



Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 11:17 am BST

PDB ID : 5JTE / pdb_00005jte
EMDB ID : EMD-8175
Title : Cryo-EM structure of an ErmBL-stalled ribosome in complex with A-, P-, and E-tRNA
Authors : Arenz, S.; Bock, L.V.; Graf, M.; Innis, C.A.; Beckmann, R.; Grubmueller, H.; Vaiana, A.C.; Wilson, D.N.
Deposited on : 2016-05-09
Resolution : 3.60 Å (reported)
Based on initial model : 5AFI

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:

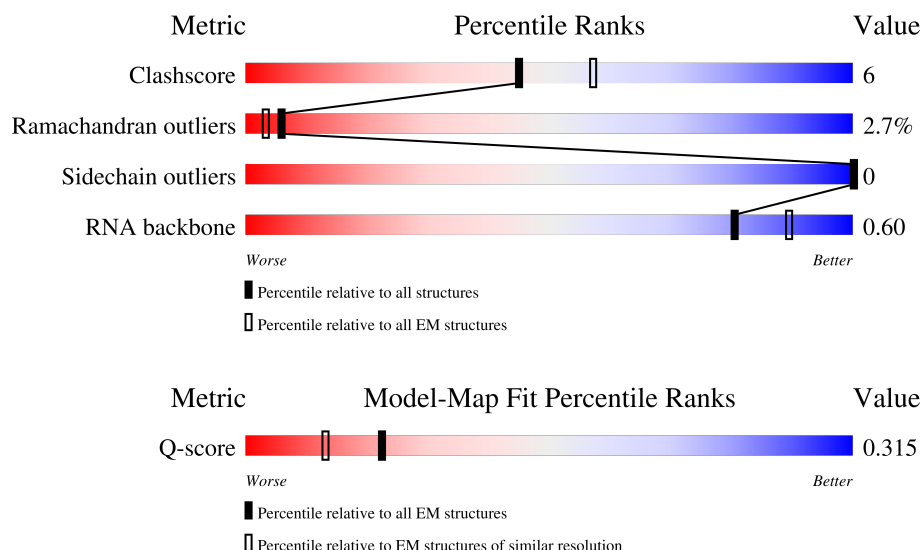
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.60 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	12797 (3.10 - 4.10)

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	1539	
2	AB	240	

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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	101	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	10	
23	AW	74	
24	AX	77	
25	AY	71	
26	BA	2897	
27	BB	120	

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Mol	Chain	Length	Quality of chain
28	BC	273	
29	BD	209	
30	BE	201	
31	BF	179	
32	BG	177	
33	BH	149	
34	BI	142	
35	BJ	142	
36	BK	123	
37	BL	144	
38	BM	136	
39	BN	127	
40	BO	117	
41	BP	115	
42	BQ	118	
43	BR	103	
44	BS	110	
45	BT	100	
46	BU	104	
47	BV	94	
48	BW	85	
49	BX	78	
50	BY	63	
51	BZ	59	
52	B0	57	

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Mol	Chain	Length	Quality of chain
53	B1	55	89% 62% 27% 9%
54	B2	46	48% 76% 24%
55	B3	65	68% 74% 25%
56	B4	38	71% 82% 18%
57	B5	9	78% 33% 67%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 146760 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1539	Total	C	N	O	P	0	0
			33015	14725	6052	10699	1539		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- 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	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- 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	98	Total	C	N	O	S	0	0
			786	493	150	142	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
			955	590	196	165	4		

- 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	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0
			710	437	143	129	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	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	10	Total	C	N	O	P	0	0
			218	98	44	66	10		

- Molecule 23 is a RNA chain called A-site Lysine tRNA Lysine.

Mol	Chain	Residues	Atoms					AltConf	Trace	
23	AW	74	Total	C	N	O	P	S	0	0
			1593	716	280	522	73	2		

- Molecule 24 is a RNA chain called P-site tRNA Aspartate.

Mol	Chain	Residues	Atoms					AltConf	Trace	
24	AX	77	Total	C	N	O	P	S	0	0
			1656	741	290	547	77	1		

- Molecule 25 is a RNA chain called E-site tRNA Valine.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	AY	71	Total	C	N	O	P	S	0	0
			1525	682	276	496	70	1		

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BA	2897	Total	C	N	O	P	0	0
			62195	27745	11446	20107	2897		

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BB	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 28 is a protein called 50S ribosomal protein L2.

