158	C
1	AA	1159	U

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Mol	Chain	Res	Type
1	AA	1167	A
1	AA	1168	U
1	AA	1171	A
1	AA	1174	G
1	AA	1175	G
1	AA	1176	A
1	AA	1184	G
1	AA	1187	G
1	AA	1196	A
1	AA	1197	A
1	AA	1211	U
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C
1	AA	1215	G
1	AA	1227	A
1	AA	1238	A
1	AA	1239	A
1	AA	1242	G
1	AA	1257	A
1	AA	1260	G
1	AA	1275	A
1	AA	1277	C
1	AA	1278	G
1	AA	1279	G
1	AA	1280	A
1	AA	1285	A
1	AA	1286	U
1	AA	1287	A
1	AA	1299	A
1	AA	1300	G
1	AA	1302	C
1	AA	1305	G
1	AA	1311	A
1	AA	1312	G
1	AA	1317	C
1	AA	1320	C
1	AA	1323	G
1	AA	1329	A
1	AA	1332	A
1	AA	1334	G
1	AA	1338	G

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Mol	Chain	Res	Type
1	AA	1340	A
1	AA	1346	A
1	AA	1353	G
1	AA	1363	A
1	AA	1364	U
1	AA	1370	G
1	AA	1378	C
1	AA	1379	G
1	AA	1381	U
1	AA	1383	C
1	AA	1396	A
1	AA	1398	A
1	AA	1404	C
1	AA	1408	A
1	AA	1419	G
1	AA	1429	A
1	AA	1441	A
1	AA	1446	A
1	AA	1447	A
1	AA	1448	C
1	AA	1452	C
1	AA	1453	G
1	AA	1487	G
1	AA	1493	A
1	AA	1494	G
1	AA	1497	G
1	AA	1503	A
1	AA	1506	U
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
22	AV	16	A
22	AV	24	A
22	AV	26	A
22	AV	27	C
22	AV	44	A
22	AV	45	C
22	AV	46	G
22	AV	49	G
22	AV	53	G
23	AW	6	G
23	AW	9	G

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Mol	Chain	Res	Type
23	AW	14	A
23	AW	16	C
23	AW	17	C
23	AW	17(A)	U
23	AW	18	G
23	AW	19	G
23	AW	20	H2U
23	AW	21	A
23	AW	22	G
23	AW	25	C
23	AW	31	G
23	AW	37	A
23	AW	47	U
23	AW	48	C
23	AW	49	G
23	AW	57	A
23	AW	59	A
23	AW	74	C
23	AW	75	C
23	AW	76	A
24	AX	5	G
24	AX	6	G
24	AX	8	4SU
24	AX	9	A
24	AX	11	C
24	AX	15	G
24	AX	16	H2U
24	AX	17	C
24	AX	18	G
24	AX	20	H2U
24	AX	22	G
24	AX	45	U
24	AX	46	7MG
24	AX	49	C
24	AX	58	A
24	AX	74	C
25	BA	10	A
25	BA	14	A
25	BA	23	G
25	BA	34	U
25	BA	35	G
25	BA	45	G

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Mol	Chain	Res	Type
25	BA	46	G
25	BA	58	G
25	BA	60	G
25	BA	62	U
25	BA	63	A
25	BA	71	A
25	BA	74	A
25	BA	75	G
25	BA	83	A
25	BA	84	A
25	BA	85	G
25	BA	99	U
25	BA	101	A
25	BA	102	U
25	BA	103	A
25	BA	110	G
25	BA	118	A
25	BA	119	A
25	BA	120	U
25	BA	122	G
25	BA	131	A
25	BA	138	U
25	BA	139	U
25	BA	140	C
25	BA	141	G
25	BA	142	A
25	BA	144	A
25	BA	149	A
25	BA	163	C
25	BA	165	A
25	BA	181	A
25	BA	196	A
25	BA	215	G
25	BA	216	A
25	BA	221	A
25	BA	222	A
25	BA	248	G
25	BA	249	C
25	BA	264	C
25	BA	265	A
25	BA	266	G
25	BA	270	A

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Mol	Chain	Res	Type
25	BA	271	G
25	BA	272	A
25	BA	276	U
25	BA	277	G
25	BA	278	A
25	BA	285	G
25	BA	291	G
25	BA	302	C
25	BA	311	A
25	BA	327	G
25	BA	329	G
25	BA	330	A
25	BA	353	C
25	BA	361	G
25	BA	362	A
25	BA	371	A
25	BA	372	G
25	BA	386	G
25	BA	396	G
25	BA	405	U
25	BA	411	G
25	BA	412	A
25	BA	424	G
25	BA	435	C
25	BA	451	U
25	BA	456	C
25	BA	457	A
25	BA	477	A
25	BA	480	A
25	BA	481	G
25	BA	491	G
25	BA	501	A
25	BA	503	A
25	BA	504	A
25	BA	505	A
25	BA	509	C
25	BA	531	C
25	BA	532	A
25	BA	533	G
25	BA	544	G
25	BA	550	U
25	BA	563	A

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Mol	Chain	Res	Type
25	BA	569	U
25	BA	573	U
25	BA	574	A
25	BA	575	A
25	BA	586	A
25	BA	603	A
25	BA	609	A
25	BA	613	A
25	BA	614	A
25	BA	615	U
25	BA	616	A
25	BA	618	G
25	BA	627	A
25	BA	637	A
25	BA	645	C
25	BA	647	G
25	BA	651	G
25	BA	654	A
25	BA	655	A
25	BA	668	A
25	BA	685	A
25	BA	686	U
25	BA	696	G
25	BA	717	C
25	BA	724	U
25	BA	730	A
25	BA	738	G
25	BA	746	PSU
25	BA	747	5MU
25	BA	757	G
25	BA	764	A
25	BA	765	C
25	BA	775	G
25	BA	776	G
25	BA	782	A
25	BA	783	A
25	BA	784	G
25	BA	785	G
25	BA	788	A
25	BA	789	A
25	BA	790	U
25	BA	805	G

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Mol	Chain	Res	Type
25	BA	812	C
25	BA	827	U
25	BA	828	U
25	BA	845	A
25	BA	846	U
25	BA	858	G
25	BA	859	G
25	BA	869	G
25	BA	878	A
25	BA	881	G
25	BA	883	G
25	BA	884	U
25	BA	885	C
25	BA	887	U
25	BA	890	C
25	BA	891	G
25	BA	892	A
25	BA	895	U
25	BA	896	A
25	BA	897	C
25	BA	898	C
25	BA	899	A
25	BA	910	A
25	BA	914	G
25	BA	931	U
25	BA	933	A
25	BA	940	G
25	BA	941	A
25	BA	945	A
25	BA	946	C
25	BA	953	G
25	BA	961	C
25	BA	974	G
25	BA	983	A
25	BA	996	A
25	BA	999	U
25	BA	1005	C
25	BA	1012	U
25	BA	1013	C
25	BA	1023	U
25	BA	1026	G
25	BA	1033	U

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Mol	Chain	Res	Type
25	BA	1040	A
25	BA	1043	C
25	BA	1045	C
25	BA	1046	A
25	BA	1047	G
25	BA	1050	A
25	BA	1055	G
25	BA	1060	U
25	BA	1061	U
25	BA	1063	G
25	BA	1064	C
25	BA	1065	U
25	BA	1066	U
25	BA	1067	A
25	BA	1068	G
25	BA	1069	A
25	BA	1070	A
25	BA	1073	A
25	BA	1074	G
25	BA	1078	U
25	BA	1083	U
25	BA	1087	G
25	BA	1088	A
25	BA	1090	A
25	BA	1107	G
25	BA	1111	A
25	BA	1112	G
25	BA	1119	U
25	BA	1122	G
25	BA	1130	U
25	BA	1132	U
25	BA	1134	A
25	BA	1135	C
25	BA	1142	A
25	BA	1170	C
25	BA	1171	G
25	BA	1173	U
25	BA	1174	U
25	BA	1175	A
25	BA	1176	U
25	BA	1177	G
25	BA	1178	C

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Mol	Chain	Res	Type
25	BA	1180	U
25	BA	1186	G
25	BA	1212	G
25	BA	1236	G
25	BA	1238	G
25	BA	1248	G
25	BA	1253	A
25	BA	1256	G
25	BA	1265	A
25	BA	1271	G
25	BA	1272	A
25	BA	1273	U
25	BA	1301	A
25	BA	1302	A
25	BA	1321	A
25	BA	1345	C
25	BA	1352	U
25	BA	1365	A
25	BA	1368	G
25	BA	1378	A
25	BA	1379	U
25	BA	1380	G
25	BA	1383	A
25	BA	1395	A
25	BA	1405	U
25	BA	1406	U
25	BA	1407	G
25	BA	1408	G
25	BA	1409	U
25	BA	1414	C
25	BA	1416	G
25	BA	1417	C
25	BA	1420	A
25	BA	1428	C
25	BA	1434	A
25	BA	1435	G
25	BA	1452	G
25	BA	1453	A
25	BA	1455	G
25	BA	1458	U
25	BA	1460	U
25	BA	1478	G

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Mol	Chain	Res	Type
25	BA	1482	G
25	BA	1483	G
25	BA	1490	A
25	BA	1493	C
25	BA	1495	A
25	BA	1497	U
25	BA	1508	A
25	BA	1509	A
25	BA	1510	G
25	BA	1515	A
25	BA	1529	G
25	BA	1534	U
25	BA	1535	A
25	BA	1536	C
25	BA	1537	G
25	BA	1554	U
25	BA	1558	C
25	BA	1559	U
25	BA	1566	A
25	BA	1569	A
25	BA	1578	U
25	BA	1580	A
25	BA	1581	G
25	BA	1583	A
25	BA	1584	U
25	BA	1589	U
25	BA	1590	A
25	BA	1592	C
25	BA	1593	A
25	BA	1594	U
25	BA	1595	C
25	BA	1596	A
25	BA	1597	A
25	BA	1608	A
25	BA	1609	A
25	BA	1610	A
25	BA	1613	G
25	BA	1619	G
25	BA	1630	A
25	BA	1647	U
25	BA	1648	U
25	BA	1649	G

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Mol	Chain	Res	Type
25	BA	1651	G
25	BA	1674	G
25	BA	1677	A
25	BA	1703	G
25	BA	1713	A
25	BA	1714	U
25	BA	1715	G
25	BA	1718	G
25	BA	1729	U
25	BA	1730	C
25	BA	1732	C
25	BA	1738	G
25	BA	1742	U
25	BA	1750	G
25	BA	1755	A
25	BA	1758	U
25	BA	1761	C
25	BA	1764	C
25	BA	1773	A
25	BA	1791	A
25	BA	1800	C
25	BA	1801	A
25	BA	1808	A
25	BA	1811	G
25	BA	1816	C
25	BA	1829	A
25	BA	1833	C
25	BA	1848	A
25	BA	1858	A
25	BA	1859	U
25	BA	1862	G
25	BA	1864	U
25	BA	1869	G
25	BA	1870	C
25	BA	1905	C
25	BA	1906	G
25	BA	1907	G
25	BA	1912	A
25	BA	1913	A
25	BA	1914	C
25	BA	1917	PSU
25	BA	1918	A

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Mol	Chain	Res	Type
25	BA	1919	A
25	BA	1929	G
25	BA	1930	G
25	BA	1931	U
25	BA	1936	A
25	BA	1938	A
25	BA	1939	5MU
25	BA	1955	U
25	BA	1960	A
25	BA	1965	C
25	BA	1966	A
25	BA	1967	C
25	BA	1970	A
25	BA	1971	U
25	BA	1972	G
25	BA	1987	A
25	BA	1991	U
25	BA	1992	G
25	BA	1993	U
25	BA	1997	C
25	BA	2002	G
25	BA	2022	U
25	BA	2023	C
25	BA	2026	U
25	BA	2031	A
25	BA	2033	A
25	BA	2043	C
25	BA	2051	A
25	BA	2052	A
25	BA	2055	C
25	BA	2056	G
25	BA	2060	A
25	BA	2061	G
25	BA	2062	A
25	BA	2063	C
25	BA	2069	G7M
25	BA	2093	G
25	BA	2095	A
25	BA	2097	A
25	BA	2099	U
25	BA	2100	G
25	BA	2101	A

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Mol	Chain	Res	Type
25	BA	2102	G
25	BA	2107	G
25	BA	2109	U
25	BA	2110	G
25	BA	2111	U
25	BA	2113	U
25	BA	2115	G
25	BA	2116	G
25	BA	2117	A
25	BA	2118	U
25	BA	2119	A
25	BA	2120	G
25	BA	2121	G
25	BA	2123	G
25	BA	2124	G
25	BA	2125	G
25	BA	2126	A
25	BA	2127	G
25	BA	2129	C
25	BA	2131	U
25	BA	2132	U
25	BA	2133	G
25	BA	2135	A
25	BA	2136	G
25	BA	2137	U
25	BA	2138	G
25	BA	2139	U
25	BA	2140	G
25	BA	2148	G
25	BA	2150	C
25	BA	2157	G
25	BA	2159	G
25	BA	2162	G
25	BA	2164	C
25	BA	2165	C
25	BA	2167	U
25	BA	2169	A
25	BA	2170	A
25	BA	2171	A
25	BA	2172	U
25	BA	2173	A
25	BA	2177	C

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Mol	Chain	Res	Type
25	BA	2181	U
25	BA	2182	U
25	BA	2183	A
25	BA	2188	U
25	BA	2189	U
25	BA	2191	A
25	BA	2192	U
25	BA	2193	G
25	BA	2194	U
25	BA	2197	U
25	BA	2198	A
25	BA	2199	A
25	BA	2203	U
25	BA	2204	G
25	BA	2211	G
25	BA	2212	A
25	BA	2213	U
25	BA	2225	A
25	BA	2226	C
25	BA	2229	U
25	BA	2238	G
25	BA	2239	G
25	BA	2245	U
25	BA	2246	G
25	BA	2250	G
25	BA	2251	OMG
25	BA	2252	G
25	BA	2268	A
25	BA	2278	A
25	BA	2283	C
25	BA	2287	A
25	BA	2294	G
25	BA	2297	A
25	BA	2305	U
25	BA	2308	G
25	BA	2309	A
25	BA	2315	G
25	BA	2322	A
25	BA	2325	G
25	BA	2333	A
25	BA	2335	A
25	BA	2336	A

