



Full wwPDB EM Validation Report ⓘ

Jun 20, 2026 – 09:30 pm BST

PDB ID : 7O1C / pdb_00007o1c
EMDB ID : EMD-12695
Title : Cryo-EM structure of an Escherichia coli TnaC(R23F)-ribosome-RF2 complex stalled in response to L-tryptophan
Authors : van der Stel, A.X.; Gordon, E.R.; Sengupta, A.; Martinez, A.K.; Klepacki, D.; Perry, T.N.; Herrero del Valle, A.; Vazquez-Laslop, N.; Sachs, M.S.; Cruz-Vera, L.R.; Innis, C.A.
Deposited on : 2021-03-29
Resolution : 2.60 Å(reported)
Based on initial model : 6TBV

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.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

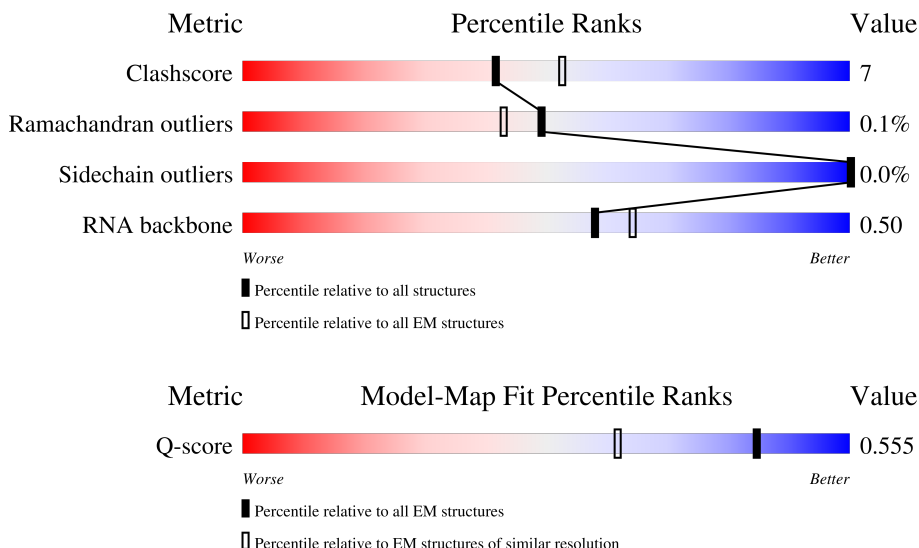
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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.



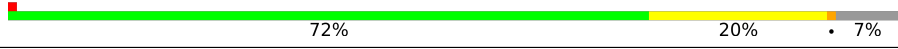
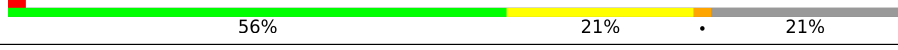
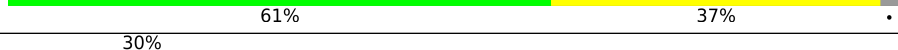
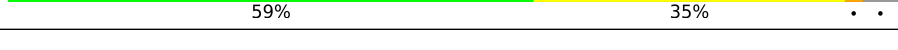
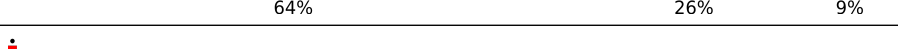
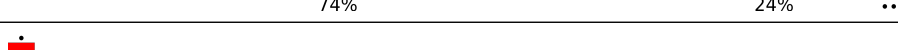
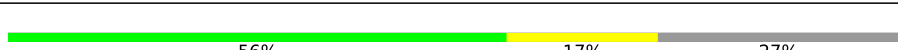
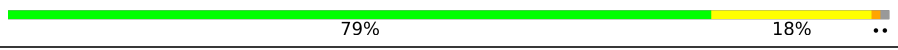
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8728 (2.10 - 3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1534	
2	AB	241	

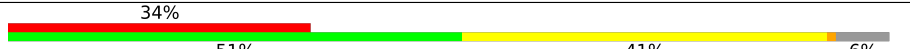
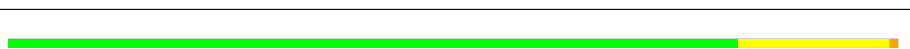
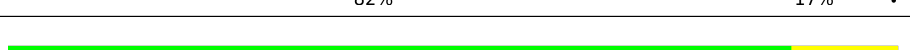
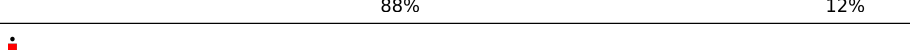
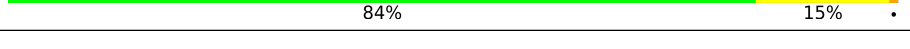
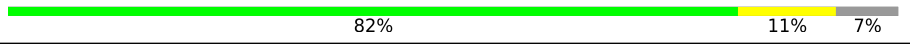
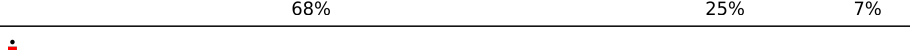
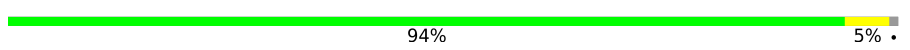
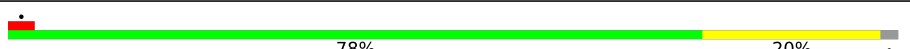
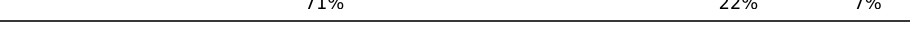
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Mol	Chain	Length	Quality of chain
3	AC	233	
4	AD	206	
5	AE	167	
6	AF	135	
7	AG	179	
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	102	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	BA	2897	
23	BB	120	
24	BC	273	
25	BD	209	
26	BE	201	
27	BF	179	

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Mol	Chain	Length	Quality of chain
28	BG	177	
29	BH	149	
30	BI	70	
31	BJ	142	
32	BK	123	
33	BL	144	
34	BM	136	
35	BN	127	
36	BO	117	
37	BP	115	
38	BQ	118	
39	BR	103	
40	BS	110	
41	BT	100	
42	BU	104	
43	BV	94	
44	BW	85	
45	BX	78	
46	BY	63	
47	BZ	59	
48	B0	57	
49	B1	55	
50	B2	46	
51	B3	65	
52	B4	38	

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Mol	Chain	Length	Quality of chain
53	B5	17	76% 18% 6%
54	B7	10	30% 60% 10%
55	B8	77	42% 40% 18%
56	B9	365	21% 60% 35% 5%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 148175 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 Ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1534	Total	C	N	O	P	0	0
			32930	14694	6041	10661	1534		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0
			1181	735	227	215	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	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	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	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AN	35	ALA	-	insertion	UNP P0AG59

- 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	55	Total	C	N	O	0	0
			455	288	86	81		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	82	Total	C	N	O	S	0	0
			656	419	125	110	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	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 22 is a RNA chain called Ribosomal RNA 23S.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BA	2897	Total	C	N	O	P	0	0
			62209	27759	11446	20107	2897		

- Molecule 23 is a RNA chain called Ribosomal RNA 5S.

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

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

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

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BH	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BI	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BK	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 33 is a protein called 50S ribosomal protein L15.

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

- Molecule 34 is a protein called 50S ribosomal protein L16.

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

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BN	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 36 is a protein called 50S ribosomal protein L18.

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

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

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

- Molecule 42 is a protein called 50S ribosomal protein L24.

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

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BW	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 45 is a protein called 50S ribosomal protein L28.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

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

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B1	51	Total	C	N	O		0	0
			414	266	76	72			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 53 is a protein called TnaC-(R23F) - Tryptophanase leader peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	B5	17	Total	C	N	O	0	0
			146	97	24	25		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B7	10	Total	C	N	O	P	0	0
			211	94	36	71	10		

- Molecule 55 is a RNA chain called P-site tRNA-Pro.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B8	77	Total	C	N	O	P	0	0
			1646	733	295	541	77		

- Molecule 56 is a protein called Peptide chain release factor RF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B9	348	Total	C	N	O	S	0	0
			2768	1705	482	571	10		

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	AA	87	Total	Mg	0
			87	87	
57	BA	243	Total	Mg	0
			243	243	
57	BB	1	Total	Mg	0
			1	1	
57	BC	1	Total	Mg	0
			1	1	
57	BD	2	Total	Mg	0
			2	2	
57	BL	3	Total	Mg	0
			3	3	
57	B8	2	Total	Mg	0
			2	2	

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
58	AA	38	Total	K	0
			38	38	
58	AM	1	Total	K	0
			1	1	
58	BA	104	Total	K	0
			104	104	
58	BB	1	Total	K	0
			1	1	
58	BC	1	Total	K	0
			1	1	
58	BD	1	Total	K	0
			1	1	

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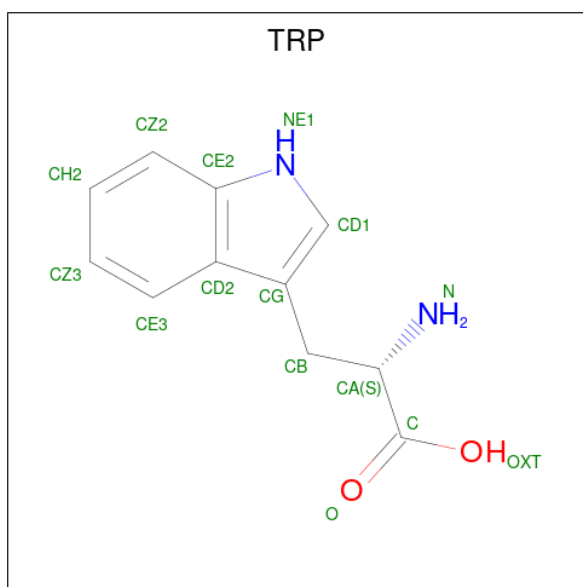
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Mol	Chain	Residues	Atoms		AltConf
58	BM	1	Total	K	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
59	AB	1	Total	Zn	0
			1	1	
59	BI	1	Total	Zn	0
			1	1	
59	B4	1	Total	Zn	0
			1	1	

- Molecule 60 is TRYPTOPHAN (CCD ID: TRP) (formula: C₁₁H₁₂N₂O₂).



Mol	Chain	Residues	Atoms				AltConf
60	BA	1	Total	C	N	O	0
			15	11	2	2	

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	AA	167	Total	O	0
			167	167	
61	AK	1	Total	O	0
			1	1	

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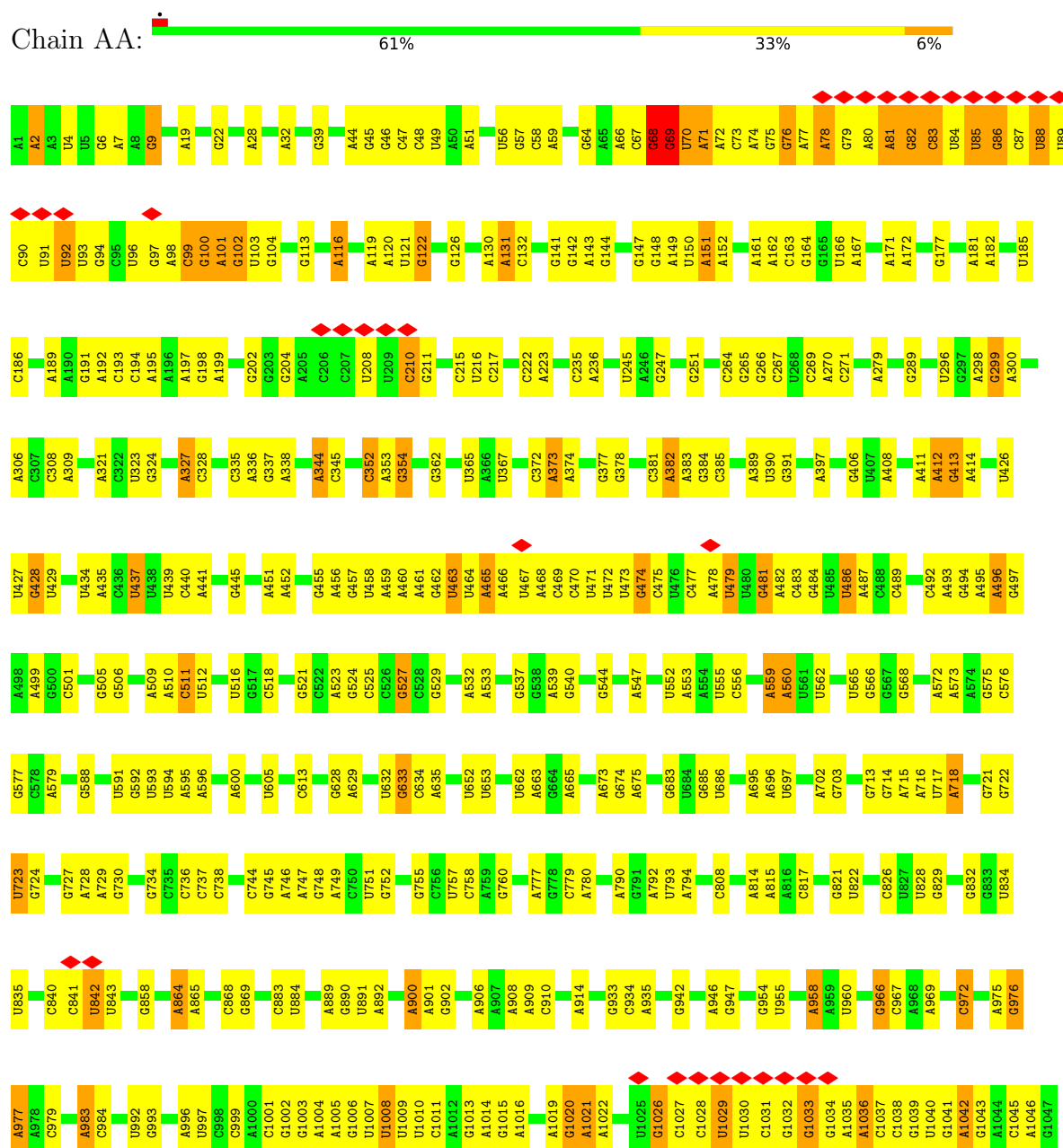
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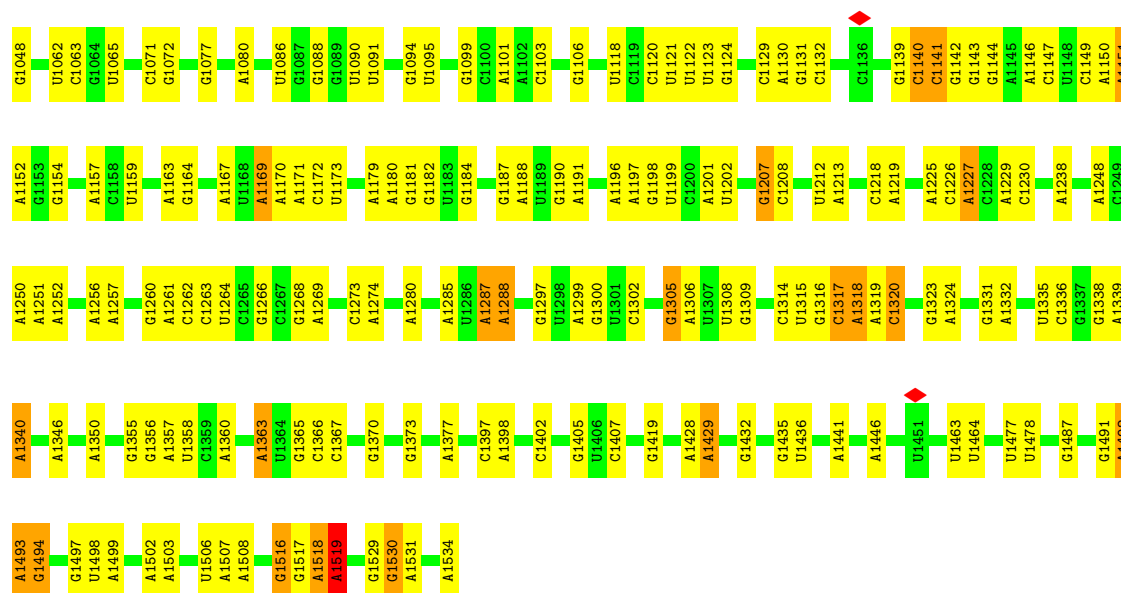
Mol	Chain	Residues	Atoms		AltConf
61	AM	1	Total 1	O 1	0
61	AN	3	Total 3	O 3	0
61	BA	617	Total 617	O 617	0
61	BC	6	Total 6	O 6	0
61	BD	2	Total 2	O 2	0
61	BN	3	Total 3	O 3	0

3 Residue-property plots

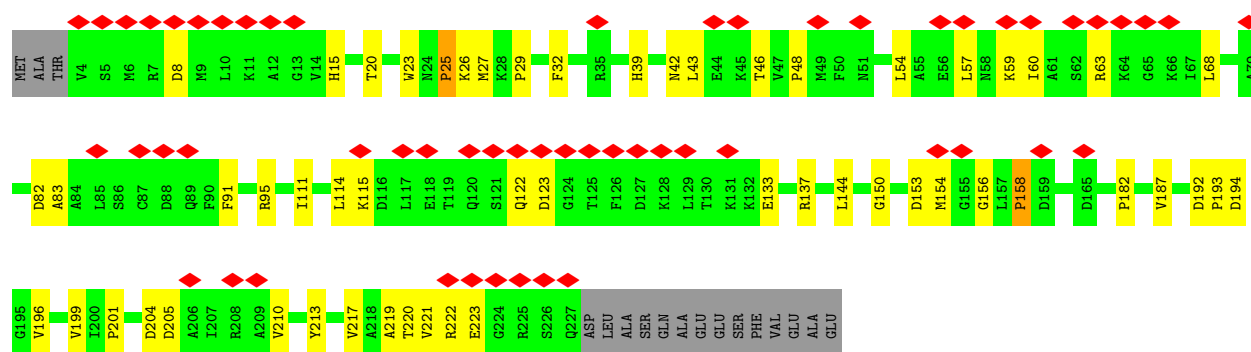
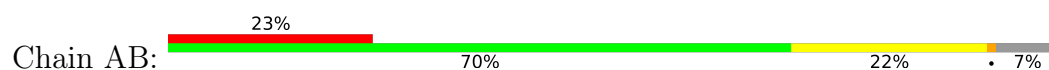
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Ribosomal RNA 16S

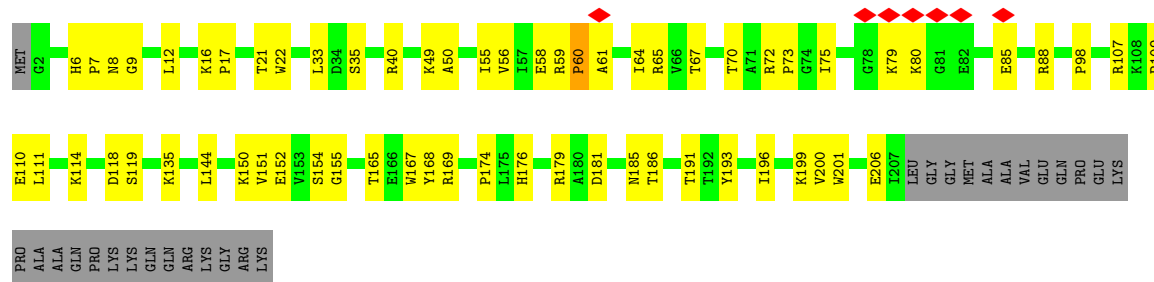




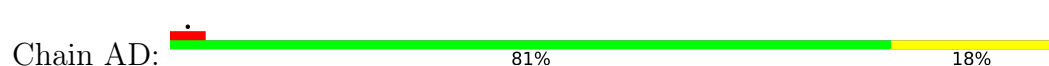
• Molecule 2: 30S ribosomal protein S2

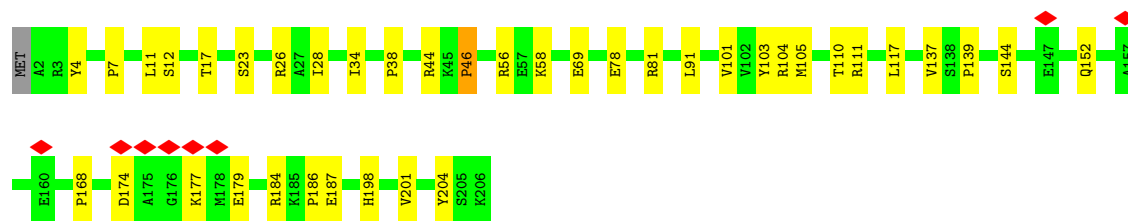


• Molecule 3: 30S ribosomal protein S3

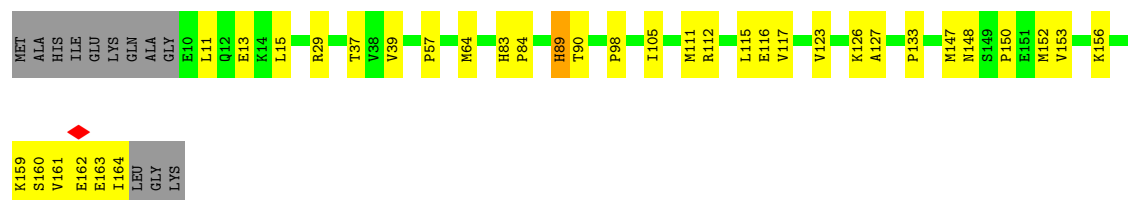
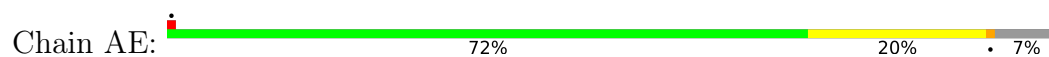


• Molecule 4: 30S ribosomal protein S4

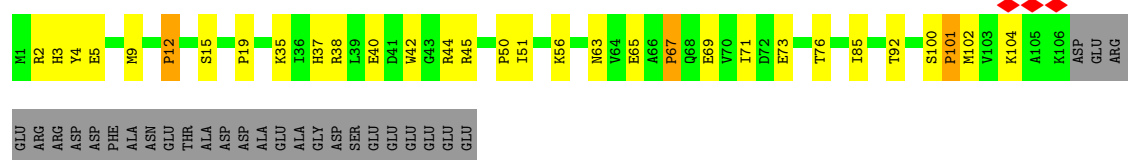




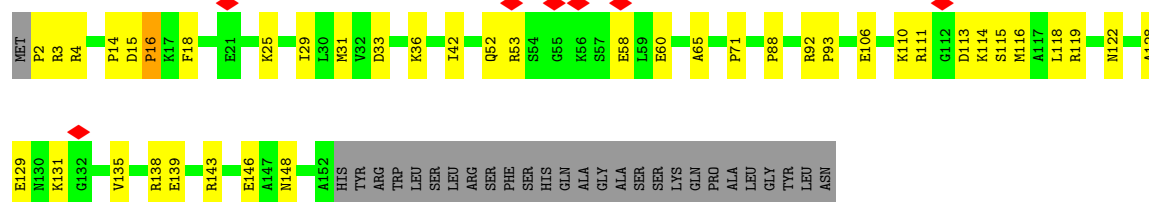
- Molecule 5: 30S ribosomal protein S5



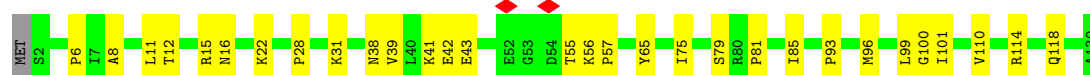
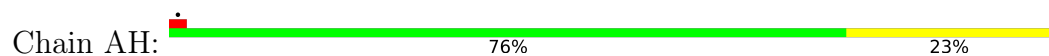
- Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7

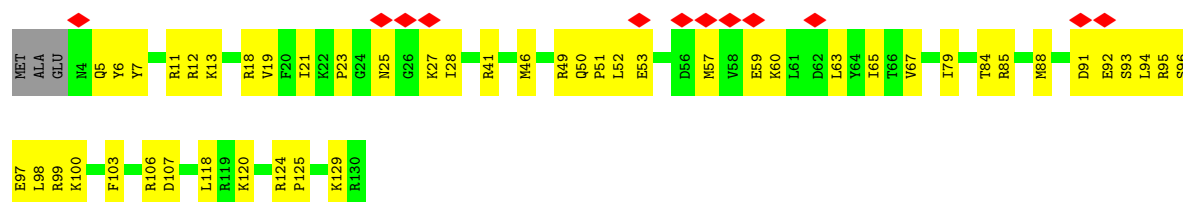


- Molecule 8: 30S ribosomal protein S8

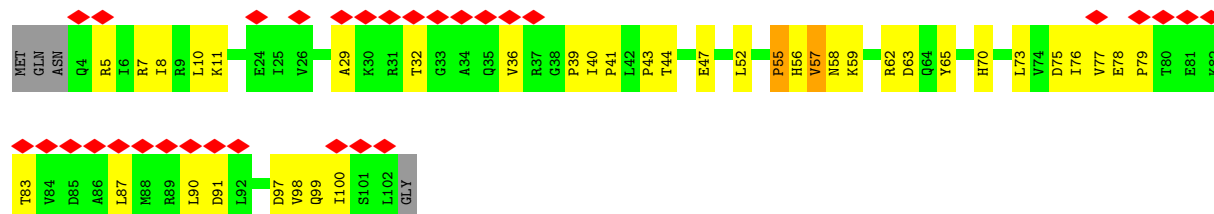


- Molecule 9: 30S ribosomal protein S9

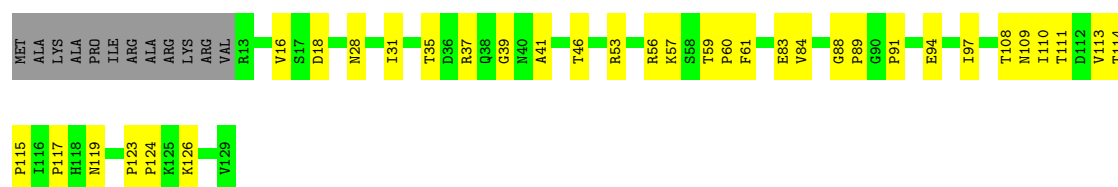




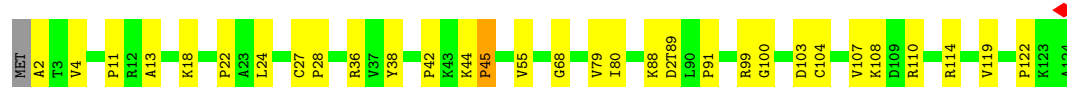
- Molecule 10: 30S ribosomal protein S10



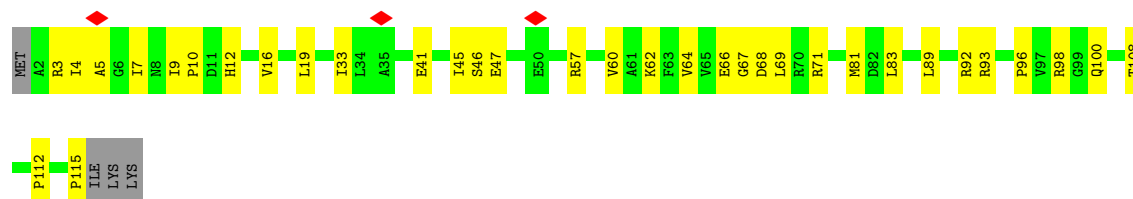
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

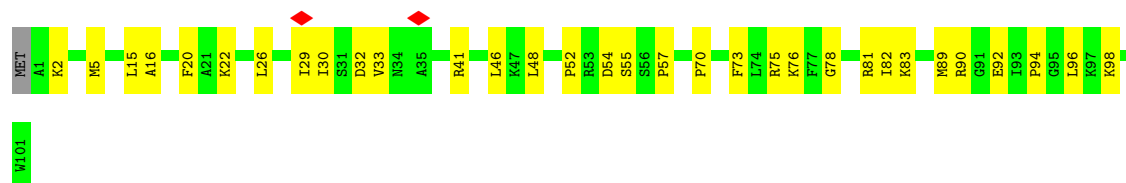


- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14





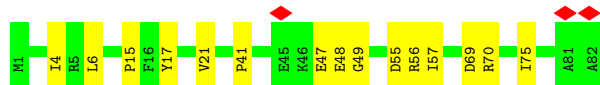
- Molecule 15: 30S ribosomal protein S15

Chain AO: 97%



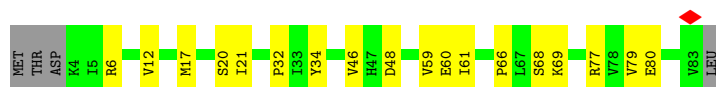
- Molecule 16: 30S ribosomal protein S16

Chain AP: 82% 18%



- Molecule 17: 30S ribosomal protein S17

Chain AQ: 74% 21% 5%



- Molecule 18: 30S ribosomal protein S18

Chain AR: 56% 17% 27%



- Molecule 19: 30S ribosomal protein S19

Chain AS: 5% 57% 30% 11%



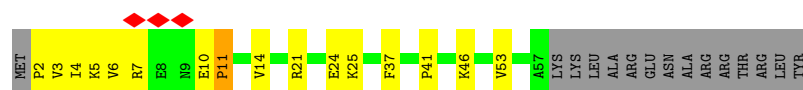
- Molecule 20: 30S ribosomal protein S20

Chain AT: 83% 16%



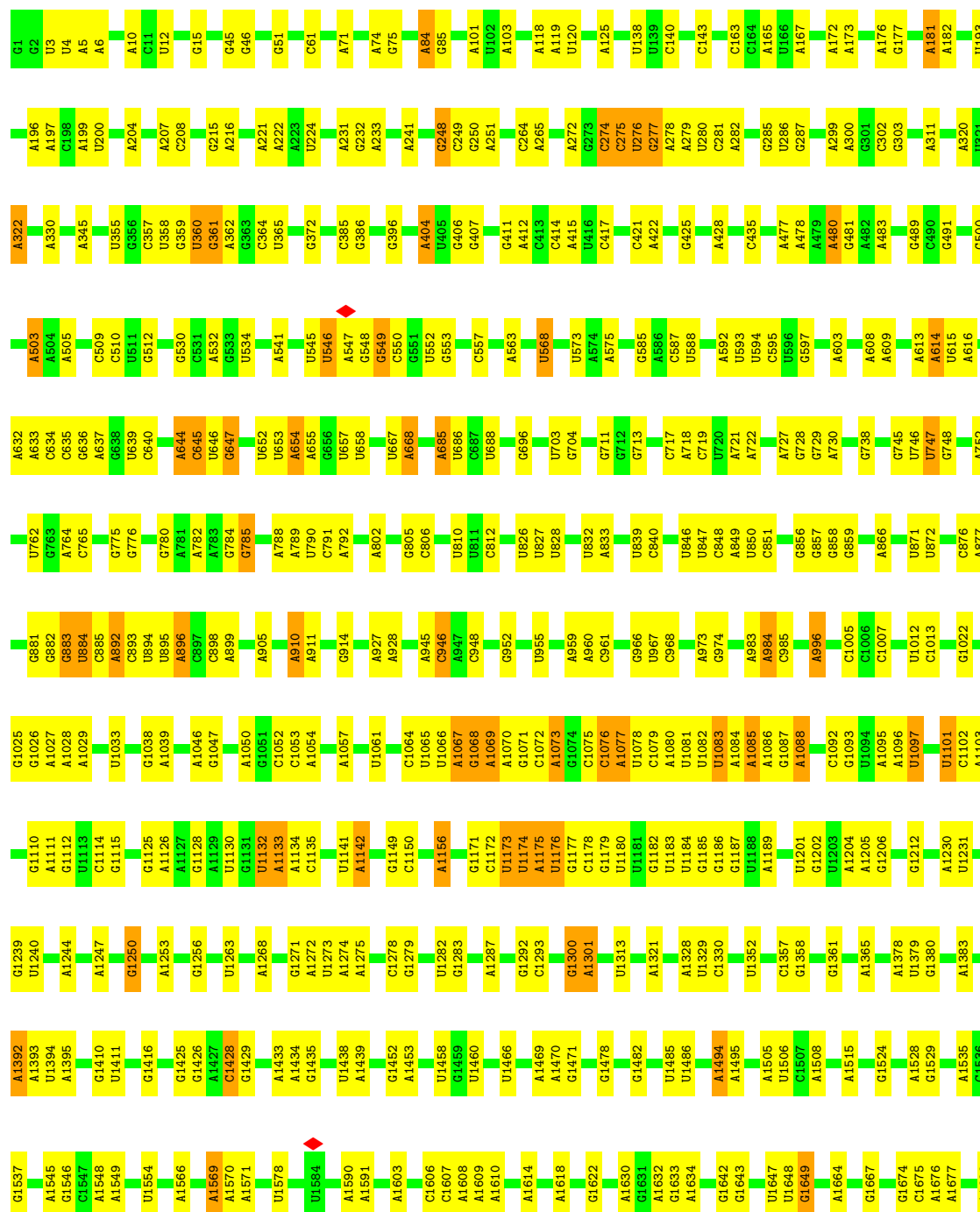
- Molecule 21: 30S ribosomal protein S21

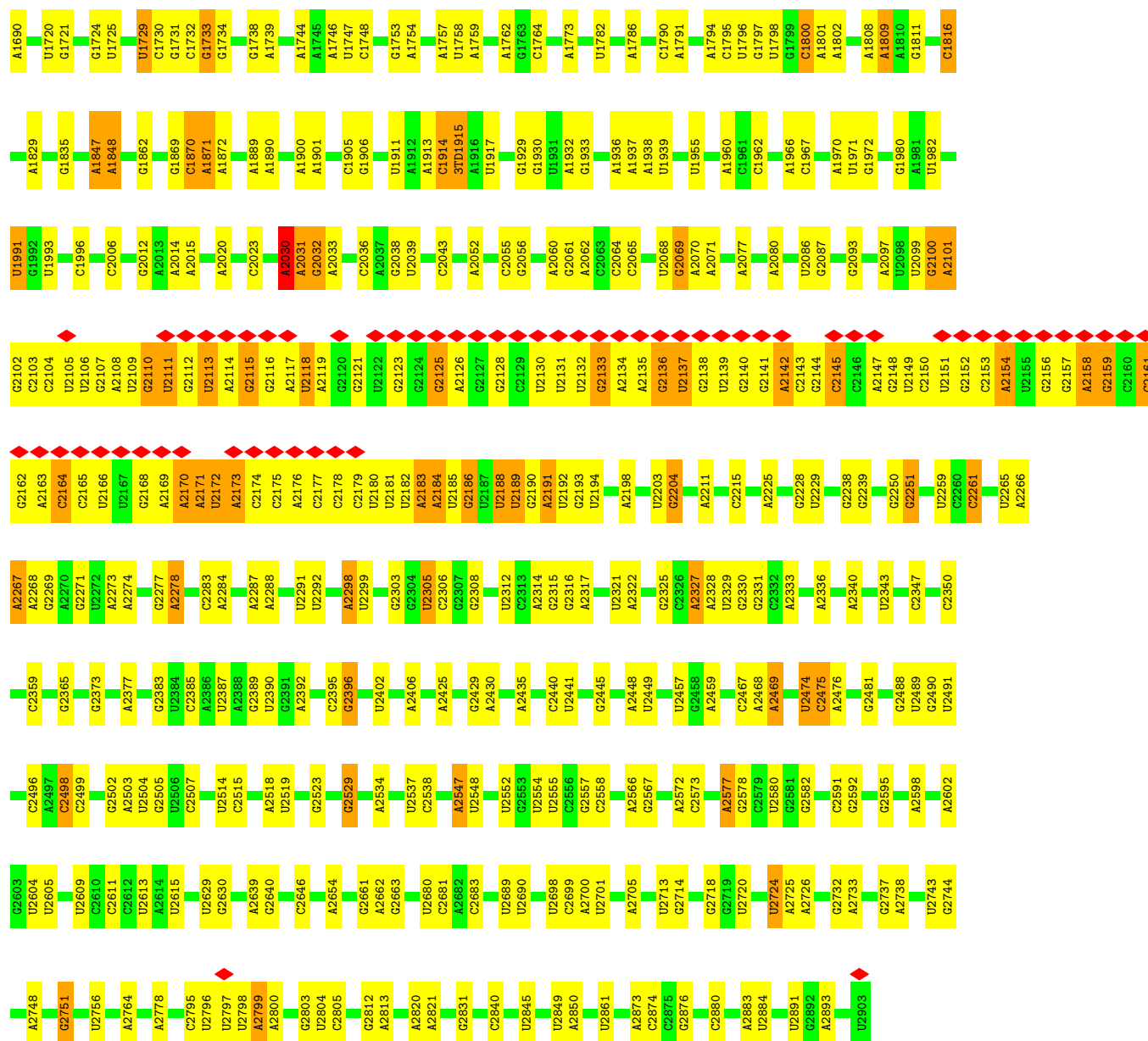
Chain AU:  56% 21% 21%



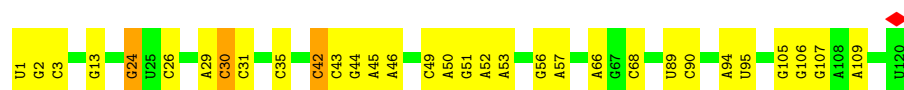
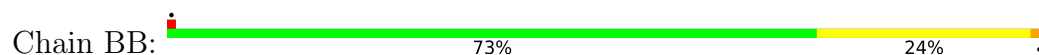
- Molecule 22: Ribosomal RNA 23S

Chain BA:  70% 26%

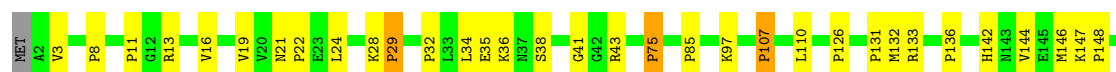
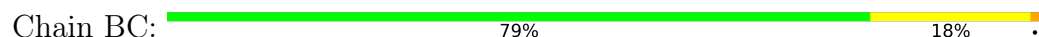




• Molecule 23: Ribosomal RNA 5S



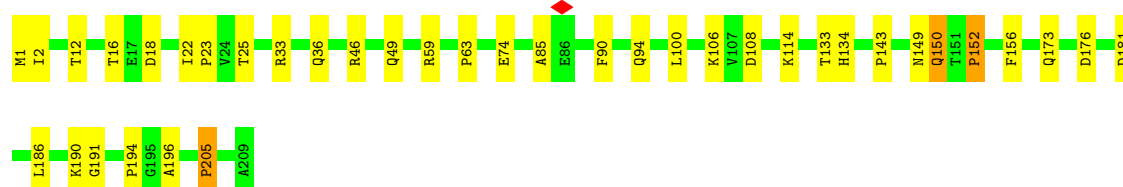
• Molecule 24: 50S ribosomal protein L2





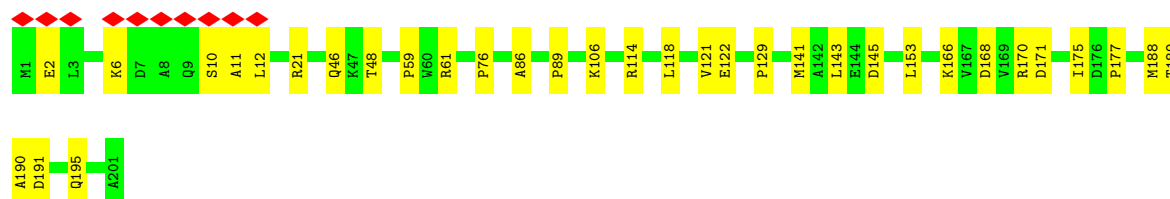
- Molecule 25: 50S ribosomal protein L3

Chain BD: 82% 17%



- Molecule 26: 50S ribosomal protein L4

Chain BE: 5% 83% 17%



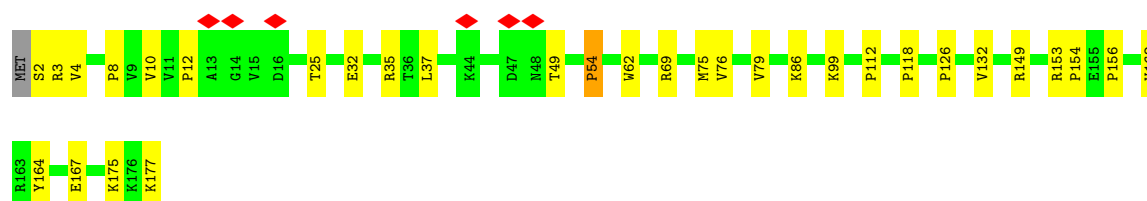
- Molecule 27: 50S ribosomal protein L5

Chain BF: 72% 27%



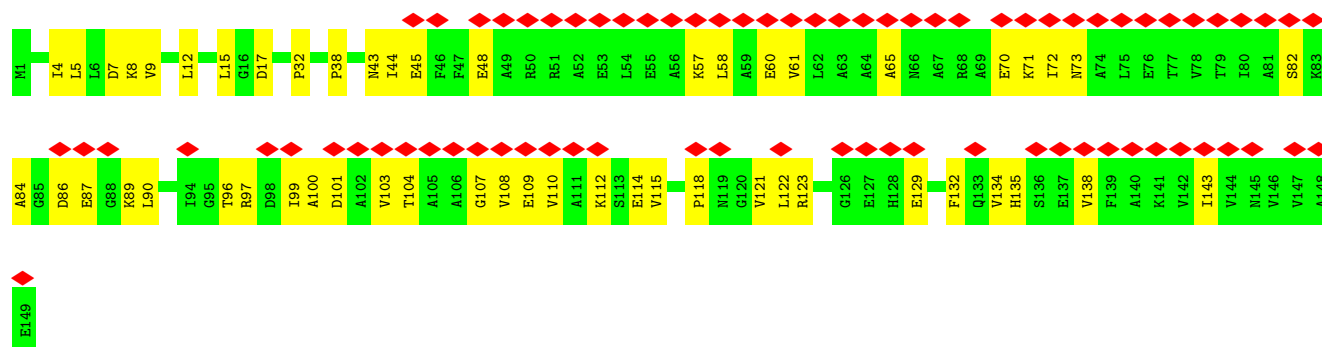
- Molecule 28: 50S ribosomal protein L6

Chain BG: 81% 18%

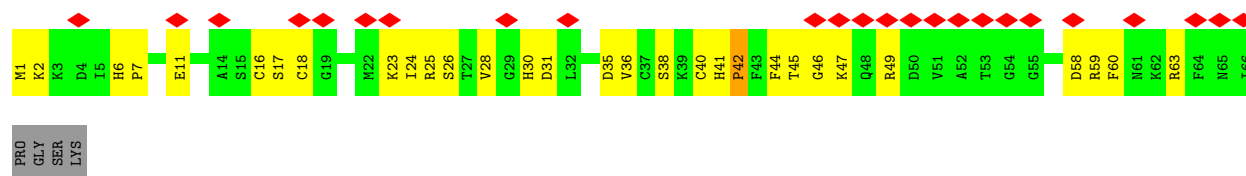


- Molecule 29: 50S ribosomal protein L9

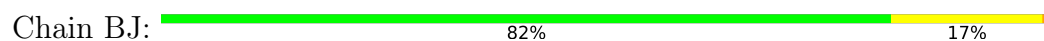
Chain BH: 51% 64% 36%



- Molecule 30: 50S ribosomal protein L31



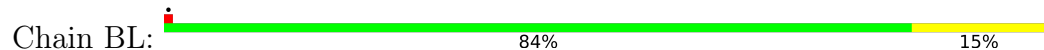
- Molecule 31: 50S ribosomal protein L13



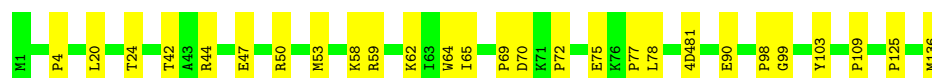
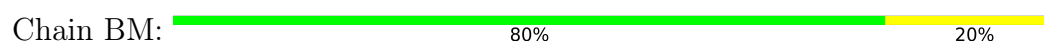
- Molecule 32: 50S ribosomal protein L14



- Molecule 33: 50S ribosomal protein L15



- Molecule 34: 50S ribosomal protein L16



• Molecule 35: 50S ribosomal protein L17

Chain BN:  82% 11% 7%

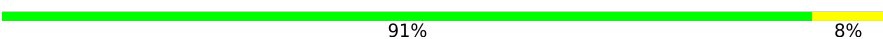
• Molecule 36: 50S ribosomal protein L18

Chain BO:  87% 13%

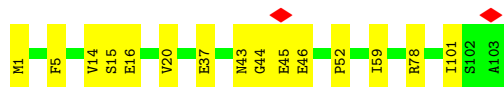
• Molecule 37: 50S ribosomal protein L19

Chain BP:  81% 18%

• Molecule 38: 50S ribosomal protein L20

Chain BQ:  91% 8%

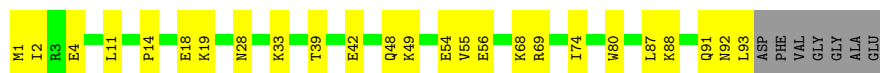
• Molecule 39: 50S ribosomal protein L21

Chain BR:  85% 15%

• Molecule 40: 50S ribosomal protein L22

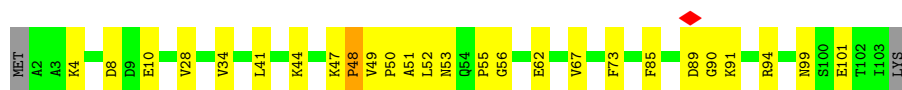
Chain BS:  81% 19%

• Molecule 41: 50S ribosomal protein L23

Chain BT:  68% 25% 7%

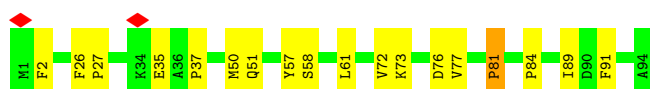
- Molecule 42: 50S ribosomal protein L24

Chain BU:  73% 24% ..