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

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

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

- Molecule 32 is a protein called 50S ribosomal protein L6.

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

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BH	47	Total	C	N	O	S	0	0
			359	233	62	63	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BI	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BK	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BL	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BM	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BW	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BY	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

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

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

- Molecule 52 is a protein called 50S ribosomal protein L32.

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

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	B1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 54 is a protein called 50S ribosomal protein L34.

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

- Molecule 55 is a protein called 50S ribosomal protein L35.

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

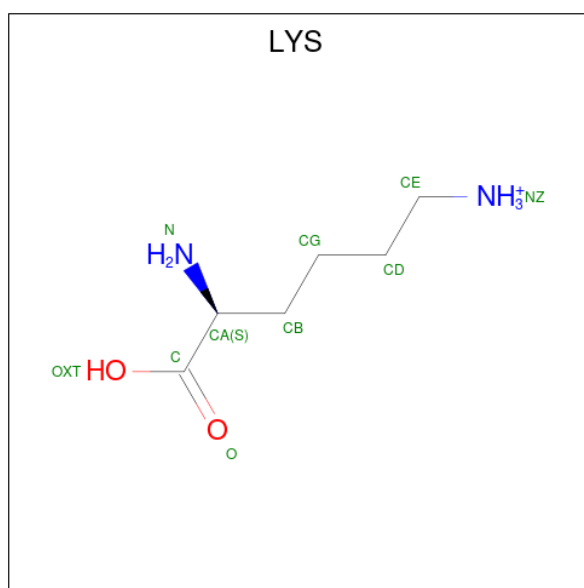
- Molecule 56 is a protein called 50S ribosomal protein L36.

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

- Molecule 57 is a protein called ErmBL.

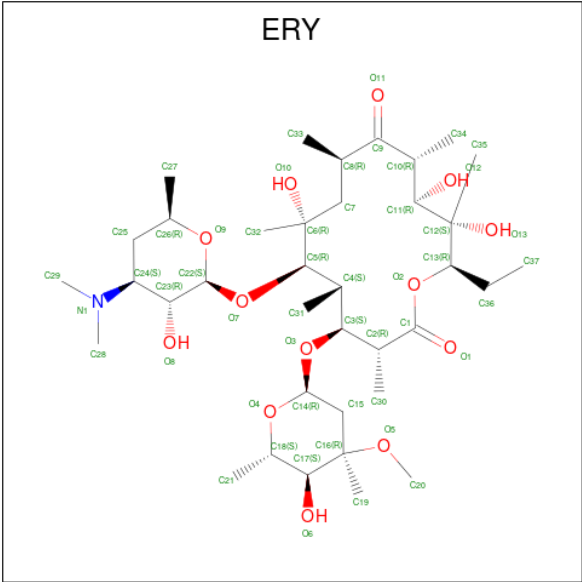
Mol	Chain	Residues	Atoms					AltConf	Trace
57	B5	9	Total	C	N	O	S	0	0
			74	46	14	13	1		

- Molecule 58 is LYSINE (CCD ID: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms				AltConf
58	AW	1	Total	C	N	O	0
			9	6	2	1	

- Molecule 59 is ERYTHROMYCIN A (CCD ID: ERY) (formula: $C_{37}H_{67}NO_{13}$).