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Mol	Chain	Res	Type
25	BA	2347	C
25	BA	2350	C
25	BA	2361	G
25	BA	2372	U
25	BA	2376	A
25	BA	2383	G
25	BA	2385	C
25	BA	2402	U
25	BA	2403	C
25	BA	2406	A
25	BA	2410	G
25	BA	2423	U
25	BA	2424	C
25	BA	2425	A
25	BA	2426	A
25	BA	2429	G
25	BA	2430	A
25	BA	2431	U
25	BA	2435	A
25	BA	2441	U
25	BA	2445	2MG
25	BA	2448	A
25	BA	2470	G
25	BA	2474	U
25	BA	2476	A
25	BA	2478	A
25	BA	2491	U
25	BA	2502	G
25	BA	2504	PSU
25	BA	2505	G
25	BA	2512	C
25	BA	2513	A
25	BA	2518	A
25	BA	2520	C
25	BA	2525	G
25	BA	2529	G
25	BA	2535	G
25	BA	2547	A
25	BA	2552	OMU
25	BA	2554	U
25	BA	2566	A
25	BA	2567	G

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Mol	Chain	Res	Type
25	BA	2573	C
25	BA	2574	G
25	BA	2585	U
25	BA	2586	U
25	BA	2602	A
25	BA	2609	U
25	BA	2610	C
25	BA	2611	C
25	BA	2613	U
25	BA	2629	U
25	BA	2630	G
25	BA	2663	G
25	BA	2671	G
25	BA	2682	A
25	BA	2689	U
25	BA	2690	U
25	BA	2714	G
25	BA	2716	C
25	BA	2726	A
25	BA	2744	G
25	BA	2748	A
25	BA	2757	A
25	BA	2762	C
25	BA	2778	A
25	BA	2791	G
25	BA	2797	U
25	BA	2798	U
25	BA	2799	G
25	BA	2801	G
25	BA	2818	U
25	BA	2820	A
25	BA	2825	G
25	BA	2849	U
25	BA	2859	G
25	BA	2861	U
25	BA	2867	G
25	BA	2872	A
25	BA	2874	C
25	BA	2879	A
25	BA	2880	C
25	BA	2883	A
25	BA	2884	U

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Mol	Chain	Res	Type
25	BA	2885	G
25	BA	2886	A
25	BA	2891	U
25	BA	2902	C
25	BA	2903	U
26	BB	13	G
26	BB	16	G
26	BB	35	C
26	BB	36	C
26	BB	45	A
26	BB	56	G
26	BB	64	G
26	BB	66	A
26	BB	89	U
26	BB	90	C
26	BB	99	A
26	BB	109	A

All (104) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	70	U
1	AA	147	G
1	AA	181	A
1	AA	182	A
1	AA	183	C
1	AA	197	A
1	AA	209	U
1	AA	428	G
1	AA	481	G
1	AA	587	G
1	AA	641	U
1	AA	701	U
1	AA	793	U
1	AA	873	A
1	AA	961	U
1	AA	991	U
1	AA	992	U
1	AA	1166	G
1	AA	1167	A
1	AA	1196	A

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Mol	Chain	Res	Type
1	AA	1211	U
1	AA	1213	A
1	AA	1214	C
1	AA	1299	A
1	AA	1363	A
1	AA	1396	A
1	AA	1447	A
22	AV	43	A
23	AW	15	G
23	AW	16	C
23	AW	18	G
23	AW	19	G
23	AW	20	H2U
23	AW	21	A
23	AW	47	U
23	AW	60	U
24	AX	19	G
25	BA	33	C
25	BA	62	U
25	BA	71	A
25	BA	101	A
25	BA	138	U
25	BA	140	C
25	BA	199	A
25	BA	271	G
25	BA	310	A
25	BA	404	A
25	BA	503	A
25	BA	549	C
25	BA	685	A
25	BA	764	A
25	BA	776	G
25	BA	784	G
25	BA	885	C
25	BA	890	C
25	BA	895	U
25	BA	984	A
25	BA	1045	C
25	BA	1060	U
25	BA	1064	C
25	BA	1067	A
25	BA	1069	A

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Mol	Chain	Res	Type
25	BA	1077	A
25	BA	1109	C
25	BA	1111	A
25	BA	1128	G
25	BA	1173	U
25	BA	1300	G
25	BA	1320	C
25	BA	1344	U
25	BA	1379	U
25	BA	1395	A
25	BA	1405	U
25	BA	1407	G
25	BA	1434	A
25	BA	1490	A
25	BA	1494	A
25	BA	1509	A
25	BA	1583	A
25	BA	1584	U
25	BA	1608	A
25	BA	1913	A
25	BA	1918	A
25	BA	2062	A
25	BA	2191	A
25	BA	2197	U
25	BA	2198	A
25	BA	2210	U
25	BA	2212	A
25	BA	2225	A
25	BA	2250	G
25	BA	2296	U
25	BA	2308	G
25	BA	2425	A
25	BA	2573	C
25	BA	2585	U
25	BA	2602	A
25	BA	2610	C
25	BA	2756	U
25	BA	2797	U
25	BA	2798	U
25	BA	2873	A
26	BB	1	U

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

53 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	$\#\|Z\| > 2$
25	2MG	BA	2445	29,25	18,26,27	2.24	7 (38%)	16,38,41	1.75	4 (25%)
24	H2U	AX	20	24	18,21,22	3.12	5 (27%)	21,30,33	1.95	5 (23%)
1	MA6	AA	1518	1	18,26,27	1.33	3 (16%)	19,38,41	4.05	2 (10%)
24	PSU	AX	32	24	18,21,22	1.01	1 (5%)	22,30,33	1.72	4 (18%)
1	2MG	AA	1207	1,62	18,26,27	2.32	7 (38%)	16,38,41	1.72	4 (25%)
25	H2U	BA	2449	25	18,21,22	2.85	5 (27%)	21,30,33	2.13	5 (23%)
1	2MG	AA	1516	1	18,26,27	2.27	7 (38%)	16,38,41	1.64	4 (25%)
24	PSU	AX	39	24	18,21,22	1.05	1 (5%)	22,30,33	1.85	5 (22%)
24	MIA	AX	37	24	22,29,32	2.86	4 (18%)	22,41,47	2.73	7 (31%)
25	OMC	BA	2498	62,25	19,22,23	2.81	7 (36%)	26,31,34	0.96	1 (3%)
25	2MA	BA	2503	62,25	17,25,26	2.59	7 (41%)	17,37,40	1.52	4 (23%)
23	5MU	AW	54	23	19,22,23	1.39	5 (26%)	28,32,35	2.11	6 (21%)
25	5MU	BA	1939	62,25	19,22,23	1.46	4 (21%)	28,32,35	2.32	6 (21%)
1	PSU	AA	516	1	18,21,22	1.14	2 (11%)	22,30,33	2.15	6 (27%)
24	3AU	AX	47	24	18,21,29	3.43	8 (44%)	26,30,43	1.72	5 (19%)
23	OMC	AW	32	23	19,22,23	2.81	8 (42%)	26,31,34	0.78	0
25	3TD	BA	1915	25	18,22,23	4.42	10 (55%)	22,32,35	2.19	4 (18%)
1	UR3	AA	1498	1	19,22,23	2.50	6 (31%)	26,32,35	1.25	2 (7%)
25	5MC	BA	1962	25	18,22,23	3.75	7 (38%)	26,32,35	1.08	4 (15%)
25	PSU	BA	2457	25	18,21,22	1.12	2 (11%)	22,30,33	2.00	5 (22%)
25	1MG	BA	745	25	18,26,27	2.60	5 (27%)	19,39,42	1.45	3 (15%)
1	5MC	AA	967	1	18,22,23	3.75	7 (38%)	26,32,35	1.04	2 (7%)
25	PSU	BA	955	25	18,21,22	1.11	2 (11%)	22,30,33	1.94	5 (22%)
1	5MC	AA	1407	1	18,22,23	3.77	7 (38%)	26,32,35	1.07	2 (7%)
25	PSU	BA	1911	25	18,21,22	1.09	1 (5%)	22,30,33	1.85	4 (18%)
23	H2U	AW	20	23	18,21,22	3.00	5 (27%)	21,30,33	2.25	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	7MG	AX	46	24	22,26,27	3.86	10 (45%)	29,39,42	2.00	9 (31%)
25	OMU	BA	2552	25	19,22,23	2.83	7 (36%)	26,31,34	1.76	4 (15%)
25	PSU	BA	2605	25	18,21,22	1.08	2 (11%)	22,30,33	1.90	4 (18%)
25	5MU	BA	747	25	19,22,23	1.40	4 (21%)	28,32,35	2.28	6 (21%)
1	2MG	AA	966	1	18,26,27	2.30	7 (38%)	16,38,41	1.75	5 (31%)
1	G7M	AA	527	1	20,26,27	2.17	8 (40%)	17,39,42	1.32	2 (11%)
23	PSU	AW	55	23	18,21,22	1.07	1 (5%)	22,30,33	1.86	6 (27%)
25	6MZ	BA	2030	25	18,25,26	1.92	2 (11%)	16,36,39	2.50	3 (18%)
24	H2U	AX	16	24	18,21,22	3.02	5 (27%)	21,30,33	2.05	5 (23%)
24	PSU	AX	55	24	18,21,22	1.05	1 (5%)	22,30,33	1.87	5 (22%)
25	PSU	BA	2580	25	18,21,22	1.09	3 (16%)	22,30,33	2.07	6 (27%)
28	MEQ	BD	150	28	8,9,10	0.89	0	5,10,12	0.55	0
25	G7M	BA	2069	25	20,26,27	2.28	8 (40%)	17,39,42	1.31	3 (17%)
23	4SU	AW	8	23	18,21,22	4.08	8 (44%)	26,30,33	2.30	5 (19%)
1	4OC	AA	1402	1,62	20,23,24	3.24	9 (45%)	26,32,35	0.97	1 (3%)
25	PSU	BA	1917	25	18,21,22	1.07	2 (11%)	22,30,33	1.87	5 (22%)
25	2MG	BA	1835	25	18,26,27	2.26	7 (38%)	16,38,41	1.79	4 (25%)
24	4SU	AX	8	24	18,21,22	4.08	8 (44%)	26,30,33	2.34	5 (19%)
36	4D4	BN	81	36	9,11,12	2.51	3 (33%)	8,13,15	0.83	0
25	OMG	BA	2251	25,23	18,26,27	2.56	8 (44%)	19,38,41	1.54	4 (21%)
12	D2T	AL	89	12	7,9,10	1.01	0	6,11,13	2.45	4 (66%)
24	5MU	AX	54	24	19,22,23	1.36	5 (26%)	28,32,35	2.06	7 (25%)
25	6MZ	BA	1618	25	18,25,26	1.86	3 (16%)	16,36,39	2.37	4 (25%)
25	PSU	BA	2604	25	18,21,22	1.05	1 (5%)	22,30,33	1.91	5 (22%)
25	PSU	BA	2504	25	18,21,22	1.04	1 (5%)	22,30,33	1.91	4 (18%)
1	MA6	AA	1519	1	18,26,27	1.33	3 (16%)	19,38,41	4.10	2 (10%)
25	PSU	BA	746	62,25	18,21,22	1.07	3 (16%)	22,30,33	1.97	7 (31%)

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
25	2MG	BA	2445	29,25	-	2/5/27/28	0/3/3/3
24	H2U	AX	20	24	-	3/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
24	PSU	AX	32	24	-	0/7/25/26	0/2/2/2
1	2MG	AA	1207	1,62	-	1/5/27/28	0/3/3/3
25	H2U	BA	2449	25	-	0/7/38/39	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
24	PSU	AX	39	24	-	0/7/25/26	0/2/2/2
24	MIA	AX	37	24	-	4/9/31/34	0/3/3/3
25	OMC	BA	2498	62,25	-	2/9/27/28	0/2/2/2
25	2MA	BA	2503	62,25	-	2/3/25/26	0/3/3/3
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2
25	5MU	BA	1939	62,25	-	2/7/25/26	0/2/2/2
1	PSU	AA	516	1	-	2/7/25/26	0/2/2/2
24	3AU	AX	47	24	-	2/7/25/35	0/2/2/2
23	OMC	AW	32	23	-	0/9/27/28	0/2/2/2
25	3TD	BA	1915	25	-	2/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
25	5MC	BA	1962	25	-	0/7/25/26	0/2/2/2
25	PSU	BA	2457	25	-	0/7/25/26	0/2/2/2
25	1MG	BA	745	25	-	0/3/25/26	0/3/3/3
1	5MC	AA	967	1	-	3/7/25/26	0/2/2/2
25	PSU	BA	955	25	-	0/7/25/26	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
25	PSU	BA	1911	25	-	1/7/25/26	0/2/2/2
23	H2U	AW	20	23	-	2/7/38/39	0/2/2/2
24	7MG	AX	46	24	-	3/7/37/38	0/3/3/3
25	OMU	BA	2552	25	-	2/9/27/28	0/2/2/2
25	PSU	BA	2605	25	-	0/7/25/26	0/2/2/2
25	5MU	BA	747	25	-	0/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	2/5/27/28	0/3/3/3
1	G7M	AA	527	1	-	1/3/25/26	0/3/3/3
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
25	6MZ	BA	2030	25	-	2/5/27/28	0/3/3/3
24	H2U	AX	16	24	-	3/7/38/39	0/2/2/2
24	PSU	AX	55	24	-	1/7/25/26	0/2/2/2
25	PSU	BA	2580	25	-	0/7/25/26	0/2/2/2
28	MEQ	BD	150	28	-	2/8/9/11	-
25	G7M	BA	2069	25	-	2/3/25/26	0/3/3/3
23	4SU	AW	8	23	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4OC	AA	1402	1,62	-	0/9/29/30	0/2/2/2
25	PSU	BA	1917	25	-	2/7/25/26	0/2/2/2
25	2MG	BA	1835	25	-	0/5/27/28	0/3/3/3
24	4SU	AX	8	24	-	2/7/25/26	0/2/2/2
36	4D4	BN	81	36	-	7/11/12/14	-
25	OMG	BA	2251	25,23	-	1/5/27/28	0/3/3/3
12	D2T	AL	89	12	-	1/7/12/14	-
24	5MU	AX	54	24	-	0/7/25/26	0/2/2/2
25	6MZ	BA	1618	25	-	2/5/27/28	0/3/3/3
25	PSU	BA	2604	25	-	0/7/25/26	0/2/2/2
25	PSU	BA	2504	25	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	3/7/29/30	0/3/3/3
25	PSU	BA	746	62,25	-	2/7/25/26	0/2/2/2