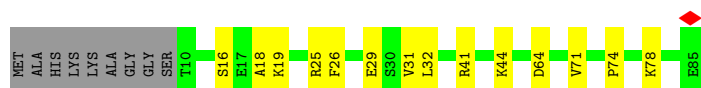
- Molecule 43: 50S ribosomal protein L25

Chain BV:  81% 18% .

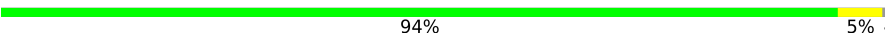


- Molecule 44: 50S ribosomal protein L27

Chain BW:  73% 16% 11%



- Molecule 45: 50S ribosomal protein L28

Chain BX:  94% 5% .



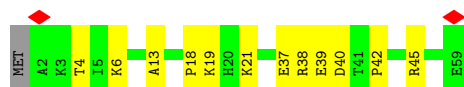
- Molecule 46: 50S ribosomal protein L29

Chain BY:  90% 8% .



- Molecule 47: 50S ribosomal protein L30

Chain BZ:  78% 20% .



- Molecule 48: 50S ribosomal protein L32

Chain B0:  81% 18% .



- Molecule 49: 50S ribosomal protein L33

Chain B1: 71% 22% 7%



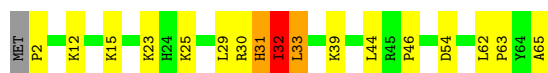
- Molecule 50: 50S ribosomal protein L34

Chain B2: 87% 13%



- Molecule 51: 50S ribosomal protein L35

Chain B3: 72% 22% ...



- Molecule 52: 50S ribosomal protein L36

Chain B4: 87% 13%



- Molecule 53: TnaC-(R23F) - Tryptophanase leader peptide

Chain B5: 76% 18% 6%



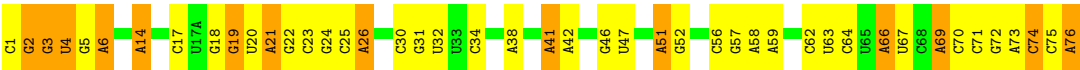
- Molecule 54: mRNA

Chain B7: 30% 60% 10%

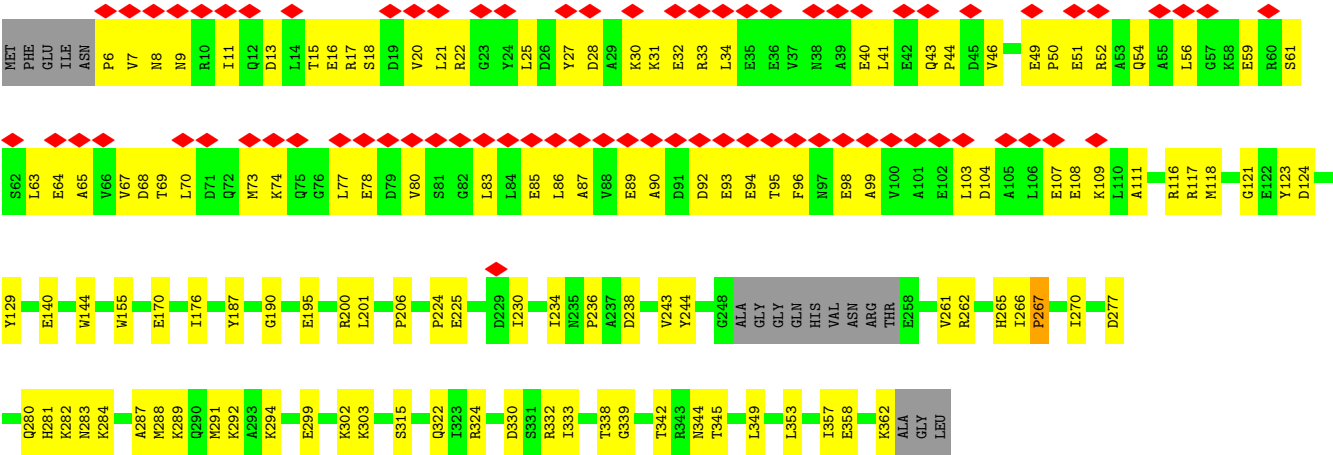


- Molecule 55: P-site tRNA-Pro

Chain B8: 42% 40% 18%



● Molecule 56: Peptide chain release factor RF2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	113840	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA, FEI TITAN KRIOS	Depositor
Voltage (kV)	200, 300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40, 44	Depositor
Minimum defocus (nm)	-1000, -400	Depositor
Maximum defocus (nm)	-2000, -1600	Depositor
Magnification	55127, 59880	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.112	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	370.056, 370.056, 370.056	wwPDB
Map dimensions	408, 408, 408	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.907, 0.907, 0.907	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.70	0/36593	0.75	7/57081 (0.0%)
2	AB	0.80	7/1784 (0.4%)	0.53	0/2403
3	AC	0.84	7/1651 (0.4%)	0.58	2/2225 (0.1%)
4	AD	0.78	6/1665 (0.4%)	0.46	0/2227
5	AE	0.87	5/1157 (0.4%)	0.54	0/1557
6	AF	0.98	5/881 (0.6%)	0.54	0/1189
7	AG	0.95	7/1195 (0.6%)	0.54	0/1602
8	AH	0.92	5/989 (0.5%)	0.59	0/1326
9	AI	0.73	3/1034 (0.3%)	0.54	0/1375
10	AJ	1.04	7/805 (0.9%)	0.56	0/1089
11	AK	1.10	7/893 (0.8%)	0.60	0/1205
12	AL	1.15	9/960 (0.9%)	0.61	0/1286
13	AM	0.93	5/892 (0.6%)	0.57	0/1193
14	AN	0.88	4/811 (0.5%)	0.56	0/1081
15	AO	0.44	0/722	0.42	0/964
16	AP	0.74	2/659 (0.3%)	0.53	0/884
17	AQ	0.77	2/657 (0.3%)	0.52	0/881
18	AR	0.92	2/462 (0.4%)	0.56	0/621
19	AS	1.07	5/672 (0.7%)	0.59	0/904
20	AT	0.59	1/676 (0.1%)	0.42	0/895
21	AU	1.09	4/472 (0.8%)	0.53	0/627
22	BA	0.93	5/69120 (0.0%)	0.81	4/107824 (0.0%)
23	BB	0.75	0/2872	0.68	0/4478
24	BC	1.27	19/2121 (0.9%)	0.65	0/2852
25	BD	1.03	8/1576 (0.5%)	0.57	0/2119
26	BE	0.89	6/1571 (0.4%)	0.57	0/2113
27	BF	0.87	6/1434 (0.4%)	0.51	0/1926
28	BG	1.01	8/1343 (0.6%)	0.53	1/1816 (0.1%)
29	BH	0.69	3/1121 (0.3%)	0.48	0/1515
30	BI	0.78	2/531 (0.4%)	0.50	0/709
31	BJ	1.06	6/1152 (0.5%)	0.57	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	BK	1.08	5/955 (0.5%)	0.64	0/1279
33	BL	0.96	4/1062 (0.4%)	0.64	0/1413
34	BM	1.15	7/1081 (0.6%)	0.65	0/1443
35	BN	1.07	4/958 (0.4%)	0.66	0/1281
36	BO	0.78	2/910 (0.2%)	0.56	1/1219 (0.1%)
37	BP	0.96	4/929 (0.4%)	0.56	0/1242
38	BQ	0.85	0/960	0.59	0/1278
39	BR	0.86	3/829 (0.4%)	0.61	0/1107
40	BS	0.86	2/864 (0.2%)	0.57	0/1156
41	BT	0.75	1/744 (0.1%)	0.60	0/994
42	BU	0.94	3/787 (0.4%)	0.61	0/1051
43	BV	1.03	4/766 (0.5%)	0.61	0/1025
44	BW	0.88	1/587 (0.2%)	0.62	0/776
45	BX	0.95	2/635 (0.3%)	0.60	0/848
46	BY	0.60	0/502	0.52	0/667
47	BZ	1.00	2/453 (0.4%)	0.62	0/605
48	B0	0.89	1/450 (0.2%)	0.60	0/599
49	B1	1.02	2/421 (0.5%)	0.70	0/561
50	B2	0.99	1/380 (0.3%)	0.65	0/498
51	B3	1.23	4/513 (0.8%)	0.82	1/676 (0.1%)
52	B4	1.00	1/303 (0.3%)	0.68	0/397
53	B5	1.38	2/151 (1.3%)	1.05	0/205
54	B7	0.61	1/233 (0.4%)	0.84	1/358 (0.3%)
55	B8	0.75	14/1839 (0.8%)	0.69	1/2866 (0.0%)
56	B9	0.71	8/2806 (0.3%)	0.51	1/3778 (0.0%)
All	All	0.88	234/158589 (0.1%)	0.73	19/236840 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	AE	0	1
51	B3	0	1
All	All	0	2

All (234) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	892	A	C2'-C1'	-16.38	1.28	1.53
22	BA	892	A	O4'-C1'	14.53	1.63	1.41