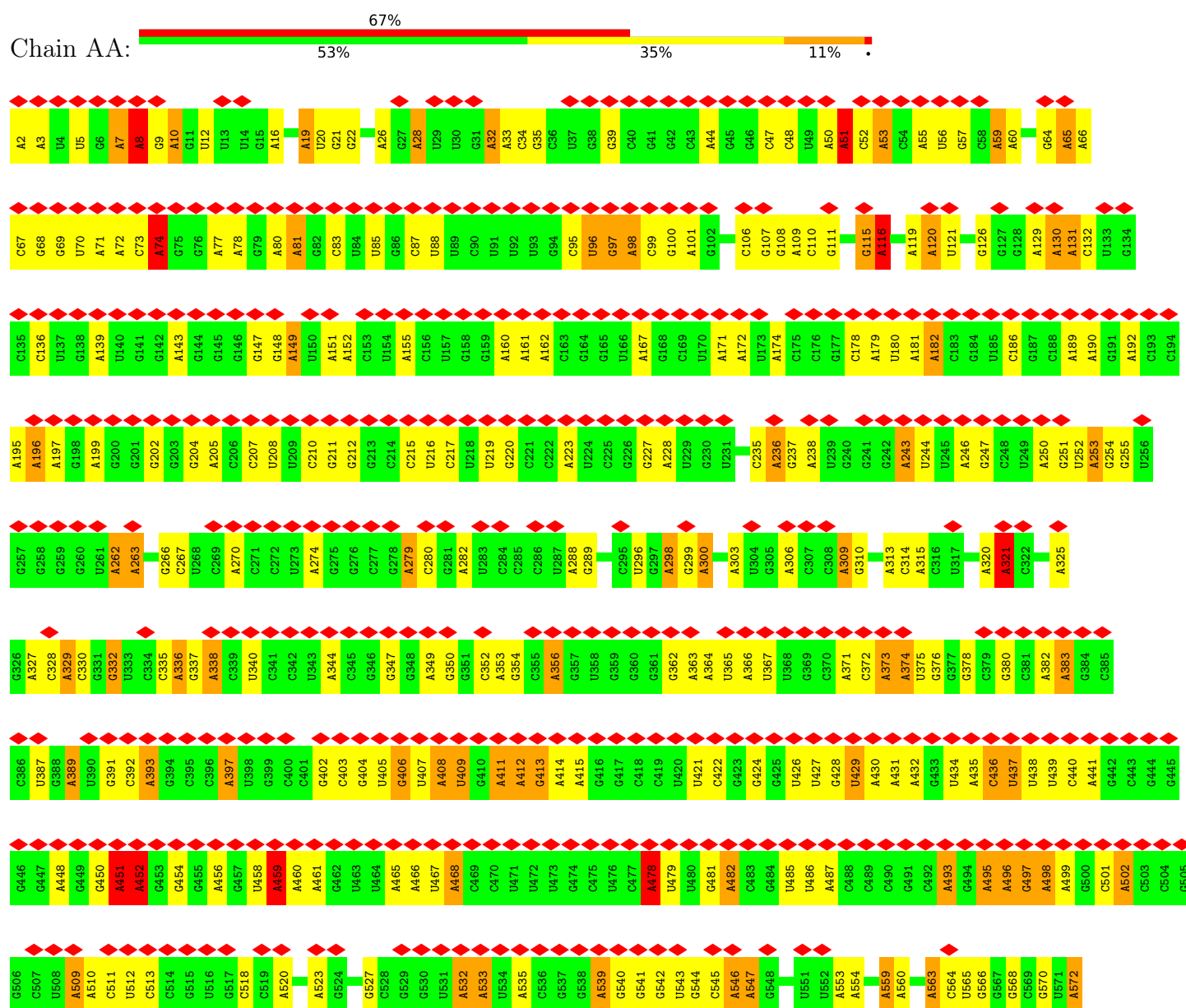


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
59	BA	1	51	37	1	13	0

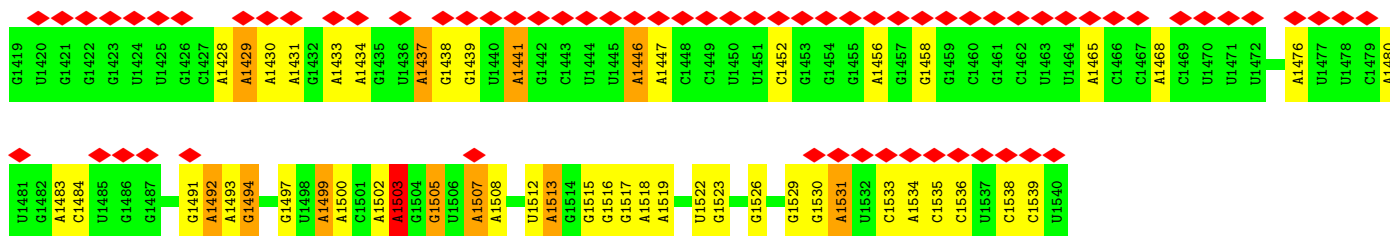
3 Residue-property plots

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