All (252) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1915	3TD	C6-C5	11.77	1.49	1.35
24	AX	37	MIA	C13-C14	9.69	1.60	1.32
25	BA	1915	3TD	C2-N1	9.63	1.49	1.37
1	AA	1407	5MC	C6-C5	9.59	1.50	1.34
24	AX	20	H2U	C2-N1	9.57	1.49	1.35
23	AW	20	H2U	C2-N1	9.32	1.48	1.35
24	AX	16	H2U	C2-N1	9.27	1.48	1.35
1	AA	967	5MC	C6-C5	9.23	1.49	1.34
23	AW	8	4SU	C4-N3	9.23	1.47	1.37
25	BA	1962	5MC	C6-C5	9.19	1.49	1.34
24	AX	46	7MG	C8-N9	9.12	1.51	1.46
24	AX	8	4SU	C4-N3	9.08	1.47	1.37
25	BA	2449	H2U	C2-N1	8.27	1.47	1.35
24	AX	46	7MG	C5-N7	7.94	1.44	1.35
24	AX	37	MIA	C6-N6	7.74	1.48	1.34
24	AX	47	3AU	C2-N1	7.63	1.50	1.38
24	AX	8	4SU	C2-N1	7.59	1.50	1.38
25	BA	745	1MG	C2-N3	7.53	1.48	1.34
23	AW	8	4SU	C2-N1	7.39	1.50	1.38
24	AX	47	3AU	C6-C5	7.07	1.51	1.35
1	AA	967	5MC	C4-N3	7.04	1.46	1.34
25	BA	1962	5MC	C4-N3	7.03	1.46	1.34
25	BA	2503	2MA	C2-N3	6.97	1.46	1.31
1	AA	1407	5MC	C4-N3	6.66	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	20	H2U	C2-N3	6.63	1.49	1.38
1	AA	1402	4OC	C4-N3	6.53	1.44	1.32
23	AW	8	4SU	C2-N3	6.48	1.49	1.38
24	AX	47	3AU	C2-N3	6.48	1.49	1.38
24	AX	8	4SU	C2-N3	6.45	1.49	1.38
25	BA	1962	5MC	C2-N3	6.40	1.49	1.36
1	AA	967	5MC	C2-N3	6.30	1.49	1.36
1	AA	1407	5MC	C2-N3	6.28	1.49	1.36
25	BA	2552	OMU	C2-N3	6.27	1.49	1.38
24	AX	16	H2U	C2-N3	6.27	1.49	1.38
25	BA	2030	6MZ	C6-N6	6.26	1.45	1.35
25	BA	1618	6MZ	C6-N6	6.19	1.45	1.35
1	AA	1402	4OC	C6-C5	6.19	1.49	1.35
23	AW	20	H2U	C2-N3	6.18	1.49	1.38
1	AA	1498	UR3	C2-N1	6.15	1.47	1.38
25	BA	2449	H2U	C2-N3	6.08	1.48	1.38
24	AX	8	4SU	C6-C5	6.01	1.49	1.35
23	AW	8	4SU	C6-C5	6.00	1.49	1.35
25	BA	2498	OMC	C2-N3	5.95	1.48	1.36
23	AW	32	OMC	C2-N3	5.94	1.48	1.36
25	BA	1915	3TD	C6-N1	5.87	1.46	1.36
36	BN	81	4D4	CZ-NE	5.86	1.44	1.33
24	AX	46	7MG	C4-N3	5.84	1.48	1.34
25	BA	2552	OMU	C6-C5	5.84	1.48	1.35
24	AX	46	7MG	C2-N3	5.84	1.47	1.33
1	AA	1498	UR3	C6-C5	5.73	1.48	1.35
25	BA	2498	OMC	C6-C5	5.65	1.48	1.35
1	AA	1402	4OC	C2-N3	5.65	1.47	1.36
23	AW	32	OMC	C6-C5	5.62	1.48	1.35
23	AW	8	4SU	C4-S4	-5.57	1.57	1.68
24	AX	8	4SU	C5-C4	5.57	1.49	1.42
24	AX	46	7MG	C4-N9	5.52	1.44	1.37
24	AX	8	4SU	C4-S4	-5.43	1.58	1.68
23	AW	8	4SU	C5-C4	5.42	1.49	1.42
25	BA	1962	5MC	C4-N4	5.26	1.47	1.34
1	AA	1407	5MC	C4-N4	5.19	1.47	1.34
25	BA	2251	OMG	C2-N2	5.17	1.46	1.34
1	AA	967	5MC	C4-N4	5.15	1.47	1.34
25	BA	745	1MG	C2-N2	5.12	1.43	1.34
25	BA	2503	2MA	C4-N3	5.11	1.49	1.37
24	AX	20	H2U	C4-N3	5.10	1.46	1.37
24	AX	47	3AU	C4-N3	5.07	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1915	3TD	C1'-C5	-5.05	1.38	1.50
25	BA	2251	OMG	C4-N3	5.00	1.49	1.37
1	AA	1402	4OC	O2-C2	-5.00	1.14	1.23
25	BA	2251	OMG	C2-N3	4.92	1.45	1.33
25	BA	2552	OMU	C2-N1	4.92	1.46	1.38
1	AA	1407	5MC	C6-N1	4.85	1.46	1.38
1	AA	967	5MC	C6-N1	4.82	1.46	1.38
24	AX	46	7MG	C2-N2	4.81	1.45	1.34
24	AX	16	H2U	C4-N3	4.78	1.45	1.37
25	BA	1962	5MC	C6-N1	4.78	1.46	1.38
23	AW	20	H2U	C4-N3	4.73	1.45	1.37
1	AA	966	2MG	C2-N2	4.68	1.43	1.33
23	AW	32	OMC	C4-N4	4.68	1.44	1.33
1	AA	1402	4OC	C4-N4	4.68	1.45	1.35
25	BA	2069	G7M	C2-N3	4.67	1.44	1.33
25	BA	2498	OMC	C4-N4	4.67	1.44	1.33
25	BA	2498	OMC	C4-N3	4.63	1.43	1.34
23	AW	32	OMC	C4-N3	4.61	1.43	1.34
25	BA	745	1MG	C4-N3	4.44	1.48	1.37
25	BA	2069	G7M	C2-N2	4.42	1.44	1.34
25	BA	2449	H2U	C4-N3	4.42	1.45	1.37
1	AA	1498	UR3	C2-N3	4.40	1.47	1.39
1	AA	1516	2MG	C2-N2	4.37	1.43	1.33
1	AA	527	G7M	C2-N3	4.36	1.43	1.33
1	AA	1207	2MG	C2-N2	4.36	1.43	1.33
25	BA	2069	G7M	C4-N3	4.35	1.47	1.37
25	BA	1962	5MC	C2-N1	4.32	1.49	1.40
25	BA	1915	3TD	C2-N3	4.30	1.48	1.38
1	AA	1407	5MC	C2-N1	4.26	1.49	1.40
1	AA	527	G7M	C2-N2	4.17	1.44	1.34
25	BA	2445	2MG	C2-N2	4.17	1.42	1.33
25	BA	1835	2MG	C2-N2	4.11	1.42	1.33
1	AA	527	G7M	C4-N3	4.10	1.47	1.37
24	AX	46	7MG	C2-N1	4.05	1.47	1.37
1	AA	1402	4OC	C5-C4	4.03	1.49	1.40
1	AA	967	5MC	C2-N1	4.02	1.48	1.40
23	AW	32	OMC	C2-N1	4.00	1.48	1.40
1	AA	966	2MG	C6-N1	3.97	1.43	1.37
25	BA	2552	OMU	O4-C4	-3.95	1.16	1.24
25	BA	2498	OMC	C2-N1	3.92	1.48	1.40
24	AX	46	7MG	C5-C6	3.91	1.53	1.43
25	BA	1835	2MG	C6-N1	3.90	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1207	2MG	C6-N1	3.85	1.43	1.37
25	BA	2552	OMU	C4-N3	3.78	1.45	1.38
1	AA	1516	2MG	C2-N1	3.77	1.42	1.36
1	AA	1516	2MG	C6-N1	3.76	1.43	1.37
1	AA	966	2MG	C2-N1	3.72	1.42	1.36
1	AA	1207	2MG	C4-N3	3.70	1.46	1.37
1	AA	966	2MG	C4-N3	3.70	1.46	1.37
25	BA	2445	2MG	C4-N3	3.69	1.46	1.37
25	BA	1835	2MG	C2-N1	3.68	1.42	1.36
25	BA	1835	2MG	C4-N3	3.66	1.46	1.37
1	AA	1207	2MG	C2-N1	3.65	1.42	1.36
25	BA	2445	2MG	C6-N1	3.64	1.43	1.37
25	BA	1835	2MG	O6-C6	-3.63	1.15	1.23
25	BA	2552	OMU	O2-C2	-3.61	1.16	1.23
1	AA	1402	4OC	C2-N1	3.61	1.47	1.40
24	AX	46	7MG	O6-C6	-3.61	1.16	1.23
25	BA	2445	2MG	O6-C6	-3.59	1.16	1.23
1	AA	1516	2MG	O6-C6	-3.55	1.16	1.23
1	AA	1207	2MG	O6-C6	-3.52	1.16	1.23
25	BA	2445	2MG	C2-N1	3.51	1.42	1.36
25	BA	2069	G7M	C6-N1	3.51	1.43	1.37
25	BA	1915	3TD	O2-C2	-3.49	1.16	1.23
25	BA	1939	5MU	C4-N3	-3.43	1.32	1.38
25	BA	2251	OMG	C6-N1	3.41	1.43	1.37
24	AX	47	3AU	C6-N1	3.39	1.46	1.38
1	AA	1516	2MG	C4-N3	3.39	1.45	1.37
1	AA	966	2MG	O6-C6	-3.35	1.16	1.23
25	BA	2503	2MA	C6-N1	3.29	1.45	1.38
24	AX	8	4SU	O2-C2	-3.27	1.17	1.23
1	AA	1207	2MG	C5-C4	-3.27	1.34	1.43
1	AA	527	G7M	C6-N1	3.26	1.42	1.37
36	BN	81	4D4	CZ-NH2	3.25	1.45	1.32
23	AW	8	4SU	O2-C2	-3.24	1.17	1.23
24	AX	46	7MG	C6-N1	3.22	1.44	1.38
24	AX	55	PSU	C6-C5	3.21	1.39	1.35
1	AA	1402	4OC	CM4-N4	3.19	1.51	1.45
25	BA	747	5MU	C4-N3	-3.19	1.32	1.38
25	BA	2251	OMG	C5-C4	-3.18	1.35	1.43
24	AX	39	PSU	C6-C5	3.17	1.39	1.35
1	AA	1518	MA6	C5-C4	-3.16	1.32	1.40
23	AW	55	PSU	C6-C5	3.15	1.39	1.35
25	BA	2030	6MZ	C5-C4	-3.15	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1516	2MG	C5-C4	-3.15	1.35	1.43
25	BA	2445	2MG	C5-C4	-3.14	1.35	1.43
1	AA	1519	MA6	C5-C4	-3.14	1.32	1.40
25	BA	1835	2MG	C5-C4	-3.09	1.35	1.43
24	AX	8	4SU	C6-N1	3.08	1.45	1.38
1	AA	966	2MG	C5-C4	-3.07	1.35	1.43
23	AW	32	OMC	O2-C2	-3.06	1.18	1.23
25	BA	1618	6MZ	C5-C4	-3.05	1.32	1.40
25	BA	1915	3TD	O4-C4	-3.05	1.16	1.23
23	AW	8	4SU	C6-N1	3.04	1.45	1.38
25	BA	2498	OMC	O2-C2	-3.04	1.18	1.23
24	AX	47	3AU	O4-C4	-2.93	1.18	1.24
25	BA	2503	2MA	C5-C4	-2.93	1.35	1.43
24	AX	32	PSU	C6-C5	2.91	1.38	1.35
25	BA	1939	5MU	C6-N1	-2.89	1.33	1.38
1	AA	967	5MC	O2-C2	-2.88	1.18	1.23
1	AA	516	PSU	C6-C5	2.88	1.38	1.35
25	BA	1911	PSU	C6-C5	2.88	1.38	1.35
25	BA	2498	OMC	C6-N1	2.86	1.44	1.38
25	BA	747	5MU	C6-N1	-2.85	1.33	1.38
24	AX	47	3AU	C5-C4	2.83	1.49	1.43
1	AA	1402	4OC	C6-N1	2.83	1.44	1.38
25	BA	2504	PSU	C6-C5	2.82	1.38	1.35
25	BA	1939	5MU	C2-N3	-2.82	1.32	1.38
23	AW	54	5MU	C4-N3	-2.81	1.33	1.38
24	AX	54	5MU	C4-N3	-2.80	1.33	1.38
25	BA	2604	PSU	C6-C5	2.80	1.38	1.35
25	BA	2445	2MG	C5-C6	2.78	1.53	1.47
1	AA	1407	5MC	O2-C2	-2.77	1.18	1.23
25	BA	1917	PSU	C6-C5	2.74	1.38	1.35
1	AA	1519	MA6	C10-N6	2.74	1.52	1.45
1	AA	1518	MA6	C2-N3	2.72	1.36	1.32
24	AX	37	MIA	C5-C4	-2.71	1.33	1.40
1	AA	1518	MA6	C10-N6	2.71	1.51	1.45
23	AW	32	OMC	C6-N1	2.70	1.44	1.38
1	AA	1207	2MG	C5-C6	2.69	1.52	1.47
25	BA	1962	5MC	O2-C2	-2.69	1.18	1.23
25	BA	2251	OMG	C5-C6	2.67	1.52	1.47
25	BA	955	PSU	C6-C5	2.67	1.38	1.35
1	AA	1498	UR3	O4-C4	-2.65	1.17	1.23
1	AA	527	G7M	C5-C6	2.64	1.52	1.45
25	BA	2503	2MA	CM2-C2	2.64	1.56	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	2069	G7M	C5-C6	2.64	1.52	1.45
25	BA	1915	3TD	C10-N3	2.63	1.51	1.47
25	BA	2580	PSU	C6-C5	2.62	1.38	1.35
1	AA	1516	2MG	C5-C6	2.62	1.52	1.47
25	BA	2449	H2U	O4-C4	-2.60	1.18	1.23
25	BA	2449	H2U	O2-C2	-2.59	1.18	1.23
25	BA	1835	2MG	C5-C6	2.57	1.52	1.47
24	AX	47	3AU	O2-C2	-2.56	1.18	1.23
25	BA	2457	PSU	C6-C5	2.54	1.38	1.35
1	AA	527	G7M	O6-C6	-2.54	1.18	1.23
25	BA	2069	G7M	O6-C6	-2.53	1.18	1.23
25	BA	2069	G7M	C2-N1	2.52	1.43	1.37
1	AA	966	2MG	C5-C6	2.52	1.52	1.47
24	AX	54	5MU	C6-N1	-2.51	1.33	1.38
25	BA	747	5MU	C2-N3	-2.51	1.33	1.38
25	BA	1915	3TD	C4-N3	2.50	1.45	1.40
1	AA	1519	MA6	C2-N3	2.50	1.36	1.32
25	BA	746	PSU	C6-C5	2.47	1.38	1.35
25	BA	2503	2MA	C2-N1	2.47	1.44	1.36
23	AW	54	5MU	C6-N1	-2.43	1.33	1.38
1	AA	1498	UR3	O2-C2	-2.43	1.18	1.22
1	AA	1498	UR3	C6-N1	2.41	1.43	1.38
25	BA	2251	OMG	C2-N1	2.41	1.43	1.37
25	BA	1939	5MU	C6-C5	2.41	1.38	1.34
25	BA	2251	OMG	O6-C6	-2.40	1.18	1.23
24	AX	16	H2U	O2-C2	-2.39	1.18	1.23
25	BA	747	5MU	C6-C5	2.39	1.38	1.34
25	BA	745	1MG	C5-C4	-2.38	1.37	1.43
23	AW	54	5MU	C6-C5	2.36	1.38	1.34
25	BA	2605	PSU	C6-C5	2.36	1.38	1.35
23	AW	20	H2U	O2-C2	-2.34	1.18	1.23
36	BN	81	4D4	CZ-NH1	-2.34	1.25	1.34
1	AA	527	G7M	C2-N1	2.34	1.43	1.37
25	BA	2605	PSU	C4-C5	-2.32	1.37	1.44
24	AX	20	H2U	O2-C2	-2.30	1.18	1.23
24	AX	37	MIA	C2-N3	2.30	1.35	1.32
24	AX	54	5MU	C2-N3	-2.29	1.33	1.38
25	BA	746	PSU	C4-C5	-2.27	1.37	1.44
25	BA	2069	G7M	C5-C4	-2.27	1.34	1.39
25	BA	2552	OMU	C6-N1	2.27	1.43	1.38
25	BA	1915	3TD	O4'-C1'	-2.27	1.40	1.43
23	AW	54	5MU	C2-N3	-2.25	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	16	H2U	O4-C4	-2.23	1.18	1.23
1	AA	516	PSU	C4-C5	-2.22	1.37	1.44
23	AW	54	5MU	C4-C5	2.21	1.48	1.44
24	AX	54	5MU	C6-C5	2.18	1.38	1.34
1	AA	527	G7M	C5-C4	-2.17	1.34	1.39
25	BA	1618	6MZ	C2-N3	2.16	1.35	1.32
25	BA	746	PSU	O4'-C1'	-2.12	1.40	1.43
24	AX	20	H2U	O4-C4	-2.10	1.19	1.23
23	AW	20	H2U	O4-C4	-2.09	1.19	1.23
25	BA	2457	PSU	C4-C5	-2.09	1.38	1.44
25	BA	955	PSU	C4-C5	-2.08	1.38	1.44
25	BA	2503	2MA	C8-N7	2.08	1.38	1.35
23	AW	32	OMC	C5-C4	2.08	1.47	1.42
25	BA	2580	PSU	O4'-C1'	-2.07	1.41	1.43
25	BA	2580	PSU	C4-C5	-2.07	1.38	1.44
25	BA	1917	PSU	O4'-C1'	-2.06	1.41	1.43
24	AX	54	5MU	C4-C5	2.02	1.48	1.44
25	BA	745	1MG	C5-C6	2.01	1.53	1.47