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	B5	24	PRO	N-CD	12.07	1.64	1.47
5	AE	57	PRO	N-CD	11.47	1.63	1.47
56	B9	267	PRO	N-CD	11.47	1.63	1.47
56	B9	6	PRO	N-CD	11.42	1.63	1.47
13	AM	115	PRO	N-CD	11.39	1.63	1.47
21	AU	2	PRO	N-CD	11.36	1.63	1.47
6	AF	67	PRO	N-CD	11.27	1.63	1.47
10	AJ	79	PRO	N-CD	11.24	1.63	1.47
10	AJ	39	PRO	N-CD	11.23	1.63	1.47
4	AD	139	PRO	N-CD	11.20	1.63	1.47
2	AB	158	PRO	N-CD	11.20	1.63	1.47
7	AG	2	PRO	N-CD	11.19	1.63	1.47
9	AI	23	PRO	N-CD	11.17	1.63	1.47
42	BU	55	PRO	N-CD	11.14	1.63	1.47
4	AD	38	PRO	N-CD	11.12	1.63	1.47
9	AI	51	PRO	N-CD	11.11	1.63	1.47
27	BF	139	PRO	N-CD	11.08	1.63	1.47
56	B9	236	PRO	N-CD	11.08	1.63	1.47
6	AF	19	PRO	N-CD	11.07	1.63	1.47
29	BH	38	PRO	N-CD	11.07	1.63	1.47
10	AJ	41	PRO	N-CD	11.06	1.63	1.47
3	AC	17	PRO	N-CD	11.06	1.63	1.47
28	BG	8	PRO	N-CD	11.05	1.63	1.47
7	AG	16	PRO	N-CD	11.05	1.63	1.47
42	BU	48	PRO	N-CD	11.04	1.63	1.47
7	AG	14	PRO	N-CD	11.04	1.63	1.47
4	AD	186	PRO	N-CD	11.03	1.63	1.47
42	BU	50	PRO	N-CD	11.03	1.63	1.47
56	B9	44	PRO	N-CD	11.02	1.63	1.47
27	BF	109	PRO	N-CD	11.01	1.63	1.47
2	AB	48	PRO	N-CD	10.99	1.63	1.47
19	AS	30	PRO	N-CD	10.99	1.63	1.47
12	AL	122	PRO	N-CD	10.99	1.63	1.47
28	BG	112	PRO	N-CD	10.98	1.63	1.47
4	AD	168	PRO	N-CD	10.97	1.63	1.47
7	AG	71	PRO	N-CD	10.96	1.63	1.47
13	AM	10	PRO	N-CD	10.96	1.63	1.47
19	AS	9	PRO	N-CD	10.95	1.63	1.47
2	AB	182	PRO	N-CD	10.93	1.63	1.47
29	BH	118	PRO	N-CD	10.93	1.63	1.47
21	AU	11	PRO	N-CD	10.92	1.63	1.47
12	AL	22	PRO	N-CD	10.91	1.63	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AD	46	PRO	N-CD	10.90	1.63	1.47
3	AC	60	PRO	N-CD	10.90	1.63	1.47
7	AG	93	PRO	N-CD	10.89	1.62	1.47
5	AE	150	PRO	N-CD	10.89	1.62	1.47
3	AC	73	PRO	N-CD	10.88	1.62	1.47
56	B9	224	PRO	N-CD	10.88	1.62	1.47
14	AN	94	PRO	N-CD	10.88	1.62	1.47
30	BI	42	PRO	N-CD	10.88	1.62	1.47
13	AM	112	PRO	N-CD	10.87	1.62	1.47
47	BZ	42	PRO	N-CD	10.86	1.62	1.47
49	B1	31	PRO	N-CD	10.86	1.62	1.47
6	AF	101	PRO	N-CD	10.85	1.62	1.47
28	BG	156	PRO	N-CD	10.83	1.62	1.47
32	BK	72	PRO	N-CD	10.82	1.62	1.47
2	AB	193	PRO	N-CD	10.81	1.62	1.47
12	AL	91	PRO	N-CD	10.81	1.62	1.47
24	BC	126	PRO	N-CD	10.81	1.62	1.47
12	AL	11	PRO	N-CD	10.80	1.62	1.47
19	AS	42	PRO	N-CD	10.80	1.62	1.47
13	AM	96	PRO	N-CD	10.80	1.62	1.47
3	AC	98	PRO	N-CD	10.79	1.62	1.47
24	BC	131	PRO	N-CD	10.78	1.62	1.47
34	BM	72	PRO	N-CD	10.77	1.62	1.47
56	B9	50	PRO	N-CD	10.77	1.62	1.47
34	BM	4	PRO	N-CD	10.77	1.62	1.47
33	BL	119	PRO	N-CD	10.76	1.62	1.47
51	B3	2	PRO	N-CD	10.76	1.62	1.47
2	AB	29	PRO	N-CD	10.76	1.62	1.47
26	BE	129	PRO	N-CD	10.76	1.62	1.47
12	AL	45	PRO	N-CD	10.74	1.62	1.47
3	AC	174	PRO	N-CD	10.73	1.62	1.47
30	BI	7	PRO	N-CD	10.72	1.62	1.47
28	BG	126	PRO	N-CD	10.72	1.62	1.47
3	AC	109	PRO	N-CD	10.71	1.62	1.47
8	AH	93	PRO	N-CD	10.71	1.62	1.47
19	AS	59	PRO	N-CD	10.71	1.62	1.47
18	AR	41	PRO	N-CD	10.70	1.62	1.47
27	BF	176	PRO	N-CD	10.70	1.62	1.47
8	AH	28	PRO	N-CD	10.70	1.62	1.47
10	AJ	43	PRO	N-CD	10.70	1.62	1.47
19	AS	76	PRO	N-CD	10.69	1.62	1.47
7	AG	88	PRO	N-CD	10.69	1.62	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	B9	206	PRO	N-CD	10.68	1.62	1.47
14	AN	52	PRO	N-CD	10.68	1.62	1.47
43	BV	27	PRO	N-CD	10.67	1.62	1.47
9	AI	125	PRO	N-CD	10.66	1.62	1.47
6	AF	50	PRO	N-CD	10.66	1.62	1.47
4	AD	7	PRO	N-CD	10.66	1.62	1.47
24	BC	32	PRO	N-CD	10.65	1.62	1.47
28	BG	154	PRO	N-CD	10.64	1.62	1.47
11	AK	123	PRO	N-CD	10.64	1.62	1.47
16	AP	41	PRO	N-CD	10.62	1.62	1.47
8	AH	57	PRO	N-CD	10.62	1.62	1.47
2	AB	25	PRO	N-CD	10.62	1.62	1.47
14	AN	70	PRO	N-CD	10.62	1.62	1.47
32	BK	94	PRO	N-CD	10.61	1.62	1.47
35	BN	39	PRO	N-CD	10.60	1.62	1.47
6	AF	12	PRO	N-CD	10.59	1.62	1.47
29	BH	32	PRO	N-CD	10.59	1.62	1.47
36	BO	42	PRO	N-CD	10.59	1.62	1.47
17	AQ	66	PRO	N-CD	10.57	1.62	1.47
26	BE	177	PRO	N-CD	10.57	1.62	1.47
34	BM	77	PRO	N-CD	10.57	1.62	1.47
11	AK	89	PRO	N-CD	10.56	1.62	1.47
11	AK	91	PRO	N-CD	10.56	1.62	1.47
43	BV	84	PRO	N-CD	10.56	1.62	1.47
28	BG	54	PRO	N-CD	10.55	1.62	1.47
5	AE	84	PRO	N-CD	10.55	1.62	1.47
2	AB	201	PRO	N-CD	10.55	1.62	1.47
17	AQ	32	PRO	N-CD	10.54	1.62	1.47
27	BF	84	PRO	N-CD	10.53	1.62	1.47
32	BK	48	PRO	N-CD	10.53	1.62	1.47
37	BP	18	PRO	N-CD	10.53	1.62	1.47
24	BC	218	PRO	N-CD	10.52	1.62	1.47
51	B3	63	PRO	N-CD	10.51	1.62	1.47
28	BG	118	PRO	N-CD	10.51	1.62	1.47
37	BP	22	PRO	N-CD	10.51	1.62	1.47
14	AN	57	PRO	N-CD	10.50	1.62	1.47
18	AR	69	PRO	N-CD	10.50	1.62	1.47
35	BN	109	PRO	N-CD	10.50	1.62	1.47
11	AK	115	PRO	N-CD	10.49	1.62	1.47
11	AK	124	PRO	N-CD	10.49	1.62	1.47
25	BD	23	PRO	N-CD	10.49	1.62	1.47
24	BC	231	PRO	N-CD	10.48	1.62	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	BR	52	PRO	N-CD	10.48	1.62	1.47
24	BC	22	PRO	N-CD	10.48	1.62	1.47
5	AE	98	PRO	N-CD	10.47	1.62	1.47
21	AU	41	PRO	N-CD	10.47	1.62	1.47
48	B0	8	PRO	N-CD	10.47	1.62	1.47
24	BC	148	PRO	N-CD	10.46	1.62	1.47
35	BN	85	PRO	N-CD	10.46	1.62	1.47
8	AH	6	PRO	N-CD	10.44	1.62	1.47
28	BG	12	PRO	N-CD	10.44	1.62	1.47
43	BV	37	PRO	N-CD	10.44	1.62	1.47
20	AT	56	PRO	N-CD	10.43	1.62	1.47
45	BX	12	PRO	N-CD	10.41	1.62	1.47
11	AK	117	PRO	N-CD	10.41	1.62	1.47
8	AH	81	PRO	N-CD	10.39	1.62	1.47
11	AK	60	PRO	N-CD	10.39	1.62	1.47
24	BC	8	PRO	N-CD	10.39	1.62	1.47
31	BJ	46	PRO	N-CD	10.39	1.62	1.47
47	BZ	18	PRO	N-CD	10.38	1.62	1.47
27	BF	29	PRO	N-CD	10.37	1.62	1.47
3	AC	7	PRO	N-CD	10.36	1.62	1.47
10	AJ	55	PRO	N-CD	10.36	1.62	1.47
25	BD	63	PRO	N-CD	10.36	1.62	1.47
24	BC	227	PRO	N-CD	10.35	1.62	1.47
51	B3	46	PRO	N-CD	10.34	1.62	1.47
26	BE	89	PRO	N-CD	10.32	1.62	1.47
32	BK	120	PRO	N-CD	10.31	1.62	1.47
31	BJ	8	PRO	N-CD	10.31	1.62	1.47
49	B1	41	PRO	N-CD	10.31	1.62	1.47
34	BM	125	PRO	N-CD	10.30	1.62	1.47
25	BD	152	PRO	N-CD	10.30	1.62	1.47
32	BK	102	PRO	N-CD	10.30	1.62	1.47
41	BT	14	PRO	N-CD	10.27	1.62	1.47
5	AE	133	PRO	N-CD	10.26	1.62	1.47
31	BJ	110	PRO	N-CD	10.25	1.62	1.47
24	BC	107	PRO	N-CD	10.25	1.62	1.47
43	BV	81	PRO	N-CD	10.24	1.62	1.47
34	BM	109	PRO	N-CD	10.21	1.62	1.47
40	BS	87	PRO	N-CD	10.21	1.62	1.47
31	BJ	137	PRO	N-CD	10.20	1.62	1.47
33	BL	8	PRO	N-CD	10.19	1.62	1.47
12	AL	42	PRO	N-CD	10.19	1.62	1.47
12	AL	28	PRO	N-CD	10.16	1.61	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BD	143	PRO	N-CD	10.16	1.61	1.47
37	BP	79	PRO	N-CD	10.15	1.61	1.47
27	BF	65	PRO	N-CD	10.14	1.61	1.47
44	BW	74	PRO	N-CD	10.14	1.61	1.47
52	B4	31	PRO	N-CD	10.13	1.61	1.47
35	BN	50	PRO	N-CD	10.12	1.61	1.47
40	BS	80	PRO	N-CD	10.12	1.61	1.47
24	BC	11	PRO	N-CD	10.11	1.61	1.47
24	BC	29	PRO	N-CD	10.10	1.61	1.47
50	B2	7	PRO	N-CD	10.10	1.61	1.47
34	BM	69	PRO	N-CD	10.09	1.61	1.47
36	BO	32	PRO	N-CD	10.09	1.61	1.47
26	BE	59	PRO	N-CD	10.07	1.61	1.47
25	BD	205	PRO	N-CD	10.07	1.61	1.47
25	BD	194	PRO	N-CD	10.01	1.61	1.47
16	AP	15	PRO	N-CD	9.99	1.61	1.47
24	BC	247	PRO	N-CD	9.98	1.61	1.47
24	BC	85	PRO	N-CD	9.93	1.61	1.47
24	BC	75	PRO	N-CD	9.89	1.61	1.47
33	BL	56	PRO	N-CD	9.86	1.61	1.47
24	BC	136	PRO	N-CD	9.81	1.61	1.47
31	BJ	113	PRO	N-CD	9.79	1.61	1.47
24	BC	244	PRO	N-CD	9.79	1.61	1.47
26	BE	76	PRO	N-CD	9.76	1.61	1.47
45	BX	31	PRO	N-CD	9.74	1.61	1.47
34	BM	98	PRO	N-CD	9.67	1.61	1.47
31	BJ	97	PRO	N-CD	9.66	1.61	1.47
22	BA	892	A	C4'-O4'	-9.65	1.31	1.45
33	BL	62	PRO	N-CD	9.40	1.60	1.47
7	AG	2	PRO	N-CA	-9.25	1.33	1.47
51	B3	2	PRO	N-CA	-9.13	1.33	1.47
13	AM	115	PRO	N-CA	-9.06	1.33	1.47
21	AU	2	PRO	N-CA	-9.00	1.33	1.47
25	BD	152	PRO	N-CA	-8.83	1.32	1.47
56	B9	6	PRO	N-CA	-8.54	1.34	1.47
39	BR	52	PRO	N-CA	-8.19	1.33	1.47
12	AL	45	PRO	N-CA	-8.15	1.33	1.47
22	BA	2449	U	C5-C6	8.15	1.50	1.34
10	AJ	39	PRO	N-CA	-7.88	1.33	1.47
53	B5	24	PRO	N-CA	-7.20	1.36	1.47
25	BD	152	PRO	CG-CD	-6.76	1.33	1.51
55	B8	59	A	C6-N6	6.68	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	B8	58	A	C6-N6	6.68	1.47	1.33
55	B8	73	A	C6-N6	6.66	1.47	1.33
55	B8	51	A	C6-N6	6.65	1.47	1.33
55	B8	6	A	C6-N6	6.64	1.47	1.33
55	B8	42	A	C6-N6	6.63	1.47	1.33
54	B7	9	A	C6-N6	6.62	1.47	1.33
55	B8	26	A	C6-N6	6.60	1.47	1.33
55	B8	76	A	C6-N6	6.60	1.47	1.33
55	B8	14	A	C6-N6	6.58	1.47	1.33
55	B8	38	A	C6-N6	6.57	1.47	1.33
55	B8	66	A	C6-N6	6.56	1.47	1.33
55	B8	21	A	C6-N6	6.52	1.47	1.33
55	B8	41	A	C6-N6	6.46	1.46	1.33
55	B8	69	A	C6-N6	6.38	1.46	1.33
12	AL	45	PRO	CG-CD	-6.08	1.35	1.51
10	AJ	39	PRO	CG-CD	-6.02	1.35	1.51
22	BA	892	A	C3'-O3'	-5.93	1.33	1.42
39	BR	52	PRO	CG-CD	-5.89	1.35	1.51
24	BC	132	MET	CA-C	-5.26	1.45	1.52
37	BP	100	LEU	CA-C	-5.12	1.45	1.52
24	BC	231	PRO	CG-CD	-5.07	1.33	1.50
26	BE	76	PRO	CG-CD	-5.05	1.33	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	69	G	C5'-C4'-O4'	10.37	125.35	109.80
22	BA	826	U	OP1-P-O3'	-10.08	77.76	108.00
1	AA	116	A	OP2-P-O3'	-8.60	82.21	108.00
1	AA	69	G	O5'-C5'-C4'	-8.51	98.74	111.50
54	B7	10	U	O5'-P-OP1	-7.97	84.10	108.00
1	AA	116	A	OP1-P-O3'	-7.96	84.11	108.00
3	AC	107	ARG	NE-CZ-NH2	7.22	125.70	119.20
55	B8	74	C	OP1-P-O3'	-6.91	87.26	108.00
22	BA	826	U	OP2-P-O3'	-6.62	88.13	108.00
3	AC	107	ARG	CG-CD-NE	6.23	125.72	112.00
56	B9	46	VAL	N-CA-C	-5.91	107.53	113.20
36	BO	32	PRO	CA-N-CD	-5.69	104.04	112.00
22	BA	752	A	N1-C6-N6	-5.50	102.12	118.60
51	B3	32	ILE	CG1-CB-CG2	-5.46	94.31	110.70
22	BA	512	G	O4'-C1'-N9	5.44	116.36	108.20
1	AA	69	G	O4'-C1'-N9	5.37	116.55	108.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BG	156	PRO	CA-N-CD	-5.19	104.73	112.00
1	AA	68	G	C4-N9-C1'	5.06	141.68	126.50
1	AA	69	G	C1'-O4'-C4'	-5.06	104.84	109.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AE	89	HIS	Peptide
51	B3	31	HIS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32930	0	16583	460	0
2	AB	1753	0	1780	36	0
3	AC	1624	0	1696	37	0
4	AD	1643	0	1707	21	0
5	AE	1144	0	1185	21	0
6	AF	862	0	864	23	0
7	AG	1181	0	1238	28	0
8	AH	979	0	1031	18	0
9	AI	1022	0	1070	42	0
10	AJ	795	0	836	25	0
11	AK	877	0	887	19	0
12	AL	957	0	1017	20	0
13	AM	883	0	941	29	0
14	AN	799	0	841	27	0
15	AO	714	0	734	2	0
16	AP	649	0	666	8	0
17	AQ	648	0	691	10	0
18	AR	455	0	478	10	0
19	AS	656	0	680	25	0
20	AT	670	0	719	9	0
21	AU	465	0	491	11	0
22	BA	62209	0	31287	441	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	BB	2569	0	1301	19	0
24	BC	2082	0	2154	28	0
25	BD	1566	0	1618	20	0
26	BE	1552	0	1619	20	0
27	BF	1410	0	1444	38	0
28	BG	1323	0	1371	15	0
29	BH	1110	0	1148	32	0
30	BI	522	0	520	24	0
31	BJ	1129	0	1162	16	0
32	BK	946	0	1023	6	0
33	BL	1053	0	1128	15	0
34	BM	1075	0	1155	15	0
35	BN	945	0	989	7	0
36	BO	900	0	935	8	0
37	BP	917	0	962	13	0
38	BQ	947	0	1019	11	0
39	BR	816	0	839	8	0
40	BS	857	0	922	12	0
41	BT	738	0	807	17	0
42	BU	779	0	831	18	0
43	BV	753	0	780	12	0
44	BW	580	0	594	11	0
45	BX	625	0	652	2	0
46	BY	501	0	531	4	0
47	BZ	449	0	488	8	0
48	B0	444	0	458	7	0
49	B1	414	0	442	6	0
50	B2	377	0	418	3	0
51	B3	504	0	572	17	0
52	B4	302	0	340	3	0
53	B5	146	0	139	5	0
54	B7	211	0	110	5	0
55	B8	1646	0	831	26	0
56	B9	2768	0	2666	90	0
57	AA	87	0	0	0	0
57	B8	2	0	0	0	0
57	BA	243	0	0	0	0
57	BB	1	0	0	0	0
57	BC	1	0	0	0	0
57	BD	2	0	0	0	0
57	BL	3	0	0	0	0
58	AA	38	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	AM	1	0	0	0	0
58	BA	104	0	0	0	0
58	BB	1	0	0	0	0
58	BC	1	0	0	0	0
58	BD	1	0	0	0	0
58	BM	1	0	0	0	0
59	AB	1	0	0	0	0
59	B4	1	0	0	0	0
59	BI	1	0	0	0	0
60	BA	15	0	9	0	0
61	AA	167	0	0	0	0
61	AK	1	0	0	0	0
61	AM	1	0	0	0	0
61	AN	3	0	0	0	0
61	BA	617	0	0	3	0
61	BC	6	0	0	0	0
61	BD	2	0	0	0	0
61	BN	3	0	0	0	0
All	All	148175	0	99399	1663	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1663) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:B8:1:C:H5'	56:B9:282:LYS:NZ	1.70	1.05
22:BA:2185:U:C4	22:BA:2186:G:O6	2.13	1.00
1:AA:1088:G:N2	1:AA:1167:A:H61	1.59	1.00
1:AA:1026:G:C6	1:AA:1035:A:N6	2.32	0.98
22:BA:884:U:O4	22:BA:892:A:C5	2.21	0.93
1:AA:1088:G:H21	1:AA:1167:A:H61	0.96	0.92
1:AA:445:G:H1	1:AA:489:C:H5	1.20	0.90
1:AA:100:G:H4'	1:AA:101:A:O5'	1.71	0.89
22:BA:2107:G:H1	22:BA:2182:U:H3	1.17	0.89
1:AA:1026:G:N1	1:AA:1035:A:C6	2.41	0.89
8:AH:12:THR:HG22	8:AH:15:ARG:HH12	1.37	0.89
55:B8:1:C:H5'	56:B9:282:LYS:HZ3	1.33	0.88
1:AA:1026:G:C6	1:AA:1035:A:C6	2.62	0.87
1:AA:1088:G:H21	1:AA:1167:A:N6	1.74	0.86
1:AA:49:U:C5	1:AA:365:U:O4	2.30	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:81:A:H2	1:AA:88:U:H3	1.21	0.84
1:AA:208:U:H3	1:AA:211:G:H1	1.24	0.84
1:AA:1026:G:N1	1:AA:1035:A:C5	2.46	0.84
1:AA:49:U:C4	1:AA:365:U:O4	2.31	0.83
1:AA:9:G:OP2	5:AE:126:LYS:NZ	2.13	0.82
12:AL:114:ARG:HB2	12:AL:119:VAL:HB	1.62	0.82
1:AA:81:A:O2'	1:AA:82:G:N7	2.13	0.82
11:AK:88:GLY:H	11:AK:114:THR:HG22	1.44	0.82
13:AM:7:ILE:HD11	27:BF:112:ARG:HA	1.62	0.81
1:AA:100:G:C5	1:AA:102:G:C5	2.67	0.81
22:BA:2068:U:H3	22:BA:2430:A:H2	1.25	0.81
22:BA:2103:C:C4	22:BA:2104:C:N4	2.49	0.81
56:B9:117:ARG:HH12	56:B9:362:LYS:HE2	1.46	0.80
6:AF:3:HIS:ND1	6:AF:65:GLU:OE2	2.14	0.80
1:AA:1320:C:OP2	19:AS:3:ARG:NH2	2.15	0.79
1:AA:49:U:O4	1:AA:365:U:O4	2.00	0.79
29:BH:96:THR:HG23	29:BH:115:VAL:HB	1.63	0.79
22:BA:548:G:O2'	22:BA:549:G:O4'	2.01	0.79
22:BA:2611:C:OP2	61:BA:3402:HOH:O	2.00	0.79
1:AA:70:U:O2	1:AA:71:A:N6	2.13	0.79
11:AK:109:ASN:HB3	21:AU:5:LYS:HD3	1.65	0.79
2:AB:122:GLN:NE2	2:AB:123:ASP:OD1	2.17	0.78
22:BA:2840:C:H5''	35:BN:53:THR:HG21	1.64	0.78
29:BH:97:ARG:HB2	29:BH:112:LYS:HE3	1.66	0.77
47:BZ:6:LYS:NZ	47:BZ:37:GLU:HG3	1.98	0.77
1:AA:1305:G:H21	1:AA:1332:A:H2	1.30	0.77
22:BA:2185:U:O4	22:BA:2186:G:O6	2.02	0.77
22:BA:2639:A:O3'	31:BJ:96:ARG:NH1	2.17	0.77
22:BA:1172:C:N4	22:BA:1178:C:O2	2.17	0.77
30:BI:18:CYS:HB3	30:BI:40:CYS:SG	2.24	0.77
10:AJ:65:TYR:HB3	14:AN:96:LEU:HD11	1.65	0.77
1:AA:81:A:C2	1:AA:88:U:N3	2.51	0.76
22:BA:2185:U:N3	22:BA:2186:G:O6	2.18	0.76
22:BA:2189:U:H2'	22:BA:2190:G:H8	1.49	0.76
23:BB:31:C:O2	23:BB:53:A:N6	2.18	0.76
15:AO:89:ARG:NH2	22:BA:713:G:N7	2.34	0.76
22:BA:285:G:H1	22:BA:355:U:H3	1.32	0.76
22:BA:1250:G:H5''	38:BQ:6:ARG:HD3	1.66	0.76
34:BM:47:GLU:OE1	34:BM:50:ARG:NH1	2.19	0.76
22:BA:2188:U:O2'	22:BA:2189:U:O4'	2.04	0.76
27:BF:80:ARG:HH22	55:B8:56:C:N4	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:456:A:H61	1:AA:475:C:H42	1.34	0.75
1:AA:1397:C:OP2	5:AE:29:ARG:NH2	2.19	0.75
1:AA:1350:A:OP2	9:AI:120:LYS:NZ	2.19	0.75
23:BB:1:U:H2'	23:BB:2:G:H8	1.51	0.75
3:AC:35:SER:OG	3:AC:59:ARG:NH2	2.19	0.75
7:AG:106:GLU:O	7:AG:110:LYS:NZ	2.20	0.75
22:BA:2141:G:H2'	22:BA:2142:A:H8	1.51	0.75
24:BC:107:PRO:HD2	24:BC:110:LEU:HD22	1.69	0.75
55:B8:1:C:H5'	56:B9:282:LYS:HZ1	1.48	0.75
31:BJ:95:ARG:HE	31:BJ:96:ARG:HG3	1.51	0.75
3:AC:6:HIS:HB3	14:AN:89:MET:HE2	1.69	0.74
22:BA:358:U:H2'	22:BA:359:G:H8	1.50	0.74
1:AA:85:U:OP2	1:AA:86:G:N2	2.20	0.74
10:AJ:52:LEU:HD11	10:AJ:59:LYS:HA	1.70	0.74
28:BG:164:TYR:HB2	28:BG:167:GLU:HB2	1.66	0.74
8:AH:114:ARG:O	8:AH:118:GLN:NE2	2.21	0.74
5:AE:159:LYS:NZ	8:AH:42:GLU:O	2.20	0.74
12:AL:68:GLY:O	12:AL:99:ARG:NH1	2.21	0.74
9:AI:19:VAL:HG22	9:AI:65:ILE:HG12	1.69	0.74
1:AA:100:G:H22	1:AA:152:A:H1'	1.53	0.74
22:BA:280:U:O4	22:BA:360:U:O2	2.05	0.74
13:AM:89:LEU:HD12	13:AM:93:ARG:HH22	1.53	0.73
1:AA:717:U:H4'	11:AK:119:ASN:HD22	1.51	0.73
2:AB:15:HIS:HB3	2:AB:43:LEU:HD11	1.70	0.73
10:AJ:5:ARG:HG3	10:AJ:77:VAL:HG12	1.68	0.73
22:BA:2103:C:N4	22:BA:2104:C:N4	2.36	0.73
23:BB:42:C:OP2	30:BI:2:LYS:NZ	2.15	0.73
26:BE:61:ARG:NH2	53:B5:9:THR:OG1	2.22	0.73
1:AA:1130:A:OP1	9:AI:18:ARG:NH2	2.20	0.73
22:BA:2140:G:H1	22:BA:2151:U:H3	1.36	0.73
10:AJ:47:GLU:OE2	14:AN:76:LYS:NZ	2.22	0.73
1:AA:100:G:H2'	1:AA:102:G:H8	1.54	0.72
1:AA:1516:2MG:N2	1:AA:1519:MA6:OP2	2.20	0.72
1:AA:1363:A:O2'	1:AA:1365:G:N7	2.22	0.72
4:AD:12:SER:OG	4:AD:17:THR:O	2.07	0.72
1:AA:96:U:H2'	1:AA:97:G:H8	1.55	0.72
22:BA:545:U:O2	22:BA:548:G:N1	2.18	0.72
56:B9:25:LEU:HD21	56:B9:116:ARG:HG3	1.70	0.72
1:AA:635:A:O3'	17:AQ:6:ARG:NH1	2.23	0.72
22:BA:1607:C:N4	22:BA:1622:G:OP2	2.24	0.71
1:AA:68:G:H8	1:AA:69:G:O3'	1.74	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:746:A:H2'	1:AA:747:A:C8	2.25	0.71
1:AA:97:G:H2'	1:AA:98:A:O4'	1.91	0.71
3:AC:9:GLY:HA2	3:AC:12:LEU:HG	1.72	0.71
27:BF:142:ASP:OD2	27:BF:145:LYS:NZ	2.24	0.71
1:AA:437:U:H5'	4:AD:152:GLN:HE22	1.56	0.71
29:BH:15:LEU:HD21	29:BH:58:LEU:HD11	1.72	0.71
1:AA:840:C:N4	1:AA:842:U:O2'	2.24	0.71
22:BA:1083:U:O2	22:BA:1085:A:N7	2.23	0.71
27:BF:126:GLY:O	27:BF:158:THR:OG1	2.09	0.70
1:AA:68:G:H2'	1:AA:70:U:H5'	1.73	0.70
22:BA:2190:G:H2'	22:BA:2191:A:H8	1.56	0.70
32:BK:71:ARG:NH2	32:BK:123:LEU:O	2.21	0.70
22:BA:2138:G:O6	22:BA:2154:A:N6	2.25	0.70
22:BA:2831:G:OP2	25:BD:59:ARG:NH2	2.24	0.70
51:B3:32:ILE:HD12	51:B3:32:ILE:H	1.56	0.70
55:B8:18:G:O2'	55:B8:57:G:N2	2.24	0.70
22:BA:884:U:C4	22:BA:892:A:N7	2.60	0.69
22:BA:884:U:O4	22:BA:892:A:N7	2.24	0.69
9:AI:88:MET:HE1	9:AI:95:ARG:HA	1.75	0.69
33:BL:82:LEU:HD22	33:BL:90:VAL:HG21	1.75	0.69
56:B9:41:LEU:HD21	56:B9:56:LEU:HB3	1.75	0.69
1:AA:202:G:O2'	1:AA:467:U:O4	2.10	0.68
22:BA:2188:U:H2'	22:BA:2189:U:C6	2.28	0.68
56:B9:270:ILE:HD12	56:B9:294:LYS:HG2	1.76	0.68
14:AN:15:LEU:HD23	14:AN:54:ASP:HB2	1.75	0.68
2:AB:82:ASP:OD1	2:AB:83:ALA:N	2.27	0.68
22:BA:1847:A:HO2'	22:BA:1848:A:H8	1.40	0.68
8:AH:96:MET:HG3	8:AH:99:LEU:HB2	1.76	0.68
1:AA:460:A:H2'	1:AA:461:A:C8	2.28	0.68
22:BA:2141:G:H2'	22:BA:2142:A:C8	2.29	0.68
1:AA:1103:C:OP1	2:AB:95:ARG:NH2	2.27	0.68
1:AA:910:C:OP2	12:AL:18:LYS:NZ	2.26	0.67
14:AN:26:LEU:HD11	14:AN:48:LEU:HD13	1.76	0.67
22:BA:1102:C:H2'	22:BA:1103:A:H8	1.59	0.67
19:AS:25:SER:HB3	19:AS:28:LYS:HZ1	1.60	0.67
22:BA:2190:G:H2'	22:BA:2191:A:C8	2.29	0.67
22:BA:2261:C:OP1	44:BW:19:LYS:NZ	2.26	0.67
27:BF:140:GLU:OE2	30:BI:26:SER:OG	2.09	0.67
42:BU:89:ASP:OD1	42:BU:90:GLY:N	2.22	0.67
1:AA:96:U:H2'	1:AA:97:G:C8	2.30	0.67
3:AC:40:ARG:NH1	3:AC:55:ILE:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:B9:287:ALA:O	56:B9:291:MET:N	2.28	0.67
22:BA:2102:G:N2	22:BA:2188:U:O2	2.29	0.66
1:AA:100:G:O2'	1:AA:102:G:OP2	2.12	0.66
1:AA:463:U:H2'	1:AA:464:U:C2	2.31	0.66
1:AA:76:G:H1	1:AA:93:U:H3	1.43	0.66
22:BA:1667:G:O2'	22:BA:1991:U:O4	2.12	0.66
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.30	0.66
1:AA:1530:G:O6	21:AU:46:LYS:NZ	2.28	0.66
1:AA:64:G:C2	1:AA:69:G:C4	2.84	0.66
1:AA:102:G:C5	1:AA:103:U:C5	2.83	0.66
9:AI:59:GLU:HG2	9:AI:60:LYS:HD3	1.77	0.66
1:AA:100:G:H2'	1:AA:102:G:C8	2.31	0.66
10:AJ:63:ASP:OD1	14:AN:98:LYS:NZ	2.28	0.66
23:BB:43:C:O2	27:BF:92:ARG:NH2	2.29	0.66
1:AA:544:G:OP1	4:AD:56:ARG:NH2	2.28	0.65
2:AB:114:LEU:HD13	2:AB:144:LEU:HD22	1.78	0.65
13:AM:66:GLU:HG3	13:AM:67:GLY:H	1.60	0.65
22:BA:1847:A:O2'	22:BA:1848:A:H8	1.79	0.65
22:BA:2611:C:OP2	61:BA:3404:HOH:O	2.14	0.65
22:BA:541:A:N6	22:BA:553:G:O6	2.29	0.65
33:BL:123:ARG:NH1	33:BL:143:GLU:OE1	2.30	0.65
1:AA:1251:A:H2'	1:AA:1252:A:C8	2.31	0.65
31:BJ:114:LEU:HG	31:BJ:118:MET:HE3	1.79	0.65
19:AS:30:PRO:HA	19:AS:48:THR:HG23	1.79	0.65
22:BA:1729:U:O2'	22:BA:1731:G:N2	2.29	0.65
22:BA:2102:G:H1	22:BA:2188:U:H3	1.44	0.65
22:BA:2377:A:O2'	36:BO:117:PHE:O	2.13	0.65
35:BN:2:ARG:HD2	35:BN:2:ARG:O	1.96	0.65
51:B3:31:HIS:C	51:B3:33:LEU:H	2.05	0.65
13:AM:4:ILE:HG22	13:AM:5:ALA:H	1.61	0.64
22:BA:2171:A:O2'	22:BA:2173:A:OP1	2.13	0.64
30:BI:46:GLY:HA2	30:BI:49:ARG:CZ	2.27	0.64
34:BM:62:LYS:HD2	34:BM:64:TRP:CZ2	2.32	0.64
47:BZ:6:LYS:HZ3	47:BZ:37:GLU:HG3	1.62	0.64
56:B9:87:ALA:HA	56:B9:92:ASP:HB3	1.78	0.64
1:AA:100:G:OP1	20:AT:5:LYS:NZ	2.30	0.64
1:AA:102:G:C6	1:AA:103:U:C4	2.86	0.64
8:AH:96:MET:HB3	8:AH:100:GLY:H	1.62	0.64
9:AI:25:ASN:H	9:AI:27:LYS:NZ	1.95	0.64
22:BA:2299:U:OP2	27:BF:71:ARG:NH1	2.30	0.64
25:BD:1:MET:HE3	25:BD:205:PRO:HG3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1033:G:H2'	1:AA:1034:G:C8	2.32	0.64
5:AE:111:MET:HE2	5:AE:127:ALA:HB2	1.78	0.64
11:AK:84:VAL:HB	11:AK:110:ILE:HG22	1.80	0.64
22:BA:2113:U:OP2	22:BA:2115:G:N2	2.30	0.64
56:B9:342:THR:HG22	56:B9:344:ASN:H	1.62	0.64
22:BA:2134:A:O2'	22:BA:2135:A:O4'	2.11	0.64
33:BL:62:PRO:HB2	51:B3:30:ARG:HH11	1.63	0.64
2:AB:26:LYS:NZ	2:AB:194:ASP:OD2	2.31	0.64
6:AF:40:GLU:OE1	6:AF:100:SER:OG	2.15	0.64
19:AS:19:VAL:O	19:AS:23:VAL:HG23	1.98	0.64
22:BA:2469:A:N6	22:BA:2481:G:O2'	2.31	0.64
42:BU:4:LYS:O	42:BU:94:ARG:NH2	2.31	0.64
1:AA:1130:A:H2'	1:AA:1131:G:H8	1.61	0.64
34:BM:75:GLU:HG2	34:BM:90:GLU:HG3	1.79	0.64
42:BU:28:VAL:HG22	42:BU:34:VAL:HG12	1.79	0.64
43:BV:58:SER:O	43:BV:73:LYS:NZ	2.31	0.64
1:AA:100:G:O4'	1:AA:101:A:C8	2.51	0.64
1:AA:100:G:C4	1:AA:102:G:C8	2.86	0.64
2:AB:219:ALA:O	2:AB:222:ARG:N	2.31	0.64
22:BA:534:U:O2'	38:BQ:49:ASP:OD2	2.11	0.64
28:BG:2:SER:OG	28:BG:3:ARG:N	2.26	0.64
1:AA:100:G:O2'	1:AA:102:G:O5'	2.16	0.64
41:BT:39:THR:OG1	41:BT:42:GLU:OE1	2.11	0.64
1:AA:537:G:OP1	12:AL:110:ARG:NH2	2.31	0.64
22:BA:2305:U:H5''	27:BF:131:GLY:HA3	1.79	0.64
56:B9:358:GLU:OE1	56:B9:358:GLU:N	2.31	0.64
42:BU:34:VAL:HG13	42:BU:67:VAL:HG22	1.79	0.63
1:AA:67:C:C4	1:AA:69:G:C4	2.86	0.63
9:AI:106:ARG:NH1	9:AI:107:ASP:O	2.31	0.63
1:AA:28:A:O2'	1:AA:296:U:OP1	2.14	0.63
1:AA:68:G:C8	1:AA:69:G:O3'	2.50	0.63
1:AA:459:A:H2'	1:AA:460:A:C8	2.33	0.63
5:AE:148:ASN:HB2	5:AE:152:MET:SD	2.38	0.63
17:AQ:17:MET:HG3	17:AQ:20:SER:HB2	1.80	0.63
54:B7:1:C:H2'	54:B7:2:G:H8	1.61	0.63
1:AA:67:C:C5	1:AA:69:G:C4	2.87	0.63
22:BA:2161:C:O2'	22:BA:2173:A:O5'	2.16	0.63
56:B9:31:LYS:HA	56:B9:34:LEU:HD12	1.81	0.63
1:AA:1169:A:H2'	1:AA:1170:A:C8	2.34	0.63
24:BC:133:ARG:CZ	29:BH:123:ARG:HH12	2.12	0.62
56:B9:116:ARG:NH1	56:B9:117:ARG:HG2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:67:C:N4	1:AA:69:G:C2	2.66	0.62
22:BA:946:C:OP2	61:BA:3401:HOH:O	0.62	0.62
48:B0:52:ARG:NH2	48:B0:54:VAL:HG12	2.14	0.62
1:AA:1340:A:HO2'	55:B8:31:G:HO2'	1.47	0.62
22:BA:1101:U:O2'	52:B4:12:ARG:NH2	2.32	0.62
22:BA:2359:C:O2'	51:B3:54:ASP:OD1	2.18	0.62
23:BB:51:G:OP1	36:BO:63:LYS:NZ	2.22	0.62
29:BH:5:LEU:HD13	29:BH:17:ASP:HB2	1.82	0.62
22:BA:884:U:O4	22:BA:892:A:C6	2.52	0.62
1:AA:1350:A:O2'	7:AG:33:ASP:OD1	2.17	0.62
22:BA:1065:U:H3	22:BA:1073:A:H61	1.47	0.62
22:BA:2116:G:N7	22:BA:2165:C:N4	2.47	0.62
2:AB:114:LEU:HB2	2:AB:144:LEU:CD2	2.29	0.62
22:BA:2799:A:O2'	22:BA:2800:A:H5''	2.00	0.62
16:AP:48:GLU:HG3	16:AP:49:GLY:H	1.63	0.62
22:BA:2109:U:O2	22:BA:2180:U:O4	2.17	0.62
56:B9:22:ARG:HE	56:B9:70:LEU:HD13	1.65	0.62
7:AG:138:ARG:NH2	7:AG:139:GLU:OE2	2.31	0.61
56:B9:118:MET:HE1	56:B9:187:TYR:HB3	1.81	0.61
1:AA:1077:G:N2	1:AA:1080:A:OP2	2.31	0.61
1:AA:1180:A:OP2	9:AI:99:ARG:NH2	2.32	0.61
22:BA:1753:G:OP1	37:BP:93:ARG:NH1	2.34	0.61
1:AA:492:C:H2'	1:AA:493:A:C8	2.34	0.61
1:AA:1152:A:OP1	10:AJ:70:HIS:ND1	2.26	0.61
6:AF:44:ARG:HD2	6:AF:56:LYS:HG3	1.81	0.61
22:BA:1649:G:O2'	35:BN:106:ASP:OD2	2.05	0.61
1:AA:68:G:C6	1:AA:100:G:O6	2.54	0.61
46:BY:10:SER:OG	46:BY:13:GLU:OE1	2.16	0.61
9:AI:12:ARG:HG3	9:AI:13:LYS:H	1.65	0.61
22:BA:2134:A:H1'	22:BA:2159:G:H1'	1.83	0.61
1:AA:64:G:C4	1:AA:69:G:C6	2.89	0.61
22:BA:1914:C:N4	56:B9:315:SER:O	2.24	0.61
56:B9:15:THR:O	56:B9:18:SER:OG	2.19	0.61
56:B9:170:GLU:HA	56:B9:176:ILE:HA	1.81	0.61
3:AC:49:LYS:O	3:AC:72:ARG:NH1	2.34	0.61
7:AG:118:LEU:O	7:AG:122:ASN:ND2	2.33	0.61
22:BA:358:U:H2'	22:BA:359:G:C8	2.33	0.61
29:BH:82:SER:HB2	29:BH:90:LEU:HD11	1.82	0.61
56:B9:333:ILE:HG13	56:B9:345:THR:HG22	1.82	0.61
1:AA:382:A:H2'	1:AA:383:A:C8	2.36	0.61
5:AE:163:GLU:HB3	8:AH:114:ARG:HH22	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.81	0.61
41:BT:56:GLU:OE1	41:BT:56:GLU:N	2.33	0.61
43:BV:2:PHE:HB3	43:BV:50:MET:HE3	1.82	0.61
1:AA:1266:G:N2	1:AA:1269:A:OP2	2.32	0.61
9:AI:46:MET:O	9:AI:50:GLN:HG3	2.01	0.61
11:AK:108:THR:O	21:AU:6:VAL:HG12	2.01	0.61
22:BA:2316:G:H2'	22:BA:2317:A:H8	1.66	0.61
29:BH:84:ALA:HB2	29:BH:90:LEU:HD12	1.83	0.61
1:AA:673:A:H2'	1:AA:674:G:C8	2.36	0.60
2:AB:23:TRP:CZ3	2:AB:25:PRO:HA	2.35	0.60
22:BA:2118:U:O2	22:BA:2145:C:N4	2.34	0.60
41:BT:1:MET:HG2	41:BT:2:ILE:N	2.16	0.60
1:AA:462:G:C5	1:AA:463:U:C4	2.89	0.60
1:AA:481:G:O2'	1:AA:483:C:N4	2.34	0.60
9:AI:129:LYS:NZ	55:B8:34:C:OP2	2.27	0.60
22:BA:1469:A:H2'	22:BA:1470:A:C8	2.36	0.60
30:BI:11:GLU:OE2	30:BI:23:LYS:HD2	2.01	0.60
3:AC:9:GLY:H	14:AN:89:MET:HE3	1.66	0.60
22:BA:2180:U:H2'	22:BA:2181:U:H6	1.66	0.60
56:B9:69:THR:HG23	56:B9:109:LYS:HE3	1.83	0.60
1:AA:100:G:C6	1:AA:102:G:C4	2.89	0.60
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.66	0.60
4:AD:58:LYS:NZ	4:AD:69:GLU:OE1	2.34	0.60
32:BK:121:GLU:OE1	37:BP:65:SER:OG	2.17	0.60
26:BE:168:ASP:OD2	26:BE:170:ARG:NH1	2.31	0.60
1:AA:458:U:H2'	1:AA:459:A:C8	2.36	0.60
2:AB:114:LEU:HB2	2:AB:144:LEU:HD22	1.84	0.60
22:BA:2365:G:N7	51:B3:39:LYS:NZ	2.47	0.60
34:BM:20:LEU:HD13	43:BV:81:PRO:HG2	1.84	0.60
56:B9:74:LYS:O	56:B9:78:GLU:HG3	2.02	0.60
22:BA:636:G:OP1	33:BL:129:LYS:NZ	2.32	0.60
1:AA:337:G:H2'	1:AA:338:A:C8	2.36	0.60
5:AE:153:VAL:HG23	5:AE:156:LYS:HE3	1.84	0.60
22:BA:881:G:N2	22:BA:895:U:O2	2.34	0.60
56:B9:15:THR:HA	56:B9:77:LEU:HD13	1.83	0.60
1:AA:171:A:H2'	1:AA:172:A:C8	2.37	0.59
10:AJ:36:VAL:HG22	10:AJ:76:ILE:HD12	1.82	0.59
22:BA:1022:G:O6	31:BJ:68:LYS:NZ	2.30	0.59
3:AC:110:GLU:HB2	3:AC:144:LEU:HD12	1.83	0.59
1:AA:147:G:H2'	1:AA:148:G:C8	2.37	0.59
22:BA:1064:C:H2'	22:BA:1065:U:C6	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2103:C:N4	22:BA:2104:C:H41	1.95	0.59
29:BH:135:HIS:HB3	29:BH:138:VAL:HG22	1.84	0.59
36:BO:50:ALA:O	36:BO:81:ARG:NH2	2.35	0.59
5:AE:161:VAL:HG22	5:AE:162:GLU:H	1.67	0.59
1:AA:1305:G:N2	1:AA:1331:G:H1'	2.17	0.59
4:AD:174:ASP:OD2	4:AD:177:LYS:NZ	2.35	0.59
11:AK:111:THR:HG23	21:AU:3:VAL:HB	1.83	0.59
16:AP:6:LEU:HB3	16:AP:17:TYR:HB3	1.84	0.59
41:BT:11:LEU:O	46:BY:29:ARG:NH1	2.34	0.59
1:AA:72:A:H2'	1:AA:73:C:O4'	2.03	0.59
1:AA:235:C:H2'	1:AA:236:A:C8	2.38	0.59
1:AA:1316:G:N2	1:AA:1318:A:H3'	2.17	0.59
22:BA:585:G:N7	38:BQ:6:ARG:NH1	2.51	0.59
34:BM:78:LEU:HD12	56:B9:281:HIS:CD2	2.38	0.59
1:AA:1250:A:H2'	1:AA:1251:A:C8	2.38	0.59
22:BA:884:U:N3	22:BA:892:A:C8	2.71	0.59
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.38	0.59
2:AB:32:PHE:HB2	2:AB:42:ASN:HB2	1.85	0.59
55:B8:2:G:O2'	55:B8:3:G:H2'	2.02	0.59
14:AN:32:ASP:OD1	14:AN:33:VAL:N	2.36	0.58
1:AA:126:G:OP1	1:AA:605:U:O2'	2.19	0.58
14:AN:29:ILE:HG13	14:AN:30:ILE:HD12	1.85	0.58
1:AA:79:G:H2'	1:AA:80:A:C8	2.38	0.58
1:AA:79:G:H2'	1:AA:80:A:H8	1.69	0.58
1:AA:100:G:O2'	1:AA:102:G:P	2.61	0.58
1:AA:713:G:H2'	1:AA:714:G:C8	2.38	0.58
1:AA:457:G:N2	1:AA:475:C:C2	2.72	0.58
1:AA:1026:G:O6	1:AA:1035:A:N6	2.37	0.58
22:BA:1156:A:C8	38:BQ:51:ARG:HG2	2.39	0.58
22:BA:1798:U:OP2	24:BC:271:ARG:NH2	2.36	0.58
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.52	0.58
2:AB:54:LEU:HG	2:AB:220:THR:HG21	1.85	0.58
14:AN:46:LEU:HD11	19:AS:13:LEU:HD13	1.85	0.58
22:BA:2798:U:H4'	22:BA:2799:A:H5'	1.86	0.58
51:B3:31:HIS:ND1	51:B3:32:ILE:HD12	2.19	0.58
1:AA:64:G:C2	1:AA:70:U:C4	2.91	0.58
22:BA:2100:G:H3'	22:BA:2101:A:H8	1.69	0.58
22:BA:2250:G:O2'	22:BA:2496:C:OP1	2.22	0.58
26:BE:6:LYS:HB3	26:BE:121:VAL:HG12	1.85	0.58
50:B2:24:THR:HG23	50:B2:27:GLY:H	1.68	0.58
1:AA:1038:C:H2'	1:AA:1039:G:H8	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2327:A:H2'	22:BA:2328:A:C8	2.38	0.58
56:B9:80:VAL:HG11	56:B9:103:LEU:HD13	1.84	0.58
1:AA:76:G:C4	1:AA:77:A:C8	2.92	0.58
31:BJ:95:ARG:HH21	31:BJ:96:ARG:HD2	1.68	0.58
1:AA:632:U:H5''	1:AA:633:G:C8	2.39	0.57
1:AA:1130:A:H2'	1:AA:1131:G:C8	2.39	0.57
49:B1:29:THR:HG23	49:B1:30:LYS:HG2	1.84	0.57
1:AA:465:A:O2'	1:AA:466:A:O4'	2.19	0.57
8:AH:22:LYS:O	8:AH:65:TYR:OH	2.13	0.57
22:BA:597:G:O2'	33:BL:11:GLY:O	2.21	0.57
1:AA:469:C:H2'	1:AA:470:C:C6	2.39	0.57
1:AA:1491:G:H5'	1:AA:1492:A:OP2	2.04	0.57
25:BD:46:ARG:NH1	25:BD:85:ALA:O	2.37	0.57
56:B9:7:VAL:HG23	56:B9:8:ASN:H	1.68	0.57
46:BY:10:SER:H	46:BY:13:GLU:CD	2.12	0.57
22:BA:1086:A:O2'	22:BA:1087:G:N7	2.37	0.57
47:BZ:40:ASP:OD1	47:BZ:45:ARG:HD3	2.03	0.57
1:AA:68:G:H5'	1:AA:171:A:H1'	1.87	0.57
1:AA:524:G:H2'	1:AA:525:C:C6	2.39	0.57
22:BA:2139:U:H2'	22:BA:2140:G:C8	2.40	0.57
40:BS:66:ILE:H	40:BS:66:ILE:HD12	1.69	0.57
56:B9:22:ARG:NE	56:B9:70:LEU:HD13	2.19	0.57
14:AN:2:LYS:HD2	14:AN:5:MET:HE2	1.86	0.57
22:BA:278:A:H2	22:BA:361:G:N3	2.03	0.57
27:BF:56:ASP:OD1	27:BF:57:LEU:N	2.38	0.57
1:AA:68:G:OP2	1:AA:69:G:H4'	2.05	0.57
1:AA:1071:C:H2'	1:AA:1072:G:H8	1.69	0.57
2:AB:210:VAL:HA	2:AB:213:TYR:HD2	1.70	0.57
22:BA:871:U:H2'	22:BA:872:U:C6	2.40	0.57
26:BE:2:GLU:OE2	26:BE:12:LEU:N	2.38	0.57
27:BF:98:GLU:OE2	30:BI:25:ARG:HD3	2.04	0.57
56:B9:28:ASP:O	56:B9:32:GLU:N	2.32	0.57
56:B9:265:HIS:CD2	56:B9:267:PRO:HD2	2.40	0.57
34:BM:42:THR:HG22	34:BM:44:ARG:H	1.70	0.57
56:B9:243:VAL:HG12	56:B9:261:VAL:HG12	1.87	0.57
22:BA:857:G:H2'	22:BA:858:G:O4'	2.05	0.57
22:BA:2104:C:H2'	22:BA:2105:U:C6	2.39	0.57
24:BC:142:HIS:ND1	24:BC:193:GLY:O	2.35	0.57
1:AA:728:A:H2'	1:AA:729:A:C8	2.40	0.56
22:BA:1082:U:H2'	22:BA:1083:U:C6	2.39	0.56
1:AA:49:U:O4	1:AA:365:U:C4	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:67:C:C6	1:AA:69:G:H1'	2.41	0.56
9:AI:91:ASP:OD1	9:AI:92:GLU:N	2.37	0.56
22:BA:1292:G:H2'	22:BA:1293:C:C6	2.40	0.56
24:BC:16:VAL:HG22	24:BC:206:GLY:HA3	1.86	0.56
1:AA:49:U:H5	1:AA:365:U:O4	1.86	0.56
1:AA:78:A:H2'	1:AA:79:G:C8	2.41	0.56
1:AA:100:G:C5	1:AA:101:A:C6	2.93	0.56
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.40	0.56
22:BA:2170:A:H1'	22:BA:2171:A:C8	2.40	0.56
56:B9:94:GLU:O	56:B9:98:GLU:N	2.32	0.56
1:AA:70:U:H1'	1:AA:71:A:N7	2.20	0.56
2:AB:23:TRP:HZ3	2:AB:25:PRO:HA	1.70	0.56
56:B9:83:LEU:HB3	56:B9:95:THR:HG21	1.87	0.56
8:AH:38:ASN:O	8:AH:41:LYS:N	2.36	0.56
20:AT:36:TYR:O	20:AT:39:ILE:N	2.39	0.56
22:BA:2328:A:H2'	22:BA:2329:U:C6	2.40	0.56
22:BA:2107:G:H2'	22:BA:2108:A:C8	2.41	0.56
1:AA:100:G:C6	1:AA:102:G:C5	2.93	0.56
1:AA:208:U:O2	1:AA:211:G:O6	2.23	0.56
1:AA:64:G:N3	1:AA:69:G:C5	2.74	0.56
1:AA:87:C:H2'	1:AA:88:U:H4'	1.87	0.56
1:AA:1124:G:H4'	10:AJ:40:ILE:HD11	1.88	0.56
3:AC:114:LYS:HB2	3:AC:185:ASN:HD22	1.71	0.56
22:BA:2661:G:H2'	22:BA:2662:A:C8	2.41	0.56
25:BD:1:MET:HE1	25:BD:100:LEU:HD21	1.86	0.56
39:BR:37:GLU:O	39:BR:37:GLU:HG2	2.06	0.56
56:B9:230:ILE:HG23	56:B9:299:GLU:HG2	1.86	0.56
22:BA:1729:U:O2	22:BA:1731:G:N2	2.36	0.56
41:BT:2:ILE:HD13	41:BT:42:GLU:HG3	1.87	0.56
8:AH:39:VAL:HG21	8:AH:110:VAL:HG12	1.88	0.55
14:AN:26:LEU:HA	14:AN:30:ILE:HD13	1.86	0.55
22:BA:2331:G:OP1	44:BW:44:LYS:NZ	2.39	0.55
22:BA:1278:C:H2'	22:BA:1279:G:H8	1.71	0.55
22:BA:1738:G:O2'	22:BA:1739:A:H8	1.89	0.55
22:BA:1870:C:H2'	22:BA:1871:A:C8	2.41	0.55
22:BA:703:U:H2'	22:BA:704:G:O4'	2.05	0.55
1:AA:64:G:N2	1:AA:69:G:H2'	2.21	0.55
1:AA:469:C:H2'	1:AA:470:C:H6	1.71	0.55
1:AA:808:C:OP2	15:AO:48:LYS:NZ	2.39	0.55
22:BA:1178:C:H2'	22:BA:1179:G:H8	1.72	0.55
31:BJ:21:THR:HG22	31:BJ:61:LYS:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BK:40:LYS:HD3	32:BK:58:LEU:O	2.06	0.55
37:BP:34:GLU:OE2	37:BP:39:ARG:NE	2.39	0.55
40:BS:12:SER:O	40:BS:101:SER:OG	2.22	0.55
56:B9:33:ARG:HD2	56:B9:63:LEU:HD21	1.87	0.55
1:AA:71:A:C2	1:AA:101:A:C5	2.94	0.55
1:AA:933:G:OP1	7:AG:4:ARG:NH1	2.38	0.55
22:BA:1800:C:H5'	24:BC:146:MET:HE1	1.89	0.55
1:AA:279:A:H5'	1:AA:279:A:C8	2.41	0.55
1:AA:279:A:H5'	1:AA:279:A:H8	1.71	0.55
1:AA:662:U:H2'	1:AA:663:A:C8	2.41	0.55
1:AA:714:G:H2'	1:AA:715:A:C8	2.41	0.55
22:BA:1980:G:O2'	22:BA:1982:U:OP2	2.24	0.55
24:BC:181:MET:HB2	24:BC:268:VAL:HB	1.89	0.55
22:BA:552:U:H2'	22:BA:553:G:H8	1.71	0.55
22:BA:2140:G:H2'	22:BA:2141:G:O4'	2.07	0.55
56:B9:330:ASP:OD2	56:B9:332:ARG:NH1	2.39	0.55
1:AA:100:G:C6	1:AA:102:G:C2	2.95	0.55
1:AA:718:A:C2	18:AR:38:LYS:HE2	2.41	0.55
11:AK:31:ILE:HG23	11:AK:46:THR:HG22	1.88	0.55
25:BD:133:THR:HG22	25:BD:134:HIS:H	1.72	0.55
51:B3:32:ILE:O	51:B3:32:ILE:HG22	2.05	0.55
2:AB:43:LEU:HA	2:AB:46:THR:HG22	1.88	0.55
37:BP:2:SER:O	37:BP:2:SER:OG	2.24	0.55
22:BA:1614:A:C2	40:BS:93:ALA:HB2	2.42	0.55
1:AA:100:G:C5	1:AA:102:G:C4	2.95	0.54
3:AC:186:THR:HG23	3:AC:199:LYS:HG2	1.89	0.54
5:AE:116:GLU:OE2	5:AE:117:VAL:HG23	2.06	0.54
22:BA:545:U:O2'	22:BA:546:U:O4'	2.24	0.54
41:BT:33:LYS:HG3	41:BT:80:TRP:CE3	2.42	0.54
55:B8:46:G:H2'	55:B8:47:U:H5'	1.89	0.54
56:B9:8:ASN:HA	56:B9:11:ILE:HD12	1.89	0.54
1:AA:575:G:O2'	1:AA:821:G:OP2	2.21	0.54
1:AA:1179:A:OP2	9:AI:99:ARG:NH1	2.40	0.54
22:BA:848:C:H2'	22:BA:849:A:C8	2.42	0.54
22:BA:2068:U:N3	22:BA:2430:A:H2	2.01	0.54
27:BF:140:GLU:HA	30:BI:28:VAL:HG22	1.89	0.54
32:BK:12:ASP:OD2	32:BK:14:SER:OG	2.25	0.54
1:AA:73:C:C2	1:AA:74:A:C8	2.95	0.54
27:BF:110:ARG:HH22	27:BF:139:PRO:HB3	1.73	0.54
51:B3:31:HIS:O	51:B3:33:LEU:N	2.39	0.54
1:AA:1001:C:H2'	1:AA:1002:G:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:3:HIS:HB2	6:AF:92:THR:O	2.08	0.54
22:BA:996:A:O3'	38:BQ:91:ASP:OD1	2.26	0.54
1:AA:81:A:H2	1:AA:88:U:N3	1.97	0.54
1:AA:91:U:H2'	1:AA:92:U:C6	2.43	0.54
3:AC:135:LYS:HD3	3:AC:168:TYR:CD2	2.42	0.54
22:BA:2100:G:C5	22:BA:2101:A:C5	2.95	0.54
22:BA:2152:G:H2'	22:BA:2153:C:C6	2.42	0.54
31:BJ:140:LEU:HG	31:BJ:142:ILE:HB	1.88	0.54
1:AA:1492:A:H5'	12:AL:44:LYS:HD2	1.88	0.54
22:BA:2130:U:O2'	22:BA:2133:G:O2'	2.24	0.54
22:BA:2191:A:H2'	22:BA:2192:U:C6	2.42	0.54
29:BH:7:ASP:OD1	29:BH:8:LYS:N	2.40	0.54
22:BA:1177:G:H2'	22:BA:1178:C:C6	2.42	0.54
30:BI:30:HIS:CG	30:BI:31:ASP:H	2.26	0.54
3:AC:79:LYS:HD2	3:AC:80:LYS:HG3	1.89	0.54
9:AI:7:TYR:HE1	9:AI:18:ARG:HB2	1.72	0.54
22:BA:634:C:H2'	22:BA:635:C:C6	2.43	0.54
56:B9:288:MET:HG3	56:B9:289:LYS:HD2	1.90	0.54
1:AA:66:A:C6	1:AA:67:C:C5	2.96	0.54
1:AA:1360:A:OP2	14:AN:75:ARG:NH2	2.41	0.54
17:AQ:12:VAL:HG23	17:AQ:59:VAL:HG21	1.90	0.54
29:BH:9:VAL:HG11	29:BH:12:LEU:HD12	1.90	0.54
19:AS:6:LYS:HZ2	30:BI:63:ARG:HD3	1.73	0.54
28:BG:25:THR:OG1	28:BG:32:GLU:OE2	2.26	0.54
1:AA:757:U:OP1	1:AA:822:U:O2'	2.26	0.53
3:AC:16:LYS:NZ	3:AC:181:ASP:OD1	2.41	0.53
12:AL:45:PRO:HB2	54:B7:10:U:N3	2.22	0.53
22:BA:2102:G:H2'	22:BA:2103:C:O4'	2.08	0.53
28:BG:86:LYS:HG2	28:BG:132:VAL:HG12	1.90	0.53
19:AS:42:PRO:HD3	30:BI:60:PHE:CE2	2.43	0.53
20:AT:54:MET:HE2	20:AT:79:LEU:HD12	1.89	0.53
22:BA:1292:G:H2'	22:BA:1293:C:H6	1.72	0.53
22:BA:2876:G:OP1	37:BP:2:SER:N	2.41	0.53
33:BL:73:ILE:HB	33:BL:106:GLU:OE1	2.08	0.53
37:BP:88:ARG:NH2	37:BP:110:ILE:O	2.37	0.53
1:AA:1035:A:H2'	1:AA:1035:A:N3	2.22	0.53
34:BM:50:ARG:HG3	34:BM:65:ILE:HD11	1.89	0.53
1:AA:215:C:H2'	1:AA:216:U:C6	2.44	0.53
6:AF:44:ARG:HB3	6:AF:56:LYS:HE3	1.89	0.53
22:BA:2204:G:OP2	24:BC:147:LYS:NZ	2.34	0.53
54:B7:2:G:N2	54:B7:3:C:O4'	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:98:A:H2'	1:AA:99:C:O4'	2.09	0.53
1:AA:389:A:H3'	1:AA:390:U:H6	1.74	0.53
6:AF:42:TRP:CH2	6:AF:102:MET:HG3	2.44	0.53
7:AG:65:ALA:HB2	7:AG:128:ALA:HB2	1.91	0.53
22:BA:2267:A:H5''	22:BA:2268:A:H5'	1.89	0.53
2:AB:27:MET:HE1	2:AB:187:VAL:HG12	1.90	0.53
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.91	0.53
16:AP:55:ASP:OD1	16:AP:56:ARG:N	2.42	0.53
1:AA:1229:A:O2'	55:B8:30:C:OP1	2.27	0.53
19:AS:18:LYS:HD3	19:AS:31:LEU:HD11	1.91	0.53
22:BA:364:C:H2'	22:BA:365:U:C6	2.43	0.53
22:BA:1085:A:O2'	22:BA:1086:A:O4'	2.14	0.53
55:B8:71:C:H2'	55:B8:72:G:C8	2.44	0.53
1:AA:539:A:H2'	1:AA:540:G:C8	2.44	0.53
22:BA:404:A:N6	22:BA:421:C:O2'	2.41	0.53
27:BF:115:ARG:O	30:BI:47:LYS:NZ	2.42	0.53
56:B9:353:LEU:O	56:B9:357:ILE:HG12	2.08	0.53
1:AA:100:G:N2	1:AA:152:A:H1'	2.22	0.53
1:AA:1317:C:O2	19:AS:37:ARG:NH2	2.37	0.53
3:AC:72:ARG:O	3:AC:75:ILE:HG22	2.09	0.53
1:AA:70:U:O5'	1:AA:70:U:H6	1.93	0.52
1:AA:71:A:N1	1:AA:72:A:C5	2.77	0.52
1:AA:1477:U:H2'	1:AA:1478:U:C6	2.44	0.52
22:BA:545:U:O2'	22:BA:546:U:O5'	2.26	0.52
41:BT:28:ASN:ND2	41:BT:88:LYS:O	2.42	0.52
11:AK:59:THR:HG22	11:AK:61:PHE:H	1.75	0.52
13:AM:66:GLU:O	13:AM:69:LEU:N	2.43	0.52
22:BA:1202:G:O6	22:BA:1244:A:N6	2.42	0.52
39:BR:5:PHE:HB3	39:BR:59:ILE:HD12	1.91	0.52
1:AA:738:C:OP1	6:AF:2:ARG:NH2	2.43	0.52
3:AC:56:VAL:HG22	3:AC:67:THR:HB	1.92	0.52
5:AE:115:LEU:HD13	5:AE:123:VAL:HG11	1.92	0.52
7:AG:143:ARG:O	7:AG:146:GLU:HG3	2.09	0.52
19:AS:6:LYS:NZ	30:BI:63:ARG:HD3	2.24	0.52
22:BA:1072:C:N4	22:BA:1093:G:O6	2.43	0.52
22:BA:1149:G:H2'	22:BA:1150:C:C6	2.45	0.52
23:BB:43:C:H5''	30:BI:1:MET:SD	2.50	0.52
56:B9:195:GLU:OE1	56:B9:324:ARG:NH1	2.42	0.52
1:AA:70:U:C5	1:AA:94:G:C8	2.97	0.52
7:AG:111:ARG:HB2	7:AG:119:ARG:HG3	1.91	0.52
10:AJ:7:ARG:NH2	10:AJ:75:ASP:OD2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:181:A:H2'	22:BA:182:A:C8	2.45	0.52
22:BA:1738:G:HO2'	22:BA:1739:A:H8	1.57	0.52
22:BA:2185:U:N3	22:BA:2186:G:C6	2.78	0.52
22:BA:2284:A:OP1	49:B1:5:ILE:HB	2.10	0.52
22:BA:500:G:N1	22:BA:503:A:OP2	2.40	0.52
22:BA:639:U:H2'	22:BA:640:C:C6	2.44	0.52
22:BA:2110:G:H8	22:BA:2110:G:OP2	1.92	0.52
24:BC:29:PRO:HG2	24:BC:34:LEU:HD11	1.91	0.52
31:BJ:19:ASP:OD2	31:BJ:58:ASN:ND2	2.42	0.52
1:AA:972:C:OP2	10:AJ:59:LYS:NZ	2.39	0.52
11:AK:35:THR:HG22	11:AK:41:ALA:HA	1.91	0.52
22:BA:2101:A:H2'	22:BA:2102:G:C8	2.45	0.52
22:BA:2191:A:H2'	22:BA:2192:U:H6	1.75	0.52
22:BA:2316:G:H2'	22:BA:2317:A:C8	2.44	0.52
41:BT:55:VAL:HG12	41:BT:87:LEU:HD23	1.91	0.52
1:AA:68:G:C8	1:AA:69:G:O2'	2.60	0.52
4:AD:44:ARG:HG3	4:AD:46:PRO:HD3	1.92	0.52
10:AJ:29:ALA:O	10:AJ:32:THR:OG1	2.27	0.52
22:BA:483:A:OP1	42:BU:47:LYS:NZ	2.39	0.52
22:BA:1073:A:H4'	22:BA:2474:U:H4'	1.91	0.52
48:B0:53:LYS:HE3	48:B0:56:ALA:HA	1.92	0.52
22:BA:1548:A:H2'	22:BA:1549:A:C8	2.45	0.52
22:BA:1746:A:H2'	22:BA:1747:U:C6	2.45	0.52
23:BB:106:G:H2'	23:BB:107:G:O4'	2.10	0.52
56:B9:65:ALA:O	56:B9:69:THR:OG1	2.21	0.52
56:B9:87:ALA:HB1	56:B9:96:PHE:HB2	1.92	0.52
1:AA:457:G:N2	1:AA:474:G:H22	2.08	0.52
1:AA:461:A:H2'	1:AA:462:G:C8	2.45	0.52
1:AA:1147:C:O2	9:AI:18:ARG:NH1	2.43	0.52
22:BA:1172:C:H5''	22:BA:1173:U:C2	2.45	0.52
22:BA:1494:A:H2'	22:BA:1495:A:C8	2.45	0.52
22:BA:2163:A:H3'	22:BA:2164:C:H4'	1.91	0.52
47:BZ:6:LYS:HZ1	47:BZ:37:GLU:HG3	1.73	0.52
1:AA:191:G:H2'	1:AA:192:A:C8	2.45	0.52
1:AA:1314:C:H2'	1:AA:1315:U:C6	2.45	0.52
1:AA:1507:A:H2'	1:AA:1508:A:C8	2.44	0.52
5:AE:11:LEU:HD23	5:AE:39:VAL:HG22	1.92	0.52
47:BZ:37:GLU:O	47:BZ:38:ARG:NH1	2.42	0.52
22:BA:1102:C:C2	22:BA:1103:A:C8	2.98	0.51
29:BH:97:ARG:HE	29:BH:112:LYS:HZ1	1.57	0.51
1:AA:208:U:O4	1:AA:211:G:N2	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:908:A:H2'	1:AA:909:A:C8	2.45	0.51
17:AQ:79:VAL:HG23	17:AQ:80:GLU:OE1	2.10	0.51
22:BA:172:A:H2'	22:BA:173:A:H8	1.75	0.51
22:BA:882:G:N2	22:BA:883:G:O6	2.43	0.51
29:BH:61:VAL:O	29:BH:65:ALA:N	2.39	0.51
51:B3:31:HIS:O	51:B3:33:LEU:HG	2.10	0.51
1:AA:100:G:N9	1:AA:102:G:C8	2.79	0.51
1:AA:166:U:H2'	1:AA:167:A:H8	1.75	0.51
1:AA:568:G:O6	12:AL:2:ALA:HB2	2.10	0.51
1:AA:826:C:O2	8:AH:16:ASN:ND2	2.43	0.51
2:AB:57:LEU:HD21	2:AB:217:VAL:HG13	1.91	0.51
6:AF:73:GLU:HA	6:AF:76:THR:HB	1.93	0.51
12:AL:79:VAL:N	12:AL:103:ASP:OD2	2.41	0.51
22:BA:849:A:H2'	22:BA:850:U:C6	2.45	0.51
27:BF:147:ASP:OD1	27:BF:147:ASP:N	2.40	0.51
44:BW:26:PHE:H	44:BW:29:GLU:HG3	1.74	0.51
1:AA:384:G:H2'	1:AA:385:C:C6	2.45	0.51
1:AA:1007:U:O2'	1:AA:1008:U:H5'	2.11	0.51
4:AD:58:LYS:HD2	4:AD:204:TYR:OH	2.11	0.51
22:BA:281:C:H2'	22:BA:282:A:C8	2.46	0.51
22:BA:881:G:H21	22:BA:896:A:N6	2.08	0.51
22:BA:2020:A:H5'	48:B0:9:THR:CG2	2.40	0.51
26:BE:10:SER:OG	26:BE:11:ALA:N	2.39	0.51
29:BH:99:ILE:HD11	29:BH:122:LEU:HD11	1.91	0.51
13:AM:68:ASP:OD1	13:AM:69:LEU:N	2.43	0.51
22:BA:414:C:H2'	22:BA:415:A:C8	2.45	0.51
25:BD:12:THR:OG1	37:BP:9:GLU:OE2	2.17	0.51
55:B8:66:A:H2'	55:B8:67:U:C6	2.46	0.51
1:AA:100:G:N1	1:AA:102:G:N3	2.58	0.51
1:AA:142:G:H3'	1:AA:143:A:H8	1.76	0.51
1:AA:555:U:H2'	1:AA:556:C:C6	2.46	0.51
22:BA:587:C:C2	33:BL:19:LEU:HD12	2.46	0.51
55:B8:62:C:H2'	55:B8:63:U:C6	2.45	0.51
1:AA:92:U:H2'	1:AA:93:U:C6	2.44	0.51
22:BA:2101:A:H2'	22:BA:2102:G:O4'	2.11	0.51
22:BA:2102:G:C2	22:BA:2103:C:H1'	2.46	0.51
22:BA:2125:G:N1	22:BA:2171:A:OP1	2.36	0.51
56:B9:118:MET:HE3	56:B9:190:GLY:HA3	1.92	0.51
1:AA:486:U:H2'	1:AA:487:A:H8	1.75	0.51
13:AM:3:ARG:NH2	13:AM:7:ILE:HB	2.26	0.51
13:AM:81:MET:HE1	13:AM:92:ARG:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2305:U:H2'	22:BA:2306:C:C6	2.46	0.51
38:BQ:58:ARG:O	38:BQ:62:ILE:HG12	2.11	0.51
1:AA:1207:2MG:HM23	1:AA:1208:C:H1'	1.93	0.51
5:AE:161:VAL:HG13	5:AE:163:GLU:OE1	2.11	0.51
22:BA:1085:A:H2'	22:BA:1086:A:C4	2.46	0.51
22:BA:2151:U:H2'	22:BA:2152:G:C8	2.46	0.51
23:BB:1:U:H2'	23:BB:2:G:C8	2.39	0.51
51:B3:62:LEU:HB3	51:B3:65:ALA:HB2	1.93	0.51
53:B5:8:VAL:HG22	53:B5:9:THR:H	1.76	0.51
56:B9:99:ALA:O	56:B9:103:LEU:N	2.34	0.51
1:AA:66:A:C6	1:AA:67:C:C4	2.99	0.51
1:AA:78:A:H2'	1:AA:79:G:H8	1.76	0.51
1:AA:166:U:H2'	1:AA:167:A:C8	2.46	0.51
1:AA:1151:A:H5''	10:AJ:44:THR:HG23	1.93	0.51
2:AB:8:ASP:OD1	2:AB:8:ASP:N	2.40	0.51
12:AL:55:VAL:HG11	12:AL:80:ILE:HD11	1.93	0.51
14:AN:20:PHE:C	14:AN:22:LYS:H	2.19	0.51
14:AN:92:GLU:N	14:AN:92:GLU:OE1	2.44	0.51
22:BA:2180:U:H2'	22:BA:2181:U:C6	2.45	0.51
22:BA:2343:U:HO2'	22:BA:2373:G:HO2'	1.55	0.51
22:BA:2523:G:HO2'	22:BA:2764:A:HO2'	1.59	0.51
34:BM:136:MET:SD	43:BV:76:ASP:HA	2.51	0.51
37:BP:27:GLU:HG3	37:BP:87:LYS:HE2	1.93	0.51
39:BR:1:MET:HE3	39:BR:101:ILE:HB	1.92	0.51
1:AA:632:U:H5''	1:AA:633:G:H8	1.76	0.50
1:AA:1297:G:N2	7:AG:114:LYS:HB3	2.26	0.50
22:BA:1092:C:H2'	22:BA:1093:G:C8	2.46	0.50
40:BS:1:MET:SD	40:BS:3:THR:OG1	2.69	0.50
7:AG:18:PHE:CZ	7:AG:58:GLU:HG2	2.46	0.50
7:AG:135:VAL:O	7:AG:139:GLU:HG2	2.11	0.50
22:BA:248:G:H5'	22:BA:250:G:N7	2.26	0.50
22:BA:748:G:C8	40:BS:89:ALA:HB1	2.46	0.50
22:BA:2143:C:H2'	22:BA:2144:G:O4'	2.11	0.50
24:BC:35:GLU:HG2	24:BC:36:LYS:H	1.75	0.50
37:BP:5:ILE:O	37:BP:9:GLU:HG2	2.10	0.50
1:AA:83:C:O2'	1:AA:85:U:N3	2.41	0.50
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.46	0.50
5:AE:105:ILE:HD13	5:AE:116:GLU:HB3	1.93	0.50
6:AF:37:HIS:CD2	6:AF:65:GLU:HG2	2.46	0.50
22:BA:1485:U:H2'	22:BA:1486:U:H6	1.77	0.50
22:BA:2273:A:H2'	22:BA:2274:A:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:BV:51:GLN:OE1	43:BV:57:TYR:OH	2.29	0.50
1:AA:1314:C:H2'	1:AA:1315:U:H6	1.76	0.50
16:AP:47:GLU:HG2	16:AP:48:GLU:O	2.11	0.50
28:BG:35:ARG:HB3	28:BG:75:MET:HE1	1.93	0.50
56:B9:200:ARG:NE	56:B9:322:GLN:OE1	2.44	0.50
1:AA:1118:U:OP1	9:AI:11:ARG:HD2	2.11	0.50
22:BA:1073:A:H8	22:BA:1073:A:O5'	1.95	0.50
22:BA:2101:A:N1	22:BA:2102:G:C6	2.80	0.50
22:BA:2683:C:O2	32:BK:70:ARG:NH2	2.44	0.50
25:BD:90:PHE:HD2	25:BD:94:GLN:NE2	2.09	0.50
27:BF:80:ARG:HH22	55:B8:56:C:H42	1.56	0.50
28:BG:175:LYS:HE2	28:BG:177:LYS:HB3	1.94	0.50
30:BI:36:VAL:HG11	30:BI:41:HIS:HD2	1.76	0.50
1:AA:100:G:C6	1:AA:102:G:C6	2.99	0.50
1:AA:1463:U:H2'	1:AA:1464:U:C6	2.47	0.50
7:AG:42:ILE:HD12	7:AG:116:MET:HB3	1.94	0.50
22:BA:1847:A:O2'	22:BA:1848:A:C8	2.55	0.50
4:AD:101:VAL:HG11	4:AD:137:VAL:HG21	1.94	0.50
18:AR:37:GLY:O	18:AR:63:ARG:NH2	2.44	0.50
22:BA:728:G:H4'	24:BC:13:ARG:HD3	1.94	0.50
22:BA:1361:G:O2'	22:BA:2215:C:O2'	2.28	0.50
27:BF:102:ARG:HG3	30:BI:24:ILE:HD11	1.94	0.50
1:AA:1130:A:O2'	9:AI:5:GLN:NE2	2.40	0.50
5:AE:153:VAL:HG11	8:AH:99:LEU:HD22	1.94	0.50
9:AI:7:TYR:CE1	9:AI:18:ARG:HB2	2.47	0.50
22:BA:2291:U:H2'	22:BA:2292:U:C6	2.46	0.50
46:BY:3:ALA:HB2	46:BY:52:ARG:HD3	1.93	0.50
1:AA:68:G:OP2	1:AA:69:G:O5'	2.30	0.50
1:AA:976:G:OP2	1:AA:1358:U:O2'	2.29	0.50
1:AA:1029:U:H3'	1:AA:1031:C:C6	2.46	0.50
19:AS:4:SER:OG	19:AS:5:LEU:N	2.41	0.50
19:AS:64:ASP:OD2	19:AS:65:GLU:N	2.45	0.50
22:BA:1796:U:H2'	22:BA:1797:G:C8	2.47	0.50
22:BA:2014:A:H2'	22:BA:2015:A:C8	2.47	0.50
24:BC:35:GLU:HG2	24:BC:36:LYS:N	2.27	0.50
56:B9:129:TYR:HE1	56:B9:225:GLU:HG3	1.76	0.50
1:AA:633:G:H2'	1:AA:634:C:H6	1.76	0.49
13:AM:12:HIS:ND1	13:AM:12:HIS:O	2.45	0.49
22:BA:172:A:H2'	22:BA:173:A:C8	2.47	0.49
22:BA:2331:G:P	44:BW:44:LYS:NZ	2.85	0.49
55:B8:3:G:H4'	55:B8:4:U:OP1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:B9:234:ILE:H	56:B9:292:LYS:HZ3	1.60	0.49
1:AA:1013:G:N2	1:AA:1016:A:OP2	2.44	0.49
10:AJ:8:ILE:HG22	10:AJ:100:ILE:HA	1.94	0.49
22:BA:910:A:H2'	22:BA:911:A:C8	2.47	0.49
22:BA:2108:A:H2	22:BA:2181:U:H3	1.56	0.49
25:BD:181:ASP:HB3	25:BD:186:LEU:HB2	1.95	0.49
31:BJ:26:GLY:O	31:BJ:30:THR:HG23	2.12	0.49
56:B9:30:LYS:HE2	56:B9:63:LEU:HD23	1.93	0.49
22:BA:285:G:H2'	22:BA:286:U:C6	2.48	0.49
22:BA:286:U:H2'	22:BA:287:G:H8	1.77	0.49
22:BA:1095:A:H2'	22:BA:1096:A:C8	2.47	0.49
22:BA:1590:A:H2'	22:BA:1591:A:C8	2.47	0.49
29:BH:129:GLU:HG3	29:BH:143:ILE:HD12	1.95	0.49
1:AA:102:G:C4	1:AA:103:U:C6	3.01	0.49
1:AA:1038:C:H2'	1:AA:1039:G:C8	2.46	0.49
3:AC:154:SER:HB3	3:AC:165:THR:HG23	1.95	0.49
8:AH:11:LEU:HD22	8:AH:75:ILE:HD11	1.93	0.49
10:AJ:59:LYS:HE2	10:AJ:62:ARG:NH2	2.26	0.49
20:AT:28:MET:HE1	20:AT:67:ILE:HG21	1.94	0.49
25:BD:16:THR:OG1	25:BD:18:ASP:OD1	2.25	0.49
27:BF:105:THR:HA	30:BI:38:SER:HB3	1.93	0.49
48:B0:38:HIS:ND1	48:B0:39:LEU:O	2.45	0.49
55:B8:23:C:H2'	55:B8:24:G:C8	2.46	0.49
1:AA:66:A:N1	1:AA:67:C:C4	2.81	0.49