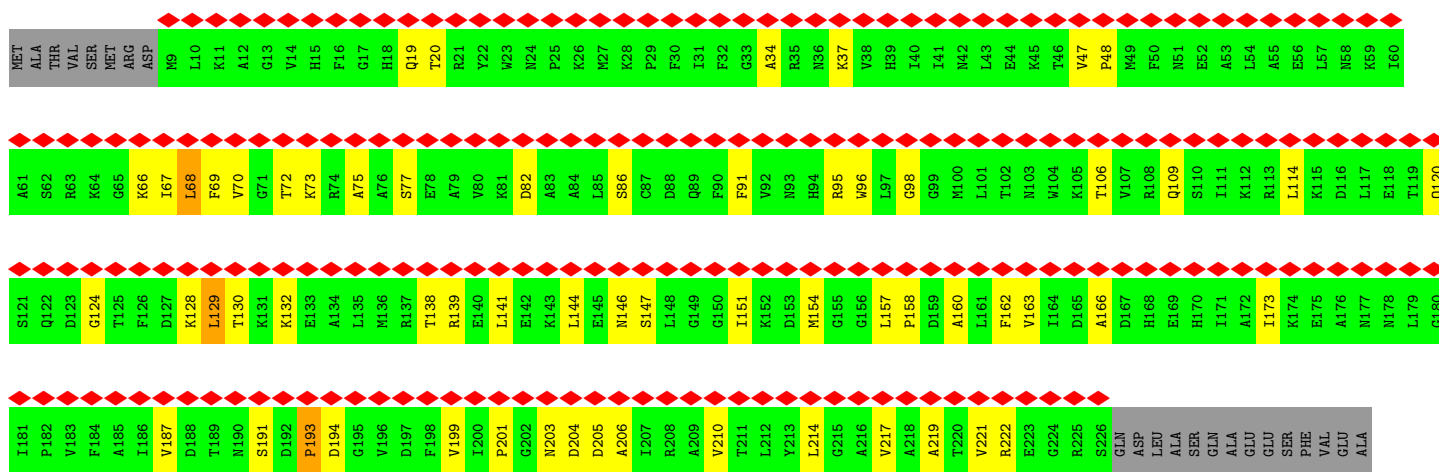
• Molecule 1: 16S ribosomal RNA



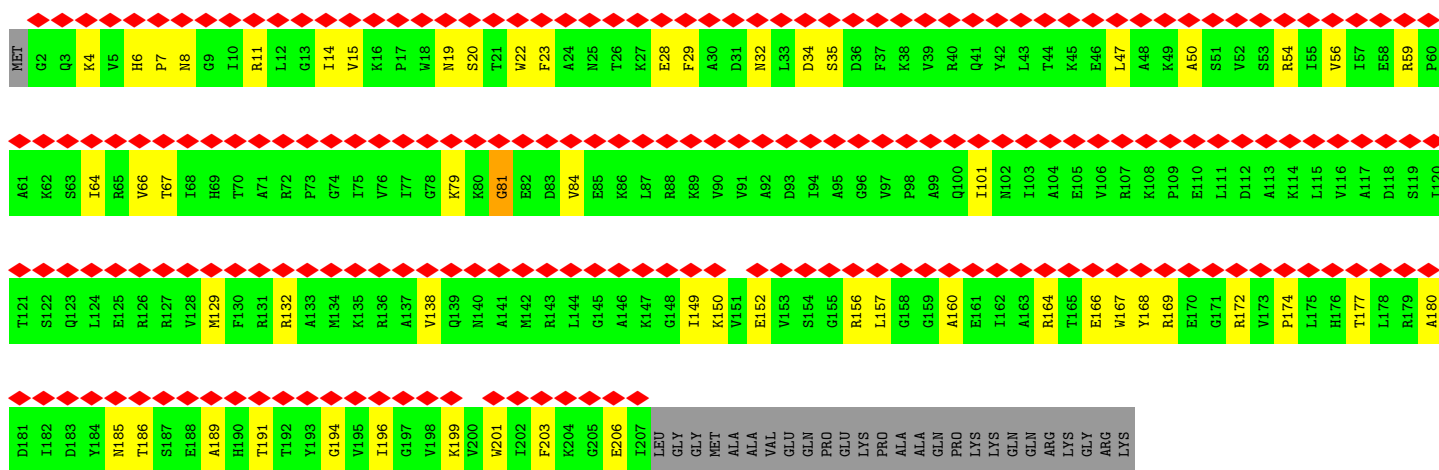




• Molecule 2: 30S ribosomal protein S2



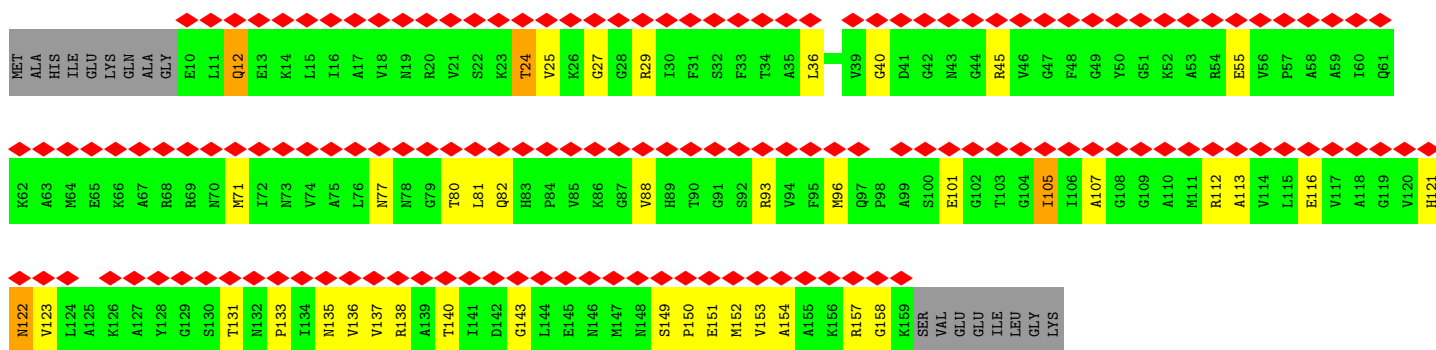