All (220) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1519	MA6	N1-C6-N6	-16.64	99.54	117.06
1	AA	1518	MA6	N1-C6-N6	-16.52	99.67	117.06
24	AX	8	4SU	C4-N3-C2	-8.27	119.31	127.34
24	AX	37	MIA	C12-C13-C14	-8.16	111.27	127.14
23	AW	8	4SU	C4-N3-C2	-8.08	119.49	127.34
23	AW	20	H2U	C4-N3-C2	-7.43	119.63	125.79
25	BA	2449	H2U	C4-N3-C2	-7.37	119.67	125.79
24	AX	16	H2U	C4-N3-C2	-7.16	119.86	125.79
25	BA	1915	3TD	N1-C2-N3	6.93	121.61	116.14
25	BA	2030	6MZ	C9-N6-C6	-6.86	116.97	122.87
24	AX	20	H2U	C4-N3-C2	-6.68	120.25	125.79
25	BA	1618	6MZ	C9-N6-C6	-6.22	117.51	122.87
25	BA	1939	5MU	C4-N3-C2	-5.85	119.77	127.35
25	BA	747	5MU	C4-N3-C2	-5.73	119.93	127.35
24	AX	8	4SU	C5-C4-N3	5.68	119.96	114.69
25	BA	1618	6MZ	N3-C2-N1	-5.68	119.81	128.68
1	AA	1518	MA6	N3-C2-N1	-5.65	119.85	128.68
1	AA	1519	MA6	N3-C2-N1	-5.64	119.87	128.68
24	AX	37	MIA	N3-C2-N1	-5.57	119.98	128.68
25	BA	1939	5MU	N3-C2-N1	5.57	122.28	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AW	8	4SU	C5-C4-N3	5.54	119.83	114.69
25	BA	2030	6MZ	N3-C2-N1	-5.48	120.11	128.68
25	BA	2552	OMU	C4-N3-C2	-5.36	119.51	126.58
25	BA	747	5MU	N3-C2-N1	5.36	122.00	114.89
23	AW	54	5MU	C4-N3-C2	-5.16	120.67	127.35
24	AX	54	5MU	C4-N3-C2	-5.12	120.72	127.35
24	AX	46	7MG	C5-C6-N1	5.12	120.02	110.99
25	BA	2605	PSU	C4-N3-C2	-5.12	118.96	126.34
25	BA	2457	PSU	N1-C2-N3	5.06	120.86	115.13
1	AA	516	PSU	C4-N3-C2	-5.03	119.09	126.34
24	AX	47	3AU	C4-N3-C2	-5.01	119.97	126.58
1	AA	516	PSU	N1-C2-N3	5.01	120.81	115.13
25	BA	955	PSU	N1-C2-N3	5.01	120.80	115.13
25	BA	2604	PSU	N1-C2-N3	4.99	120.79	115.13
25	BA	2457	PSU	C4-N3-C2	-4.99	119.15	126.34
25	BA	955	PSU	C4-N3-C2	-4.97	119.17	126.34
25	BA	1939	5MU	C5-C6-N1	-4.95	118.24	123.34
25	BA	2580	PSU	C4-N3-C2	-4.84	119.36	126.34
25	BA	1911	PSU	C4-N3-C2	-4.83	119.38	126.34
25	BA	2580	PSU	N1-C2-N3	4.81	120.58	115.13
25	BA	1939	5MU	C5-C4-N3	4.80	119.41	115.31
25	BA	1917	PSU	N1-C2-N3	4.80	120.57	115.13
24	AX	54	5MU	N3-C2-N1	4.79	121.25	114.89
25	BA	2504	PSU	C4-N3-C2	-4.79	119.44	126.34
25	BA	2604	PSU	C4-N3-C2	-4.77	119.46	126.34
25	BA	1911	PSU	N1-C2-N3	4.76	120.52	115.13
25	BA	1915	3TD	C4-N3-C2	-4.74	119.46	124.61
23	AW	54	5MU	N3-C2-N1	4.74	121.18	114.89
24	AX	55	PSU	N1-C2-N3	4.71	120.47	115.13
24	AX	39	PSU	C4-N3-C2	-4.70	119.57	126.34
24	AX	55	PSU	C4-N3-C2	-4.69	119.59	126.34
25	BA	747	5MU	C5-C4-N3	4.68	119.30	115.31
25	BA	2504	PSU	N1-C2-N3	4.65	120.40	115.13
24	AX	39	PSU	N1-C2-N3	4.65	120.40	115.13
25	BA	746	PSU	C4-N3-C2	-4.61	119.69	126.34
25	BA	2605	PSU	N1-C2-N3	4.57	120.31	115.13
25	BA	747	5MU	C5-C6-N1	-4.56	118.65	123.34
24	AX	32	PSU	C4-N3-C2	-4.55	119.78	126.34
23	AW	54	5MU	C5-C4-N3	4.53	119.18	115.31
23	AW	55	PSU	C4-N3-C2	-4.50	119.85	126.34
1	AA	1498	UR3	C4-N3-C2	-4.46	120.37	124.56
24	AX	54	5MU	C5-C4-N3	4.45	119.11	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BA	1917	PSU	C4-N3-C2	-4.45	119.93	126.34
24	AX	37	MIA	C15-C14-C13	-4.41	109.90	122.65
24	AX	46	7MG	C2-N3-C4	4.39	120.12	112.30
24	AX	47	3AU	N3-C2-N1	4.37	120.69	114.89
24	AX	32	PSU	N1-C2-N3	4.36	120.07	115.13
25	BA	1835	2MG	CM2-N2-C2	-4.30	114.36	123.86
25	BA	746	PSU	N1-C2-N3	4.24	119.93	115.13
25	BA	745	1MG	C5-C6-N1	4.12	120.09	113.90
25	BA	1939	5MU	O4-C4-C5	-4.09	120.16	124.90
24	AX	8	4SU	N3-C2-N1	4.09	120.32	114.89
23	AW	55	PSU	N1-C2-N3	4.09	119.76	115.13
25	BA	747	5MU	O4-C4-C5	-4.06	120.20	124.90
23	AW	8	4SU	N3-C2-N1	3.98	120.17	114.89
25	BA	2552	OMU	N3-C2-N1	3.94	120.12	114.89
24	AX	37	MIA	C16-C14-C13	-3.91	111.36	122.65
24	AX	54	5MU	O4-C4-C5	-3.90	120.38	124.90
1	AA	1207	2MG	C5-C6-N1	3.90	120.84	113.95
24	AX	46	7MG	C5-C4-N3	-3.90	120.70	128.13
25	BA	2030	6MZ	C2-N1-C6	3.89	119.93	116.59
23	AW	54	5MU	C5-C6-N1	-3.88	119.35	123.34
23	AW	54	5MU	O4-C4-C5	-3.84	120.45	124.90
25	BA	2445	2MG	C5-C6-N1	3.84	120.74	113.95
25	BA	1835	2MG	C5-C6-N1	3.76	120.59	113.95
25	BA	2503	2MA	C5-C6-N1	3.67	120.35	114.02
1	AA	966	2MG	C5-C6-N1	3.66	120.42	113.95
23	AW	20	H2U	N3-C2-N1	3.66	120.52	116.65
25	BA	2445	2MG	CM2-N2-C2	-3.63	115.85	123.86
12	AL	89	D2T	CB1-SB-CB	3.59	108.94	102.44
25	BA	2552	OMU	C5-C4-N3	3.56	120.16	114.84
1	AA	1516	2MG	C5-C6-N1	3.52	120.17	113.95
25	BA	2251	OMG	C5-C6-N1	3.52	120.16	113.95
23	AW	8	4SU	C5-C4-S4	-3.52	119.93	124.47
24	AX	37	MIA	C2-N1-C6	3.52	119.61	116.59
25	BA	747	5MU	O2-C2-N1	-3.50	118.13	122.79
24	AX	54	5MU	C5-C6-N1	-3.50	119.74	123.34
1	AA	1516	2MG	CM2-N2-C2	-3.39	116.36	123.86
24	AX	8	4SU	C5-C4-S4	-3.38	120.12	124.47
1	AA	1207	2MG	CM2-N2-C2	-3.34	116.49	123.86
24	AX	46	7MG	C5-C4-N9	3.32	110.66	106.35
1	AA	1407	5MC	C5-C6-N1	-3.28	119.96	123.34
24	AX	16	H2U	N3-C2-N1	3.28	120.12	116.65
1	AA	527	G7M	C2-N1-C6	-3.20	119.20	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AX	20	H2U	N3-C2-N1	3.20	120.04	116.65
24	AX	47	3AU	C5-C4-N3	3.16	119.57	114.84
12	AL	89	D2T	OD2-CG-CB	3.14	119.93	113.15
25	BA	2449	H2U	N3-C2-N1	3.10	119.94	116.65
25	BA	1915	3TD	C6-C5-C4	3.10	120.36	118.22
25	BA	1939	5MU	O2-C2-N1	-3.09	118.69	122.79
24	AX	55	PSU	O2-C2-N1	-3.07	119.41	122.79
25	BA	2604	PSU	O2-C2-N1	-3.06	119.42	122.79
25	BA	1618	6MZ	C2-N1-C6	3.06	119.22	116.59
25	BA	1917	PSU	C6-N1-C2	-3.05	119.57	122.68
25	BA	2503	2MA	C8-N7-C5	3.04	108.78	102.99
1	AA	967	5MC	C5-C6-N1	-3.02	120.23	123.34
25	BA	2251	OMG	C8-N7-C5	2.98	108.66	102.99
25	BA	2449	H2U	C5-C4-N3	2.97	119.98	116.65
25	BA	2069	G7M	C2-N1-C6	-2.93	119.70	125.10
1	AA	516	PSU	O2-C2-N1	-2.91	119.59	122.79
25	BA	2457	PSU	O2-C2-N1	-2.90	119.59	122.79
25	BA	2552	OMU	O4-C4-C5	-2.90	120.05	125.16
1	AA	516	PSU	O4'-C1'-C2'	2.90	109.23	105.14
25	BA	2251	OMG	C2-N1-C6	-2.86	119.84	125.10
24	AX	16	H2U	C5-C4-N3	2.86	119.86	116.65
1	AA	1207	2MG	C8-N7-C5	2.85	108.42	102.99
25	BA	2449	H2U	O2-C2-N1	-2.85	119.53	123.11
25	BA	2445	2MG	C8-N7-C5	2.84	108.41	102.99
24	AX	46	7MG	C4-C5-N7	2.84	109.47	105.53
25	BA	2580	PSU	O4'-C1'-C2'	2.83	109.14	105.14
24	AX	46	7MG	C2-N1-C6	-2.83	119.93	125.10
24	AX	39	PSU	O2-C2-N1	-2.81	119.69	122.79
24	AX	47	3AU	O4-C4-C5	-2.80	120.24	125.16
24	AX	20	H2U	C5-C6-N1	2.79	120.82	111.61
23	AW	20	H2U	C5-C4-N3	2.78	119.77	116.65
25	BA	1835	2MG	C8-N7-C5	2.75	108.23	102.99
25	BA	1917	PSU	O2-C2-N1	-2.72	119.80	122.79
25	BA	746	PSU	O2'-C2'-C3'	2.69	120.52	111.82
23	AW	20	H2U	O2-C2-N1	-2.69	119.73	123.11
1	AA	966	2MG	C8-N7-C5	2.68	108.09	102.99
1	AA	516	PSU	C6-N1-C2	-2.68	119.95	122.68
24	AX	16	H2U	C5-C6-N1	2.66	120.36	111.61
25	BA	745	1MG	C8-N7-C5	2.60	107.94	102.99
25	BA	2449	H2U	C5-C6-N1	2.60	120.18	111.61
1	AA	527	G7M	N2-C2-N1	2.60	122.25	116.71
25	BA	2580	PSU	O2-C2-N1	-2.60	119.93	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BA	2503	2MA	CM2-C2-N1	2.59	121.98	116.23
1	AA	966	2MG	O6-C6-C5	-2.58	119.34	124.37
25	BA	2580	PSU	C6-N1-C2	-2.57	120.05	122.68
24	AX	46	7MG	O6-C6-C5	-2.57	121.23	127.54
23	AW	55	PSU	O2-C2-N1	-2.55	119.98	122.79
25	BA	2069	G7M	N2-C2-N1	2.54	122.13	116.71
25	BA	2605	PSU	O2-C2-N1	-2.54	119.99	122.79
25	BA	2498	OMC	O3'-C3'-C2'	2.53	118.35	111.17
1	AA	966	2MG	CM2-N2-C2	-2.51	118.32	123.86
25	BA	2504	PSU	O2-C2-N1	-2.50	120.04	122.79
23	AW	20	H2U	C5-C6-N1	2.50	119.84	111.61
1	AA	1516	2MG	C8-N7-C5	2.49	107.74	102.99
25	BA	2604	PSU	C6-N1-C2	-2.45	120.18	122.68
24	AX	20	H2U	C5-C4-N3	2.44	119.39	116.65
25	BA	746	PSU	C6-C5-C4	2.43	119.90	118.20
25	BA	1962	5MC	C5-C6-N1	-2.43	120.84	123.34
25	BA	955	PSU	O2-C2-N1	-2.42	120.13	122.79
24	AX	37	MIA	C16-C14-C15	-2.42	109.27	114.60
25	BA	2580	PSU	C3'-C2'-C1'	2.40	104.43	101.64
1	AA	1402	4OC	C6-C5-C4	2.39	119.89	116.96
24	AX	54	5MU	O2-C2-N1	-2.38	119.63	122.79
25	BA	2457	PSU	C6-N1-C2	-2.37	120.26	122.68
24	AX	39	PSU	C6-N1-C2	-2.36	120.27	122.68
1	AA	1207	2MG	O6-C6-C5	-2.34	119.81	124.37
25	BA	746	PSU	C3'-C2'-C1'	2.34	104.36	101.64
25	BA	955	PSU	C6-N1-C2	-2.33	120.30	122.68
1	AA	1516	2MG	O6-C6-C5	-2.33	119.81	124.37
24	AX	16	H2U	O2-C2-N1	-2.32	120.20	123.11
25	BA	1911	PSU	O2-C2-N1	-2.31	120.24	122.79
25	BA	746	PSU	O2-C2-N1	-2.30	120.25	122.79
24	AX	32	PSU	O2-C2-N1	-2.29	120.27	122.79
1	AA	966	2MG	O3'-C3'-C4'	2.28	117.66	111.05
25	BA	745	1MG	O6-C6-C5	-2.28	120.16	124.19
24	AX	55	PSU	C6-N1-C2	-2.27	120.36	122.68
23	AW	55	PSU	C3'-C2'-C1'	2.26	104.27	101.64
23	AW	8	4SU	O2-C2-N1	-2.25	119.79	122.79
25	BA	1835	2MG	O6-C6-C5	-2.25	119.97	124.37
25	BA	1915	3TD	O4'-C1'-C2'	2.25	108.31	105.14
25	BA	2503	2MA	N1-C2-N3	-2.23	119.36	123.06
1	AA	516	PSU	C3'-C2'-C1'	2.23	104.24	101.64
23	AW	54	5MU	O2-C2-N1	-2.22	119.83	122.79
25	BA	1618	6MZ	C3'-C2'-C1'	2.21	104.31	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AX	20	H2U	O2-C2-N1	-2.18	120.37	123.11
25	BA	1917	PSU	O4'-C1'-C2'	2.18	108.22	105.14
24	AX	55	PSU	C6-C5-C4	2.18	119.72	118.20
25	BA	1911	PSU	C6-N1-C2	-2.15	120.48	122.68
12	AL	89	D2T	CB-CA-N	2.14	113.67	109.10
24	AX	8	4SU	O2-C2-N1	-2.13	119.95	122.79
25	BA	1962	5MC	C1'-N1-C6	-2.13	117.58	121.12
24	AX	46	7MG	N9-C4-N3	2.12	128.64	125.47
25	BA	2457	PSU	O4'-C1'-C2'	2.12	108.13	105.14
25	BA	2504	PSU	C6-N1-C2	-2.12	120.52	122.68
23	AW	55	PSU	C6-N1-C2	-2.09	120.55	122.68
25	BA	2445	2MG	O6-C6-C5	-2.09	120.29	124.37
1	AA	967	5MC	CM5-C5-C6	-2.08	120.07	122.85
25	BA	2069	G7M	N1-C2-N3	-2.07	119.46	123.32
12	AL	89	D2T	O-C-CA	-2.06	119.37	124.78
1	AA	1407	5MC	CM5-C5-C6	-2.06	120.10	122.85
25	BA	2605	PSU	C6-N1-C2	-2.06	120.58	122.68
23	AW	55	PSU	O4'-C1'-C2'	2.04	108.02	105.14
24	AX	46	7MG	N9-C8-N7	2.04	106.29	103.38
25	BA	1962	5MC	C1'-N1-C2	2.04	122.97	118.42
24	AX	39	PSU	C6-C5-C4	2.02	119.61	118.20
25	BA	1962	5MC	CM5-C5-C6	-2.02	120.15	122.85
1	AA	1498	UR3	C1'-N1-C2	2.02	120.40	116.99
24	AX	47	3AU	O2-C2-N1	-2.02	120.10	122.79
25	BA	2604	PSU	C6-C5-C4	2.02	119.61	118.20
23	AW	20	H2U	O5'-C5'-C4'	2.01	115.84	108.99
25	BA	2251	OMG	O6-C6-C5	-2.01	120.44	124.37
25	BA	746	PSU	C6-N1-C2	-2.01	120.63	122.68
24	AX	32	PSU	C6-N1-C2	-2.01	120.63	122.68
25	BA	955	PSU	C6-C5-C4	2.01	119.60	118.20
24	AX	37	MIA	C12-N6-C6	-2.00	119.58	122.55
24	AX	54	5MU	C5M-C5-C4	2.00	120.97	118.77