1:AA:122:G:H8	1:AA:122:G:OP2	1.94	0.49
1:AA:565:U:OP2	1:AA:566:G:O2'	2.27	0.49
2:AB:68:LEU:HD13	2:AB:158:PRO:HG3	1.94	0.49
13:AM:16:VAL:HB	13:AM:41:GLU:HG2	1.94	0.49
22:BA:480:A:OP2	42:BU:44:LYS:HE2	2.12	0.49
22:BA:1102:C:H2'	22:BA:1103:A:C8	2.44	0.49
22:BA:1545:A:H2'	22:BA:1546:G:O4'	2.12	0.49
22:BA:2141:G:O2'	22:BA:2142:A:H5'	2.13	0.49
31:BJ:31:GLU:HG2	31:BJ:142:ILE:HG13	1.93	0.49
1:AA:344:A:H5''	1:AA:345:C:H5	1.77	0.49
1:AA:695:A:H2'	1:AA:696:A:C8	2.47	0.49
1:AA:744:C:H2'	1:AA:745:G:H8	1.78	0.49
22:BA:634:C:H2'	22:BA:635:C:H6	1.76	0.49
29:BH:121:VAL:O	29:BH:121:VAL:HG12	2.12	0.49
49:B1:35:GLU:OE2	49:B1:48:ILE:HD12	2.13	0.49
1:AA:86:G:H1'	1:AA:87:C:C5	2.47	0.49
1:AA:1120:C:H2'	1:AA:1121:U:H6	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:179:ARG:NH1	3:AC:206:GLU:OE1	2.46	0.49
16:AP:57:ILE:HG21	16:AP:75:ILE:HD11	1.95	0.49
22:BA:281:C:H2'	22:BA:282:A:H8	1.78	0.49
22:BA:1676:A:H1'	25:BD:133:THR:HG21	1.95	0.49
23:BB:29:A:H2'	23:BB:30:C:C6	2.48	0.49
1:AA:1129:C:H5''	9:AI:18:ARG:NH2	2.27	0.49
2:AB:154:MET:HE3	2:AB:156:GLY:O	2.13	0.49
39:BR:15:SER:OG	39:BR:16:GLU:N	2.45	0.49
41:BT:92:ASN:OD1	41:BT:93:LEU:N	2.46	0.49
44:BW:71:VAL:HG22	44:BW:78:LYS:HD2	1.93	0.49
51:B3:29:LEU:HD11	51:B3:44:LEU:HB2	1.94	0.49
56:B9:104:ASP:O	56:B9:108:GLU:HG2	2.12	0.49
22:BA:1485:U:H2'	22:BA:1486:U:C6	2.47	0.49
22:BA:2116:G:O6	22:BA:2171:A:N6	2.45	0.49
27:BF:80:ARG:H	27:BF:83:TYR:HD2	1.60	0.49
3:AC:56:VAL:CG2	3:AC:67:THR:HB	2.43	0.48
6:AF:51:ILE:HD11	6:AF:85:ILE:HD12	1.95	0.48
22:BA:1028:A:N6	22:BA:1125:G:H2'	2.28	0.48
22:BA:2639:A:H2'	22:BA:2640:G:O4'	2.11	0.48
33:BL:62:PRO:HG2	51:B3:25:LYS:HD3	1.94	0.48
41:BT:88:LYS:HB2	41:BT:91:GLN:OE1	2.12	0.48
1:AA:100:G:N2	1:AA:152:A:O2'	2.46	0.48
1:AA:652:U:O4	1:AA:752:G:O2'	2.30	0.48
1:AA:1142:G:H2'	1:AA:1143:G:O4'	2.12	0.48
1:AA:1355:G:H2'	1:AA:1356:G:H8	1.78	0.48
9:AI:84:THR:HG23	9:AI:98:LEU:HD22	1.94	0.48
22:BA:645:C:H2'	22:BA:647:G:N7	2.28	0.48
22:BA:2646:C:OP2	22:BA:2732:G:O2'	2.31	0.48
25:BD:152:PRO:HG3	25:BD:156:PHE:CZ	2.48	0.48
27:BF:111:ILE:HB	27:BF:114:PHE:HB2	1.95	0.48
56:B9:7:VAL:HG23	56:B9:8:ASN:N	2.29	0.48
1:AA:451:A:H61	1:AA:481:G:H5'	1.78	0.48
1:AA:1287:A:H2'	1:AA:1288:A:C8	2.48	0.48
8:AH:79:SER:HB2	8:AH:85:ILE:H	1.78	0.48
14:AN:32:ASP:O	14:AN:41:ARG:NH2	2.46	0.48
22:BA:652:U:OP1	22:BA:654:A:N6	2.45	0.48
22:BA:1392:A:H5'	22:BA:1392:A:C8	2.48	0.48
22:BA:2106:U:H2'	22:BA:2107:G:C8	2.49	0.48
42:BU:51:ALA:C	42:BU:53:ASN:H	2.21	0.48
1:AA:56:U:H2'	1:AA:57:G:C8	2.49	0.48
1:AA:299:G:H2'	1:AA:300:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:628:G:H2'	1:AA:629:A:C8	2.48	0.48
1:AA:1036:A:H2'	1:AA:1037:C:C6	2.49	0.48
5:AE:83:HIS:CE1	5:AE:147:MET:HG3	2.48	0.48
22:BA:5:A:H2'	22:BA:6:A:C8	2.48	0.48
22:BA:608:A:H2'	22:BA:609:A:C8	2.48	0.48
24:BC:41:GLY:O	24:BC:43:ARG:NH1	2.47	0.48
1:AA:216:U:H2'	1:AA:217:C:C6	2.48	0.48
1:AA:308:C:H2'	1:AA:309:A:H8	1.79	0.48
1:AA:1530:G:H2'	1:AA:1531:A:C8	2.48	0.48
2:AB:133:GLU:O	2:AB:137:ARG:HG2	2.13	0.48
4:AD:101:VAL:HG22	4:AD:105:MET:HE3	1.95	0.48
7:AG:36:LYS:HG3	9:AI:41:ARG:HH22	1.79	0.48
13:AM:83:LEU:HD21	19:AS:74:PHE:HE1	1.79	0.48
28:BG:10:VAL:HA	28:BG:49:THR:HG22	1.94	0.48
33:BL:141:LYS:NZ	33:BL:143:GLU:OE2	2.46	0.48
34:BM:58:LYS:C	34:BM:59:ARG:HG3	2.39	0.48
41:BT:54:GLU:HG3	41:BT:88:LYS:HG3	1.94	0.48
55:B8:23:C:H2'	55:B8:24:G:H8	1.76	0.48
1:AA:100:G:H21	1:AA:152:A:H4'	1.78	0.48
1:AA:745:G:H2'	1:AA:746:A:C8	2.48	0.48
1:AA:1010:U:H2'	1:AA:1011:C:C6	2.48	0.48
9:AI:28:ILE:HG12	9:AI:63:LEU:HD12	1.94	0.48
22:BA:959:A:H2'	22:BA:960:A:C8	2.48	0.48
22:BA:1428:C:C5	22:BA:1569:A:H5''	2.48	0.48
22:BA:2111:U:H5''	22:BA:2145:C:N3	2.29	0.48
24:BC:251:GLN:NE2	24:BC:252:THR:O	2.46	0.48
30:BI:44:PHE:CD2	30:BI:45:THR:HG23	2.48	0.48
1:AA:996:A:H2'	1:AA:997:U:C6	2.48	0.48
1:AA:1129:C:H5''	9:AI:18:ARG:HH22	1.78	0.48
3:AC:150:LYS:HG3	3:AC:201:TRP:CE3	2.48	0.48
29:BH:96:THR:HG22	29:BH:112:LYS:HA	1.94	0.48
55:B8:19:G:H4'	55:B8:20:U:OP2	2.13	0.48
1:AA:977:A:O2'	1:AA:979:C:OP2	2.31	0.48
3:AC:151:VAL:HG12	3:AC:200:VAL:HG22	1.95	0.48
6:AF:67:PRO:HB2	6:AF:69:GLU:OE1	2.14	0.48
10:AJ:87:LEU:HA	10:AJ:90:LEU:HD23	1.95	0.48
24:BC:36:LYS:NZ	24:BC:38:SER:OG	2.47	0.48
56:B9:11:ILE:O	56:B9:15:THR:OG1	2.26	0.48
56:B9:238:ASP:HA	56:B9:266:ILE:HD12	1.96	0.48
1:AA:1366:C:H2'	1:AA:1367:C:H6	1.79	0.48
22:BA:657:U:H2'	22:BA:658:U:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1178:C:H2'	22:BA:1179:G:C8	2.47	0.48
30:BI:30:HIS:CG	30:BI:31:ASP:N	2.80	0.48
1:AA:1297:G:H21	7:AG:114:LYS:HB3	1.79	0.48
22:BA:2314:A:H2'	22:BA:2315:G:C8	2.48	0.48
26:BE:189:THR:OG1	26:BE:191:ASP:OD1	2.30	0.48
42:BU:51:ALA:O	42:BU:52:LEU:HD23	2.14	0.48
22:BA:541:A:C6	22:BA:553:G:C6	3.02	0.47
22:BA:2176:A:H2'	22:BA:2177:C:C6	2.49	0.47
24:BC:3:VAL:HG12	24:BC:19:VAL:HG22	1.96	0.47
42:BU:10:GLU:OE1	42:BU:73:PHE:HB3	2.14	0.47
56:B9:155:TRP:CD1	56:B9:353:LEU:HB2	2.48	0.47
1:AA:150:U:H2'	1:AA:151:A:H8	1.78	0.47
1:AA:1090:U:H2'	1:AA:1091:U:C6	2.49	0.47
13:AM:33:ILE:HD13	13:AM:60:VAL:HG22	1.96	0.47
22:BA:3:U:H2'	22:BA:4:U:C6	2.49	0.47
22:BA:1028:A:H2'	22:BA:1029:A:C8	2.49	0.47
22:BA:2680:U:O2'	22:BA:2681:C:H5'	2.13	0.47
26:BE:21:ARG:HH11	26:BE:106:LYS:HD2	1.79	0.47
56:B9:107:GLU:O	56:B9:111:ALA:N	2.31	0.47
1:AA:696:A:H2'	1:AA:697:U:H6	1.80	0.47
13:AM:64:VAL:HG13	13:AM:64:VAL:O	2.14	0.47
18:AR:70:TYR:HB2	18:AR:74:HIS:NE2	2.30	0.47
22:BA:357:C:H2'	22:BA:358:U:C6	2.49	0.47
22:BA:1932:A:H2'	22:BA:1933:G:O4'	2.14	0.47
22:BA:2182:U:H2'	22:BA:2183:A:C8	2.49	0.47
22:BA:2795:C:H2'	22:BA:2796:U:C6	2.49	0.47
40:BS:23:LEU:O	40:BS:27:LYS:NZ	2.47	0.47
1:AA:1373:G:H4'	7:AG:31:MET:HE1	1.96	0.47
21:AU:7:ARG:HB2	21:AU:10:GLU:OE2	2.14	0.47
22:BA:279:A:H8	22:BA:279:A:O5'	1.96	0.47
22:BA:1132:U:H3'	22:BA:1133:A:H5''	1.94	0.47
22:BA:2032:G:C5	25:BD:150:MEQ:HE3	2.49	0.47
22:BA:2387:U:H4'	44:BW:41:ARG:HH12	1.78	0.47
22:BA:2756:U:OP2	52:B4:19:ARG:NE	2.38	0.47
29:BH:44:ILE:HG13	29:BH:48:GLU:HB3	1.96	0.47
32:BK:38:ILE:HD11	32:BK:112:PHE:HZ	1.79	0.47
44:BW:32:LEU:HA	44:BW:64:ASP:OD1	2.14	0.47
54:B7:8:G:N1	56:B9:140:GLU:OE1	2.41	0.47
56:B9:17:ARG:O	56:B9:20:VAL:HG22	2.14	0.47
1:AA:300:A:H8	1:AA:300:A:O5'	1.97	0.47
1:AA:1151:A:O2'	1:AA:1152:A:H8	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:85:GLU:OE1	3:AC:88:ARG:NH2	2.45	0.47
22:BA:851:C:OP1	47:BZ:19:LYS:HE3	2.15	0.47
28:BG:76:VAL:HA	28:BG:79:VAL:HG22	1.96	0.47
1:AA:100:G:O6	1:AA:102:G:N1	2.46	0.47
1:AA:1039:G:H2'	1:AA:1040:U:H6	1.79	0.47
3:AC:110:GLU:O	3:AC:111:LEU:HD23	2.14	0.47
3:AC:118:ASP:OD1	3:AC:119:SER:N	2.48	0.47
5:AE:37:THR:HG21	5:AE:64:MET:HE2	1.97	0.47
22:BA:1328:A:H2'	22:BA:1330:C:C5	2.50	0.47
22:BA:2261:C:C5	44:BW:16:SER:HB3	2.49	0.47
27:BF:162:SER:OG	27:BF:165:GLU:OE1	2.25	0.47
1:AA:1187:G:H2'	1:AA:1188:A:C8	2.50	0.47
2:AB:223:GLU:OE1	2:AB:223:GLU:N	2.47	0.47
3:AC:21:THR:HB	3:AC:58:GLU:OE1	2.15	0.47
3:AC:22:TRP:HB3	3:AC:59:ARG:HB2	1.96	0.47
8:AH:55:THR:O	8:AH:56:LYS:HE2	2.14	0.47
22:BA:477:A:H2'	22:BA:478:A:C8	2.49	0.47
22:BA:632:A:H2'	22:BA:633:A:C8	2.50	0.47
22:BA:898:C:H2'	22:BA:899:A:O4'	2.15	0.47
22:BA:1078:U:H1'	22:BA:1088:A:H5'	1.97	0.47
22:BA:1433:A:H2'	22:BA:1434:A:O4'	2.14	0.47
22:BA:1747:U:H2'	22:BA:1748:C:C6	2.49	0.47
22:BA:2100:G:C6	22:BA:2190:G:C5	3.03	0.47
22:BA:2130:U:H2'	22:BA:2158:A:C6	2.50	0.47
22:BA:2172:U:OP2	22:BA:2173:A:H5''	2.15	0.47
22:BA:2577:A:H5''	22:BA:2578:G:H5'	1.96	0.47
22:BA:2845:U:H5''	37:BP:52:ASN:O	2.14	0.47
44:BW:25:ARG:HD3	44:BW:31:VAL:HG12	1.95	0.47
50:B2:31:LEU:HD22	50:B2:42:LEU:HD23	1.97	0.47
56:B9:69:THR:O	56:B9:73:MET:HG2	2.15	0.47
56:B9:144:TRP:CE3	56:B9:201:LEU:HD22	2.49	0.47
1:AA:390:U:H2'	1:AA:391:G:H8	1.80	0.47
1:AA:1071:C:H2'	1:AA:1072:G:C8	2.50	0.47
2:AB:196:VAL:HG23	2:AB:199:VAL:HG22	1.96	0.47
22:BA:876:C:H2'	22:BA:877:A:O4'	2.15	0.47
22:BA:967:U:H2'	22:BA:968:C:C6	2.50	0.47
22:BA:1182:G:H2'	22:BA:1183:U:O4'	2.14	0.47
34:BM:53:MET:HE1	34:BM:103:TYR:CG	2.50	0.47
51:B3:15:LYS:HB2	51:B3:23:LYS:HE3	1.95	0.47
9:AI:118:LEU:HD22	9:AI:124:ARG:HG2	1.97	0.47
11:AK:94:GLU:O	11:AK:97:ILE:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2640:G:P	31:BJ:96:ARG:HH11	2.38	0.47
29:BH:103:VAL:O	29:BH:107:GLY:N	2.36	0.47
38:BQ:48:ARG:HH11	38:BQ:49:ASP:CG	2.22	0.47
1:AA:185:U:H2'	1:AA:186:C:C6	2.50	0.47
17:AQ:21:ILE:HG12	17:AQ:48:ASP:HB2	1.97	0.47
22:BA:1466:U:O2'	22:BA:1546:G:O2'	2.17	0.47
25:BD:1:MET:SD	25:BD:2:ILE:N	2.88	0.47
30:BI:1:MET:HE3	30:BI:6:HIS:CD2	2.50	0.47
1:AA:100:G:O2'	1:AA:102:G:C5'	2.62	0.46
1:AA:674:G:H2'	1:AA:675:A:C8	2.50	0.46
4:AD:184:ARG:NH1	4:AD:187:GLU:OE1	2.48	0.46
6:AF:12:PRO:O	6:AF:15:SER:OG	2.22	0.46
9:AI:52:LEU:HD11	9:AI:63:LEU:HD11	1.97	0.46
9:AI:67:VAL:HG21	9:AI:79:ILE:HD11	1.97	0.46
22:BA:1038:G:H2'	22:BA:1039:A:C8	2.50	0.46
22:BA:1114:C:O2'	22:BA:1115:G:H5'	2.16	0.46
24:BC:144:VAL:HB	24:BC:154:LEU:HB2	1.97	0.46
56:B9:294:LYS:HE3	56:B9:294:LYS:HB2	1.83	0.46
1:AA:68:G:H5'	1:AA:171:A:C1'	2.45	0.46
1:AA:505:G:H2'	1:AA:506:G:H8	1.80	0.46
1:AA:1039:G:H2'	1:AA:1040:U:C6	2.51	0.46
1:AA:1356:G:H2'	1:AA:1357:A:H8	1.75	0.46
6:AF:4:TYR:CE2	6:AF:71:ILE:HG13	2.50	0.46
6:AF:101:PRO:HA	6:AF:104:LYS:HG2	1.95	0.46
22:BA:1889:A:H2'	22:BA:1890:A:C8	2.50	0.46
1:AA:208:U:H3'	1:AA:210:C:H41	1.79	0.46
1:AA:591:U:H2'	1:AA:592:G:H8	1.80	0.46
1:AA:718:A:H5'	11:AK:119:ASN:ND2	2.30	0.46
16:AP:47:GLU:OE1	16:AP:47:GLU:N	2.48	0.46
22:BA:299:A:H2'	22:BA:300:A:C8	2.50	0.46
22:BA:414:C:H2'	22:BA:415:A:H8	1.81	0.46
22:BA:1724:G:H2'	22:BA:1725:U:C6	2.50	0.46
1:AA:362:G:N2	1:AA:365:U:OP2	2.44	0.46
1:AA:1268:G:H2'	1:AA:1269:A:C8	2.50	0.46
2:AB:204:ASP:OD1	2:AB:205:ASP:N	2.48	0.46
3:AC:58:GLU:HB2	3:AC:65:ARG:HG2	1.97	0.46
4:AD:104:ARG:HH21	4:AD:111:ARG:HH12	1.64	0.46
5:AE:13:GLU:HG3	5:AE:39:VAL:HG23	1.97	0.46
14:AN:83:LYS:HA	14:AN:83:LYS:HD3	1.73	0.46
22:BA:249:C:O2	51:B3:12:LYS:NZ	2.49	0.46
22:BA:1174:U:H2'	22:BA:1175:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BU:89:ASP:C	42:BU:91:LYS:H	2.24	0.46
1:AA:72:A:C5	1:AA:73:C:C5	3.04	0.46
1:AA:100:G:C2	1:AA:102:G:C4	3.04	0.46
9:AI:25:ASN:OD1	9:AI:27:LYS:NZ	2.39	0.46
17:AQ:46:VAL:HG11	17:AQ:61:ILE:HD12	1.98	0.46
22:BA:2547:A:H2'	22:BA:2548:U:C6	2.50	0.46
22:BA:2557:G:H2'	22:BA:2558:C:C6	2.50	0.46
34:BM:58:LYS:O	34:BM:59:ARG:HG3	2.16	0.46
42:BU:62:GLU:OE1	42:BU:62:GLU:N	2.48	0.46
1:AA:100:G:C4	1:AA:102:G:N9	2.82	0.46
1:AA:834:U:H2'	1:AA:835:U:C6	2.50	0.46
10:AJ:32:THR:HB	10:AJ:83:THR:HG22	1.96	0.46
22:BA:1171:G:H3'	22:BA:1173:U:O4	2.15	0.46
22:BA:1869:G:N2	22:BA:1871:A:O2'	2.48	0.46
22:BA:2101:A:C2	22:BA:2189:U:O2	2.69	0.46
22:BA:2271:G:OP1	44:BW:18:ALA:HB1	2.16	0.46
22:BA:2803:G:H2'	22:BA:2804:U:C6	2.51	0.46
56:B9:93:GLU:HA	56:B9:96:PHE:HB3	1.97	0.46
1:AA:177:G:OP1	20:AT:60:ARG:HD2	2.15	0.46
1:AA:486:U:H2'	1:AA:487:A:C8	2.51	0.46
5:AE:112:ARG:O	5:AE:116:GLU:HG3	2.16	0.46
22:BA:1065:U:H2'	22:BA:1066:U:C6	2.51	0.46
22:BA:2595:G:N2	22:BA:2598:A:OP2	2.35	0.46
42:BU:101:GLU:OE1	42:BU:101:GLU:N	2.47	0.46
1:AA:954:G:H2'	1:AA:955:U:C6	2.50	0.46
1:AA:1428:A:H2'	1:AA:1429:A:O4'	2.16	0.46
22:BA:883:G:H2'	22:BA:883:G:N3	2.31	0.46
27:BF:10:ASP:HB2	27:BF:11:GLU:OE1	2.15	0.46
30:BI:59:ARG:HH22	30:BI:63:ARG:HH22	1.64	0.46
56:B9:95:THR:HA	56:B9:98:GLU:HB2	1.97	0.46
1:AA:64:G:H21	1:AA:69:G:H3'	1.81	0.46
1:AA:67:C:C4	1:AA:69:G:N3	2.84	0.46
1:AA:100:G:C8	1:AA:102:G:N7	2.84	0.46
1:AA:434:U:H2'	1:AA:435:A:C8	2.50	0.46
1:AA:466:A:N3	1:AA:467:U:H5	2.13	0.46
1:AA:539:A:H2'	1:AA:540:G:H8	1.80	0.46
6:AF:3:HIS:ND1	6:AF:65:GLU:CD	2.74	0.46
10:AJ:55:PRO:HA	14:AN:82:ILE:HD11	1.98	0.46
22:BA:2314:A:H2'	22:BA:2315:G:H8	1.80	0.46
23:BB:2:G:H2'	23:BB:3:C:C6	2.51	0.46
29:BH:110:VAL:HG21	29:BH:132:PHE:HE2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:BR:43:ASN:O	39:BR:46:GLU:HG3	2.16	0.46
1:AA:1014:A:C2	1:AA:1219:A:H1'	2.51	0.46
1:AA:1121:U:C2	1:AA:1122:U:C5	3.04	0.46
22:BA:613:A:H5''	22:BA:614:A:C8	2.51	0.46
26:BE:121:VAL:O	26:BE:190:ALA:N	2.49	0.46
27:BF:11:GLU:OE1	27:BF:11:GLU:N	2.49	0.46
42:BU:41:LEU:HA	42:BU:62:GLU:HA	1.98	0.46
42:BU:85:PHE:CE1	42:BU:94:ARG:HG2	2.51	0.46
56:B9:85:GLU:HG3	56:B9:89:GLU:CD	2.41	0.46
1:AA:45:G:H2'	1:AA:46:G:H8	1.82	0.45
1:AA:76:G:C6	1:AA:77:A:C5	3.04	0.45
1:AA:408:A:O3'	4:AD:23:SER:OG	2.34	0.45
1:AA:1377:A:OP1	7:AG:92:ARG:NH2	2.49	0.45
3:AC:155:GLY:O	3:AC:196:ILE:HG12	2.16	0.45
6:AF:35:LYS:HB2	6:AF:65:GLU:HB2	1.97	0.45
21:AU:11:PRO:HG2	21:AU:14:VAL:HG13	1.98	0.45
22:BA:250:G:H2'	22:BA:251:A:C8	2.51	0.45
22:BA:644:A:H2'	22:BA:645:C:O4'	2.16	0.45
22:BA:667:U:H2'	22:BA:668:A:O4'	2.15	0.45
22:BA:1067:A:O2'	22:BA:1068:G:O4'	2.34	0.45
23:BB:2:G:H2'	23:BB:3:C:H6	1.81	0.45
1:AA:210:C:H1'	1:AA:211:G:N2	2.30	0.45
1:AA:1086:U:H3	1:AA:1099:G:H22	1.64	0.45
22:BA:1079:C:H2'	22:BA:1080:A:H8	1.81	0.45
22:BA:2812:G:H2'	22:BA:2813:A:C8	2.51	0.45
24:BC:21:ASN:HB3	24:BC:24:LEU:HD13	1.98	0.45
40:BS:59:GLU:HG2	40:BS:60:HIS:N	2.30	0.45
47:BZ:13:ALA:O	47:BZ:21:LYS:HE2	2.16	0.45
49:B1:40:ASP:HB3	49:B1:43:VAL:HG12	1.98	0.45
56:B9:27:TYR:CE1	56:B9:67:VAL:HA	2.51	0.45
1:AA:64:G:N2	1:AA:70:U:C5	2.84	0.45
1:AA:100:G:C2	1:AA:102:G:H1'	2.50	0.45
1:AA:1042:A:O2'	1:AA:1043:G:O5'	2.32	0.45
1:AA:1316:G:H22	1:AA:1318:A:H3'	1.81	0.45
14:AN:90:ARG:HB2	14:AN:92:GLU:OE1	2.17	0.45
22:BA:645:C:H2'	22:BA:647:G:C8	2.52	0.45
22:BA:1201:U:H2'	22:BA:1202:G:H8	1.81	0.45
22:BA:1434:A:H2'	22:BA:1435:G:C8	2.51	0.45
25:BD:108:ASP:OD1	25:BD:173:GLN:HA	2.16	0.45
26:BE:153:LEU:HB2	26:BE:171:ASP:OD2	2.16	0.45
27:BF:8:TYR:O	27:BF:13:VAL:HG13	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1149:C:H2'	1:AA:1150:A:C8	2.51	0.45
1:AA:1305:G:N2	1:AA:1332:A:H2	2.08	0.45
22:BA:2064:C:H2'	22:BA:2065:C:C6	2.51	0.45
29:BH:86:ASP:OD1	29:BH:87:GLU:N	2.45	0.45
56:B9:118:MET:HE2	56:B9:187:TYR:HD2	1.80	0.45
56:B9:121:GLY:C	56:B9:123:TYR:H	2.25	0.45
1:AA:64:G:C4	1:AA:69:G:C5	3.05	0.45
1:AA:958:A:C6	19:AS:55:ARG:HG2	2.52	0.45
1:AA:1309:G:N7	13:AM:98:ARG:NH2	2.63	0.45
13:AM:71:ARG:NH2	27:BF:113:ASP:OD2	2.50	0.45
22:BA:884:U:H1'	22:BA:893:C:C2	2.52	0.45
22:BA:948:C:H1'	22:BA:984:A:C8	2.51	0.45
40:BS:73:LYS:HB3	40:BS:106:VAL:HB	1.98	0.45
42:BU:48:PRO:HB3	42:BU:56:GLY:H	1.81	0.45
50:B2:44:VAL:HG23	50:B2:44:VAL:O	2.17	0.45
56:B9:49:GLU:OE1	56:B9:52:ARG:NH2	2.49	0.45
1:AA:390:U:H2'	1:AA:391:G:C8	2.50	0.45
1:AA:633:G:H2'	1:AA:634:C:C6	2.51	0.45
10:AJ:10:LEU:HD23	10:AJ:98:VAL:HG12	1.98	0.45
13:AM:46:SER:OG	13:AM:47:GLU:N	2.50	0.45
22:BA:1816:C:N4	24:BC:35:GLU:OE1	2.47	0.45
22:BA:2130:U:H5''	22:BA:2133:G:OP1	2.17	0.45
41:BT:48:GLN:HE21	41:BT:55:VAL:H	1.65	0.45
56:B9:338:THR:OG1	56:B9:339:GLY:HA2	2.16	0.45
1:AA:473:U:H2'	1:AA:474:G:C8	2.50	0.45
1:AA:891:U:H2'	1:AA:892:A:H8	1.81	0.45
1:AA:1170:A:H2'	1:AA:1171:A:O4'	2.15	0.45
1:AA:1202:U:N3	14:AN:82:ILE:HG21	2.32	0.45
4:AD:117:LEU:HD23	4:AD:117:LEU:HA	1.76	0.45
9:AI:25:ASN:H	9:AI:27:LYS:HZ3	1.62	0.45
19:AS:5:LEU:HA	19:AS:5:LEU:HD13	1.74	0.45
22:BA:1425:G:H2'	22:BA:1426:G:C8	2.51	0.45
22:BA:1689:A:H2'	22:BA:1690:A:C8	2.52	0.45
22:BA:2183:A:H2'	22:BA:2184:A:C8	2.52	0.45
22:BA:2640:G:P	31:BJ:96:ARG:NH1	2.90	0.45
31:BJ:110:PRO:O	31:BJ:115:GLY:HA3	2.17	0.45
40:BS:35:ILE:O	40:BS:39:THR:HG23	2.17	0.45
52:B4:18:LYS:HE3	52:B4:21:GLY:HA2	1.98	0.45
56:B9:40:GLU:O	56:B9:43:GLN:HG2	2.16	0.45
1:AA:100:G:C4	1:AA:102:G:C4	3.05	0.45
1:AA:193:C:H2'	1:AA:194:C:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:946:A:H2'	1:AA:947:G:C8	2.51	0.45
1:AA:1009:U:H3	1:AA:1020:G:H1	1.65	0.45
1:AA:1140:C:O2'	1:AA:1141:C:O5'	2.31	0.45
6:AF:45:ARG:O	6:AF:56:LYS:HA	2.17	0.45
22:BA:1096:A:C2	22:BA:1097:U:H1'	2.52	0.45
22:BA:2100:G:H3'	22:BA:2101:A:C8	2.51	0.45
22:BA:2130:U:H4'	22:BA:2133:G:H4'	1.97	0.45
22:BA:2315:G:H2'	22:BA:2316:G:H8	1.82	0.45
24:BC:176:LEU:HD12	24:BC:180:GLU:OE1	2.16	0.45
42:BU:99:ASN:OD1	42:BU:99:ASN:N	2.50	0.45
56:B9:61:SER:HA	56:B9:64:GLU:HG3	1.99	0.45
56:B9:280:GLN:O	56:B9:284:LYS:N	2.37	0.45
1:AA:494:G:H2'	1:AA:496:A:H8	1.82	0.45
1:AA:1129:C:H4'	9:AI:18:ARG:HH22	1.81	0.45
2:AB:210:VAL:HA	2:AB:213:TYR:CD2	2.51	0.45
10:AJ:7:ARG:HG3	10:AJ:73:LEU:HD11	1.99	0.45
20:AT:43:ASP:OD1	20:AT:44:LYS:N	2.50	0.45
22:BA:359:G:C6	22:BA:360:U:C4	3.05	0.45
22:BA:2107:G:O6	22:BA:2183:A:N6	2.50	0.45
22:BA:2591:C:H2'	22:BA:2592:G:C8	2.51	0.45
27:BF:12:VAL:HA	27:BF:15:LYS:HG2	1.99	0.45
34:BM:53:MET:HE1	34:BM:103:TYR:CD2	2.52	0.45
1:AA:308:C:H2'	1:AA:309:A:C8	2.52	0.45
6:AF:9:MET:HE2	6:AF:85:ILE:HD11	1.99	0.45
22:BA:832:U:H2'	22:BA:833:A:C8	2.52	0.45
22:BA:2330:G:O3'	44:BW:44:LYS:NZ	2.44	0.45
25:BD:114:LYS:HE2	25:BD:196:ALA:HB2	1.98	0.45
55:B8:69:A:H2'	55:B8:70:C:C6	2.52	0.45
1:AA:67:C:O2	1:AA:171:A:H2	2.00	0.44
1:AA:723:U:O4	21:AU:53:VAL:HG22	2.17	0.44
1:AA:954:G:H21	1:AA:1227:A:H62	1.65	0.44
1:AA:1120:C:C2	1:AA:1121:U:C5	3.05	0.44
1:AA:1230:C:H5'	55:B8:30:C:H5''	1.99	0.44
3:AC:152:GLU:HG3	3:AC:167:TRP:HB3	1.98	0.44
18:AR:21:ILE:HG21	18:AR:55:LEU:HD23	1.99	0.44
1:AA:6:G:O2'	1:AA:298:A:H1'	2.17	0.44
1:AA:235:C:H2'	1:AA:236:A:H8	1.81	0.44
12:AL:107:VAL:HG23	12:AL:110:ARG:HB2	2.00	0.44
22:BA:359:G:C5	22:BA:360:U:C4	3.05	0.44
22:BA:952:G:C6	22:BA:966:G:C6	3.04	0.44
22:BA:1052:C:H2'	22:BA:1053:C:H6	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1357:C:H2'	22:BA:1358:G:O4'	2.17	0.44
22:BA:1632:A:H2'	22:BA:1633:G:C8	2.51	0.44
22:BA:2312:U:H5'	27:BF:85:ILE:HD11	1.98	0.44
26:BE:118:LEU:HD11	26:BE:188:MET:SD	2.58	0.44
48:B0:13:ARG:O	48:B0:17:ARG:HG3	2.16	0.44
56:B9:277:ASP:O	56:B9:283:ASN:ND2	2.47	0.44
1:AA:440:C:C2	1:AA:441:A:C8	3.05	0.44
1:AA:883:C:O2'	1:AA:884:U:H5'	2.18	0.44
22:BA:277:G:O2'	22:BA:361:G:O6	2.33	0.44
22:BA:1809:A:H8	22:BA:1809:A:O5'	2.01	0.44
29:BH:70:GLU:O	29:BH:71:LYS:HB3	2.18	0.44
29:BH:108:VAL:HG23	29:BH:109:GLU:HG3	1.99	0.44
41:BT:68:LYS:O	41:BT:74:ILE:HD12	2.17	0.44
1:AA:459:A:N1	1:AA:460:A:C6	2.85	0.44
1:AA:718:A:H2	18:AR:38:LYS:HE2	1.81	0.44
1:AA:908:A:H2'	1:AA:909:A:H8	1.82	0.44
1:AA:1118:U:OP1	9:AI:11:ARG:NH1	2.43	0.44
2:AB:60:ILE:HA	2:AB:63:ARG:HH12	1.82	0.44
7:AG:115:SER:O	7:AG:119:ARG:HB2	2.17	0.44
22:BA:274:C:C5	22:BA:275:C:N3	2.85	0.44
22:BA:541:A:N1	22:BA:553:G:C6	2.85	0.44
22:BA:1076:C:H2'	22:BA:1077:A:C8	2.52	0.44
22:BA:1079:C:H2'	22:BA:1080:A:C8	2.53	0.44
22:BA:1282:U:H2'	22:BA:1283:G:O4'	2.17	0.44
1:AA:751:U:H2'	1:AA:752:G:O4'	2.17	0.44
2:AB:192:ASP:OD1	2:AB:192:ASP:N	2.51	0.44
6:AF:38:ARG:NE	6:AF:63:ASN:OD1	2.49	0.44
9:AI:98:LEU:HD23	9:AI:103:PHE:HD2	1.82	0.44
22:BA:848:C:H2'	22:BA:849:A:H8	1.82	0.44
22:BA:1505:A:H2'	22:BA:1506:U:O4'	2.17	0.44
22:BA:2724:U:H2'	22:BA:2725:A:C8	2.53	0.44
25:BD:36:GLN:HB3	25:BD:49:GLN:HE21	1.83	0.44
28:BG:149:ARG:HA	28:BG:162:VAL:HG13	1.99	0.44
42:BU:48:PRO:HB3	42:BU:56:GLY:N	2.32	0.44
1:AA:198:G:H2'	1:AA:199:A:H8	1.83	0.44
1:AA:868:C:H2'	1:AA:869:G:O4'	2.17	0.44
1:AA:1181:G:O2'	1:AA:1182:G:N7	2.48	0.44
1:AA:1318:A:H1'	19:AS:37:ARG:NH1	2.32	0.44
22:BA:372:G:C8	45:BX:61:LYS:HD2	2.52	0.44
22:BA:1085:A:C8	22:BA:1086:A:C6	3.05	0.44
22:BA:1729:U:C2	22:BA:1731:G:N2	2.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2123:G:C6	22:BA:2176:A:N6	2.86	0.44
29:BH:134:VAL:HG23	29:BH:138:VAL:HG23	1.99	0.44
35:BN:16:HIS:CD2	35:BN:16:HIS:O	2.70	0.44
1:AA:113:G:H1'	1:AA:354:G:H5'	1.99	0.44
1:AA:1014:A:H2'	1:AA:1015:G:C8	2.53	0.44
1:AA:1040:U:H2'	1:AA:1041:G:H8	1.83	0.44
1:AA:1171:A:H2'	1:AA:1172:C:H6	1.83	0.44
1:AA:1308:U:OP2	13:AM:100:GLN:NE2	2.49	0.44
1:AA:1435:G:H2'	1:AA:1436:U:C6	2.53	0.44
7:AG:113:ASP:OD2	7:AG:122:ASN:ND2	2.47	0.44
9:AI:6:TYR:HB2	9:AI:21:ILE:HD11	2.00	0.44
11:AK:37:ARG:NH1	11:AK:83:GLU:OE2	2.51	0.44
17:AQ:77:ARG:NH1	17:AQ:79:VAL:HG12	2.33	0.44
22:BA:856:G:H2'	22:BA:857:G:C8	2.53	0.44
22:BA:2038:G:H2'	22:BA:2039:U:O4'	2.17	0.44
37:BP:6:LYS:O	37:BP:10:GLN:HG2	2.17	0.44
51:B3:29:LEU:HD11	51:B3:44:LEU:CB	2.47	0.44
55:B8:63:U:H2'	55:B8:64:C:C6	2.53	0.44
56:B9:27:TYR:HE1	56:B9:67:VAL:HA	1.83	0.44
1:AA:131:A:H2'	1:AA:132:C:C6	2.53	0.44
1:AA:715:A:H2'	1:AA:716:A:C8	2.53	0.44
1:AA:890:G:O2'	1:AA:906:A:N6	2.51	0.44
1:AA:1020:G:H2'	1:AA:1021:A:C8	2.53	0.44
1:AA:1120:C:H2'	1:AA:1121:U:C6	2.53	0.44
1:AA:1202:U:C2	14:AN:82:ILE:HG21	2.53	0.44
8:AH:12:THR:HG22	8:AH:15:ARG:NH1	2.19	0.44
9:AI:60:LYS:HE2	9:AI:60:LYS:HB2	1.82	0.44
22:BA:176:A:O2'	22:BA:177:G:H5'	2.18	0.44
22:BA:1733:G:H2'	22:BA:1734:G:H8	1.83	0.44
22:BA:2554:U:H2'	22:BA:2555:U:C6	2.52	0.44
41:BT:4:GLU:HG2	41:BT:49:LYS:HE2	1.99	0.44
49:B1:5:ILE:HG23	49:B1:28:ARG:NH1	2.32	0.44
49:B1:17:THR:HG21	49:B1:42:VAL:HG13	2.00	0.44
1:AA:1340:A:O2'	55:B8:32:U:H5'	2.18	0.44
16:AP:69:ASP:OD1	16:AP:70:ARG:N	2.51	0.44
19:AS:29:LYS:HG2	19:AS:30:PRO:HD2	2.00	0.44
22:BA:320:A:O2'	22:BA:322:A:OP2	2.33	0.44
22:BA:2099:U:H2'	22:BA:2100:G:O4'	2.17	0.44
22:BA:2113:U:H3'	22:BA:2115:G:N2	2.33	0.44
26:BE:48:THR:HG22	26:BE:86:ALA:HB3	1.99	0.44
27:BF:137:ILE:HG13	27:BF:138:PHE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BH:101:ASP:O	29:BH:104:THR:OG1	2.22	0.44
38:BQ:48:ARG:NH1	38:BQ:49:ASP:OD1	2.51	0.44
1:AA:45:G:H2'	1:AA:46:G:C8	2.52	0.43
1:AA:389:A:H3'	1:AA:390:U:C6	2.53	0.43
1:AA:1010:U:H2'	1:AA:1011:C:H6	1.82	0.43
9:AI:97:GLU:H	9:AI:97:GLU:CD	2.26	0.43
17:AQ:60:GLU:OE1	17:AQ:77:ARG:NH2	2.51	0.43
20:AT:44:LYS:NZ	20:AT:87:ALA:OXT	2.38	0.43
22:BA:1175:A:H1'	22:BA:1176:U:C6	2.53	0.43
22:BA:1796:U:H2'	22:BA:1797:G:H8	1.83	0.43
22:BA:2181:U:H2'	22:BA:2182:U:O4'	2.18	0.43
25:BD:22:ILE:HG23	25:BD:190:LYS:HG3	2.00	0.43
36:BO:110:ALA:O	36:BO:115:LEU:HB3	2.17	0.43
1:AA:102:G:N3	1:AA:151:A:H2	2.16	0.43
1:AA:270:A:H2'	1:AA:271:C:C6	2.52	0.43
1:AA:462:G:C6	1:AA:463:U:C4	3.06	0.43
1:AA:683:G:N2	11:AK:39:GLY:O	2.51	0.43
2:AB:144:LEU:HD23	2:AB:144:LEU:O	2.18	0.43
8:AH:8:ALA:O	8:AH:12:THR:HG23	2.19	0.43
10:AJ:52:LEU:HB2	14:AN:81:ARG:HD2	1.99	0.43
18:AR:22:ASP:OD2	18:AR:24:LYS:HE2	2.18	0.43
22:BA:810:U:C4	33:BL:29:LYS:O	2.71	0.43
22:BA:1027:A:C2	22:BA:2488:G:H5'	2.53	0.43
22:BA:2185:U:H2'	22:BA:2186:G:C8	2.53	0.43
23:BB:42:C:C6	27:BF:66:LEU:HB2	2.53	0.43
39:BR:14:VAL:HG12	39:BR:20:VAL:HG11	2.00	0.43
39:BR:44:GLY:O	39:BR:45:GLU:HG2	2.16	0.43
43:BV:26:PHE:HE2	43:BV:89:ILE:HG12	1.82	0.43
56:B9:31:LYS:HD2	56:B9:34:LEU:HD12	1.99	0.43
1:AA:73:C:H2'	1:AA:74:A:O4'	2.18	0.43
1:AA:149:A:H2'	1:AA:150:U:C6	2.53	0.43
1:AA:269:C:H2'	1:AA:270:A:C8	2.53	0.43
4:AD:4:TYR:CE2	4:AD:11:LEU:HD11	2.53	0.43
7:AG:113:ASP:O	7:AG:119:ARG:NH2	2.48	0.43
22:BA:45:G:H5''	22:BA:46:G:O5'	2.18	0.43
22:BA:1250:G:H5''	38:BQ:6:ARG:CD	2.44	0.43
22:BA:2193:G:H2'	22:BA:2194:U:C6	2.53	0.43
22:BA:2251:OMG:HM23	22:BA:2251:OMG:H1'	1.73	0.43
24:BC:267:ILE:HG21	24:BC:270:ARG:HD2	1.98	0.43
27:BF:14:LYS:O	27:BF:18:THR:HG23	2.17	0.43
55:B8:62:C:H2'	55:B8:63:U:H6	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:B9:9:ASN:O	56:B9:13:ASP:N	2.50	0.43
56:B9:33:ARG:HD2	56:B9:63:LEU:HD11	1.99	0.43
1:AA:71:A:C6	1:AA:101:A:C6	3.06	0.43
1:AA:461:A:C6	1:AA:462:G:O6	2.72	0.43
22:BA:839:U:H2'	22:BA:840:C:C6	2.53	0.43
22:BA:1278:C:H2'	22:BA:1279:G:C8	2.53	0.43
22:BA:2108:A:N1	22:BA:2181:U:O4	2.51	0.43
22:BA:2113:U:P	22:BA:2115:G:H1	2.42	0.43
22:BA:2298:A:N6	22:BA:2321:U:O4	2.52	0.43
1:AA:66:A:C5	1:AA:67:C:C5	3.07	0.43
1:AA:100:G:C2	1:AA:101:A:C2	3.06	0.43
1:AA:451:A:H1'	1:AA:452:A:C2	2.54	0.43
1:AA:696:A:H2'	1:AA:697:U:C6	2.54	0.43
1:AA:1405:G:O2'	1:AA:1518:MA6:O2'	2.36	0.43
3:AC:60:PRO:O	3:AC:61:ALA:C	2.61	0.43
13:AM:89:LEU:HA	13:AM:92:ARG:HG2	2.00	0.43
19:AS:36:ARG:NH2	19:AS:75:ALA:O	2.51	0.43
22:BA:548:G:H2'	22:BA:548:G:N3	2.33	0.43
22:BA:1570:A:H2'	22:BA:1571:A:C8	2.54	0.43
22:BA:1590:A:H2'	22:BA:1591:A:H8	1.83	0.43
22:BA:1720:U:H2'	22:BA:1721:G:O4'	2.17	0.43
22:BA:2265:U:OP2	22:BA:2266:A:O2'	2.36	0.43
24:BC:75:PRO:HG2	24:BC:97:LYS:HG3	2.00	0.43
1:AA:460:A:C6	1:AA:461:A:C6	3.06	0.43
1:AA:779:C:H2'	1:AA:780:A:O4'	2.18	0.43
1:AA:1048:G:H4'	14:AN:2:LYS:NZ	2.34	0.43
1:AA:1315:U:O2	1:AA:1360:A:H2	2.02	0.43
2:AB:20:THR:HG22	2:AB:39:HIS:CD2	2.54	0.43
3:AC:9:GLY:N	14:AN:89:MET:HE3	2.31	0.43
22:BA:893:C:H2'	22:BA:894:U:O4'	2.19	0.43
22:BA:2389:G:H5''	22:BA:2390:U:O4'	2.19	0.43
27:BF:73:SER:OG	27:BF:80:ARG:HA	2.19	0.43
30:BI:16:CYS:SG	30:BI:17:SER:N	2.92	0.43
31:BJ:49:ASP:CG	31:BJ:121:LYS:HZ3	2.27	0.43
56:B9:124:ASP:O	56:B9:187:TYR:HA	2.18	0.43
1:AA:67:C:N4	1:AA:69:G:C6	2.87	0.43
1:AA:162:A:H8	1:AA:162:A:O5'	1.99	0.43
1:AA:1121:U:H2'	1:AA:1122:U:H6	1.84	0.43
1:AA:1141:C:H2'	1:AA:1142:G:H8	1.83	0.43
3:AC:59:ARG:CZ	3:AC:64:ILE:HD12	2.49	0.43
13:AM:19:LEU:HD23	13:AM:19:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:66:GLU:HG3	13:AM:67:GLY:N	2.31	0.43
22:BA:593:U:H2'	22:BA:594:U:C6	2.53	0.43
22:BA:685:A:H5''	22:BA:788:A:H62	1.84	0.43
22:BA:2700:A:H2'	22:BA:2701:U:C6	2.53	0.43
26:BE:61:ARG:NH2	53:B5:9:THR:HG1	2.15	0.43
33:BL:78:ARG:HG2	33:BL:113:ALA:HB3	2.00	0.43
34:BM:136:MET:HE3	43:BV:57:TYR:CD1	2.53	0.43
37:BP:13:MET:HE2	37:BP:55:LEU:N	2.33	0.43
55:B8:51:A:H2'	55:B8:52:G:C8	2.54	0.43
1:AA:1306:A:O2'	13:AM:108:THR:HG21	2.18	0.43
21:AU:4:ILE:O	21:AU:4:ILE:HG13	2.18	0.43
22:BA:568:U:H1'	22:BA:2030:6MZ:H9C1	2.00	0.43
24:BC:28:LYS:HA	24:BC:28:LYS:HD3	1.86	0.43
1:AA:445:G:N1	1:AA:489:C:H5	2.00	0.43
1:AA:1143:G:H2'	1:AA:1144:G:H8	1.84	0.43
2:AB:111:ILE:O	2:AB:114:LEU:HB3	2.19	0.43
2:AB:219:ALA:O	2:AB:221:VAL:N	2.52	0.43
22:BA:1179:G:H2'	22:BA:1180:U:C6	2.54	0.43
22:BA:1816:C:H41	24:BC:35:GLU:CD	2.26	0.43
22:BA:2514:U:H2'	22:BA:2515:C:C6	2.53	0.43
53:B5:8:VAL:C	53:B5:10:SER:H	2.26	0.43
1:AA:335:C:H2'	1:AA:336:A:C8	2.54	0.43
1:AA:457:G:H22	1:AA:474:G:N2	2.16	0.43
1:AA:466:A:O2'	1:AA:467:U:H6	2.01	0.43
1:AA:591:U:OP1	8:AH:31:LYS:NZ	2.48	0.43
1:AA:1493:A:H4'	1:AA:1494:G:OP1	2.18	0.43
19:AS:28:LYS:HE2	19:AS:28:LYS:HB2	1.89	0.43
22:BA:285:G:H2'	22:BA:286:U:H6	1.83	0.43
22:BA:422:A:H8	22:BA:422:A:O5'	2.01	0.43
22:BA:2174:C:H2'	22:BA:2175:C:C6	2.54	0.43
22:BA:2720:U:OP1	37:BP:53:ARG:NH2	2.52	0.43
34:BM:70:ASP:OD1	34:BM:70:ASP:N	2.52	0.43
42:BU:49:VAL:HG22	42:BU:51:ALA:H	1.83	0.43
56:B9:338:THR:H	56:B9:339:GLY:HA2	1.83	0.43
1:AA:412:A:O2'	1:AA:414:A:H5'	2.19	0.42
1:AA:471:U:H2'	1:AA:472:U:C6	2.54	0.42
1:AA:473:U:C2	1:AA:474:G:C8	3.07	0.42
12:AL:36:ARG:HG2	12:AL:38:TYR:CD1	2.53	0.42
22:BA:2139:U:O4	22:BA:2152:G:O6	2.37	0.42
25:BD:33:ARG:HH22	25:BD:74:GLU:HG3	1.84	0.42
26:BE:191:ASP:O	26:BE:195:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:B9:21:LEU:HB2	56:B9:25:LEU:HD12	2.01	0.42
14:AN:98:LYS:HE3	14:AN:98:LYS:HB3	1.79	0.42
18:AR:38:LYS:HB2	18:AR:38:LYS:HE3	1.72	0.42
22:BA:1870:C:O2'	22:BA:1871:A:O4'	2.37	0.42
22:BA:2031:A:C6	22:BA:2498:OMC:H1'	2.54	0.42
22:BA:2537:U:H2'	22:BA:2538:C:C6	2.54	0.42
23:BB:49:C:H2'	23:BB:50:A:C8	2.54	0.42
24:BC:247:PRO:HG2	24:BC:248:TRP:CZ3	2.54	0.42
29:BH:4:ILE:HD13	29:BH:43:ASN:HB2	2.01	0.42
41:BT:18:GLU:HG2	41:BT:19:LYS:N	2.34	0.42
43:BV:72:VAL:HB	43:BV:91:PHE:HB3	2.01	0.42
1:AA:100:G:C4	1:AA:101:A:C6	3.08	0.42
5:AE:160:SER:HA	5:AE:164:ILE:HD11	2.01	0.42
7:AG:60:GLU:OE1	7:AG:60:GLU:N	2.47	0.42
10:AJ:77:VAL:HG23	10:AJ:78:GLU:OE1	2.18	0.42
11:AK:28:ASN:O	11:AK:57:LYS:HE3	2.19	0.42
22:BA:280:U:C4	22:BA:360:U:O2	2.71	0.42
22:BA:1068:G:C8	22:BA:1069:A:N7	2.88	0.42
22:BA:1175:A:C8	22:BA:1176:U:N3	2.87	0.42
22:BA:2149:U:H2'	22:BA:2150:C:C6	2.54	0.42
29:BH:4:ILE:HA	29:BH:17:ASP:O	2.19	0.42
1:AA:75:G:C5	1:AA:76:G:C8	3.07	0.42
1:AA:193:C:H2'	1:AA:194:C:C6	2.53	0.42
1:AA:264:C:H2'	1:AA:265:G:O4'	2.19	0.42
1:AA:593:U:H2'	1:AA:594:U:H6	1.85	0.42
1:AA:745:G:H2'	1:AA:746:A:H8	1.83	0.42
1:AA:933:G:O6	7:AG:3:ARG:NH2	2.48	0.42
1:AA:983:A:H5''	1:AA:984:C:OP2	2.19	0.42
1:AA:1005:A:H3'	1:AA:1006:G:H8	1.83	0.42
1:AA:1009:U:H2'	1:AA:1010:U:C6	2.54	0.42
6:AF:101:PRO:N	6:AF:104:LYS:HE3	2.34	0.42
22:BA:1050:A:C2	22:BA:2751:G:C4	3.08	0.42
22:BA:2165:C:H2'	22:BA:2166:U:O4'	2.19	0.42
22:BA:2228:G:H2'	22:BA:2229:U:C6	2.54	0.42
51:B3:31:HIS:C	51:B3:33:LEU:N	2.73	0.42
1:AA:64:G:N1	1:AA:69:G:C2	2.87	0.42
1:AA:64:G:C5	1:AA:69:G:C6	3.06	0.42
1:AA:75:G:C6	1:AA:76:G:C5	3.08	0.42
1:AA:413:G:N2	1:AA:428:G:H1'	2.35	0.42
1:AA:727:G:N2	1:AA:730:G:OP2	2.43	0.42
10:AJ:56:HIS:CG	10:AJ:57:VAL:H	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:594:U:H2'	22:BA:595:C:C6	2.55	0.42
22:BA:2030:6MZ:H2	22:BA:2499:C:H5''	2.01	0.42
22:BA:2086:U:H2'	22:BA:2087:G:C8	2.54	0.42
22:BA:2467:C:H2'	22:BA:2468:A:O4'	2.18	0.42
22:BA:2698:U:H2'	22:BA:2699:C:C6	2.54	0.42
27:BF:147:ASP:OD1	27:BF:150:ARG:NH2	2.53	0.42
29:BH:84:ALA:HB1	29:BH:89:LYS:O	2.19	0.42
43:BV:35:GLU:OE1	43:BV:35:GLU:N	2.52	0.42
55:B8:25:C:H2'	55:B8:26:A:O4'	2.19	0.42
1:AA:68:G:O6	1:AA:100:G:O6	2.36	0.42
1:AA:1026:G:C6	1:AA:1027:C:N4	2.87	0.42
1:AA:1106:G:O2'	3:AC:169:ARG:NH2	2.53	0.42
1:AA:1366:C:H2'	1:AA:1367:C:C6	2.55	0.42
6:AF:42:TRP:CZ2	6:AF:102:MET:HG3	2.54	0.42
13:AM:3:ARG:HG2	13:AM:9:ILE:HG12	2.02	0.42
18:AR:38:LYS:HA	18:AR:38:LYS:HD3	1.79	0.42
22:BA:231:A:H2'	22:BA:232:G:O4'	2.20	0.42
22:BA:1007:C:OP1	31:BJ:37:ARG:NH2	2.52	0.42
22:BA:2277:G:H2'	22:BA:2278:A:H5''	2.02	0.42
28:BG:99:LYS:HG3	28:BG:99:LYS:O	2.20	0.42
45:BX:26:LYS:HA	45:BX:26:LYS:HD2	1.97	0.42
56:B9:16:GLU:O	56:B9:20:VAL:HG13	2.19	0.42
56:B9:33:ARG:CD	56:B9:63:LEU:HD11	2.50	0.42
56:B9:86:LEU:O	56:B9:90:ALA:HB3	2.20	0.42
1:AA:463:U:H2'	1:AA:464:U:N1	2.35	0.42
1:AA:744:C:H2'	1:AA:745:G:C8	2.55	0.42
1:AA:748:G:H2'	1:AA:749:A:C8	2.55	0.42
9:AI:57:MET:HA	9:AI:60:LYS:HE2	2.01	0.42
22:BA:84:A:H4'	22:BA:85:G:O5'	2.19	0.42
22:BA:207:A:H2'	22:BA:208:C:O4'	2.20	0.42
22:BA:881:G:N2	22:BA:896:A:H62	2.17	0.42
22:BA:966:G:H2'	22:BA:967:U:C6	2.55	0.42
22:BA:1081:U:H2'	22:BA:1082:U:C6	2.54	0.42
22:BA:2020:A:H5'	48:B0:9:THR:HG21	2.01	0.42
22:BA:2100:G:O6	22:BA:2189:U:C2	2.72	0.42
22:BA:2188:U:H2'	22:BA:2189:U:C5	2.55	0.42
35:BN:37:THR:HG22	35:BN:110:MET:HE1	2.00	0.42
53:B5:8:VAL:C	53:B5:10:SER:N	2.78	0.42
1:AA:1190:G:H5'	3:AC:176:HIS:NE2	2.35	0.42
1:AA:1273:C:H2'	1:AA:1274:A:O4'	2.20	0.42
1:AA:1338:G:H2'	1:AA:1339:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:28:ILE:HG12	4:AD:34:ILE:HD11	2.02	0.42
4:AD:91:LEU:HD23	4:AD:91:LEU:HA	1.82	0.42
5:AE:89:HIS:O	5:AE:90:THR:C	2.63	0.42
7:AG:129:GLU:HB3	7:AG:131:LYS:NZ	2.35	0.42
11:AK:53:ARG:HD2	11:AK:53:ARG:HA	1.75	0.42
11:AK:126:LYS:HE2	21:AU:37:PHE:HB2	2.00	0.42
12:AL:24:LEU:O	12:AL:27:CYS:HB3	2.20	0.42
22:BA:1410:G:H2'	22:BA:1411:U:C6	2.55	0.42
22:BA:1790:C:H2'	22:BA:1791:A:C5	2.54	0.42
22:BA:2130:U:H5''	22:BA:2133:G:P	2.60	0.42
29:BH:44:ILE:HG23	29:BH:45:GLU:CD	2.44	0.42
29:BH:100:ALA:O	29:BH:104:THR:HG23	2.20	0.42
43:BV:77:VAL:HG22	43:BV:89:ILE:HD12	2.01	0.42
47:BZ:4:THR:HA	47:BZ:39:GLU:HA	2.01	0.42
1:AA:67:C:N4	1:AA:69:G:N1	2.68	0.42
2:AB:59:LYS:O	2:AB:63:ARG:NH1	2.53	0.42
7:AG:42:ILE:HG21	7:AG:116:MET:HG3	2.02	0.42
9:AI:91:ASP:OD2	9:AI:94:LEU:HB2	2.20	0.42
22:BA:1470:A:H2'	22:BA:1471:G:O4'	2.20	0.42
22:BA:1762:A:H8	22:BA:1762:A:O5'	2.03	0.42
22:BA:2474:U:O2'	22:BA:2475:C:OP1	2.34	0.42
22:BA:2796:U:O2'	22:BA:2797:U:H2'	2.19	0.42
23:BB:49:C:H2'	23:BB:50:A:H8	1.85	0.42
25:BD:106:LYS:NZ	25:BD:176:ASP:OD1	2.52	0.42
27:BF:6:ASP:OD1	27:BF:7:TYR:N	2.49	0.42
27:BF:123:ASP:OD2	27:BF:127:ASN:HB2	2.19	0.42
1:AA:523:A:C2	12:AL:88:LYS:HB3	2.55	0.42
1:AA:1003:G:N2	1:AA:1005:A:O5'	2.52	0.42
6:AF:5:GLU:OE1	18:AR:23:TYR:OH	2.24	0.42
10:AJ:8:ILE:HA	10:AJ:99:GLN:O	2.20	0.42
12:AL:100:GLY:N	12:AL:104:CYS:O	2.38	0.42
22:BA:883:G:N1	22:BA:894:U:O2'	2.47	0.42
22:BA:1378:A:O2'	22:BA:1380:G:N7	2.53	0.42
22:BA:2181:U:H2'	22:BA:2182:U:H6	1.85	0.42
22:BA:2395:C:H2'	22:BA:2396:G:O4'	2.19	0.42
22:BA:2529:G:H5'	28:BG:175:LYS:HB3	2.01	0.42
29:BH:57:LYS:O	29:BH:60:GLU:HG3	2.20	0.42
1:AA:324:G:N1	1:AA:327:A:OP2	2.52	0.41
1:AA:460:A:C6	1:AA:461:A:N6	2.88	0.41
1:AA:591:U:H2'	1:AA:592:G:C8	2.54	0.41
1:AA:864:A:H2'	1:AA:865:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:999:C:N3	1:AA:1042:A:N6	2.68	0.41
1:AA:1308:U:H2'	1:AA:1309:G:H8	1.85	0.41
1:AA:1355:G:H2'	1:AA:1356:G:C8	2.55	0.41
8:AH:43:GLU:HG3	8:AH:101:ILE:HD13	2.02	0.41
12:AL:107:VAL:CG2	12:AL:110:ARG:HB2	2.49	0.41
13:AM:45:ILE:HD13	13:AM:45:ILE:HA	1.88	0.41
22:BA:138:U:H2'	22:BA:140:C:C5	2.55	0.41
22:BA:279:A:H2'	22:BA:280:U:O4'	2.20	0.41
22:BA:927:A:H2'	22:BA:928:A:C8	2.54	0.41
22:BA:1174:U:H1'	22:BA:1177:G:C2	2.55	0.41
22:BA:2012:G:OP1	40:BS:11:ARG:NH2	2.39	0.41
26:BE:122:GLU:N	26:BE:122:GLU:OE1	2.52	0.41
27:BF:163:ASP:N	27:BF:163:ASP:OD1	2.51	0.41
56:B9:21:LEU:HD11	56:B9:70:LEU:HD11	2.00	0.41
1:AA:66:A:N6	1:AA:67:C:N4	2.68	0.41
1:AA:100:G:O4'	1:AA:101:A:N9	2.53	0.41
1:AA:458:U:H2'	1:AA:459:A:H8	1.83	0.41
1:AA:1373:G:N7	9:AI:13:LYS:NZ	2.65	0.41
10:AJ:11:LYS:HB2	10:AJ:97:ASP:OD1	2.20	0.41
11:AK:16:VAL:HG12	11:AK:18:ASP:H	1.85	0.41
12:AL:36:ARG:HG2	12:AL:38:TYR:HD1	1.85	0.41
22:BA:361:G:H4'	22:BA:362:A:OP1	2.19	0.41
22:BA:780:G:C2	22:BA:785:G:O6	2.73	0.41
22:BA:1067:A:N6	56:B9:54:GLN:OE1	2.52	0.41
22:BA:1239:G:H2'	22:BA:1240:U:O4'	2.20	0.41
24:BC:157:SER:O	24:BC:160:THR:OG1	2.36	0.41
26:BE:141:MET:HB2	26:BE:143:LEU:HG	2.02	0.41
35:BN:8:ARG:HB3	35:BN:10:LEU:HG	2.01	0.41
1:AA:100:G:N1	1:AA:102:G:C4	2.88	0.41
7:AG:15:ASP:OD1	7:AG:16:PRO:HD2	2.20	0.41
9:AI:49:ARG:O	9:AI:53:GLU:HG2	2.21	0.41
10:AJ:91:ASP:OD1	10:AJ:91:ASP:N	2.49	0.41
11:AK:113:VAL:O	11:AK:113:VAL:HG12	2.20	0.41
22:BA:276:U:O2'	22:BA:277:G:O5'	2.32	0.41
22:BA:1052:C:H2'	22:BA:1053:C:C6	2.55	0.41
22:BA:1141:U:H4'	22:BA:1142:A:O4'	2.20	0.41
1:AA:426:U:H2'	1:AA:427:U:C6	2.55	0.41
1:AA:736:C:OP1	18:AR:61:ARG:NH2	2.49	0.41
2:AB:91:PHE:O	2:AB:150:GLY:HA3	2.21	0.41
2:AB:144:LEU:HD23	2:AB:144:LEU:C	2.45	0.41
19:AS:34:TRP:CD1	19:AS:52:HIS:ND1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2070:A:H2'	22:BA:2071:A:O4'	2.20	0.41
22:BA:2743:U:O2'	28:BG:153:ARG:NH1	2.52	0.41
22:BA:2804:U:H2'	22:BA:2805:C:C6	2.55	0.41
23:BB:45:A:C4	23:BB:46:A:C8	3.09	0.41
26:BE:21:ARG:HH11	26:BE:106:LYS:CD	2.33	0.41
26:BE:145:ASP:HB3	26:BE:166:LYS:HB3	2.01	0.41
27:BF:110:ARG:NH2	27:BF:139:PRO:HB3	2.34	0.41
28:BG:4:VAL:O	28:BG:69:ARG:HD2	2.20	0.41
56:B9:33:ARG:NE	56:B9:59:GLU:OE1	2.53	0.41
1:AA:2:A:H1'	1:AA:613:C:O2'	2.20	0.41
1:AA:151:A:H5''	1:AA:152:A:OP2	2.20	0.41
1:AA:352:C:O2'	1:AA:354:G:OP1	2.31	0.41
1:AA:381:C:H2'	1:AA:382:A:O4'	2.21	0.41
1:AA:441:A:H1'	1:AA:497:G:N2	2.36	0.41
1:AA:559:A:H4'	1:AA:560:A:H3'	2.03	0.41
1:AA:748:G:H2'	1:AA:749:A:H8	1.86	0.41
2:AB:153:ASP:N	2:AB:153:ASP:OD1	2.52	0.41
7:AG:52:GLN:NE2	7:AG:53:ARG:HG3	2.35	0.41
22:BA:1279:G:C6	22:BA:1292:G:C6	3.08	0.41
22:BA:1300:G:H4'	22:BA:1301:A:H5''	2.03	0.41
22:BA:1642:G:H2'	22:BA:1643:G:O4'	2.21	0.41
22:BA:2102:G:N1	22:BA:2188:U:N3	2.62	0.41
27:BF:6:ASP:OD1	27:BF:6:ASP:N	2.53	0.41
28:BG:37:LEU:HD23	28:BG:37:LEU:HA	1.88	0.41
36:BO:76:LYS:O	36:BO:80:GLU:OE1	2.39	0.41
38:BQ:76:TYR:CZ	38:BQ:80:ILE:HG13	2.55	0.41
39:BR:78:ARG:HE	39:BR:78:ARG:HB2	1.69	0.41
40:BS:7:HIS:ND1	40:BS:10:ALA:HB2	2.36	0.41
56:B9:349:LEU:HD23	56:B9:349:LEU:HA	1.84	0.41
1:AA:208:U:H3'	1:AA:210:C:N4	2.34	0.41
1:AA:383:A:O5'	1:AA:383:A:H8	2.04	0.41
1:AA:411:A:P	4:AD:26:ARG:HH12	2.43	0.41
1:AA:552:U:H2'	1:AA:553:A:H8	1.86	0.41
1:AA:954:G:H2'	1:AA:955:U:O4'	2.21	0.41
3:AC:6:HIS:CE1	3:AC:8:ASN:HB3	2.56	0.41
3:AC:33:LEU:HD23	3:AC:33:LEU:HA	1.92	0.41
5:AE:15:LEU:HD12	5:AE:37:THR:HG22	2.03	0.41
6:AF:100:SER:C	6:AF:104:LYS:HE3	2.45	0.41
9:AI:12:ARG:O	9:AI:13:LYS:C	2.63	0.41
13:AM:64:VAL:O	13:AM:69:LEU:HB2	2.20	0.41
22:BA:1528:A:H2'	22:BA:1529:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2137:U:C2	22:BA:2138:G:N7	2.88	0.41
22:BA:2189:U:C2'	22:BA:2190:G:H8	2.25	0.41
29:BH:72:ILE:HG13	29:BH:73:ASN:N	2.35	0.41
30:BI:58:ASP:OD2	30:BI:58:ASP:N	2.53	0.41
33:BL:109:LYS:HG2	33:BL:126:ARG:HB2	2.02	0.41
34:BM:24:THR:HG22	34:BM:99:GLY:O	2.20	0.41
1:AA:477:C:H2'	1:AA:479:U:O4'	2.20	0.41
1:AA:494:G:O2'	1:AA:496:A:H1'	2.20	0.41
1:AA:501:C:OP1	12:AL:114:ARG:NH2	2.49	0.41
1:AA:1320:C:N3	19:AS:36:ARG:NH1	2.69	0.41
3:AC:79:LYS:O	3:AC:80:LYS:HG3	2.20	0.41
3:AC:191:THR:HG22	3:AC:193:TYR:H	1.84	0.41
14:AN:73:PHE:CZ	14:AN:78:GLY:HA2	2.56	0.41
19:AS:29:LYS:HD2	19:AS:30:PRO:O	2.21	0.41
22:BA:729:G:C6	24:BC:207:LYS:HB2	2.56	0.41
22:BA:1185:G:H5''	22:BA:1186:G:OP1	2.21	0.41
22:BA:1794:A:H2'	22:BA:1795:C:C6	2.56	0.41
22:BA:2148:G:C2	22:BA:2149:U:C4	3.09	0.41
23:BB:94:A:H2'	23:BB:95:U:O4'	2.20	0.41
1:AA:455:G:H2'	1:AA:456:A:C8	2.56	0.41
1:AA:594:U:H2'	1:AA:595:A:O4'	2.20	0.41
1:AA:1118:U:O3'	9:AI:85:ARG:NH2	2.43	0.41
1:AA:1141:C:H2'	1:AA:1142:G:C8	2.55	0.41
1:AA:1261:A:C5	1:AA:1262:C:C5	3.09	0.41
1:AA:1263:C:H2'	1:AA:1264:U:C6	2.56	0.41
4:AD:103:TYR:CE1	4:AD:110:THR:HA	2.55	0.41
4:AD:144:SER:HB3	4:AD:179:GLU:HB2	2.02	0.41
7:AG:25:LYS:O	7:AG:29:ILE:HG12	2.20	0.41
22:BA:718:A:H2'	22:BA:719:C:O4'	2.20	0.41
22:BA:2392:A:C2	33:BL:55:MET:SD	3.13	0.41
26:BE:46:GLN:HB2	26:BE:86:ALA:HB1	2.02	0.41
1:AA:88:U:H1'	1:AA:89:U:H5	1.85	0.41
1:AA:185:U:H2'	1:AA:186:C:H6	1.84	0.41
1:AA:323:U:H2'	1:AA:324:G:O4'	2.21	0.41
1:AA:858:G:O6	1:AA:869:G:H3'	2.21	0.41
1:AA:1338:G:O2'	55:B8:41:A:H4'	2.21	0.41
3:AC:50:ALA:O	3:AC:70:THR:OG1	2.39	0.41
4:AD:198:HIS:HA	4:AD:201:VAL:HG22	2.02	0.41
13:AM:57:ARG:NH1	30:BI:35:ASP:OD2	2.54	0.41
20:AT:9:LYS:O	20:AT:13:GLN:HG3	2.21	0.41
22:BA:2178:C:H2'	22:BA:2179:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2489:U:H2'	22:BA:2490:G:O4'	2.20	0.41
23:BB:24:G:H8	23:BB:24:G:H2'	1.78	0.41
23:BB:51:G:O2'	23:BB:52:A:H5'	2.21	0.41
33:BL:57:LEU:HD22	51:B3:54:ASP:HB3	2.03	0.41
40:BS:2:GLU:HG2	40:BS:106:VAL:HG13	2.03	0.41
56:B9:27:TYR:CD1	56:B9:70:LEU:HD12	2.56	0.41
56:B9:64:GLU:HB2	56:B9:68:ASP:CG	2.46	0.41
1:AA:76:G:C5	1:AA:77:A:N7	2.89	0.41
1:AA:1006:G:H2'	1:AA:1007:U:O4'	2.21	0.41
1:AA:1163:A:H2'	1:AA:1164:G:C8	2.55	0.41
12:AL:4:VAL:CG2	17:AQ:34:TYR:HB3	2.50	0.41
12:AL:108:LYS:HA	12:AL:108:LYS:HD2	1.89	0.41
21:AU:25:LYS:HE2	21:AU:25:LYS:HA	2.03	0.41
22:BA:2137:U:H2'	22:BA:2138:G:C8	2.56	0.41
22:BA:2662:A:H8	22:BA:2662:A:O5'	2.04	0.41
27:BF:11:GLU:HG2	27:BF:12:VAL:N	2.35	0.41
28:BG:54:PRO:HG3	28:BG:62:TRP:CE2	2.56	0.41
29:BH:114:GLU:N	29:BH:114:GLU:OE2	2.54	0.41
56:B9:302:LYS:NZ	56:B9:303:LYS:HD3	2.36	0.41
1:AA:222:C:H2'	1:AA:223:A:H8	1.86	0.40
2:AB:115:LYS:HE2	2:AB:115:LYS:HB3	1.77	0.40
9:AI:96:SER:O	9:AI:100:LYS:HG2	2.20	0.40
13:AM:83:LEU:CD2	19:AS:74:PHE:HE1	2.34	0.40
22:BA:727:A:O2'	22:BA:728:G:H5'	2.22	0.40
22:BA:1230:A:H2'	22:BA:1231:U:O4'	2.22	0.40
22:BA:1394:U:H4'	22:BA:1603:A:H4'	2.04	0.40
23:BB:45:A:C8	27:BF:92:ARG:NH2	2.89	0.40
26:BE:175:ILE:O	26:BE:175:ILE:HG13	2.20	0.40
31:BJ:49:ASP:OD2	31:BJ:121:LYS:NZ	2.53	0.40
36:BO:26:LEU:HD23	36:BO:92:PHE:HD1	1.87	0.40
36:BO:56:LYS:HA	36:BO:56:LYS:HD3	1.77	0.40
38:BQ:3:ARG:HH21	38:BQ:3:ARG:HD3	1.72	0.40
43:BV:2:PHE:HB2	43:BV:61:LEU:HD22	2.03	0.40
56:B9:51:GLU:HG2	56:B9:52:ARG:N	2.36	0.40
1:AA:377:G:H2'	1:AA:378:G:H8	1.86	0.40
1:AA:511:C:C2	1:AA:512:U:C5	3.09	0.40
1:AA:900:A:H2'	1:AA:901:A:C8	2.57	0.40
1:AA:946:A:H2'	1:AA:947:G:H8	1.86	0.40
1:AA:1122:U:H2'	1:AA:1123:U:C6	2.55	0.40
9:AI:91:ASP:C	9:AI:93:SER:H	2.29	0.40
13:AM:4:ILE:HG22	13:AM:5:ALA:N	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:721:A:H2'	22:BA:722:A:C8	2.56	0.40
22:BA:1073:A:O5'	22:BA:1073:A:C8	2.73	0.40
22:BA:1438:U:H2'	22:BA:1439:A:H8	1.86	0.40
22:BA:2137:U:H2'	22:BA:2138:G:H8	1.85	0.40
22:BA:2148:G:H2'	22:BA:2149:U:C6	2.56	0.40
26:BE:21:ARG:O	26:BE:114:ARG:NH2	2.53	0.40
56:B9:64:GLU:O	56:B9:68:ASP:HB2	2.21	0.40
1:AA:69:G:N2	1:AA:102:G:C6	2.89	0.40
1:AA:102:G:C5	1:AA:103:U:C4	3.09	0.40
1:AA:373:A:H2'	1:AA:374:A:H8	1.85	0.40
1:AA:459:A:H2'	1:AA:460:A:H8	1.83	0.40
1:AA:562:U:O2'	12:AL:13:ALA:O	2.32	0.40
1:AA:737:C:H2'	1:AA:738:C:H6	1.86	0.40
13:AM:62:LYS:HE2	13:AM:62:LYS:HA	2.03	0.40
19:AS:17:LYS:HD3	19:AS:17:LYS:HA	1.91	0.40
22:BA:276:U:O2'	22:BA:277:G:O4'	2.38	0.40
22:BA:1263:U:OP1	48:B0:13:ARG:NH1	2.55	0.40
35:BN:58:ASP:OD1	35:BN:63:ARG:NH1	2.42	0.40
1:AA:66:A:N6	1:AA:104:G:C2	2.90	0.40
1:AA:457:G:N2	1:AA:474:G:H1	2.19	0.40
1:AA:457:G:H1	1:AA:474:G:H1	1.69	0.40
1:AA:685:G:O2'	1:AA:686:U:H5'	2.21	0.40
4:AD:78:GLU:OE2	4:AD:81:ARG:NE	2.45	0.40
7:AG:131:LYS:HE2	7:AG:131:LYS:HB2	1.97	0.40
13:AM:66:GLU:CG	13:AM:67:GLY:H	2.30	0.40
17:AQ:68:SER:OG	17:AQ:69:LYS:N	2.54	0.40
22:BA:1183:U:H2'	22:BA:1184:U:C6	2.57	0.40
22:BA:2101:A:C2	22:BA:2102:G:C5	3.08	0.40
22:BA:2136:G:C6	22:BA:2156:G:C2	3.10	0.40
24:BC:75:PRO:HG2	24:BC:97:LYS:CG	2.51	0.40
30:BI:42:PRO:O	30:BI:46:GLY:HA3	2.21	0.40
33:BL:131:ALA:O	33:BL:135:ILE:HG13	2.21	0.40
41:BT:69:ARG:HH11	41:BT:69:ARG:HD3	1.77	0.40
43:BV:89:ILE:HD12	43:BV:89:ILE:HG23	1.84	0.40
1:AA:195:A:OP1	20:AT:60:ARG:NH1	2.55	0.40
1:AA:459:A:N6	1:AA:460:A:N6	2.70	0.40
1:AA:1198:G:H2'	1:AA:1199:U:C6	2.57	0.40
7:AG:148:ASN:ND2	11:AK:56:ARG:HH21	2.19	0.40
14:AN:16:ALA:HA	14:AN:55:SER:HA	2.03	0.40
21:AU:21:ARG:HD2	21:AU:24:GLU:OE2	2.22	0.40
22:BA:1079:C:C2	22:BA:1080:A:C8	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1392:A:H62	41:BT:18:GLU:HG3	1.86	0.40
22:BA:2175:C:H2'	22:BA:2176:A:C8	2.57	0.40
22:BA:2737:G:H2'	22:BA:2738:A:C8	2.57	0.40
25:BD:25:THR:OG1	25:BD:191:GLY:O	2.34	0.40
36:BO:34:HIS:ND1	36:BO:53:THR:OG1	2.49	0.40
54:B7:2:G:N3	54:B7:2:G:H2'	2.35	0.40
56:B9:244:TYR:HE1	56:B9:262:ARG:HB2	1.87	0.40
56:B9:299:GLU:O	56:B9:303:LYS:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/241 (92%)	210 (95%)	12 (5%)	0	100	100
3	AC	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
4	AD	203/206 (98%)	195 (96%)	8 (4%)	0	100	100
5	AE	153/167 (92%)	144 (94%)	9 (6%)	0	100	100
6	AF	104/135 (77%)	101 (97%)	3 (3%)	0	100	100
7	AG	149/179 (83%)	135 (91%)	14 (9%)	0	100	100
8	AH	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
9	AI	125/130 (96%)	116 (93%)	9 (7%)	0	100	100
10	AJ	97/103 (94%)	89 (92%)	6 (6%)	2 (2%)	5	11
11	AK	115/129 (89%)	110 (96%)	5 (4%)	0	100	100
12	AL	120/124 (97%)	109 (91%)	11 (9%)	0	100	100
13	AM	112/118 (95%)	98 (88%)	14 (12%)	0	100	100
14	AN	99/102 (97%)	84 (85%)	15 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	AO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	AP	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
17	AQ	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
18	AR	53/75 (71%)	51 (96%)	2 (4%)	0	100	100
19	AS	80/92 (87%)	75 (94%)	5 (6%)	0	100	100
20	AT	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	AU	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
24	BC	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
25	BD	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	24	46
26	BE	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
27	BF	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
28	BG	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
29	BH	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
30	BI	64/70 (91%)	57 (89%)	7 (11%)	0	100	100
31	BJ	140/142 (99%)	140 (100%)	0	0	100	100
32	BK	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
33	BL	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
34	BM	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
35	BN	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
36	BO	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
37	BP	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
38	BQ	115/118 (98%)	115 (100%)	0	0	100	100
39	BR	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
40	BS	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
41	BT	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
42	BU	100/104 (96%)	89 (89%)	10 (10%)	1 (1%)	12	28
43	BV	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
44	BW	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
45	BX	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
46	BY	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
47	BZ	56/59 (95%)	55 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	B0	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
49	B1	49/55 (89%)	45 (92%)	4 (8%)	0	100	100
50	B2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
51	B3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	3	5
52	B4	36/38 (95%)	36 (100%)	0	0	100	100
53	B5	15/17 (88%)	13 (87%)	2 (13%)	0	100	100
56	B9	344/365 (94%)	325 (94%)	19 (6%)	0	100	100
All	All	5934/6296 (94%)	5626 (95%)	302 (5%)	6 (0%)	49	70