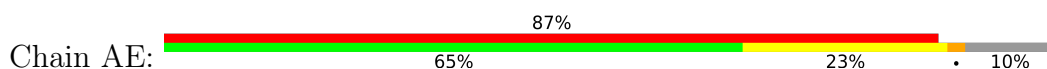
• Molecule 3: 30S ribosomal protein S3



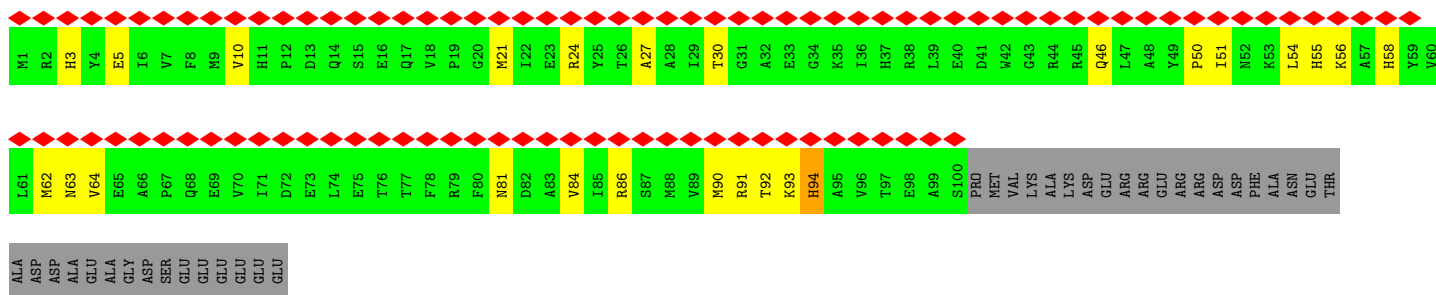
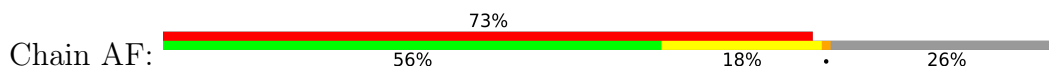
• Molecule 4: 30S ribosomal protein S4