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	966	2MG	O4'-C4'-C5'-O5'
1	AA	966	2MG	C3'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
24	AX	37	MIA	C12-C13-C14-C15
24	AX	37	MIA	C12-C13-C14-C16

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Mol	Chain	Res	Type	Atoms
24	AX	46	7MG	O4'-C4'-C5'-O5'
24	AX	46	7MG	C3'-C4'-C5'-O5'
36	BN	81	4D4	C-CA-CB-OB
36	BN	81	4D4	C-CA-CB-CG
36	BN	81	4D4	N-CA-CB-OB
36	BN	81	4D4	N-CA-CB-CG
36	BN	81	4D4	CA-CB-CG-CD
36	BN	81	4D4	OB-CB-CG-CD
23	AW	20	H2U	O4'-C4'-C5'-O5'
25	BA	746	PSU	C2'-C1'-C5-C6
25	BA	1618	6MZ	C3'-C4'-C5'-O5'
25	BA	1915	3TD	O4'-C1'-C5-C4
25	BA	1915	3TD	O4'-C1'-C5-C6
25	BA	2251	OMG	C1'-C2'-O2'-CM2
25	BA	2552	OMU	O4'-C4'-C5'-O5'
1	AA	967	5MC	O4'-C4'-C5'-O5'
1	AA	967	5MC	C3'-C4'-C5'-O5'
1	AA	1519	MA6	C3'-C4'-C5'-O5'
24	AX	8	4SU	C3'-C4'-C5'-O5'
24	AX	8	4SU	O4'-C4'-C5'-O5'
24	AX	47	3AU	C3'-C4'-C5'-O5'
24	AX	47	3AU	O4'-C4'-C5'-O5'
23	AW	20	H2U	C3'-C4'-C5'-O5'
25	BA	1618	6MZ	O4'-C4'-C5'-O5'
25	BA	1917	PSU	O4'-C4'-C5'-O5'
25	BA	2503	2MA	O4'-C4'-C5'-O5'
25	BA	2503	2MA	C3'-C4'-C5'-O5'
25	BA	2552	OMU	C3'-C4'-C5'-O5'
28	BD	150	MEQ	OE1-CD-CG-CB
28	BD	150	MEQ	NE2-CD-CG-CB
1	AA	516	PSU	C3'-C4'-C5'-O5'
25	BA	1917	PSU	C3'-C4'-C5'-O5'
25	BA	2030	6MZ	O4'-C4'-C5'-O5'
25	BA	2445	2MG	C3'-C4'-C5'-O5'
24	AX	16	H2U	O4'-C4'-C5'-O5'
25	BA	2498	OMC	O4'-C4'-C5'-O5'
1	AA	1207	2MG	O4'-C4'-C5'-O5'
1	AA	516	PSU	O4'-C4'-C5'-O5'
25	BA	2498	OMC	C3'-C4'-C5'-O5'
24	AX	37	MIA	N1-C6-N6-C12
24	AX	37	MIA	C5-C6-N6-C12
24	AX	16	H2U	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
24	AX	16	H2U	C4'-C5'-O5'-P
25	BA	2445	2MG	O4'-C4'-C5'-O5'
25	BA	1911	PSU	O4'-C4'-C5'-O5'
25	BA	2030	6MZ	C3'-C4'-C5'-O5'
25	BA	1939	5MU	O4'-C4'-C5'-O5'
24	AX	46	7MG	C4'-C5'-O5'-P
25	BA	2069	G7M	C4'-C5'-O5'-P
24	AX	55	PSU	O4'-C1'-C5-C4
36	BN	81	4D4	CG-CD-NE-CZ
12	AL	89	D2T	CG-CB-SB-CB1
24	AX	20	H2U	O4'-C1'-N1-C6
25	BA	746	PSU	O4'-C1'-C5-C6
1	AA	1519	MA6	C4'-C5'-O5'-P
25	BA	1939	5MU	C3'-C4'-C5'-O5'
25	BA	2069	G7M	O4'-C4'-C5'-O5'
24	AX	20	H2U	C2'-C1'-N1-C2
1	AA	527	G7M	C4'-C5'-O5'-P
1	AA	967	5MC	C4'-C5'-O5'-P
24	AX	20	H2U	C4'-C5'-O5'-P

There are no ring outliers.