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	BD	149	ASN
51	B3	32	ILE
51	B3	33	LEU
10	AJ	57	VAL
10	AJ	58	ASN
42	BU	8	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	186/199 (94%)	186 (100%)	0	100	100
3	AC	170/190 (90%)	170 (100%)	0	100	100
4	AD	172/173 (99%)	172 (100%)	0	100	100
5	AE	118/126 (94%)	118 (100%)	0	100	100
6	AF	92/116 (79%)	92 (100%)	0	100	100
7	AG	124/147 (84%)	124 (100%)	0	100	100
8	AH	104/105 (99%)	104 (100%)	0	100	100
9	AI	105/107 (98%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	AJ	87/90 (97%)	87 (100%)	0	100	100
11	AK	90/99 (91%)	90 (100%)	0	100	100
12	AL	102/103 (99%)	102 (100%)	0	100	100
13	AM	92/96 (96%)	92 (100%)	0	100	100
14	AN	79/84 (94%)	79 (100%)	0	100	100
15	AO	76/77 (99%)	76 (100%)	0	100	100
16	AP	65/65 (100%)	65 (100%)	0	100	100
17	AQ	74/78 (95%)	74 (100%)	0	100	100
18	AR	48/65 (74%)	48 (100%)	0	100	100
19	AS	71/79 (90%)	71 (100%)	0	100	100
20	AT	65/66 (98%)	65 (100%)	0	100	100
21	AU	48/61 (79%)	48 (100%)	0	100	100
24	BC	216/218 (99%)	216 (100%)	0	100	100
25	BD	163/163 (100%)	163 (100%)	0	100	100
26	BE	165/165 (100%)	165 (100%)	0	100	100
27	BF	148/150 (99%)	148 (100%)	0	100	100
28	BG	137/138 (99%)	137 (100%)	0	100	100
29	BH	114/114 (100%)	114 (100%)	0	100	100
30	BI	59/62 (95%)	59 (100%)	0	100	100
31	BJ	116/116 (100%)	115 (99%)	1 (1%)	70	87
32	BK	104/104 (100%)	104 (100%)	0	100	100
33	BL	103/103 (100%)	103 (100%)	0	100	100
34	BM	108/108 (100%)	108 (100%)	0	100	100
35	BN	98/103 (95%)	98 (100%)	0	100	100
36	BO	87/87 (100%)	87 (100%)	0	100	100
37	BP	99/100 (99%)	99 (100%)	0	100	100
38	BQ	89/90 (99%)	89 (100%)	0	100	100
39	BR	84/84 (100%)	84 (100%)	0	100	100
40	BS	93/93 (100%)	93 (100%)	0	100	100
41	BT	80/84 (95%)	80 (100%)	0	100	100
42	BU	83/85 (98%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	BV	78/78 (100%)	78 (100%)	0	100	100
44	BW	57/63 (90%)	57 (100%)	0	100	100
45	BX	67/68 (98%)	67 (100%)	0	100	100
46	BY	54/55 (98%)	54 (100%)	0	100	100
47	BZ	48/49 (98%)	48 (100%)	0	100	100
48	B0	47/48 (98%)	47 (100%)	0	100	100
49	B1	45/49 (92%)	45 (100%)	0	100	100
50	B2	38/38 (100%)	38 (100%)	0	100	100
51	B3	51/52 (98%)	51 (100%)	0	100	100
52	B4	34/34 (100%)	34 (100%)	0	100	100
53	B5	17/17 (100%)	16 (94%)	1 (6%)	18	38
56	B9	298/311 (96%)	298 (100%)	0	100	100
All	All	4948/5155 (96%)	4946 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	BJ	128	ASN
53	B5	24	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	94	HIS
2	AB	168	HIS
4	AD	41	HIS
4	AD	152	GLN
4	AD	198	HIS
5	AE	61	GLN
5	AE	132	ASN
6	AF	55	HIS
7	AG	130	ASN
11	AK	15	GLN
11	AK	118	HIS
11	AK	119	ASN
16	AP	26	ASN
19	AS	57	HIS