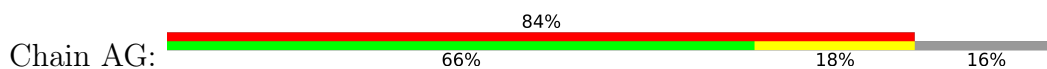
- Molecule 5: 30S ribosomal protein S5

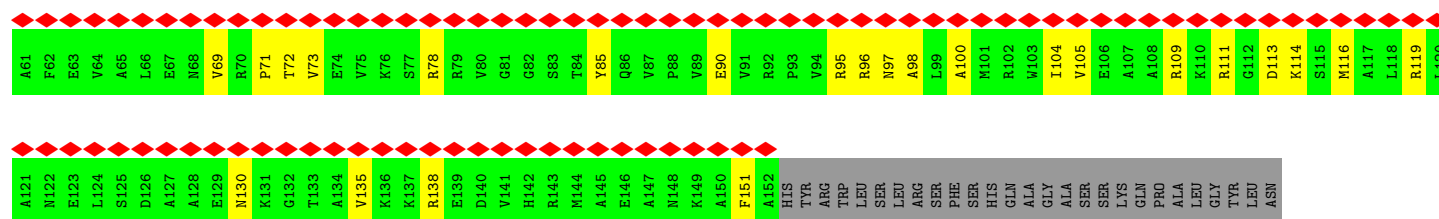


- Molecule 6: 30S ribosomal protein S6



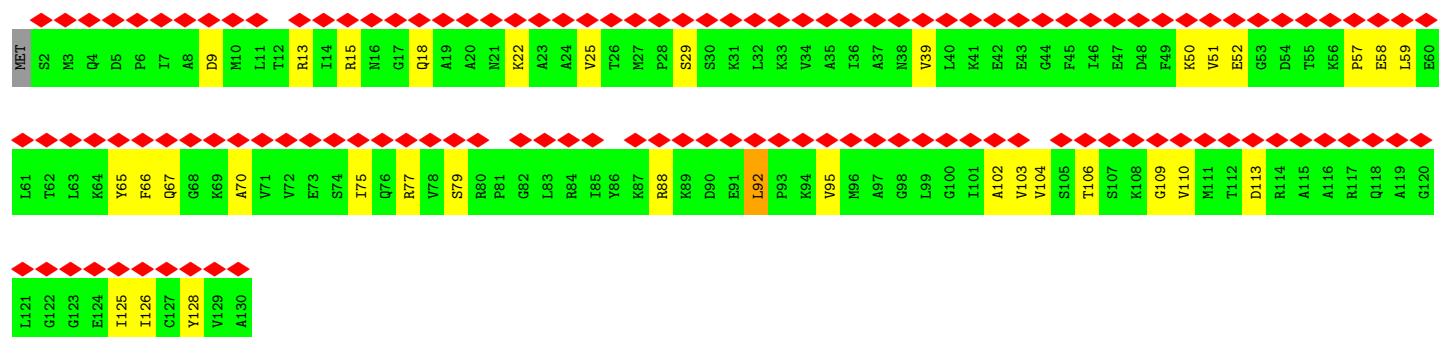
- Molecule 7: 30S ribosomal protein S7





• Molecule 8: 30S ribosomal protein S8

Chain AH: 96% 73% 25%



• Molecule 9: 30S ribosomal protein S9

Chain AI: 98% 65% 32%



• Molecule 10: 30S ribosomal protein S10

Chain AJ: 94% 52% 42% 5%

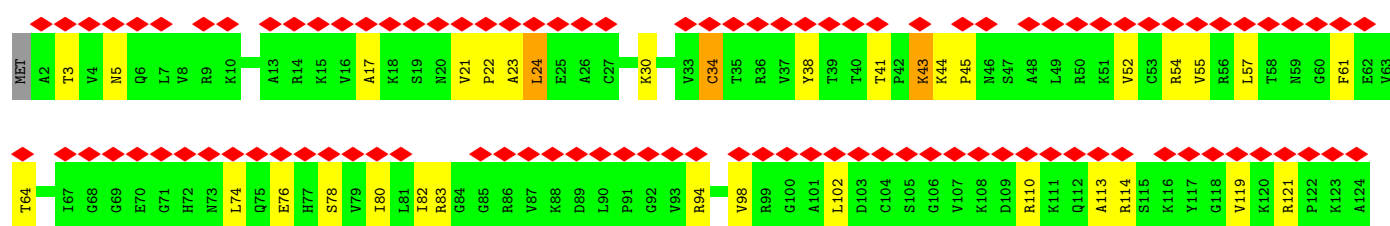
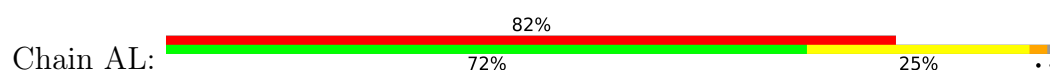