21 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1516	2MG	1	0
24	AX	37	MIA	3	0
25	BA	2503	2MA	1	0
25	BA	1915	3TD	1	0
1	AA	1498	UR3	1	0
1	AA	967	5MC	1	0
23	AW	20	H2U	2	0
25	BA	2605	PSU	1	0
1	AA	966	2MG	2	0
1	AA	527	G7M	2	0
23	AW	55	PSU	1	0
25	BA	2030	6MZ	1	0
24	AX	16	H2U	3	0
28	BD	150	MEQ	2	0
25	BA	2069	G7M	2	0
25	BA	1917	PSU	3	0
24	AX	8	4SU	1	0
25	BA	2251	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	AL	89	D2T	2	0
24	AX	54	5MU	1	0
1	AA	1519	MA6	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 492 ligands modelled in this entry, 491 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
63	PHE	AX	101	24	10,11,12	0.62	0	10,13,15	0.22	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
63	PHE	AX	101	24	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	AX	101	PHE	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
60	CD	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CD	1357:ILE	C	1358:PRO	N	1.15

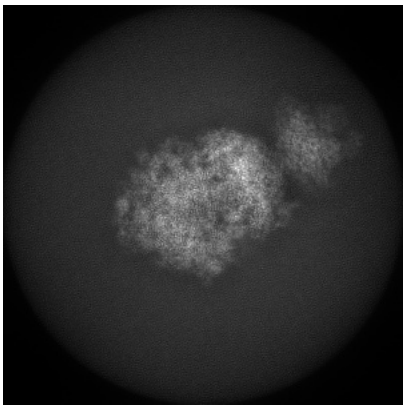
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11422. These allow visual inspection of the internal detail of the map and identification of artifacts.

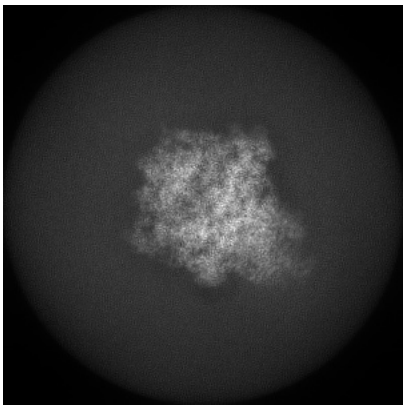
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

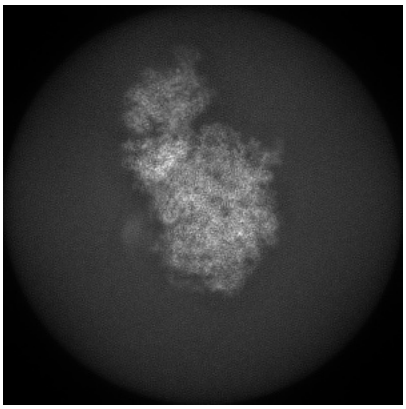
6.1.1 Primary map



X

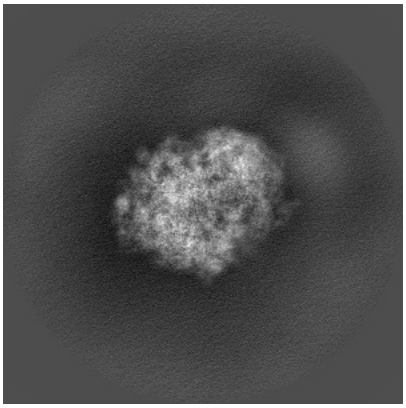


Y

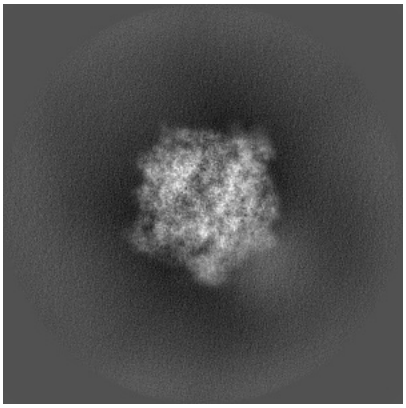


Z

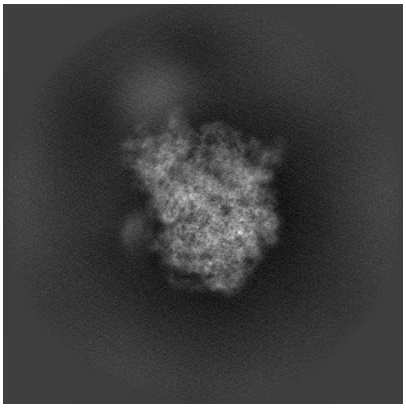
6.1.2 Raw map



X



Y

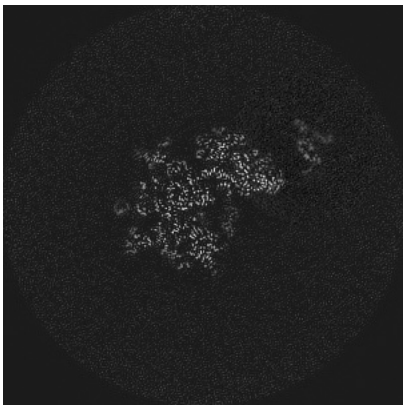


Z

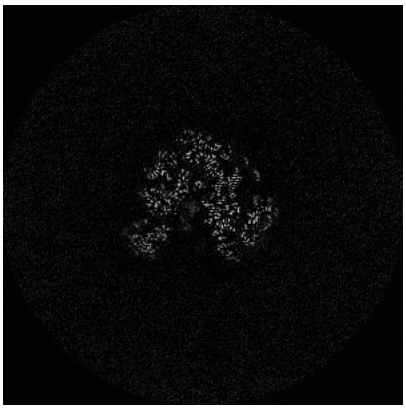
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

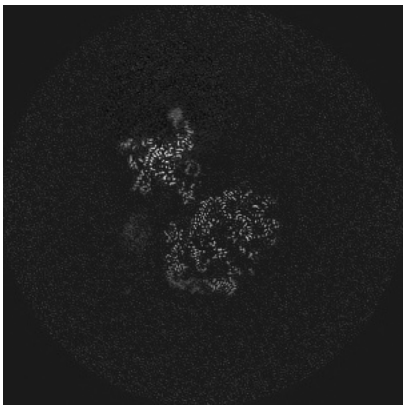
6.2.1 Primary map



X Index: 260

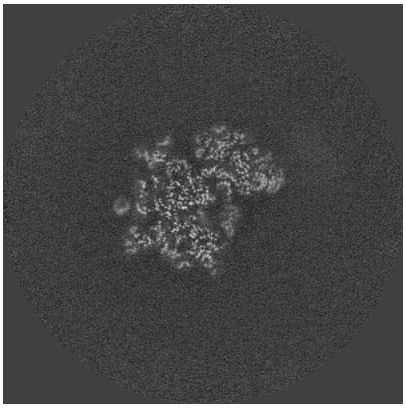


Y Index: 260

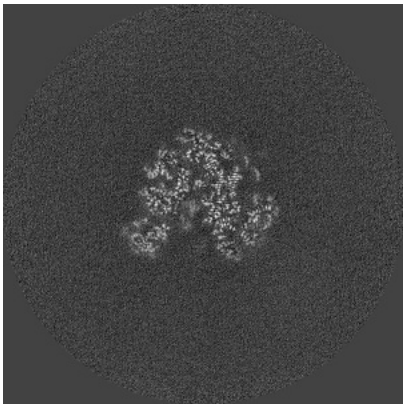


Z Index: 260

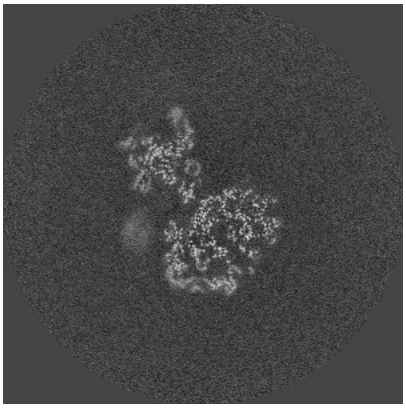
6.2.2 Raw map



X Index: 260



Y Index: 260

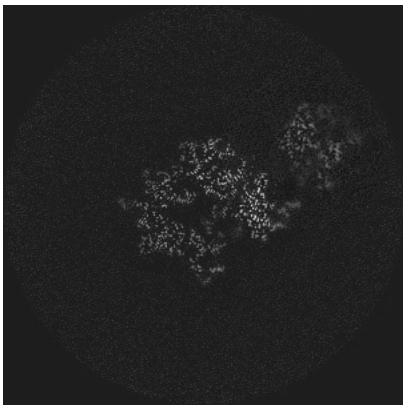


Z Index: 260

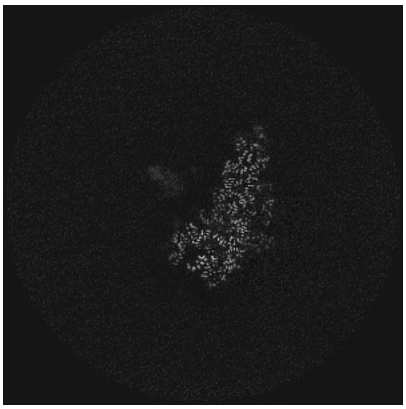
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

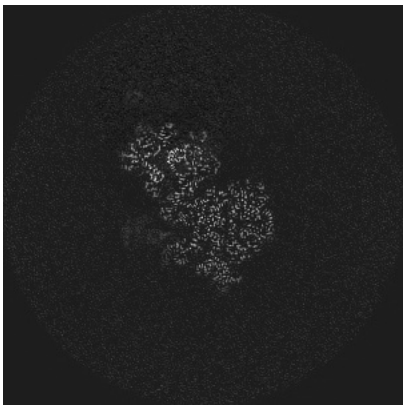
6.3.1 Primary map



X Index: 227

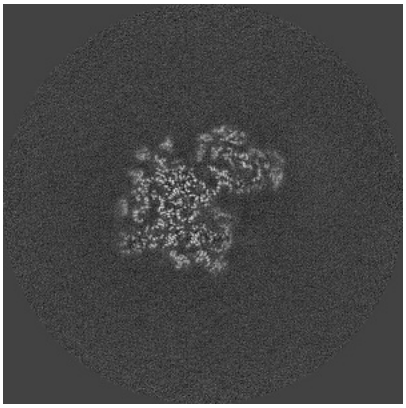


Y Index: 312

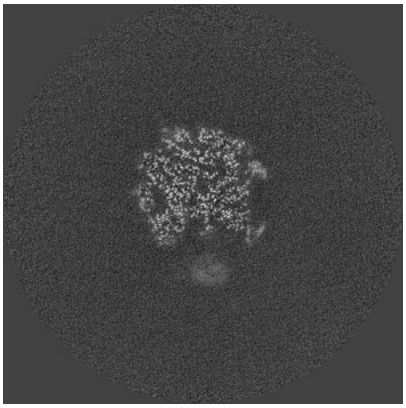


Z Index: 277

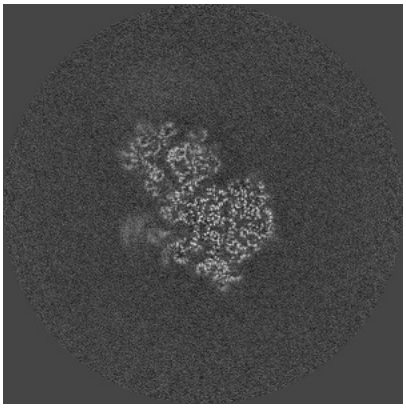
6.3.2 Raw map



X Index: 266



Y Index: 231

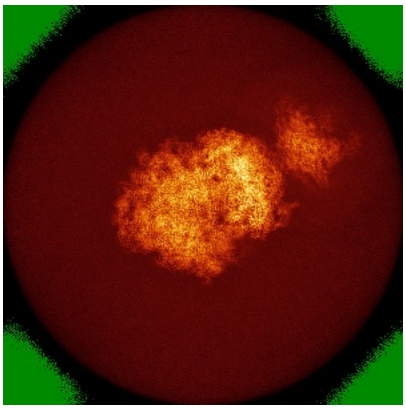


Z Index: 277

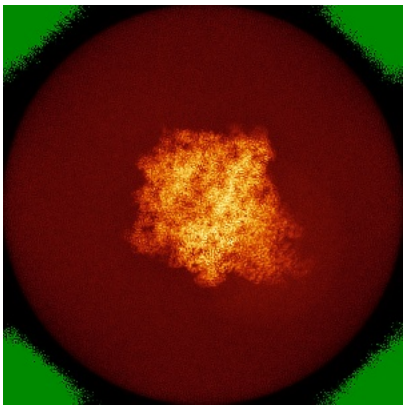
The images above show the largest variance slices of the map in three orthogonal directions.