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Mol	Chain	Res	Type
20	AT	3	ASN
20	AT	13	GLN
24	BC	25	HIS
24	BC	134	ASN
25	BD	126	ASN
26	BE	97	ASN
27	BF	52	ASN
29	BH	66	ASN
29	BH	128	HIS
32	BK	3	GLN
33	BL	93	ASN
36	BO	98	GLN
38	BQ	20	GLN
41	BT	48	GLN
43	BV	5	ASN
45	BX	23	ASN
45	BX	36	HIS
48	B0	19	HIS
50	B2	26	ASN
56	B9	214	HIS
56	B9	281	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1533/1534 (99%)	242 (15%)	8 (0%)
22	BA	2895/2897 (99%)	445 (15%)	24 (0%)
23	BB	119/120 (99%)	15 (12%)	1 (0%)
54	B7	9/10 (90%)	2 (22%)	0
55	B8	76/77 (98%)	12 (15%)	2 (2%)
All	All	4632/4638 (99%)	716 (15%)	35 (0%)

All (716) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	A
1	AA	4	U
1	AA	7	A
1	AA	9	G
1	AA	19	A
1	AA	22	G

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Mol	Chain	Res	Type
1	AA	32	A
1	AA	39	G
1	AA	44	A
1	AA	47	C
1	AA	48	C
1	AA	51	A
1	AA	58	C
1	AA	59	A
1	AA	68	G
1	AA	69	G
1	AA	70	U
1	AA	71	A
1	AA	76	G
1	AA	78	A
1	AA	81	A
1	AA	82	G
1	AA	83	C
1	AA	84	U
1	AA	85	U
1	AA	86	G
1	AA	88	U
1	AA	90	C
1	AA	92	U
1	AA	99	C
1	AA	100	G
1	AA	101	A
1	AA	102	G
1	AA	116	A
1	AA	119	A
1	AA	120	A
1	AA	121	U
1	AA	122	G
1	AA	130	A
1	AA	131	A
1	AA	141	G
1	AA	144	G
1	AA	151	A
1	AA	161	A
1	AA	163	C
1	AA	164	G
1	AA	181	A
1	AA	182	A

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Mol	Chain	Res	Type
1	AA	189	A
1	AA	197	A
1	AA	204	G
1	AA	210	C
1	AA	245	U
1	AA	247	G
1	AA	251	G
1	AA	266	G
1	AA	267	C
1	AA	289	G
1	AA	299	G
1	AA	306	A
1	AA	321	A
1	AA	327	A
1	AA	328	C
1	AA	344	A
1	AA	352	C
1	AA	353	A
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	382	A
1	AA	397	A
1	AA	406	G
1	AA	412	A
1	AA	413	G
1	AA	429	U
1	AA	437	U
1	AA	439	U
1	AA	463	U
1	AA	465	A
1	AA	468	A
1	AA	474	G
1	AA	478	A
1	AA	479	U
1	AA	481	G
1	AA	482	A
1	AA	484	G
1	AA	486	U
1	AA	495	A
1	AA	496	A

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Mol	Chain	Res	Type
1	AA	499	A
1	AA	509	A
1	AA	510	A
1	AA	511	C
1	AA	518	C
1	AA	521	G
1	AA	527	G7M
1	AA	529	G
1	AA	532	A
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	560	A
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	600	A
1	AA	633	G
1	AA	653	U
1	AA	665	A
1	AA	702	A
1	AA	703	G
1	AA	718	A
1	AA	721	G
1	AA	722	G
1	AA	723	U
1	AA	724	G
1	AA	734	G
1	AA	755	G
1	AA	758	C
1	AA	760	G
1	AA	777	A
1	AA	790	A
1	AA	792	A
1	AA	793	U
1	AA	794	A
1	AA	814	A
1	AA	815	A

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Mol	Chain	Res	Type
1	AA	817	C
1	AA	828	U
1	AA	829	G
1	AA	832	G
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	864	A
1	AA	889	A
1	AA	900	A
1	AA	902	G
1	AA	914	A
1	AA	934	C
1	AA	935	A
1	AA	942	G
1	AA	958	A
1	AA	960	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	983	A
1	AA	992	U
1	AA	993	G
1	AA	1004	A
1	AA	1008	U
1	AA	1019	A
1	AA	1020	G
1	AA	1021	A
1	AA	1022	A
1	AA	1026	G
1	AA	1028	C
1	AA	1029	U
1	AA	1030	U
1	AA	1032	G
1	AA	1033	G
1	AA	1036	A
1	AA	1042	A
1	AA	1045	C
1	AA	1046	A

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Mol	Chain	Res	Type
1	AA	1065	U
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1132	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1146	A
1	AA	1151	A
1	AA	1154	G
1	AA	1157	A
1	AA	1159	U
1	AA	1169	A
1	AA	1173	U
1	AA	1184	G
1	AA	1191	A
1	AA	1196	A
1	AA	1197	A
1	AA	1201	A
1	AA	1212	U
1	AA	1213	A
1	AA	1225	A
1	AA	1226	C
1	AA	1227	A
1	AA	1238	A
1	AA	1248	A
1	AA	1256	A
1	AA	1257	A
1	AA	1260	G
1	AA	1280	A
1	AA	1285	A
1	AA	1287	A
1	AA	1288	A
1	AA	1299	A
1	AA	1300	G
1	AA	1302	C
1	AA	1305	G
1	AA	1317	C
1	AA	1318	A
1	AA	1319	A
1	AA	1320	C

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Mol	Chain	Res	Type
1	AA	1335	U
1	AA	1336	C
1	AA	1340	A
1	AA	1346	A
1	AA	1363	A
1	AA	1370	G
1	AA	1398	A
1	AA	1419	G
1	AA	1429	A
1	AA	1432	G
1	AA	1441	A
1	AA	1446	A
1	AA	1487	G
1	AA	1492	A
1	AA	1493	A
1	AA	1494	G
1	AA	1497	G
1	AA	1499	A
1	AA	1502	A
1	AA	1503	A
1	AA	1506	U
1	AA	1517	G
1	AA	1519	MA6
1	AA	1529	G
1	AA	1530	G
1	AA	1534	A
22	BA	10	A
22	BA	12	U
22	BA	15	G
22	BA	51	G
22	BA	61	C
22	BA	71	A
22	BA	74	A
22	BA	75	G
22	BA	84	A
22	BA	101	A
22	BA	103	A
22	BA	118	A
22	BA	119	A
22	BA	120	U
22	BA	125	A
22	BA	143	C

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Mol	Chain	Res	Type
22	BA	163	C
22	BA	165	A
22	BA	167	A
22	BA	181	A
22	BA	193	U
22	BA	196	A
22	BA	197	A
22	BA	199	A
22	BA	200	U
22	BA	204	A
22	BA	215	G
22	BA	216	A
22	BA	221	A
22	BA	222	A
22	BA	224	U
22	BA	233	A
22	BA	241	A
22	BA	248	G
22	BA	264	C
22	BA	265	A
22	BA	272	A
22	BA	274	C
22	BA	275	C
22	BA	276	U
22	BA	277	G
22	BA	302	C
22	BA	303	G
22	BA	311	A
22	BA	322	A
22	BA	330	A
22	BA	345	A
22	BA	360	U
22	BA	361	G
22	BA	385	C
22	BA	386	G
22	BA	396	G
22	BA	404	A
22	BA	406	G
22	BA	407	G
22	BA	411	G
22	BA	412	A
22	BA	417	C

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Mol	Chain	Res	Type
22	BA	425	G
22	BA	428	A
22	BA	435	C
22	BA	480	A
22	BA	481	G
22	BA	489	G
22	BA	491	G
22	BA	503	A
22	BA	505	A
22	BA	509	C
22	BA	510	C
22	BA	530	G
22	BA	532	A
22	BA	546	U
22	BA	547	A
22	BA	549	G
22	BA	550	C
22	BA	557	C
22	BA	563	A
22	BA	568	U
22	BA	573	U
22	BA	575	A
22	BA	588	U
22	BA	592	A
22	BA	603	A
22	BA	614	A
22	BA	615	U
22	BA	616	A
22	BA	637	A
22	BA	644	A
22	BA	645	C
22	BA	646	U
22	BA	647	G
22	BA	653	U
22	BA	654	A
22	BA	655	A
22	BA	668	A
22	BA	685	A
22	BA	686	U
22	BA	688	U
22	BA	696	G
22	BA	711	G

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Mol	Chain	Res	Type
22	BA	717	C
22	BA	730	A
22	BA	738	G
22	BA	747	5MU
22	BA	762	U
22	BA	764	A
22	BA	765	C
22	BA	775	G
22	BA	776	G
22	BA	782	A
22	BA	784	G
22	BA	785	G
22	BA	789	A
22	BA	790	U
22	BA	791	C
22	BA	792	A
22	BA	802	A
22	BA	805	G
22	BA	806	C
22	BA	812	C
22	BA	827	U
22	BA	828	U
22	BA	846	U
22	BA	847	U
22	BA	859	G
22	BA	866	A
22	BA	883	G
22	BA	884	U
22	BA	885	C
22	BA	896	A
22	BA	905	A
22	BA	910	A
22	BA	914	G
22	BA	945	A
22	BA	946	C
22	BA	961	C
22	BA	973	A
22	BA	974	G
22	BA	983	A
22	BA	984	A
22	BA	985	C
22	BA	996	A

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Mol	Chain	Res	Type
22	BA	1005	C
22	BA	1012	U
22	BA	1013	C
22	BA	1025	G
22	BA	1026	G
22	BA	1033	U
22	BA	1046	A
22	BA	1047	G
22	BA	1054	A
22	BA	1057	A
22	BA	1061	U
22	BA	1067	A
22	BA	1068	G
22	BA	1069	A
22	BA	1070	A
22	BA	1071	G
22	BA	1073	A
22	BA	1075	C
22	BA	1076	C
22	BA	1077	A
22	BA	1083	U
22	BA	1084	A
22	BA	1085	A
22	BA	1088	A
22	BA	1097	U
22	BA	1101	U
22	BA	1110	G
22	BA	1111	A
22	BA	1112	G
22	BA	1126	A
22	BA	1128	G
22	BA	1130	U
22	BA	1132	U
22	BA	1133	A
22	BA	1134	A
22	BA	1135	C
22	BA	1142	A
22	BA	1156	A
22	BA	1173	U
22	BA	1174	U
22	BA	1175	A
22	BA	1176	U

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Mol	Chain	Res	Type
22	BA	1187	G
22	BA	1189	A
22	BA	1204	A
22	BA	1205	A
22	BA	1206	G
22	BA	1212	G
22	BA	1247	A
22	BA	1250	G
22	BA	1253	A
22	BA	1256	G
22	BA	1268	A
22	BA	1271	G
22	BA	1272	A
22	BA	1273	U
22	BA	1274	A
22	BA	1275	A
22	BA	1287	A
22	BA	1300	G
22	BA	1301	A
22	BA	1313	U
22	BA	1321	A
22	BA	1329	U
22	BA	1352	U
22	BA	1365	A
22	BA	1379	U
22	BA	1383	A
22	BA	1392	A
22	BA	1393	A
22	BA	1395	A
22	BA	1416	G
22	BA	1428	C
22	BA	1429	G
22	BA	1452	G
22	BA	1453	A
22	BA	1458	U
22	BA	1460	U
22	BA	1478	G
22	BA	1482	G
22	BA	1494	A
22	BA	1508	A
22	BA	1515	A
22	BA	1524	G

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Mol	Chain	Res	Type
22	BA	1535	A
22	BA	1537	G
22	BA	1554	U
22	BA	1566	A
22	BA	1569	A
22	BA	1578	U
22	BA	1606	C
22	BA	1608	A
22	BA	1609	A
22	BA	1610	A
22	BA	1630	A
22	BA	1634	A
22	BA	1647	U
22	BA	1648	U
22	BA	1649	G
22	BA	1664	A
22	BA	1674	G
22	BA	1675	C
22	BA	1677	A
22	BA	1729	U
22	BA	1730	C
22	BA	1732	C
22	BA	1733	G
22	BA	1744	A
22	BA	1754	A
22	BA	1757	A
22	BA	1758	U
22	BA	1759	A
22	BA	1764	C
22	BA	1773	A
22	BA	1782	U
22	BA	1786	A
22	BA	1800	C
22	BA	1801	A
22	BA	1802	A
22	BA	1808	A
22	BA	1809	A
22	BA	1811	G
22	BA	1816	C
22	BA	1829	A
22	BA	1848	A
22	BA	1862	G

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Mol	Chain	Res	Type
22	BA	1870	C
22	BA	1871	A
22	BA	1872	A
22	BA	1900	A
22	BA	1901	A
22	BA	1905	C
22	BA	1906	G
22	BA	1913	A
22	BA	1914	C
22	BA	1915	3TD
22	BA	1929	G
22	BA	1930	G
22	BA	1936	A
22	BA	1937	A
22	BA	1938	A
22	BA	1955	U
22	BA	1960	A
22	BA	1966	A
22	BA	1967	C
22	BA	1970	A
22	BA	1971	U
22	BA	1972	G
22	BA	1991	U
22	BA	1993	U
22	BA	1996	C
22	BA	2006	C
22	BA	2023	C
22	BA	2030	6MZ
22	BA	2031	A
22	BA	2032	G
22	BA	2033	A
22	BA	2036	C
22	BA	2043	C
22	BA	2052	A
22	BA	2055	C
22	BA	2056	G
22	BA	2060	A
22	BA	2061	G
22	BA	2062	A
22	BA	2069	G7M
22	BA	2077	A
22	BA	2080	A

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Mol	Chain	Res	Type
22	BA	2093	G
22	BA	2097	A
22	BA	2100	G
22	BA	2101	A
22	BA	2110	G
22	BA	2111	U
22	BA	2112	G
22	BA	2113	U
22	BA	2114	A
22	BA	2115	G
22	BA	2117	A
22	BA	2118	U
22	BA	2119	A
22	BA	2121	G
22	BA	2125	G
22	BA	2126	A
22	BA	2128	G
22	BA	2131	U
22	BA	2132	U
22	BA	2133	G
22	BA	2136	G
22	BA	2137	U
22	BA	2142	A
22	BA	2145	C
22	BA	2147	A
22	BA	2154	A
22	BA	2157	G
22	BA	2158	A
22	BA	2159	G
22	BA	2161	C
22	BA	2162	G
22	BA	2164	C
22	BA	2168	G
22	BA	2169	A
22	BA	2170	A
22	BA	2171	A
22	BA	2172	U
22	BA	2173	A
22	BA	2183	A
22	BA	2184	A
22	BA	2186	G
22	BA	2188	U

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Mol	Chain	Res	Type
22	BA	2189	U
22	BA	2191	A
22	BA	2198	A
22	BA	2203	U
22	BA	2204	G
22	BA	2211	A
22	BA	2225	A
22	BA	2238	G
22	BA	2239	G
22	BA	2259	U
22	BA	2261	C
22	BA	2267	A
22	BA	2269	G
22	BA	2278	A
22	BA	2283	C
22	BA	2287	A
22	BA	2288	A
22	BA	2298	A
22	BA	2303	G
22	BA	2305	U
22	BA	2308	G
22	BA	2322	A
22	BA	2325	G
22	BA	2327	A
22	BA	2333	A
22	BA	2336	A
22	BA	2340	A
22	BA	2347	C
22	BA	2350	C
22	BA	2383	G
22	BA	2385	C
22	BA	2396	G
22	BA	2402	U
22	BA	2406	A
22	BA	2425	A
22	BA	2429	G
22	BA	2435	A
22	BA	2440	C
22	BA	2441	U
22	BA	2448	A
22	BA	2459	A
22	BA	2469	A

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Mol	Chain	Res	Type
22	BA	2475	C
22	BA	2476	A
22	BA	2491	U
22	BA	2502	G
22	BA	2505	G
22	BA	2507	C
22	BA	2518	A
22	BA	2519	U
22	BA	2529	G
22	BA	2534	A
22	BA	2547	A
22	BA	2566	A
22	BA	2567	G
22	BA	2572	A
22	BA	2573	C
22	BA	2577	A
22	BA	2582	G
22	BA	2602	A
22	BA	2609	U
22	BA	2613	U
22	BA	2615	U
22	BA	2629	U
22	BA	2630	G
22	BA	2654	A
22	BA	2663	G
22	BA	2689	U
22	BA	2690	U
22	BA	2705	A
22	BA	2713	U
22	BA	2714	G
22	BA	2718	G
22	BA	2724	U
22	BA	2726	A
22	BA	2733	A
22	BA	2744	G
22	BA	2748	A
22	BA	2751	G
22	BA	2778	A
22	BA	2799	A
22	BA	2820	A
22	BA	2821	A
22	BA	2849	U

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Mol	Chain	Res	Type
22	BA	2850	A
22	BA	2861	U
22	BA	2873	A
22	BA	2874	C
22	BA	2880	C
22	BA	2883	A
22	BA	2884	U
22	BA	2891	U
22	BA	2893	A
23	BB	13	G
23	BB	24	G
23	BB	26	C
23	BB	30	C
23	BB	35	C
23	BB	42	C
23	BB	44	G
23	BB	56	G
23	BB	57	A
23	BB	66	A
23	BB	68	C
23	BB	89	U
23	BB	90	C
23	BB	105	G
23	BB	109	A
54	B7	4	C
54	B7	10	U
55	B8	3	G
55	B8	4	U
55	B8	5	G
55	B8	6	A
55	B8	14	A
55	B8	17	C
55	B8	19	G
55	B8	21	A
55	B8	22	G
55	B8	74	C
55	B8	75	C
55	B8	76	A

All (35) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	AA	69	G
1	AA	99	C
1	AA	100	G
1	AA	119	A
1	AA	428	G
1	AA	1225	A
1	AA	1299	A
1	AA	1493	A
22	BA	125	A
22	BA	196	A
22	BA	199	A
22	BA	276	U
22	BA	685	A
22	BA	764	A
22	BA	784	G
22	BA	984	A
22	BA	1067	A
22	BA	1175	A
22	BA	1247	A
22	BA	1253	A
22	BA	1392	A
22	BA	1608	A
22	BA	1847	A
22	BA	1900	A
22	BA	1913	A
22	BA	2158	A
22	BA	2183	A
22	BA	2211	A
22	BA	2474	U
22	BA	2518	A
22	BA	2820	A
22	BA	2873	A
23	BB	66	A
55	B8	2	G
55	B8	3	G

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

37 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$
1	5MC	AA	1407	1	18,22,23	3.14	7 (38%)	26,32,35	1.22	2 (7%)
22	G7M	BA	2069	58,22	23,26,27	2.58	6 (26%)	35,39,42	2.35	12 (34%)
22	1MG	BA	745	22	22,26,27	2.53	8 (36%)	33,39,42	1.79	8 (24%)
25	MEQ	BD	150	25	8,9,10	1.43	2 (25%)	5,10,12	1.50	1 (20%)
22	5MC	BA	1962	58,22	18,22,23	2.90	7 (38%)	26,32,35	1.10	2 (7%)
1	MA6	AA	1519	1	23,26,27	1.90	5 (21%)	34,38,41	3.48	11 (32%)
22	3TD	BA	1915	22	18,22,23	4.04	7 (38%)	22,32,35	1.75	3 (13%)
34	4D4	BM	81	34	9,11,12	2.44	4 (44%)	8,13,15	1.26	1 (12%)
1	MA6	AA	1518	1	23,26,27	1.96	7 (30%)	34,38,41	3.24	11 (32%)
1	2MG	AA	1516	1	23,26,27	2.58	7 (30%)	32,38,41	2.34	11 (34%)
22	2MA	BA	2503	57,22,58	22,25,26	3.41	9 (40%)	33,37,40	2.18	9 (27%)
1	G7M	AA	527	1,58	23,26,27	2.64	8 (34%)	35,39,42	2.28	9 (25%)
22	PSU	BA	955	22	18,21,22	3.56	6 (33%)	22,30,33	2.31	5 (22%)
22	6MZ	BA	1618	22	22,25,26	3.86	6 (27%)	30,36,39	2.70	11 (36%)
1	UR3	AA	1498	1	19,22,23	2.91	8 (42%)	26,32,35	1.43	2 (7%)
1	5MC	AA	967	1	18,22,23	3.36	7 (38%)	26,32,35	1.12	1 (3%)
22	OMU	BA	2552	57,22	19,22,23	2.56	7 (36%)	26,31,34	2.05	6 (23%)
22	5MU	BA	1939	58,22	19,22,23	1.05	3 (15%)	28,32,35	1.32	4 (14%)
22	2MG	BA	1835	22	23,26,27	2.48	7 (30%)	32,38,41	2.25	11 (34%)
22	PSU	BA	1917	22	18,21,22	3.88	6 (33%)	22,30,33	1.96	5 (22%)
22	PSU	BA	2580	22	18,21,22	3.58	7 (38%)	22,30,33	1.97	4 (18%)
22	PSU	BA	2605	22	18,21,22	3.54	8 (44%)	22,30,33	2.06	4 (18%)
12	D2T	AL	89	12	7,9,10	1.02	0	6,11,13	2.65	3 (50%)
22	PSU	BA	2604	22	18,21,22	3.40	6 (33%)	22,30,33	2.74	6 (27%)
1	PSU	AA	516	1,57	18,21,22	4.01	7 (38%)	22,30,33	1.98	6 (27%)
1	2MG	AA	1207	1,58	23,26,27	2.74	9 (39%)	32,38,41	2.21	10 (31%)
22	OMC	BA	2498	57,22	19,22,23	2.45	7 (36%)	26,31,34	0.97	2 (7%)
22	PSU	BA	746	57,22	18,21,22	3.95	8 (44%)	22,30,33	1.73	6 (27%)
22	PSU	BA	2457	57,22	18,21,22	3.44	7 (38%)	22,30,33	2.45	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PSU	BA	1911	22	18,21,22	3.98	7 (38%)	22,30,33	2.22	5 (22%)
1	4OC	AA	1402	1,57	20,23,24	2.76	8 (40%)	26,32,35	0.96	2 (7%)
22	5MU	BA	747	22	19,22,23	0.76	0	28,32,35	1.13	2 (7%)
22	6MZ	BA	2030	22	22,25,26	3.92	6 (27%)	30,36,39	2.71	10 (33%)
22	OMG	BA	2251	58,22,55	23,26,27	2.26	7 (30%)	33,38,41	1.89	12 (36%)
22	2MG	BA	2445	22	23,26,27	2.46	9 (39%)	32,38,41	2.57	12 (37%)
22	PSU	BA	2504	58,22	18,21,22	3.52	6 (33%)	22,30,33	1.74	4 (18%)
1	2MG	AA	966	1	23,26,27	2.73	7 (30%)	32,38,41	2.14	12 (37%)

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
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
22	G7M	BA	2069	58,22	-	2/7/25/26	0/3/3/3
22	1MG	BA	745	22	-	0/7/25/26	0/3/3/3
25	MEQ	BD	150	25	-	4/8/9/11	-
22	5MC	BA	1962	58,22	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	2/11/29/30	0/3/3/3
22	3TD	BA	1915	22	-	2/7/25/26	0/2/2/2
34	4D4	BM	81	34	-	2/11/12/14	-
1	MA6	AA	1518	1	-	0/11/29/30	0/3/3/3
1	2MG	AA	1516	1	-	0/9/27/28	0/3/3/3
22	2MA	BA	2503	57,22,58	-	2/7/25/26	0/3/3/3
1	G7M	AA	527	1,58	-	2/7/25/26	0/3/3/3
22	PSU	BA	955	22	-	0/7/25/26	0/2/2/2
22	6MZ	BA	1618	22	-	0/9/27/28	0/3/3/3
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
22	OMU	BA	2552	57,22	-	0/9/27/28	0/2/2/2
22	5MU	BA	1939	58,22	-	0/7/25/26	0/2/2/2
22	2MG	BA	1835	22	-	0/9/27/28	0/3/3/3
22	PSU	BA	1917	22	-	1/7/25/26	0/2/2/2
22	PSU	BA	2580	22	-	2/7/25/26	0/2/2/2
22	PSU	BA	2605	22	-	0/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	1/7/12/14	-
22	PSU	BA	2604	22	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	AA	516	1,57	-	1/7/25/26	0/2/2/2
1	2MG	AA	1207	1,58	-	0/9/27/28	0/3/3/3
22	OMC	BA	2498	57,22	-	0/9/27/28	0/2/2/2
22	PSU	BA	746	57,22	-	3/7/25/26	0/2/2/2
22	PSU	BA	2457	57,22	-	0/7/25/26	0/2/2/2
22	PSU	BA	1911	22	-	0/7/25/26	0/2/2/2
1	4OC	AA	1402	1,57	-	2/9/29/30	0/2/2/2
22	5MU	BA	747	22	-	3/7/25/26	0/2/2/2
22	6MZ	BA	2030	22	-	2/9/27/28	0/3/3/3
22	OMG	BA	2251	58,22,55	-	2/9/27/28	0/3/3/3
22	2MG	BA	2445	22	-	2/9/27/28	0/3/3/3
22	PSU	BA	2504	58,22	-	2/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	0/9/27/28	0/3/3/3