• Molecule 11: 30S ribosomal protein S11

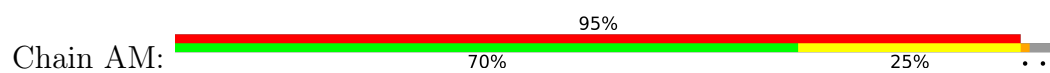
Chain AK: 88% 59% 31% 9%



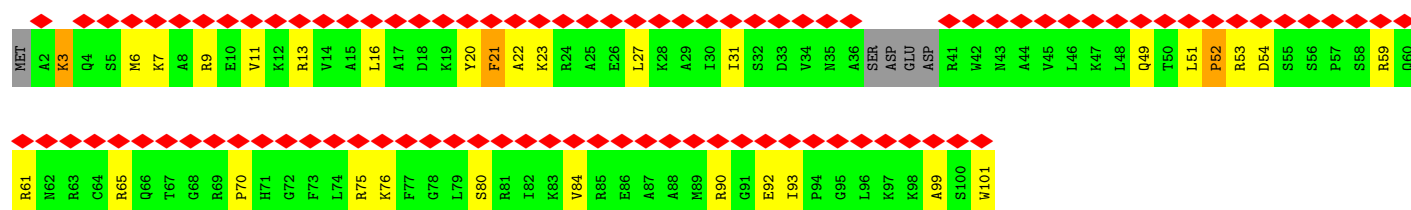
• Molecule 12: 30S ribosomal protein S12



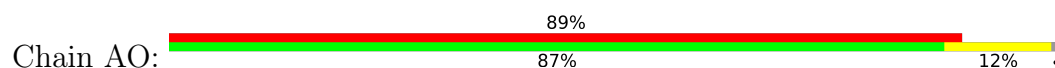
• Molecule 13: 30S ribosomal protein S13