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

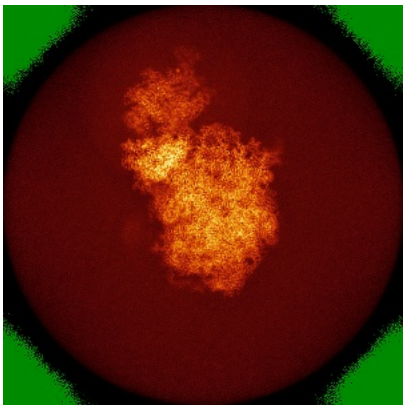
6.4.1 Primary map



X

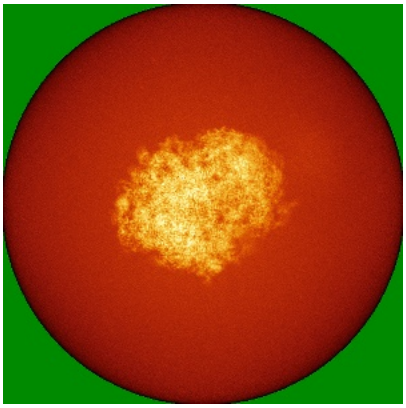


Y

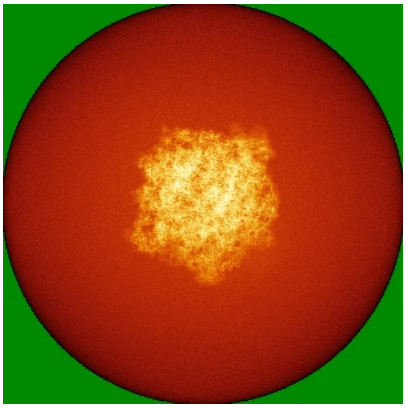


Z

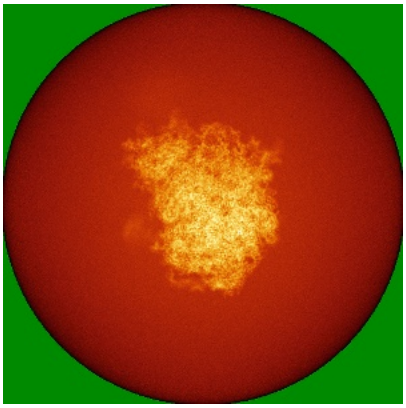
6.4.2 Raw map



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 0.5. 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.

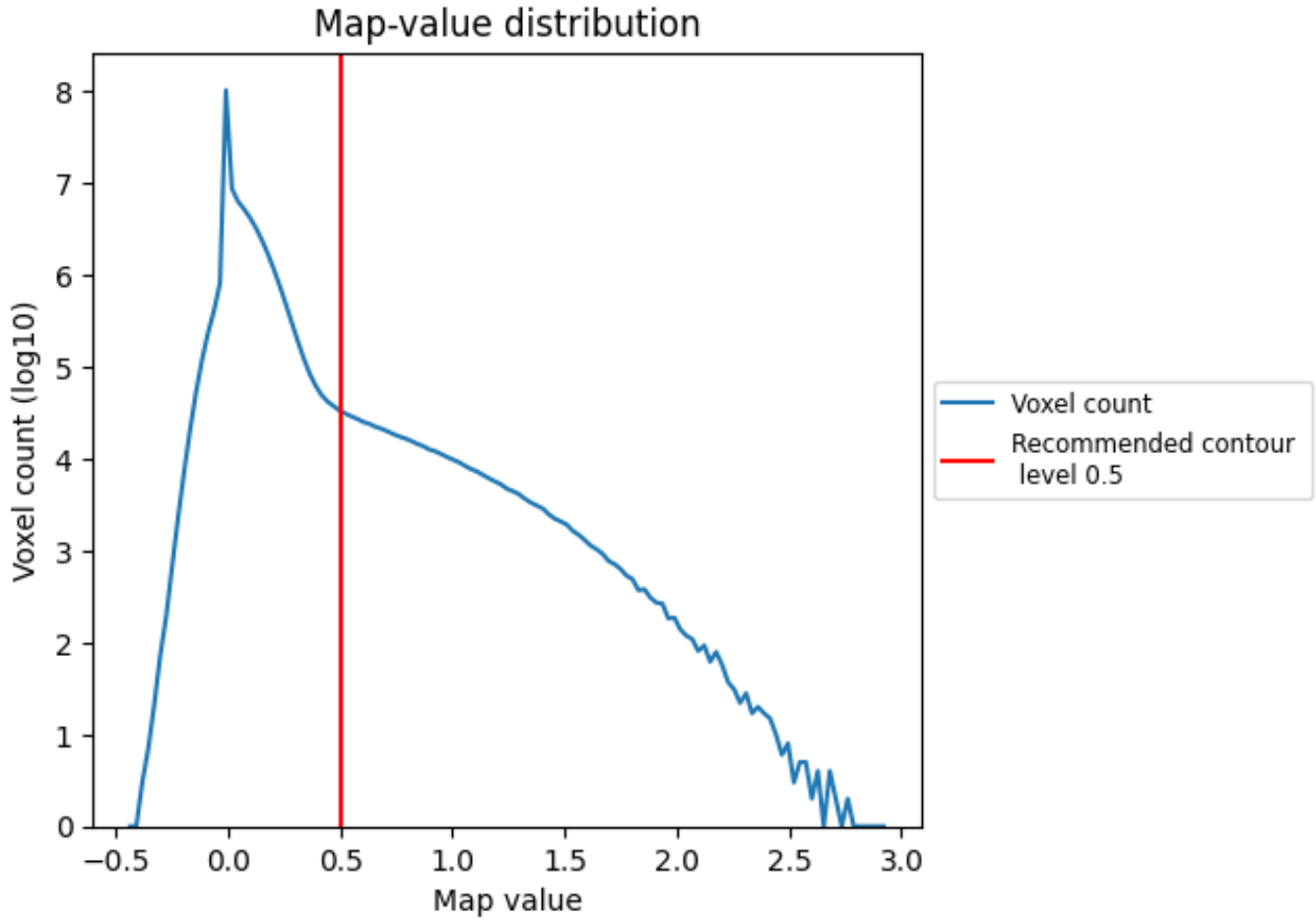
6.6 Mask visualisation (i)

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

7 Map analysis

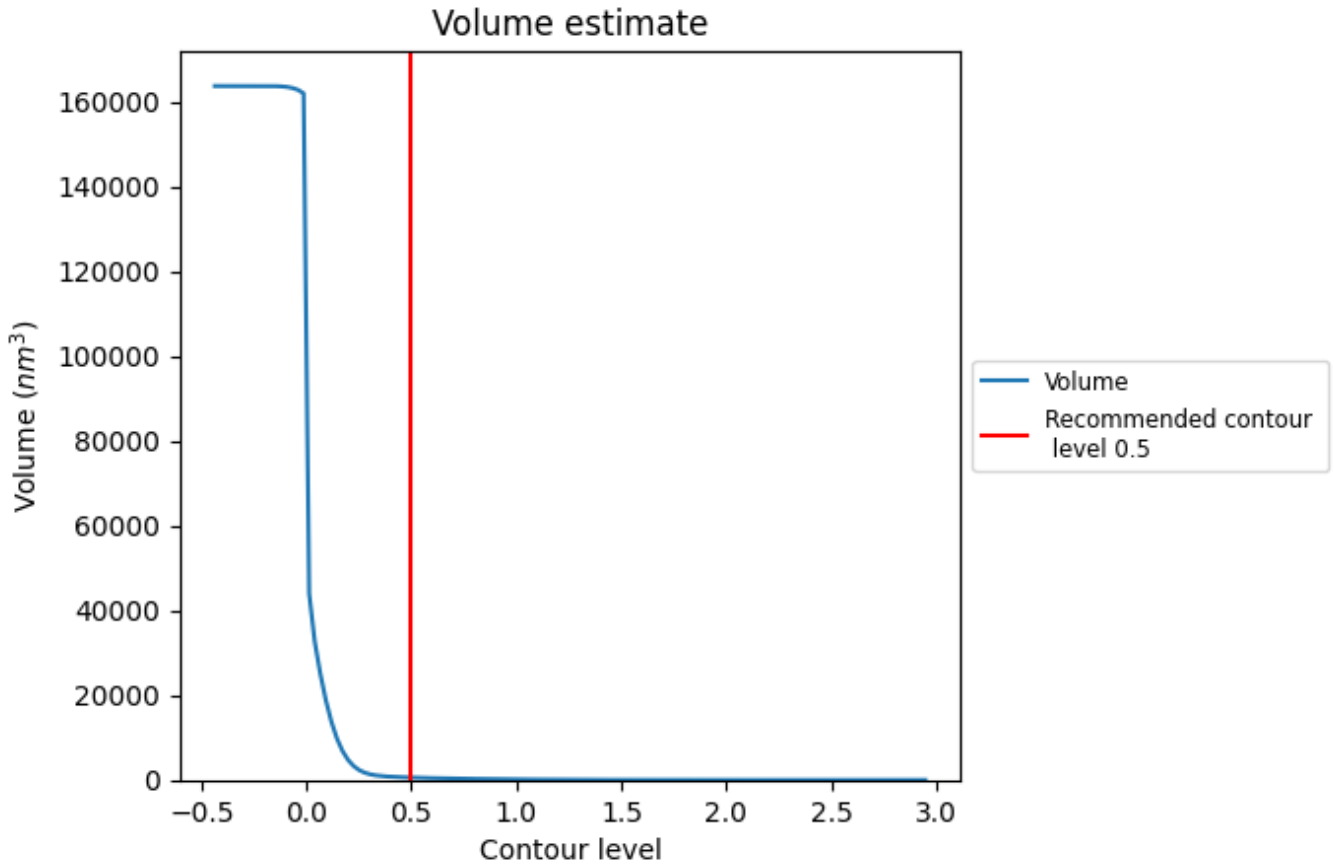
This section contains the results of statistical analysis of the map.

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.

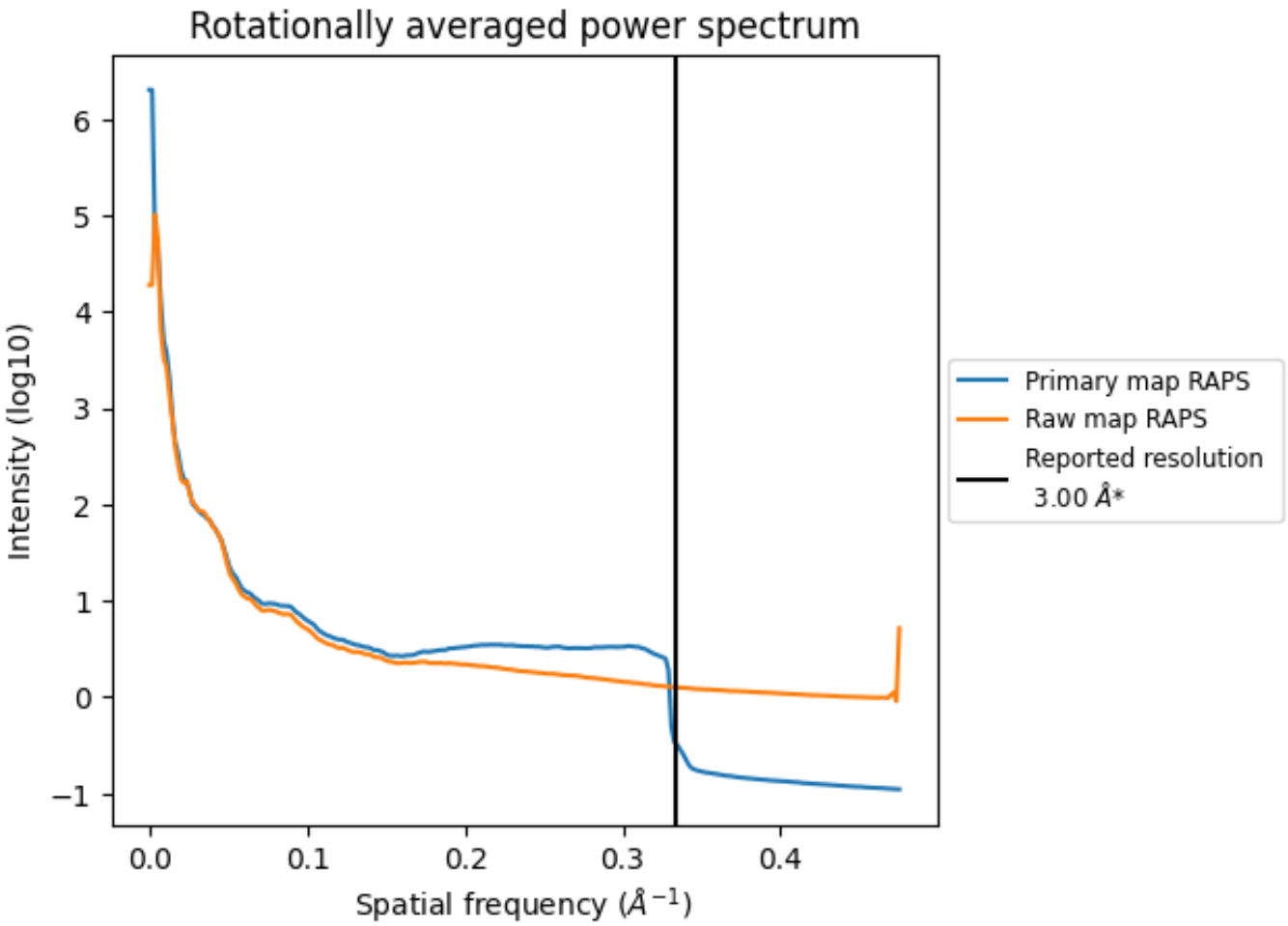
7.2 Volume estimate



The volume at the recommended contour level is 568 nm^3; this corresponds to an approximate mass of 513 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)