All (236) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2030	6MZ	C6-N6	16.40	1.52	1.34
22	BA	1618	6MZ	C6-N6	16.34	1.51	1.34
22	BA	1915	3TD	C6-C5	11.61	1.48	1.35
22	BA	1911	PSU	C6-C5	10.71	1.47	1.35
22	BA	1917	PSU	C6-C5	10.44	1.47	1.35
1	AA	516	PSU	C6-C5	10.41	1.47	1.35
22	BA	746	PSU	C6-C5	10.24	1.47	1.35
22	BA	2503	2MA	C4-N3	10.16	1.47	1.34
22	BA	2580	PSU	C6-C5	9.81	1.46	1.35
22	BA	2605	PSU	C6-C5	9.54	1.46	1.35
22	BA	2504	PSU	C6-C5	9.53	1.46	1.35
22	BA	1911	PSU	C2-N1	9.26	1.49	1.36
22	BA	955	PSU	C6-C5	9.18	1.46	1.35
22	BA	2457	PSU	C6-C5	9.15	1.46	1.35
1	AA	516	PSU	C2-N1	9.15	1.49	1.36
22	BA	2604	PSU	C6-C5	8.94	1.45	1.35
22	BA	746	PSU	C2-N1	8.88	1.48	1.36
22	BA	1917	PSU	C2-N1	8.61	1.48	1.36
1	AA	967	5MC	C6-C5	8.44	1.48	1.34
22	BA	1915	3TD	C2-N1	8.41	1.48	1.37
1	AA	1407	5MC	C6-C5	8.40	1.48	1.34
22	BA	955	PSU	C2-N1	7.86	1.47	1.36
1	AA	1498	UR3	C2-N1	7.79	1.49	1.38
22	BA	2580	PSU	C2-N1	7.78	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2504	PSU	C2-N1	7.72	1.47	1.36
22	BA	2457	PSU	C2-N1	7.69	1.47	1.36
22	BA	2604	PSU	C2-N1	7.50	1.46	1.36
22	BA	2605	PSU	C2-N1	7.40	1.46	1.36
22	BA	2069	G7M	C5-N7	-7.29	1.30	1.39
22	BA	1962	5MC	C6-C5	7.21	1.46	1.34
1	AA	1207	2MG	C2-N3	7.16	1.45	1.31
1	AA	966	2MG	C2-N3	6.93	1.45	1.31
1	AA	516	PSU	C2-N3	6.81	1.49	1.37
22	BA	746	PSU	C2-N3	6.45	1.48	1.37
22	BA	1917	PSU	C2-N3	6.39	1.48	1.37
1	AA	1516	2MG	C2-N3	6.24	1.43	1.31
1	AA	527	G7M	C5-N7	-6.22	1.32	1.39
1	AA	967	5MC	C4-N3	6.19	1.44	1.34
22	BA	1911	PSU	C2-N3	6.16	1.48	1.37
1	AA	527	G7M	C4-N3	6.14	1.48	1.34
1	AA	1207	2MG	C4-N3	6.12	1.48	1.34
22	BA	745	1MG	C4-N3	6.10	1.48	1.34
22	BA	2605	PSU	C2-N3	6.02	1.47	1.37
22	BA	1835	2MG	C2-N3	5.97	1.43	1.31
22	BA	2604	PSU	C2-N3	5.96	1.47	1.37
1	AA	1402	4OC	C6-C5	5.88	1.48	1.35
22	BA	955	PSU	C2-N3	5.87	1.47	1.37
1	AA	966	2MG	C4-N3	5.86	1.48	1.34
22	BA	745	1MG	C2-N3	5.82	1.44	1.34
1	AA	1402	4OC	C4-N3	5.76	1.42	1.32
1	AA	967	5MC	C2-N3	5.75	1.48	1.36
22	BA	2504	PSU	C2-N3	5.65	1.47	1.37
22	BA	2069	G7M	C4-N3	5.64	1.47	1.34
22	BA	2457	PSU	C2-N3	5.58	1.47	1.37
22	BA	2503	2MA	C2-N3	5.52	1.43	1.34
22	BA	2251	OMG	C4-N3	5.52	1.47	1.34
22	BA	2503	2MA	C2-N1	5.51	1.43	1.34
22	BA	2552	OMU	C2-N1	5.48	1.47	1.38
22	BA	2552	OMU	C2-N3	5.40	1.47	1.38
22	BA	1835	2MG	C4-N3	5.35	1.47	1.34
34	BM	81	4D4	CZ-NE	5.33	1.43	1.33
1	AA	527	G7M	C2-N3	5.31	1.46	1.33
22	BA	2445	2MG	C2-N3	5.31	1.42	1.31
1	AA	966	2MG	C2-N2	5.30	1.45	1.33
22	BA	2503	2MA	C6-N1	5.29	1.42	1.35
22	BA	1962	5MC	C4-N3	5.28	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1402	4OC	C2-N3	5.26	1.47	1.36
1	AA	1516	2MG	C4-N3	5.26	1.46	1.34
1	AA	1498	UR3	C6-C5	5.24	1.47	1.35
1	AA	1407	5MC	C4-N3	5.18	1.42	1.34
22	BA	1962	5MC	C2-N3	5.14	1.46	1.36
22	BA	2580	PSU	C2-N3	5.10	1.46	1.37
1	AA	1207	2MG	C2-N2	5.10	1.44	1.33
1	AA	1518	MA6	C6-N6	5.09	1.51	1.36
1	AA	1407	5MC	C2-N3	5.09	1.46	1.36
22	BA	1915	3TD	C1'-C5	-5.08	1.38	1.50
1	AA	1519	MA6	C6-N6	5.02	1.51	1.36
22	BA	2552	OMU	C6-C5	4.94	1.46	1.35
22	BA	2498	OMC	C2-N3	4.90	1.46	1.36
22	BA	2445	2MG	C4-N3	4.87	1.45	1.34
22	BA	2498	OMC	C6-C5	4.83	1.46	1.35
22	BA	1915	3TD	C6-N1	4.78	1.44	1.36
1	AA	966	2MG	C2-N1	4.63	1.44	1.36
1	AA	516	PSU	C6-N1	4.59	1.43	1.36
22	BA	2069	G7M	C2-N3	4.51	1.44	1.33
1	AA	1498	UR3	O4-C4	-4.50	1.13	1.23
1	AA	1516	2MG	C2-N2	4.45	1.43	1.33
1	AA	1207	2MG	C2-N1	4.40	1.43	1.36
22	BA	1917	PSU	C6-N1	4.39	1.43	1.36
1	AA	967	5MC	C4-N4	4.35	1.45	1.34
22	BA	1911	PSU	C6-N1	4.34	1.43	1.36
22	BA	746	PSU	C6-N1	4.27	1.43	1.36
1	AA	1498	UR3	C2-N3	4.24	1.47	1.39
22	BA	1915	3TD	C2-N3	4.22	1.48	1.38
22	BA	2445	2MG	C5-N7	-4.21	1.30	1.39
22	BA	1835	2MG	C2-N2	4.14	1.42	1.33
1	AA	1407	5MC	C4-N4	4.05	1.44	1.34
22	BA	2503	2MA	C6-N6	-3.99	1.24	1.34
1	AA	967	5MC	C6-N1	3.98	1.44	1.38
1	AA	1516	2MG	C2-N1	3.97	1.43	1.36
22	BA	2030	6MZ	C8-N9	-3.97	1.30	1.37
22	BA	745	1MG	C2-N2	3.96	1.41	1.34
22	BA	2445	2MG	C2-N2	3.95	1.42	1.33
22	BA	2251	OMG	C5-N7	-3.92	1.31	1.39
22	BA	1962	5MC	C4-N4	3.92	1.44	1.34
1	AA	1519	MA6	C5-C4	-3.92	1.31	1.39
22	BA	2498	OMC	C4-N4	3.87	1.43	1.33
1	AA	1516	2MG	C5-N7	-3.86	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	745	1MG	C5-N7	-3.85	1.31	1.39
1	AA	1518	MA6	C5-C4	-3.83	1.31	1.39
22	BA	2251	OMG	C2-N2	3.83	1.43	1.34
22	BA	1835	2MG	C5-N7	-3.82	1.31	1.39
22	BA	2503	2MA	C5-C6	3.82	1.51	1.41
1	AA	527	G7M	C2-N2	3.81	1.43	1.34
22	BA	955	PSU	C6-N1	3.81	1.42	1.36
1	AA	967	5MC	C2-N1	3.76	1.48	1.40
22	BA	2445	2MG	O6-C6	-3.76	1.16	1.23
22	BA	2498	OMC	O2-C2	-3.75	1.16	1.23
22	BA	2030	6MZ	C5-N7	-3.74	1.32	1.39
22	BA	2251	OMG	C2-N3	3.73	1.42	1.33
22	BA	2069	G7M	C4-N9	-3.71	1.28	1.38
22	BA	2580	PSU	C6-N1	3.71	1.42	1.36
22	BA	1835	2MG	O6-C6	-3.70	1.16	1.23
22	BA	2552	OMU	O4-C4	-3.69	1.17	1.24
1	AA	1407	5MC	O2-C2	-3.69	1.16	1.23
22	BA	2504	PSU	C6-N1	3.68	1.42	1.36
22	BA	2605	PSU	C6-N1	3.68	1.42	1.36
22	BA	2030	6MZ	C5-C4	-3.68	1.32	1.39
1	AA	1402	4OC	C4-N4	3.65	1.43	1.35
1	AA	527	G7M	C5-C6	3.64	1.53	1.43
22	BA	2498	OMC	C4-N3	3.62	1.41	1.34
1	AA	1518	MA6	C5-N7	-3.61	1.32	1.39
22	BA	2251	OMG	O6-C6	-3.57	1.16	1.23
22	BA	2498	OMC	C2-N1	3.56	1.47	1.40
22	BA	1618	6MZ	C5-C4	-3.54	1.32	1.39
1	AA	1407	5MC	C6-N1	3.52	1.44	1.38
1	AA	1402	4OC	C2-N1	3.47	1.47	1.40
1	AA	966	2MG	C5-N7	-3.47	1.32	1.39
22	BA	1618	6MZ	C8-N9	-3.44	1.31	1.37
22	BA	746	PSU	O4-C4	-3.43	1.17	1.23
22	BA	2552	OMU	O2-C2	-3.39	1.16	1.23
22	BA	2445	2MG	C4-N9	-3.36	1.29	1.38
22	BA	1962	5MC	O2-C2	-3.35	1.17	1.23
22	BA	2069	G7M	C2-N2	3.34	1.42	1.34
1	AA	1518	MA6	C8-N9	-3.34	1.31	1.37
1	AA	1402	4OC	C5-C4	3.31	1.47	1.40
1	AA	1207	2MG	C5-N7	-3.31	1.32	1.39
22	BA	1618	6MZ	C5-N7	-3.31	1.32	1.39
22	BA	2503	2MA	C5-N7	-3.28	1.32	1.39
1	AA	516	PSU	C4-N3	3.27	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1519	MA6	C5-N7	-3.26	1.32	1.39
1	AA	1519	MA6	C8-N9	-3.24	1.31	1.37
34	BM	81	4D4	CZ-NH2	3.19	1.45	1.32
1	AA	1498	UR3	O2-C2	-3.19	1.16	1.22
1	AA	1516	2MG	O6-C6	-3.19	1.17	1.23
22	BA	2604	PSU	C6-N1	3.17	1.41	1.36
22	BA	745	1MG	O6-C6	-3.17	1.16	1.23
22	BA	955	PSU	O4-C4	-3.15	1.17	1.23
1	AA	1516	2MG	C4-N9	-3.15	1.29	1.38
22	BA	1835	2MG	C2-N1	3.14	1.41	1.36
22	BA	2251	OMG	C4-N9	-3.12	1.29	1.38
22	BA	746	PSU	C4-N3	3.11	1.44	1.38
22	BA	2580	PSU	O4-C4	-3.10	1.17	1.23
1	AA	1402	4OC	O2-C2	-3.09	1.18	1.23
1	AA	967	5MC	O2-C2	-3.04	1.18	1.23
22	BA	2457	PSU	C6-N1	3.01	1.41	1.36
1	AA	1407	5MC	C2-N1	3.00	1.46	1.40
22	BA	1835	2MG	C4-N9	-2.99	1.30	1.38
22	BA	2580	PSU	O4'-C1'	-2.98	1.39	1.43
22	BA	2604	PSU	O4-C4	-2.93	1.18	1.23
22	BA	1917	PSU	C4-N3	2.92	1.44	1.38
1	AA	1498	UR3	C5-C4	2.90	1.51	1.43
22	BA	2030	6MZ	C6-N1	-2.88	1.30	1.35
1	AA	1207	2MG	O6-C6	-2.87	1.18	1.23
22	BA	1962	5MC	C2-N1	2.85	1.46	1.40
22	BA	2605	PSU	O4-C4	-2.84	1.18	1.23
22	BA	1911	PSU	C4-N3	2.84	1.44	1.38
1	AA	1402	4OC	C6-N1	2.82	1.44	1.38
22	BA	1911	PSU	O4-C4	-2.82	1.18	1.23
22	BA	2457	PSU	O4-C4	-2.82	1.18	1.23
22	BA	2503	2MA	C8-N7	2.80	1.36	1.31
22	BA	1962	5MC	C6-N1	2.80	1.42	1.38
22	BA	2504	PSU	O4-C4	-2.79	1.18	1.23
1	AA	527	G7M	C4-N9	-2.79	1.30	1.38
1	AA	966	2MG	O6-C6	-2.77	1.18	1.23
1	AA	527	G7M	C6-N1	2.74	1.43	1.38
22	BA	2504	PSU	C4-N3	2.69	1.43	1.38
22	BA	745	1MG	C5-C6	2.66	1.52	1.45
22	BA	1939	5MU	C4-C5	-2.64	1.40	1.44
1	AA	516	PSU	O4'-C1'	-2.61	1.40	1.43
1	AA	1498	UR3	C3U-N3	-2.60	1.42	1.47
25	BD	150	MEQ	OE1-CD	-2.60	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2445	2MG	C2-N1	2.60	1.40	1.36
22	BA	745	1MG	C4-N9	-2.59	1.31	1.38
22	BA	745	1MG	C8-N9	-2.59	1.31	1.37
22	BA	1917	PSU	O4-C4	-2.58	1.18	1.23
1	AA	1518	MA6	C6-N1	-2.57	1.29	1.34
22	BA	2445	2MG	C5-C4	-2.56	1.31	1.38
34	BM	81	4D4	CZ-NH1	-2.56	1.24	1.34
1	AA	1519	MA6	C6-N1	-2.53	1.29	1.34
22	BA	1915	3TD	O2-C2	-2.52	1.18	1.23
22	BA	955	PSU	C4-N3	2.52	1.43	1.38
22	BA	2251	OMG	C8-N9	-2.50	1.32	1.37
1	AA	966	2MG	C4-N9	-2.49	1.31	1.38
1	AA	527	G7M	C2-N1	2.46	1.43	1.37
22	BA	2605	PSU	C4-N3	2.43	1.43	1.38
22	BA	2457	PSU	O4'-C1'	-2.41	1.40	1.43
22	BA	1618	6MZ	C6-N1	-2.41	1.31	1.35
22	BA	2498	OMC	C6-N1	2.39	1.43	1.38
22	BA	2069	G7M	C5-C6	2.38	1.49	1.43
1	AA	516	PSU	O4-C4	-2.38	1.19	1.23
22	BA	2552	OMU	C4-N3	2.38	1.42	1.38
22	BA	2445	2MG	C8-N9	-2.37	1.32	1.37
22	BA	2503	2MA	C5-C4	-2.36	1.34	1.39
22	BA	1618	6MZ	C9-N6	2.28	1.49	1.45
22	BA	1915	3TD	O4-C4	-2.28	1.18	1.23
1	AA	1207	2MG	C4-N9	-2.23	1.32	1.38
25	BD	150	MEQ	CD-NE2	2.23	1.44	1.34
22	BA	1939	5MU	C5M-C5	-2.22	1.45	1.50
22	BA	746	PSU	C1'-C5	2.20	1.55	1.50
34	BM	81	4D4	OB-CB	-2.20	1.38	1.43
22	BA	2604	PSU	C4-N3	2.15	1.42	1.38
1	AA	1207	2MG	C5-C6	2.14	1.52	1.44
1	AA	1498	UR3	C6-N1	2.14	1.43	1.38
22	BA	1911	PSU	O4'-C1'	-2.14	1.40	1.43
1	AA	1518	MA6	C10-N6	-2.14	1.40	1.45
22	BA	2030	6MZ	C9-N6	2.12	1.48	1.45
22	BA	2605	PSU	O2-C2	-2.11	1.19	1.23
22	BA	1939	5MU	C4-N3	-2.11	1.34	1.38
22	BA	2552	OMU	C6-N1	2.10	1.43	1.38
1	AA	1207	2MG	C6-N1	2.09	1.42	1.38
22	BA	2457	PSU	C4-N3	2.08	1.42	1.38
22	BA	2580	PSU	C4-N3	2.06	1.42	1.38
22	BA	2605	PSU	O4'-C1'	-2.04	1.41	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	746	PSU	O4'-C1'	-2.04	1.41	1.43
1	AA	1518	MA6	C5-C6	-2.00	1.36	1.41

All (230) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1519	MA6	N1-C6-N6	-14.06	101.71	117.08
1	AA	1518	MA6	N1-C6-N6	-12.79	103.10	117.08
22	BA	2030	6MZ	C9-N6-C6	-8.27	115.75	122.87
22	BA	1618	6MZ	C9-N6-C6	-7.09	116.76	122.87
1	AA	1519	MA6	C5-C6-N6	7.09	137.64	125.30
1	AA	1518	MA6	C5-C6-N6	6.74	137.05	125.30
22	BA	2069	G7M	C1'-N9-C8	-6.69	104.14	126.74
22	BA	2445	2MG	C2-N3-C4	6.67	120.31	112.04
22	BA	1618	6MZ	N1-C2-N3	-6.59	118.29	128.60
22	BA	2604	PSU	N1-C2-N3	6.40	122.38	115.13
22	BA	2069	G7M	C1'-N9-C4	6.31	145.25	126.50
1	AA	1207	2MG	C2-N3-C4	6.30	119.85	112.04
22	BA	2604	PSU	C6-C5-C4	6.25	122.57	118.20
1	AA	527	G7M	C1'-N9-C8	-6.19	105.83	126.74
22	BA	2552	OMU	C4-N3-C2	-6.17	118.45	126.58
22	BA	2457	PSU	N1-C2-N3	6.12	122.06	115.13
1	AA	1519	MA6	N1-C2-N3	-6.01	119.20	128.60
1	AA	1516	2MG	C2-N3-C4	5.97	119.44	112.04
22	BA	2445	2MG	C2-N1-C6	-5.91	117.67	124.48
1	AA	527	G7M	C1'-N9-C4	5.90	144.01	126.50
1	AA	966	2MG	C2-N3-C4	5.89	119.34	112.04
22	BA	2604	PSU	C4-N3-C2	-5.82	117.95	126.34
22	BA	2457	PSU	C4-N3-C2	-5.79	118.00	126.34
1	AA	1516	2MG	C2-N1-C6	-5.72	117.90	124.48
22	BA	1835	2MG	C2-N3-C4	5.71	119.12	112.04
1	AA	1498	UR3	C4-N3-C2	-5.65	119.24	124.56
22	BA	2445	2MG	CM2-N2-C2	-5.61	111.46	123.86
22	BA	955	PSU	N1-C2-N3	5.58	121.45	115.13
1	AA	1518	MA6	N1-C2-N3	-5.57	119.89	128.60
22	BA	2030	6MZ	N1-C2-N3	-5.55	119.92	128.60
22	BA	2503	2MA	N9-C8-N7	-5.53	106.36	113.91
22	BA	1915	3TD	N1-C2-N3	5.46	120.45	116.14
22	BA	1911	PSU	C4-N3-C2	-5.44	118.51	126.34
22	BA	2503	2MA	C5-C4-N3	-5.41	121.10	127.19
22	BA	2605	PSU	C4-N3-C2	-5.32	118.68	126.34
22	BA	745	1MG	C5-C4-N3	-5.31	119.84	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2030	6MZ	N9-C8-N7	-5.28	106.69	113.91
22	BA	955	PSU	C4-N3-C2	-5.28	118.73	126.34
1	AA	1519	MA6	C5-C4-N3	-5.24	119.91	126.75
22	BA	1911	PSU	N1-C2-N3	5.11	120.92	115.13
22	BA	746	PSU	C4-N3-C2	-5.11	118.97	126.34
22	BA	2552	OMU	N3-C2-N1	5.11	121.67	114.89
1	AA	1518	MA6	C5-C4-N3	-5.10	120.10	126.75
22	BA	1618	6MZ	N9-C8-N7	-5.04	107.02	113.91
22	BA	1835	2MG	C2-N1-C6	-5.03	118.69	124.48
12	AL	89	D2T	CB1-SB-CB	4.91	111.32	102.44
1	AA	1207	2MG	C5-C4-N3	-4.81	120.67	128.46
22	BA	2445	2MG	C5-C4-N3	-4.74	120.77	128.46
22	BA	2580	PSU	N1-C2-N3	4.74	120.50	115.13
22	BA	1618	6MZ	C5-C4-N3	-4.69	120.63	126.75
22	BA	1917	PSU	N1-C2-N3	4.65	120.40	115.13
22	BA	2604	PSU	O2-C2-N1	-4.65	117.67	122.79
1	AA	516	PSU	C4-N3-C2	-4.61	119.69	126.34
1	AA	1516	2MG	C5-C4-N3	-4.59	121.01	128.46
22	BA	1917	PSU	C4-N3-C2	-4.53	119.81	126.34
22	BA	2605	PSU	N1-C2-N3	4.53	120.26	115.13
1	AA	1519	MA6	N9-C8-N7	-4.50	107.76	113.91
22	BA	2504	PSU	C4-N3-C2	-4.50	119.86	126.34
1	AA	966	2MG	C5-C4-N3	-4.48	121.19	128.46
1	AA	1407	5MC	C5-C6-N1	-4.45	118.76	123.34
22	BA	1835	2MG	C5-C4-N3	-4.44	121.25	128.46
1	AA	1207	2MG	C2-N1-C6	-4.42	119.40	124.48
22	BA	2030	6MZ	C5-C4-N3	-4.40	121.01	126.75
22	BA	2580	PSU	C4-N3-C2	-4.33	120.11	126.34
22	BA	2457	PSU	C6-C5-C4	4.27	121.19	118.20
22	BA	1915	3TD	C4-N3-C2	-4.24	120.00	124.61
1	AA	516	PSU	N1-C2-N3	4.20	119.88	115.13
22	BA	1911	PSU	C6-C5-C4	4.17	121.11	118.20
22	BA	1835	2MG	CM2-N2-C2	-4.14	114.71	123.86
22	BA	2503	2MA	N3-C2-N1	-4.14	118.11	125.72
1	AA	527	G7M	C2-N3-C4	4.14	119.67	112.30
22	BA	2069	G7M	O6-C6-C5	-4.12	118.76	128.06
22	BA	955	PSU	C6-N1-C2	-4.10	118.49	122.68
22	BA	2251	OMG	C5-C4-N3	-4.09	121.82	128.46
1	AA	527	G7M	C5-C6-N1	4.08	120.30	111.79
1	AA	1518	MA6	N9-C8-N7	-4.07	108.35	113.91
22	BA	2069	G7M	C5-C6-N1	4.07	120.29	111.79
1	AA	516	PSU	C6-C5-C4	4.04	121.03	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1518	MA6	C4-C5-C6	4.03	120.39	115.88
22	BA	955	PSU	C6-C5-C4	4.01	121.00	118.20
22	BA	2504	PSU	N1-C2-N3	3.96	119.61	115.13
22	BA	2251	OMG	C2-N3-C4	3.93	119.30	112.30
22	BA	2580	PSU	C6-N1-C2	-3.91	118.68	122.68
1	AA	966	2MG	C2-N1-C6	-3.89	120.00	124.48
22	BA	1618	6MZ	C2-N3-C4	3.86	120.88	111.75
1	AA	1519	MA6	C2-N3-C4	3.86	120.87	111.75
1	AA	1516	2MG	CM2-N2-C2	-3.83	115.41	123.86
22	BA	2605	PSU	C6-C5-C4	3.78	120.84	118.20
22	BA	1917	PSU	C6-N1-C2	-3.77	118.82	122.68
22	BA	745	1MG	N9-C4-N3	3.77	133.50	125.94
22	BA	2457	PSU	O2-C2-N1	-3.70	118.72	122.79
1	AA	527	G7M	C5-C4-N3	-3.69	121.07	128.15
22	BA	2604	PSU	C6-N1-C2	-3.68	118.92	122.68
22	BA	2251	OMG	N9-C8-N7	-3.59	106.62	113.39
22	BA	746	PSU	N1-C2-N3	3.58	119.19	115.13
22	BA	2251	OMG	C1'-N9-C8	-3.58	116.50	126.70
1	AA	1518	MA6	N3-C4-N9	3.57	132.97	127.08
22	BA	2030	6MZ	C4-N9-C8	3.57	109.59	105.73
22	BA	2030	6MZ	C5-N7-C8	3.56	108.57	103.51
22	BA	2552	OMU	C5-C4-N3	3.55	120.15	114.84
22	BA	2457	PSU	C6-N1-C2	-3.53	119.08	122.68
22	BA	2503	2MA	CM2-C2-N1	3.53	122.66	117.15
1	AA	966	2MG	C1'-N9-C8	-3.51	116.71	126.70
22	BA	2503	2MA	C5-N7-C8	3.48	108.45	103.51
1	AA	1518	MA6	C2-N1-C6	3.47	119.94	111.75
22	BA	2445	2MG	C5-C6-N1	3.47	121.99	113.19
1	AA	1519	MA6	C2-N1-C6	3.45	119.90	111.75
1	AA	1207	2MG	C1'-N9-C8	-3.42	116.95	126.70
22	BA	745	1MG	C2-N3-C4	3.42	119.67	111.98
1	AA	1518	MA6	C2-N3-C4	3.42	119.82	111.75
22	BA	2069	G7M	C2-N3-C4	3.40	118.36	112.30
22	BA	2445	2MG	N9-C8-N7	-3.40	106.99	113.39
1	AA	1516	2MG	O6-C6-C5	-3.37	117.67	126.60
22	BA	745	1MG	N9-C8-N7	-3.35	107.09	113.39
22	BA	2445	2MG	C1'-N9-C8	-3.32	117.24	126.70
1	AA	527	G7M	C2-N1-C6	-3.31	119.06	125.10
1	AA	967	5MC	C5-C6-N1	-3.31	119.94	123.34
22	BA	1618	6MZ	C4-N9-C8	3.31	109.31	105.73
1	AA	966	2MG	N9-C8-N7	-3.28	107.22	113.39
22	BA	2503	2MA	C4-N9-C8	3.27	109.27	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1516	2MG	N9-C8-N7	-3.27	107.23	113.39
22	BA	2030	6MZ	C2-N3-C4	3.26	119.46	111.75
22	BA	1835	2MG	C1'-N9-C8	-3.25	117.45	126.70
1	AA	1519	MA6	N3-C4-N9	3.22	132.39	127.08
1	AA	527	G7M	O6-C6-C5	-3.22	120.80	128.06
1	AA	1519	MA6	C4-C5-C6	3.22	119.48	115.88
22	BA	1835	2MG	C5-C6-N1	3.19	121.30	113.19
22	BA	1917	PSU	C6-C5-C4	3.17	120.42	118.20
22	BA	2503	2MA	N3-C4-N9	3.16	131.37	126.99
12	AL	89	D2T	OD2-CG-CB	3.15	119.96	113.15
22	BA	1618	6MZ	C5-N7-C8	3.15	107.98	103.51
22	BA	1939	5MU	C4-N3-C2	-3.10	123.34	127.35
22	BA	2503	2MA	N6-C6-N1	3.10	121.41	117.03
22	BA	1911	PSU	C6-N1-C2	-3.08	119.53	122.68
22	BA	1835	2MG	N9-C8-N7	-3.07	107.62	113.39
22	BA	1618	6MZ	N3-C4-N9	3.06	132.12	127.08
22	BA	747	5MU	C4-N3-C2	-3.05	123.41	127.35
22	BA	2030	6MZ	N3-C4-N9	3.04	132.10	127.08
1	AA	1207	2MG	N9-C8-N7	-3.03	107.69	113.39
1	AA	1519	MA6	C5-N7-C8	3.03	107.81	103.51
1	AA	1516	2MG	C5-C6-N1	3.01	120.83	113.19
22	BA	1939	5MU	C6-C5-C4	3.00	120.54	118.03
22	BA	2030	6MZ	C4-C5-C6	2.98	119.12	116.81
22	BA	2069	G7M	CN7-N7-C5	2.97	130.46	126.77
22	BA	1962	5MC	C5-C6-N1	-2.95	120.30	123.34
22	BA	745	1MG	C5-C6-N1	2.94	120.58	114.91
22	BA	1962	5MC	CM5-C5-C6	-2.90	118.97	122.85
1	AA	516	PSU	C6-N1-C2	-2.88	119.74	122.68
1	AA	1516	2MG	C1'-N9-C8	-2.87	118.54	126.70
1	AA	1207	2MG	C5-C6-N1	2.86	120.46	113.19
22	BA	2069	G7M	C2-N1-C6	-2.86	119.89	125.10
22	BA	1939	5MU	C5-C4-N3	2.83	117.73	115.31
1	AA	527	G7M	N9-C8-N7	-2.83	105.22	112.21
1	AA	1207	2MG	C1'-N9-C4	2.78	134.77	126.50
22	BA	1835	2MG	O6-C6-C5	-2.78	119.22	126.60
22	BA	2445	2MG	O6-C6-C5	-2.78	119.23	126.60
22	BA	2504	PSU	C6-C5-C4	2.77	120.13	118.20
22	BA	2069	G7M	C5-C4-N3	-2.77	122.84	128.15
22	BA	2580	PSU	C6-C5-C4	2.75	120.12	118.20
22	BA	2069	G7M	N9-C8-N7	-2.75	105.42	112.21
1	AA	966	2MG	C1'-N9-C4	2.73	134.62	126.50
22	BA	1618	6MZ	C4-N9-C1'	-2.72	120.11	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	527	G7M	N9-C4-N3	2.71	131.39	125.94
1	AA	1207	2MG	N9-C4-N3	2.69	131.34	125.94
22	BA	2251	OMG	C2-N1-C6	-2.69	120.20	125.10
22	BA	2445	2MG	C1'-N9-C4	2.68	134.47	126.50
22	BA	2251	OMG	C5-C6-N1	2.68	119.99	113.19
22	BA	1618	6MZ	C4-C5-C6	2.65	118.86	116.81
1	AA	966	2MG	N1-C2-N3	-2.62	119.90	123.95
22	BA	955	PSU	O2-C2-N1	-2.62	119.91	122.79
22	BA	2552	OMU	O2-C2-N1	-2.61	119.31	122.79
1	AA	1207	2MG	O6-C6-C5	-2.61	119.68	126.60
1	AA	1518	MA6	C5-N7-C8	2.61	107.22	103.51
22	BA	746	PSU	O2-C2-N1	-2.56	119.97	122.79
22	BA	1835	2MG	C1'-N9-C4	2.56	134.10	126.50
1	AA	1207	2MG	N1-C2-N3	-2.53	120.03	123.95
1	AA	966	2MG	C5-C6-N1	2.53	119.61	113.19
1	AA	966	2MG	O6-C6-C5	-2.51	119.93	126.60
22	BA	2251	OMG	N9-C4-N3	2.50	130.96	125.94
22	BA	2069	G7M	CN7-N7-C8	-2.47	121.03	124.84
22	BA	2251	OMG	O6-C6-C5	-2.46	120.06	126.60
22	BA	747	5MU	C6-C5-C4	2.44	120.07	118.03
1	AA	966	2MG	N9-C4-N3	2.42	130.80	125.94
22	BA	2504	PSU	C6-N1-C2	-2.42	120.21	122.68
25	BD	150	MEQ	CG-CD-NE2	2.42	119.64	116.29
22	BA	2552	OMU	O4-C4-C5	-2.39	120.95	125.16
22	BA	2030	6MZ	C4-N9-C1'	-2.39	120.90	126.59
1	AA	516	PSU	O4'-C1'-C2'	2.39	108.51	105.14
1	AA	516	PSU	O2-C2-N1	-2.39	120.16	122.79
1	AA	1519	MA6	C4-N9-C8	2.38	108.31	105.73
22	BA	2251	OMG	C1'-N9-C4	2.36	133.50	126.50
22	BA	2069	G7M	N2-C2-N1	2.35	121.72	116.71
22	BA	1835	2MG	N9-C4-N3	2.34	130.63	125.94
22	BA	1939	5MU	C5-C6-N1	-2.33	120.94	123.34
1	AA	966	2MG	CM2-N2-C2	-2.33	118.73	123.86
22	BA	746	PSU	C5-C4-N3	2.31	121.81	116.58
1	AA	1518	MA6	C4-N9-C8	2.30	108.22	105.73
22	BA	2552	OMU	C2'-C1'-N1	-2.30	109.77	114.22
22	BA	2498	OMC	O2-C2-N3	-2.27	118.64	122.33
22	BA	746	PSU	C6-N1-C2	-2.26	120.37	122.68
1	AA	1407	5MC	CM5-C5-C6	-2.25	119.84	122.85
22	BA	2069	G7M	N9-C4-N3	2.25	130.45	125.94
34	BM	81	4D4	CB-CA-C	-2.23	108.21	111.77
22	BA	2445	2MG	N1-C2-N3	-2.23	120.51	123.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1402	4OC	CM4-N4-C4	-2.21	118.12	122.45
1	AA	1516	2MG	C1'-N9-C4	2.20	133.04	126.50
22	BA	1917	PSU	O2-C2-N1	-2.19	120.38	122.79
22	BA	2503	2MA	C5-C6-N6	-2.18	118.68	123.43
1	AA	1516	2MG	N9-C4-N3	2.17	130.30	125.94
1	AA	1498	UR3	C3U-N3-C2	2.16	121.10	117.31
22	BA	745	1MG	C1'-N9-C4	-2.15	120.11	126.50
22	BA	745	1MG	C2-N1-C6	-2.14	119.21	120.95
22	BA	745	1MG	C8-N7-C5	2.14	108.11	104.24
1	AA	966	2MG	C8-N7-C5	2.12	108.08	104.24
22	BA	2445	2MG	N9-C4-N3	2.11	130.18	125.94
22	BA	2605	PSU	C6-N1-C2	-2.10	120.53	122.68
22	BA	1915	3TD	C6-C5-C4	2.10	119.67	118.22
1	AA	1402	4OC	C6-C5-C4	2.09	119.52	116.96
22	BA	1618	6MZ	C5-C6-N1	2.07	120.41	118.20
22	BA	2251	OMG	N2-C2-N1	2.07	121.11	116.71
22	BA	2251	OMG	C8-N9-C4	2.06	109.97	106.05
22	BA	1835	2MG	N1-C2-N3	-2.05	120.78	123.95
22	BA	746	PSU	O4-C4-C5	-2.05	118.68	124.05
12	AL	89	D2T	OD2-CG-OD1	-2.05	119.44	124.09
22	BA	2604	PSU	C5-C6-N1	-2.03	119.07	122.11
1	AA	1516	2MG	C8-N7-C5	2.02	107.90	104.24
22	BA	2251	OMG	C8-N7-C5	2.02	107.90	104.24
22	BA	2498	OMC	C6-C5-C4	2.01	120.74	117.50
22	BA	2445	2MG	C8-N7-C5	2.01	107.87	104.24
22	BA	1911	PSU	O4'-C1'-C2'	2.00	107.97	105.14

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	O4'-C4'-C5'-O5'
1	AA	527	G7M	C3'-C4'-C5'-O5'
25	BD	150	MEQ	O-C-CA-CB
22	BA	746	PSU	C2'-C1'-C5-C4
22	BA	747	5MU	C3'-C4'-C5'-O5'
22	BA	1915	3TD	C3'-C4'-C5'-O5'
22	BA	1915	3TD	O4'-C4'-C5'-O5'
22	BA	2251	OMG	C1'-C2'-O2'-CM2
22	BA	2504	PSU	O4'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
22	BA	747	5MU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
22	BA	2030	6MZ	O4'-C4'-C5'-O5'
22	BA	2030	6MZ	C3'-C4'-C5'-O5'
22	BA	2504	PSU	C3'-C4'-C5'-O5'
22	BA	2580	PSU	O4'-C4'-C5'-O5'
1	AA	1402	4OC	O4'-C4'-C5'-O5'
1	AA	1519	MA6	C3'-C4'-C5'-O5'
22	BA	2445	2MG	C3'-C4'-C5'-O5'
1	AA	1402	4OC	C3'-C4'-C5'-O5'
22	BA	2580	PSU	C3'-C4'-C5'-O5'
25	BD	150	MEQ	OE1-CD-CG-CB
25	BD	150	MEQ	NE2-CD-CG-CB
22	BA	2445	2MG	O4'-C4'-C5'-O5'
22	BA	2503	2MA	O4'-C4'-C5'-O5'
12	AL	89	D2T	CG-CB-SB-CB1
22	BA	2069	G7M	C4'-C5'-O5'-P
25	BD	150	MEQ	N-CA-CB-CG
22	BA	747	5MU	C4'-C5'-O5'-P
34	BM	81	4D4	OB-CB-CG-CD
22	BA	746	PSU	O4'-C4'-C5'-O5'
22	BA	2069	G7M	O4'-C4'-C5'-O5'
22	BA	746	PSU	O4'-C1'-C5'-C6
1	AA	516	PSU	O4'-C4'-C5'-O5'
22	BA	1917	PSU	O4'-C4'-C5'-O5'
22	BA	2503	2MA	C3'-C4'-C5'-O5'
34	BM	81	4D4	O-C-CA-CB
22	BA	2251	OMG	C4'-C5'-O5'-P

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	BD	150	MEQ	1	0
1	AA	1519	MA6	1	0
1	AA	1518	MA6	1	0
1	AA	1516	2MG	1	0
1	AA	1207	2MG	1	0
22	BA	2498	OMC	1	0
22	BA	2030	6MZ	2	0
22	BA	2251	OMG	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 490 ligands modelled in this entry, 489 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	$\# Z > 2$
60	TRP	BA	3001	-	14,16,16	0.71	1 (7%)	20,22,22	0.87	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	TRP	BA	3001	-	-	0/8/8/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BA	3001	TRP	OXT-C	-2.11	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	3001	TRP	OXT-C-O	-2.32	118.81	124.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	BA	2
54	B7	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	885:C	O3'	892:A	P	13.97
1	BA	2099:U	O3'	2100:G	P	3.25
1	B7	7:U	O3'	8:G	P	2.92

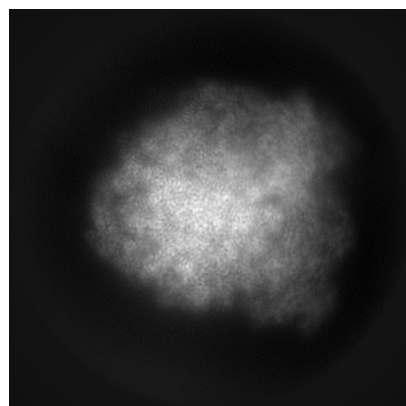
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12695. These allow visual inspection of the internal detail of the map and identification of artifacts.