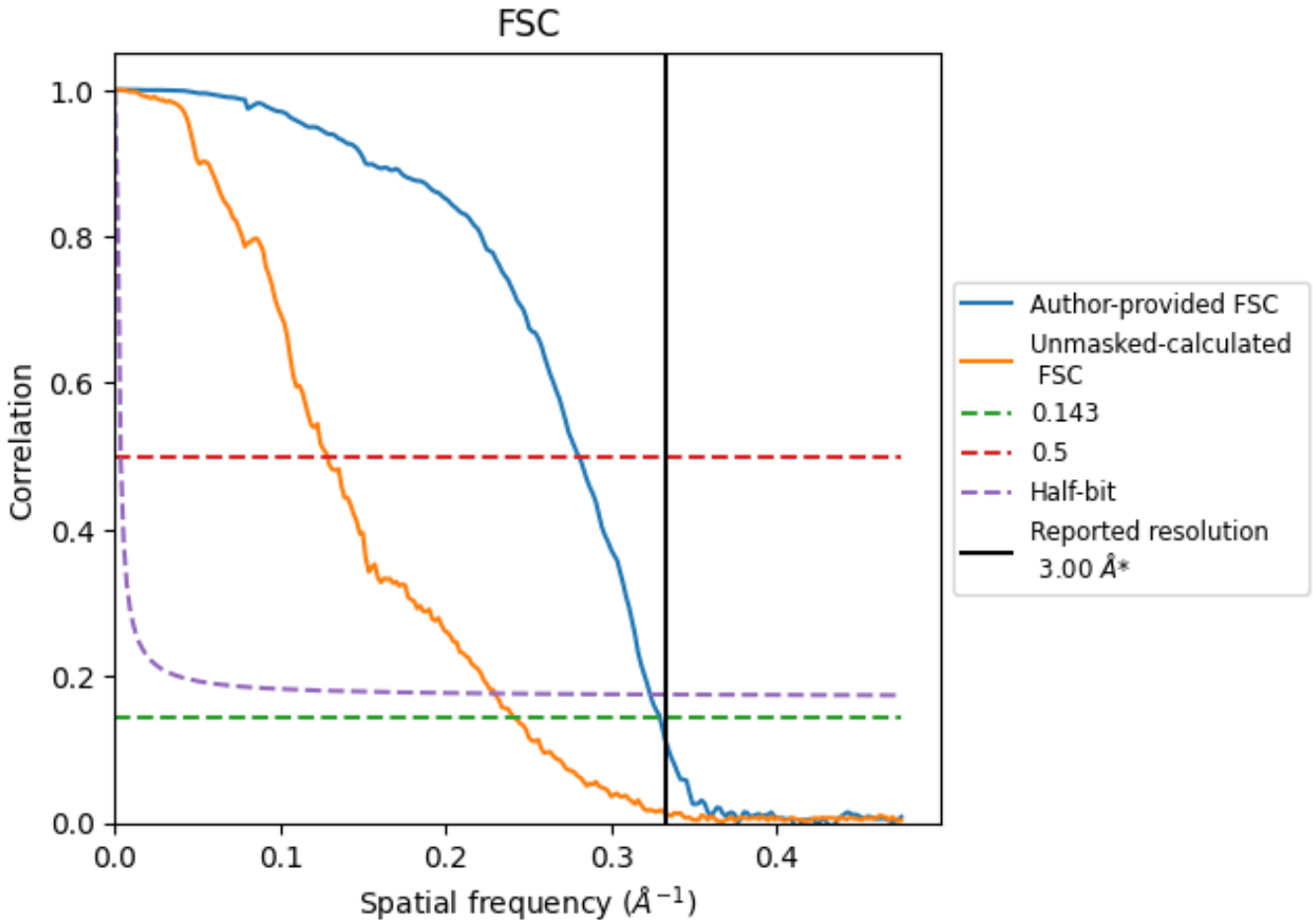


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

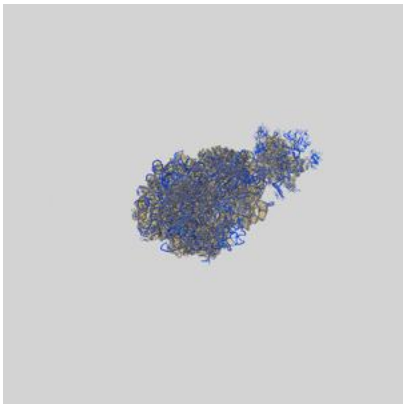
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.04	3.57	3.09
Unmasked-calculated*	4.14	7.79	4.35

*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 4.14 differs from the reported value 3.0 by more than 10 %

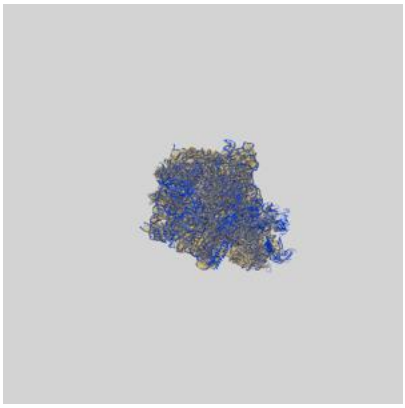
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11422 and PDB model 6ZTO. Per-residue inclusion information can be found in section 3 on page 17.

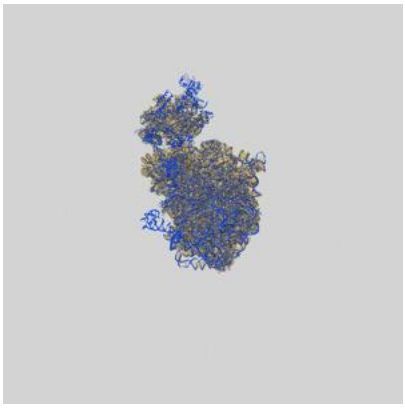
9.1 Map-model overlay



X



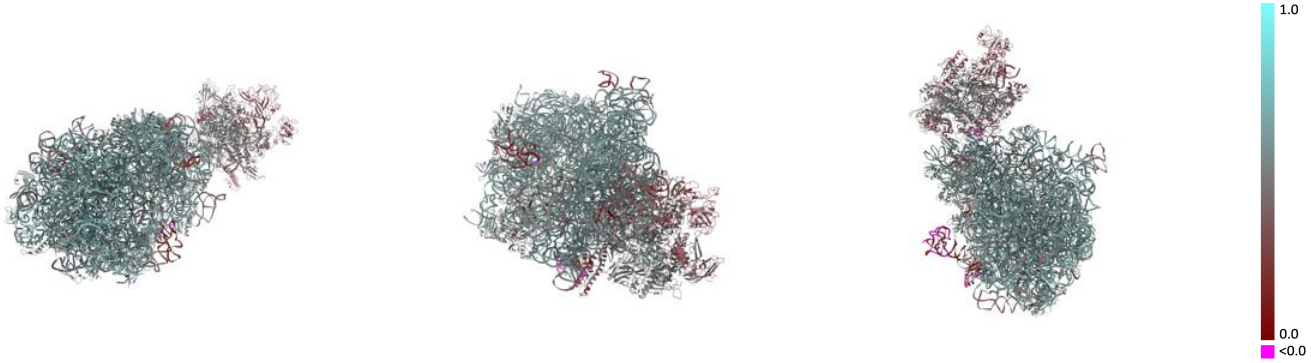
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

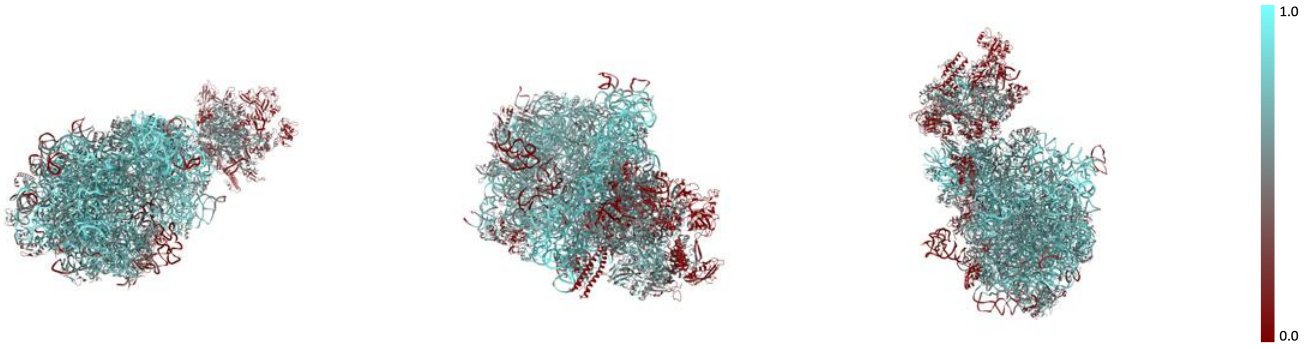
9.2 Q-score mapped to coordinate model (i)



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.

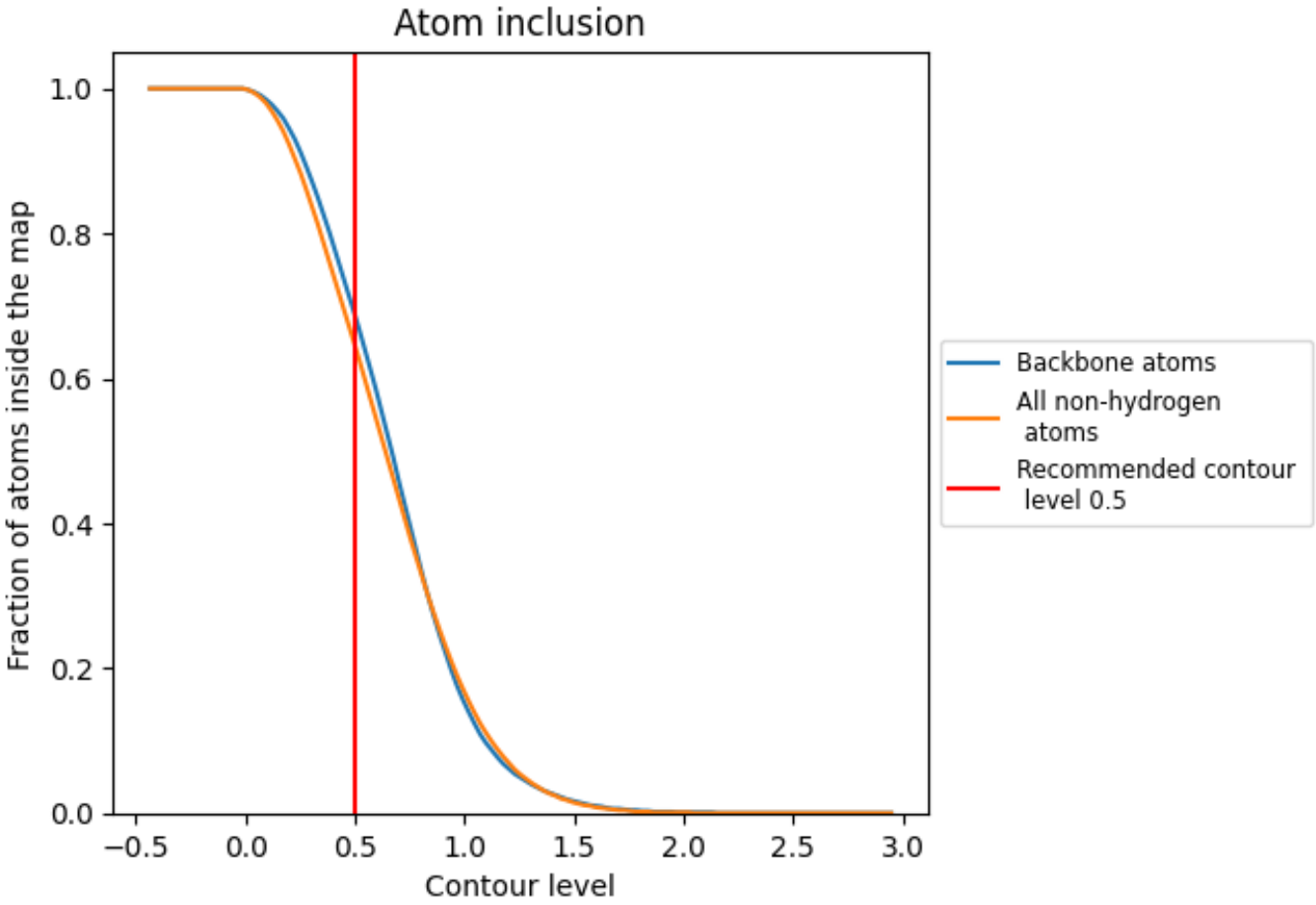
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 64% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6450	0.5460
AA	0.8620	0.5860
AB	0.2100	0.4730
AC	0.7040	0.5730
AD	0.5130	0.5360
AE	0.6160	0.5630
AF	0.4440	0.5200
AG	0.5630	0.5210
AH	0.6200	0.5740
AI	0.7820	0.5750
AJ	0.5570	0.5130
AK	0.5130	0.5450
AL	0.6510	0.5840
AM	0.6830	0.5500
AN	0.7830	0.5840
AO	0.5730	0.5670
AP	0.6920	0.5750
AQ	0.6120	0.5610
AR	0.4900	0.4890
AS	0.7710	0.5720
AT	0.6730	0.5650
AU	0.2410	0.4870
AV	0.4910	0.4780
AW	0.4880	0.5310
AX	0.2890	0.5250
B1	0.5790	0.5800
B2	0.6030	0.5850
B3	0.1590	0.5180
B4	0.7200	0.6100
B5	0.6820	0.6140
B6	0.6640	0.5950
B7	0.0670	0.4020
BA	0.7310	0.5750
BB	0.6990	0.5900
BC	0.6560	0.6040

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Chain	Atom inclusion	Q-score
BD	0.6460	0.5980
BE	0.5100	0.5700
BF	0.2480	0.4980
BG	0.3540	0.5290
BH	0.0320	0.2420
BK	0.6590	0.5930
BL	0.6120	0.5920
BM	0.5930	0.5850
BN	0.6300	0.6000
BO	0.7020	0.6090
BP	0.5320	0.5620
BQ	0.5880	0.5860
BR	0.6840	0.6000
BS	0.5970	0.5870
BT	0.6080	0.5860
BU	0.4880	0.5470
BV	0.4720	0.5520
BW	0.5430	0.5580
BX	0.6440	0.6050
BY	0.6010	0.5930
BZ	0.4440	0.5440
CA	0.4020	0.4420
CB	0.2010	0.4110
CC	0.4240	0.4390
CD	0.3200	0.4040
CE	0.0000	0.1650
CN	0.1570	0.2800
CT	0.3750	0.3590