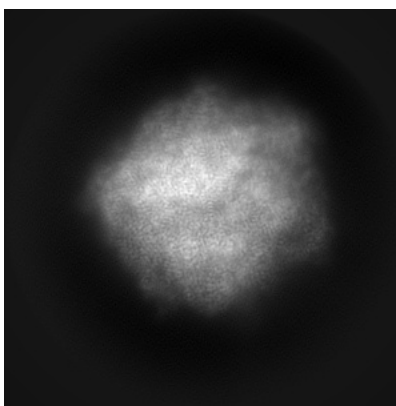
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

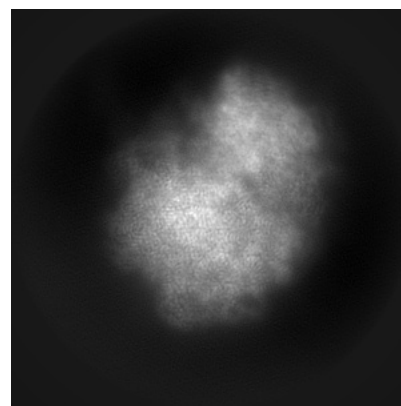
6.1.1 Primary map



X

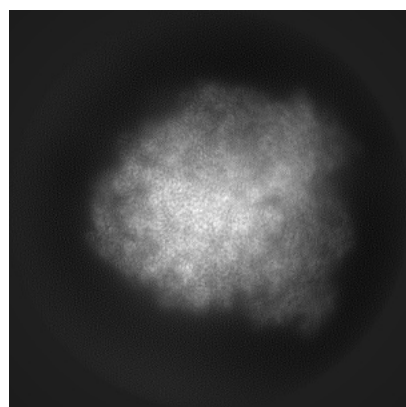


Y

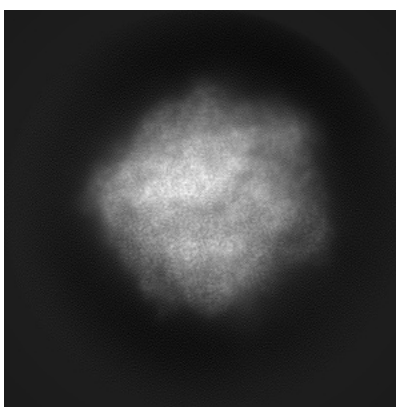


Z

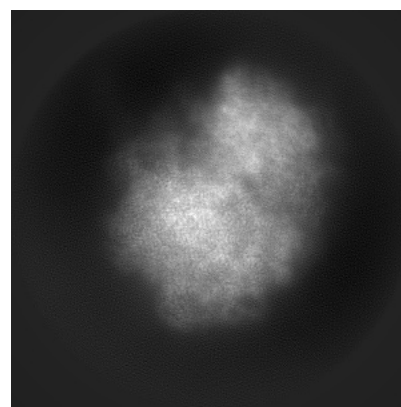
6.1.2 Raw map



X



Y

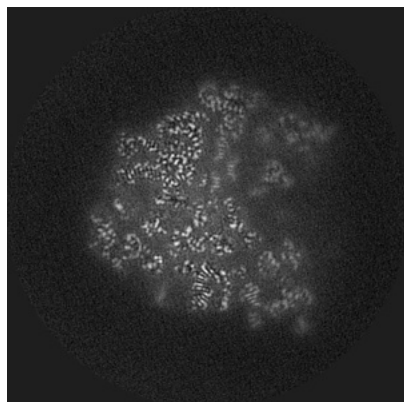


Z

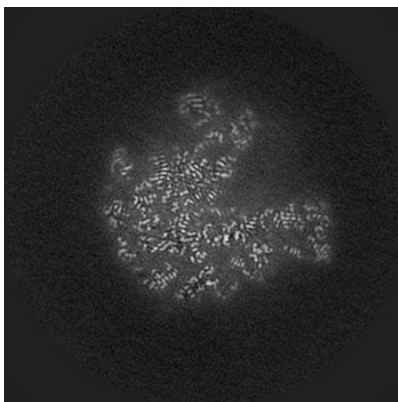
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

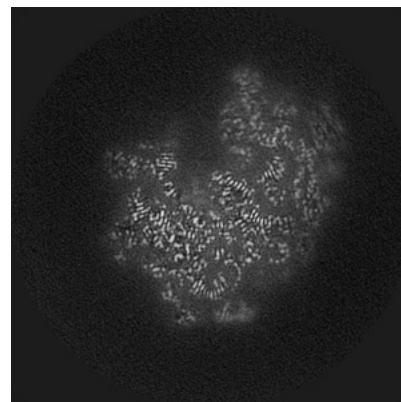
6.2.1 Primary map



X Index: 204

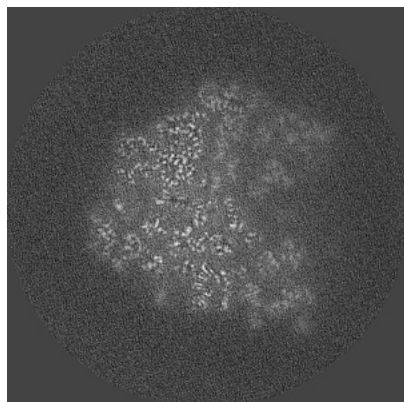


Y Index: 204

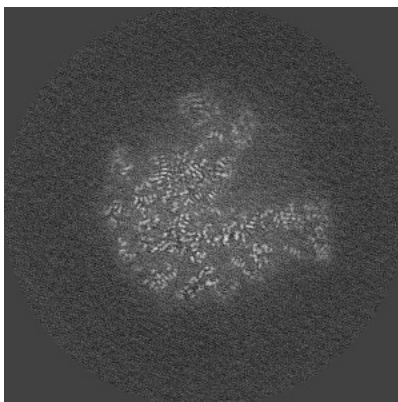


Z Index: 204

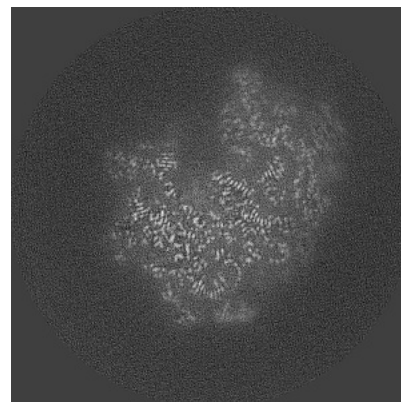
6.2.2 Raw map



X Index: 204



Y Index: 204

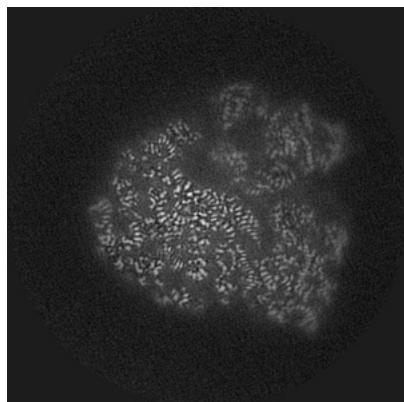


Z Index: 204

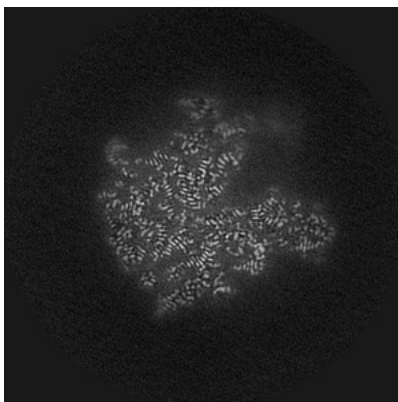
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

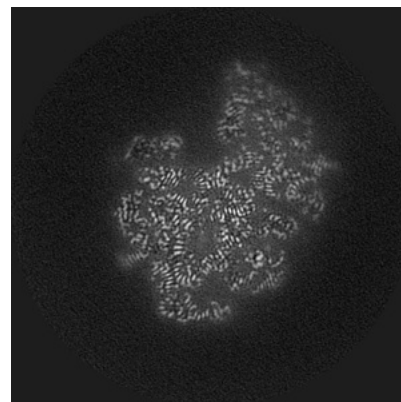
6.3.1 Primary map



X Index: 219

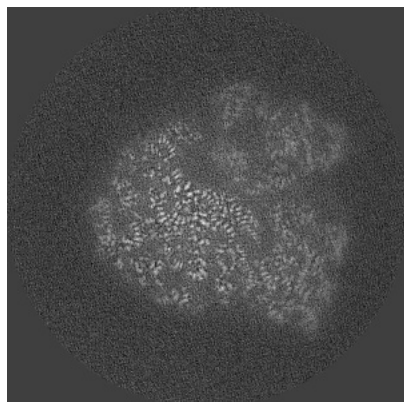


Y Index: 195

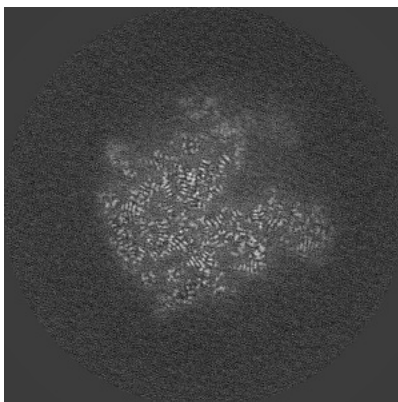


Z Index: 188

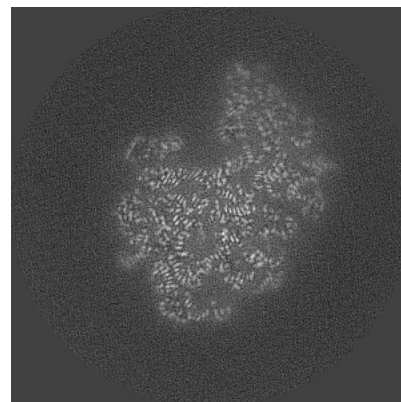
6.3.2 Raw map



X Index: 219



Y Index: 196

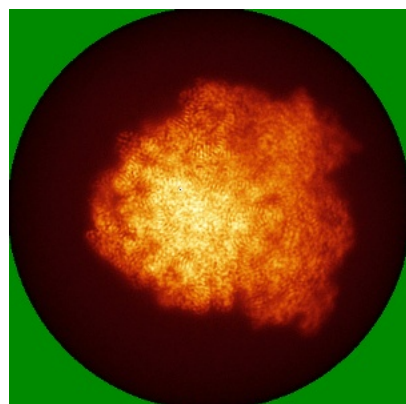


Z Index: 187

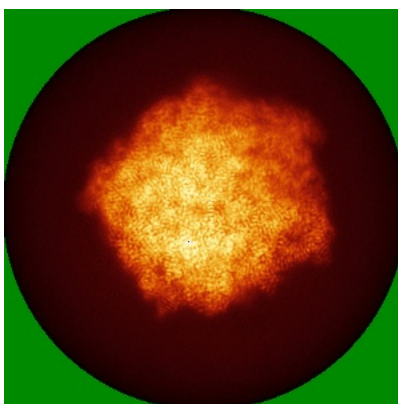
The images above show the largest variance slices of the map in three orthogonal directions.

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

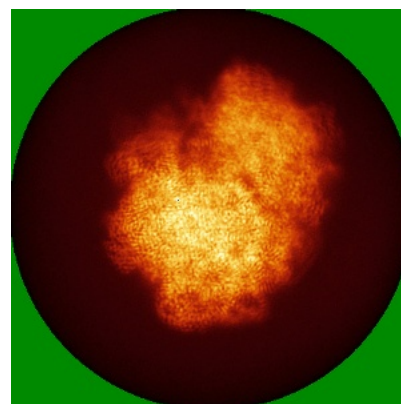
6.4.1 Primary map



X

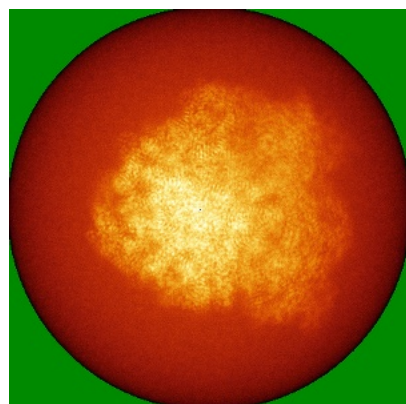


Y

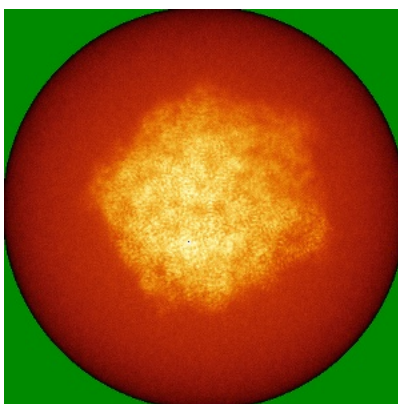


Z

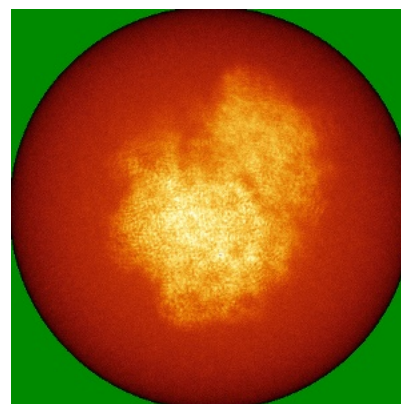
6.4.2 Raw map



X



Y

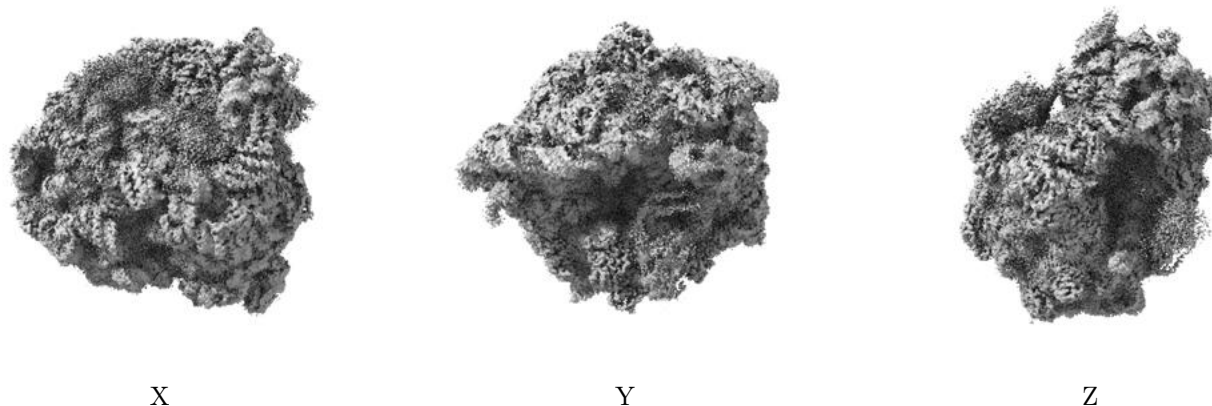


Z

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

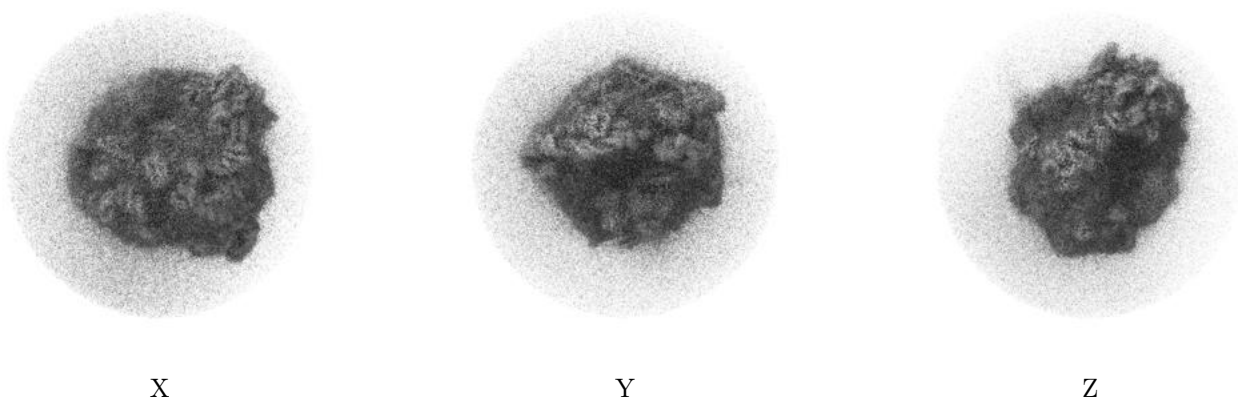
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

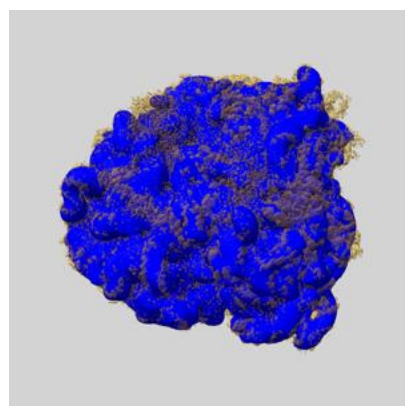
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

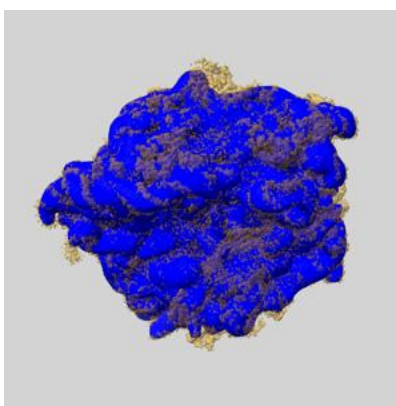
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

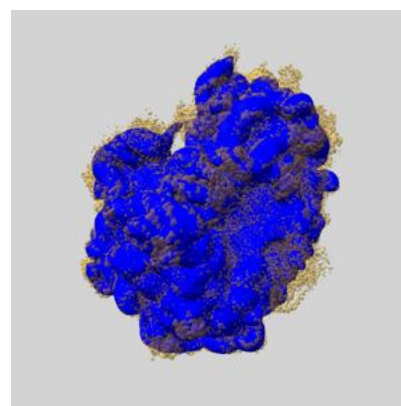
6.6.1 emd_12695_msk_1.map [i](#)



X



Y

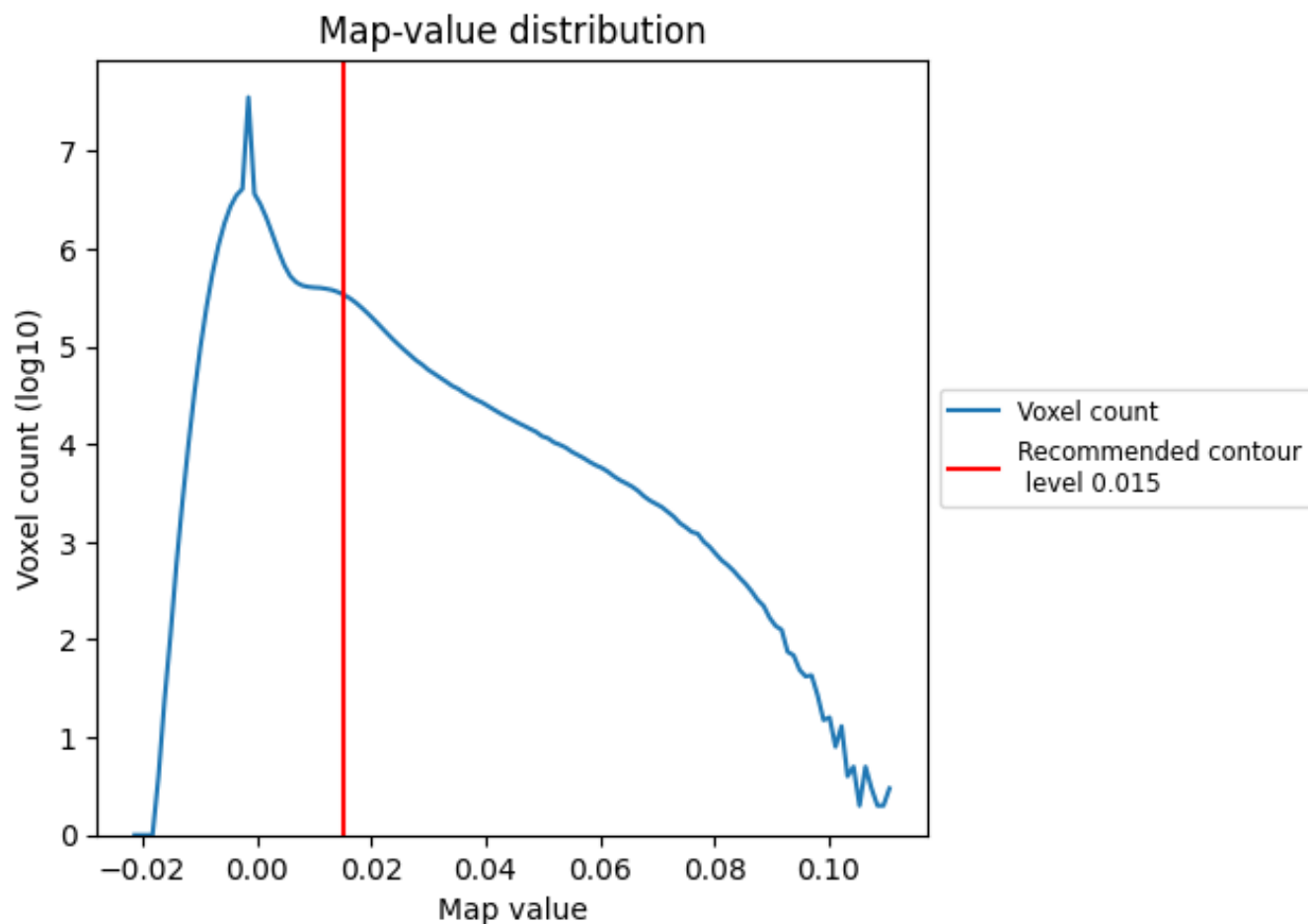


Z

7 Map analysis [i](#)

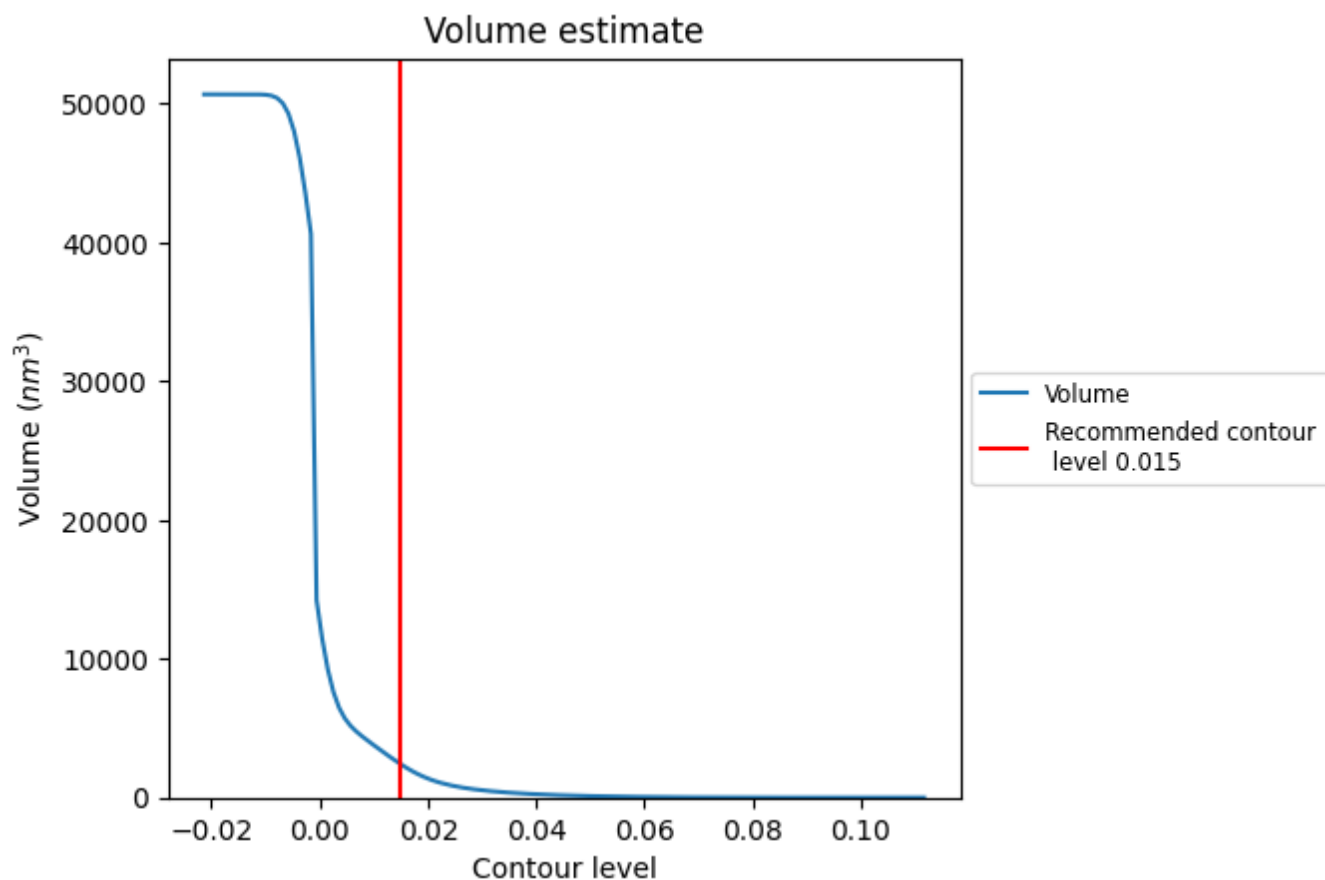
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

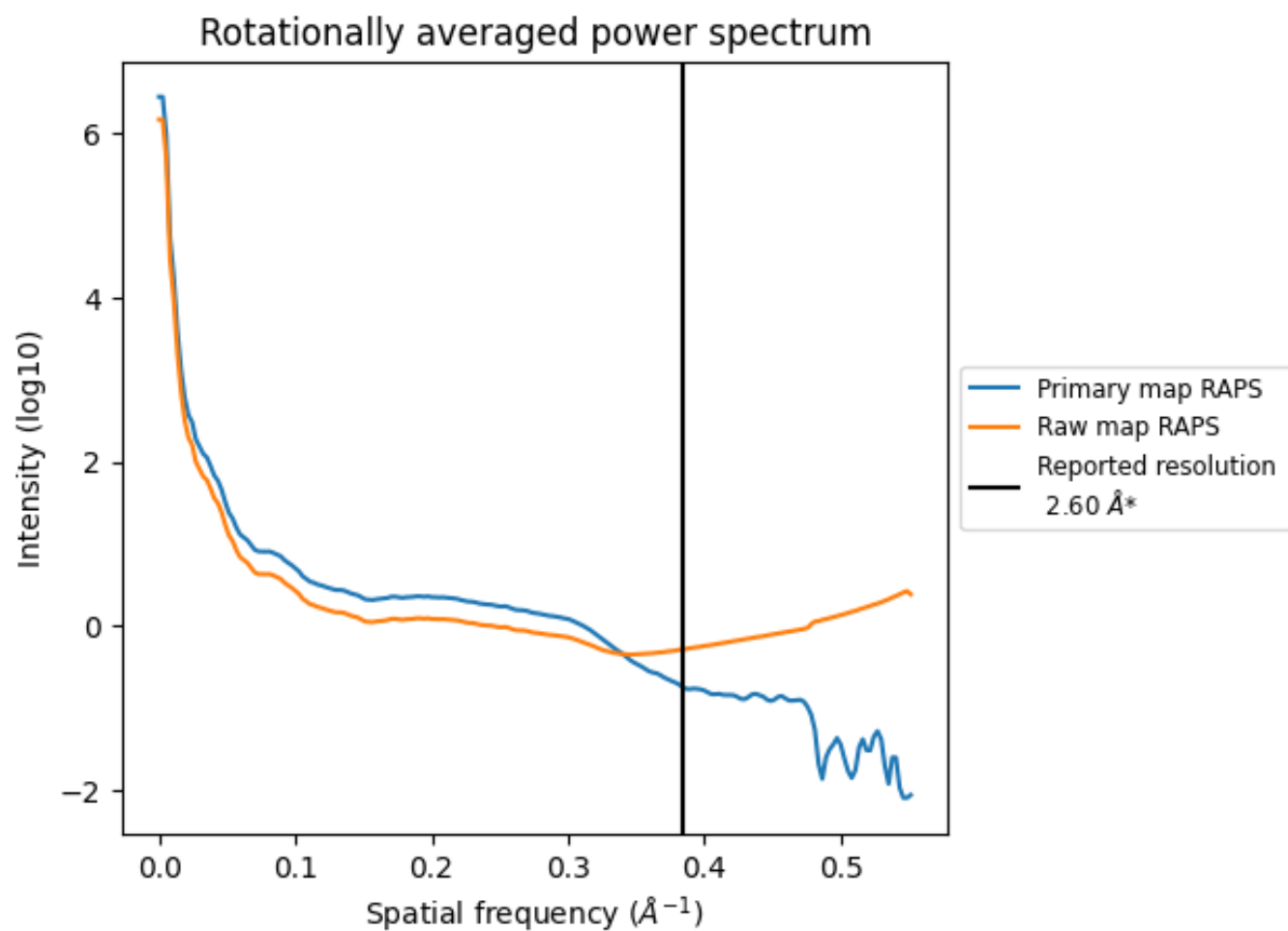
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2396 nm³; this corresponds to an approximate mass of 2165 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

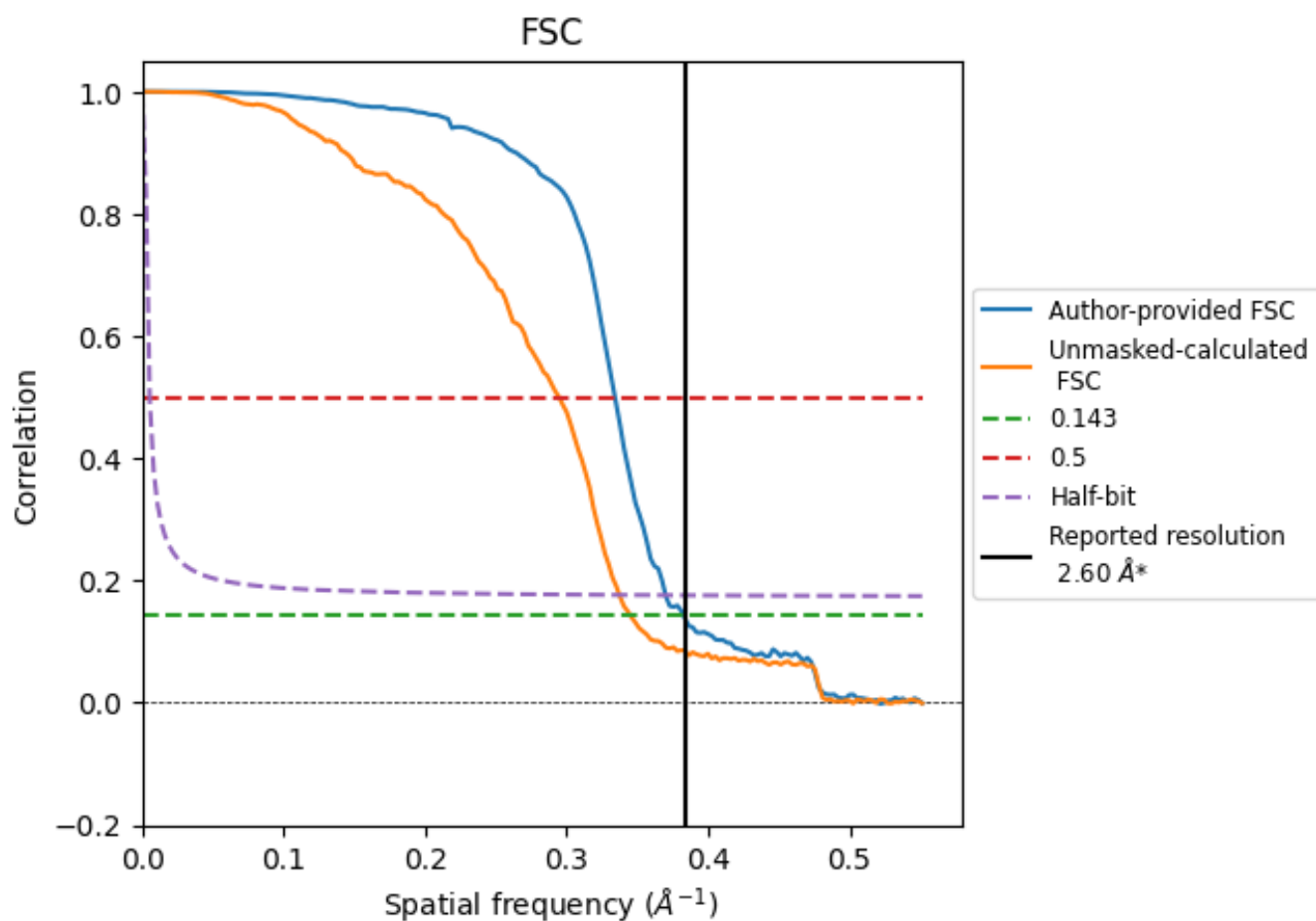


*Reported resolution corresponds to spatial frequency of $0.385 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

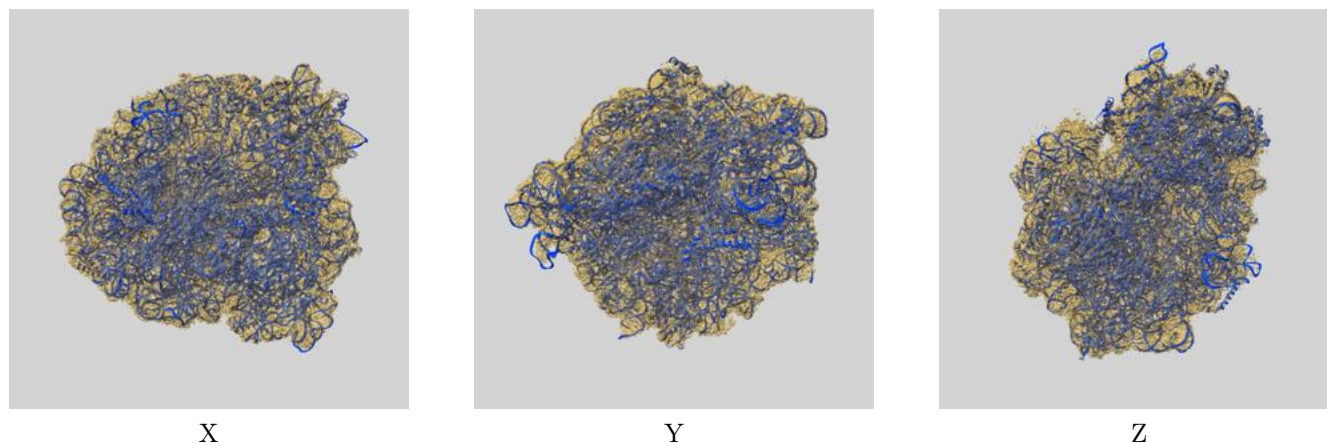
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.61	2.99	2.70
Unmasked-calculated*	2.90	3.39	2.96

*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 2.90 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

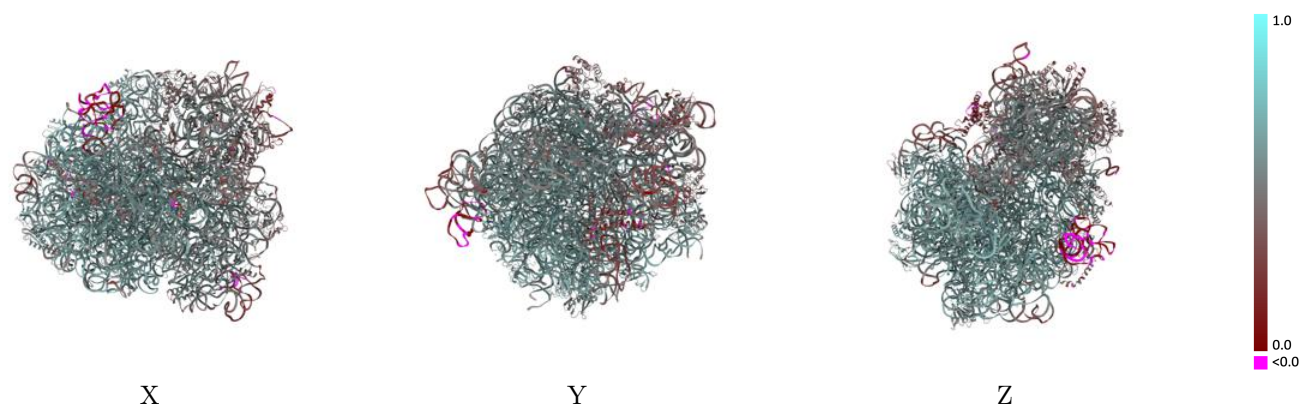
This section contains information regarding the fit between EMDB map EMD-12695 and PDB model 7O1C. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

9.1 Map-model overlay [i](#)



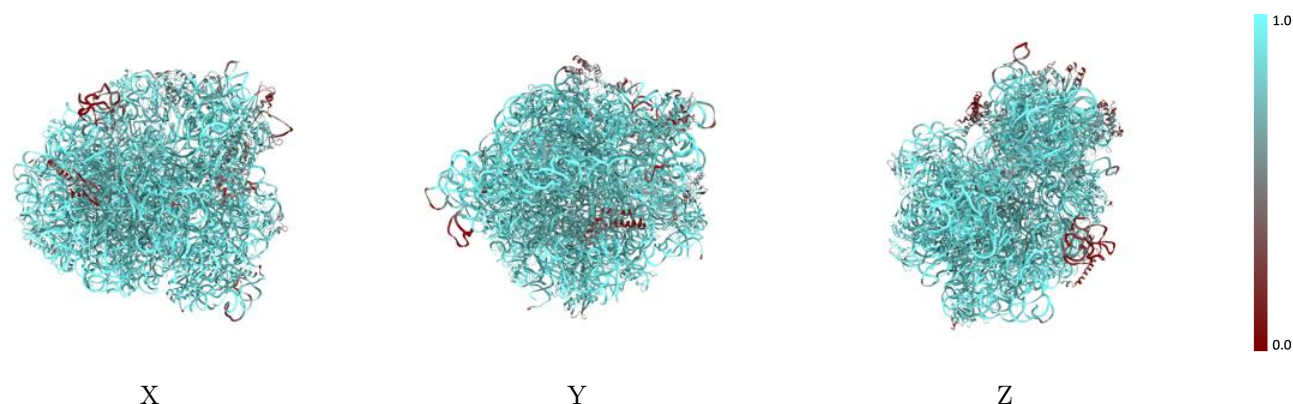
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



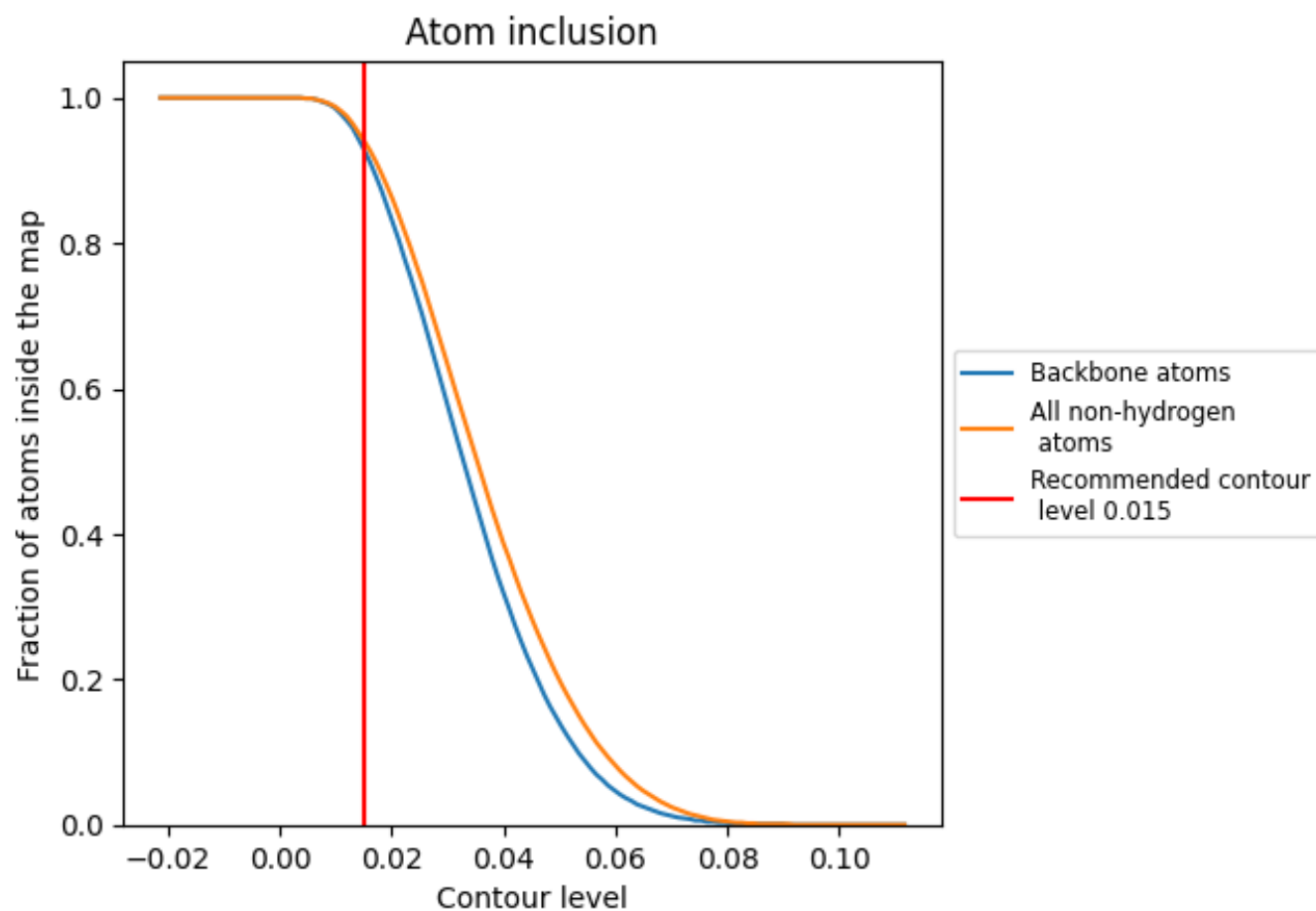
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 94% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9410	 0.5550
AA	 0.9590	 0.5270
AB	 0.5960	 0.3870
AC	 0.8500	 0.4360
AD	 0.8410	 0.4500
AE	 0.9450	 0.5100
AF	 0.8810	 0.4910
AG	 0.8140	 0.4290
AH	 0.9090	 0.5090
AI	 0.7840	 0.4280
AJ	 0.6360	 0.3580
AK	 0.9530	 0.5230
AL	 0.9760	 0.5520
AM	 0.8510	 0.4580
AN	 0.9040	 0.4500
AO	 0.9360	 0.5230
AP	 0.9120	 0.4960
AQ	 0.9450	 0.5040
AR	 0.9540	 0.5240
AS	 0.8330	 0.4340
AT	 0.9340	 0.5270
AU	 0.8760	 0.4540
B0	 0.9740	 0.6090
B1	 0.9800	 0.5780
B2	 1.0000	 0.6340
B3	 1.0000	 0.6300
B4	 0.9930	 0.6200
B5	 1.0000	 0.5670
B7	 1.0000	 0.5200
B8	 0.9990	 0.4730
B9	 0.7580	 0.3640
BA	 0.9710	 0.5970
BB	 0.9840	 0.5930
BC	 0.9970	 0.6310
BD	 0.9730	 0.6200



Continued on next page...

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Chain	Atom inclusion	Q-score
BE	 0.8800	 0.5710
BF	 0.9070	 0.4950
BG	 0.8610	 0.5360
BH	 0.4520	 0.3840
BI	 0.5510	 0.3810
BJ	 0.9810	 0.6150
BK	 0.9910	 0.6060
BL	 0.9570	 0.5940
BM	 0.9950	 0.6130
BN	 0.9910	 0.6310
BO	 0.9280	 0.5730
BP	 0.9720	 0.6060
BQ	 0.9880	 0.6250
BR	 0.9250	 0.5830
BS	 0.9800	 0.6040
BT	 0.9650	 0.5770
BU	 0.9200	 0.5460
BV	 0.9210	 0.5930
BW	 0.9810	 0.6060
BX	 0.9870	 0.6060
BY	 0.9180	 0.5440
BZ	 0.9430	 0.5870