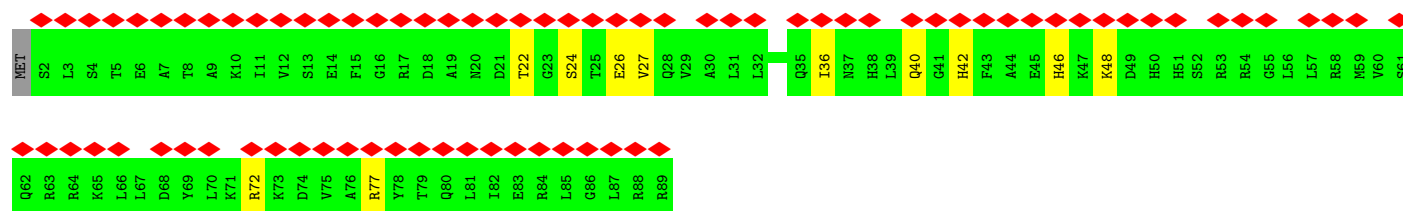


• Molecule 14: 30S ribosomal protein S14

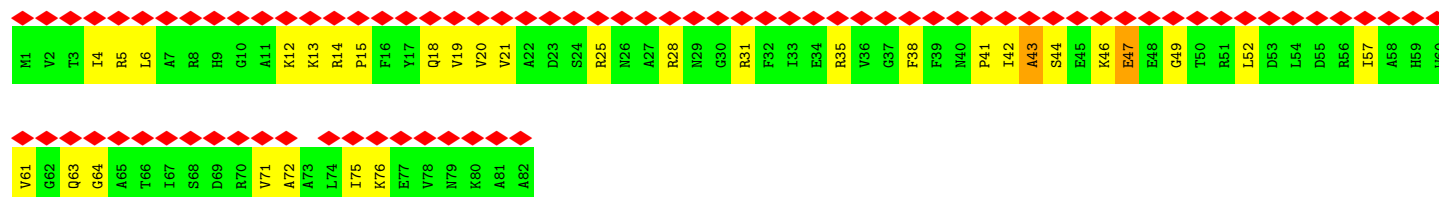


• Molecule 15: 30S ribosomal protein S15

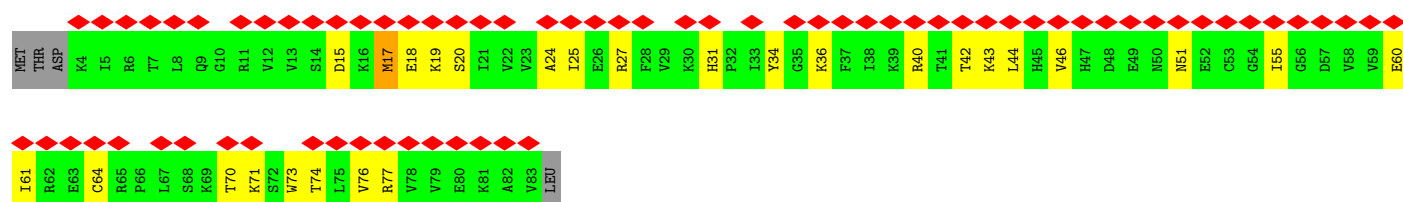
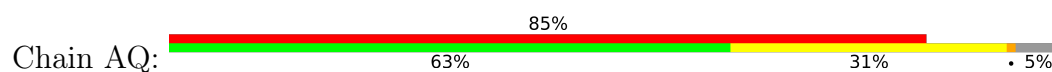




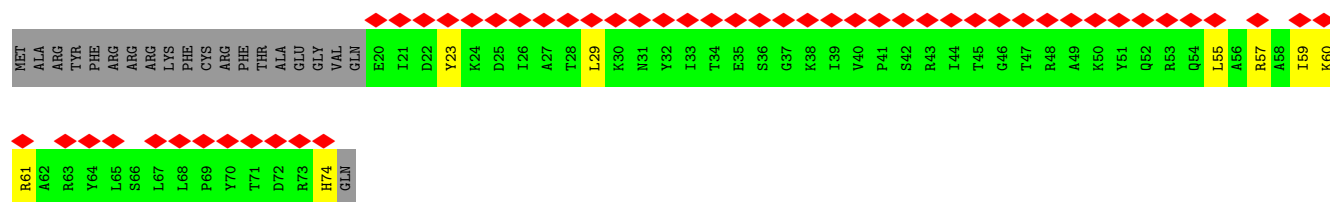
• Molecule 16: 30S ribosomal protein S16



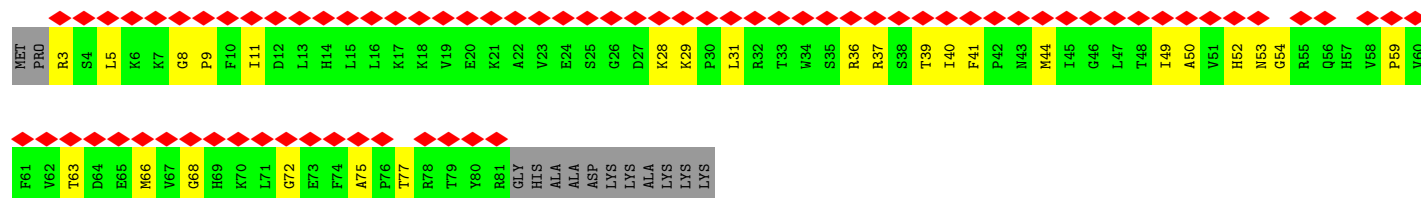
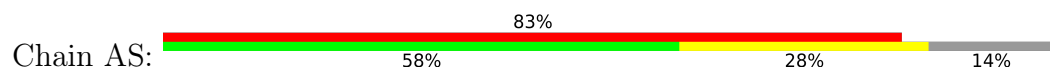
• Molecule 17: 30S ribosomal protein S17



• Molecule 18: 30S ribosomal protein S18

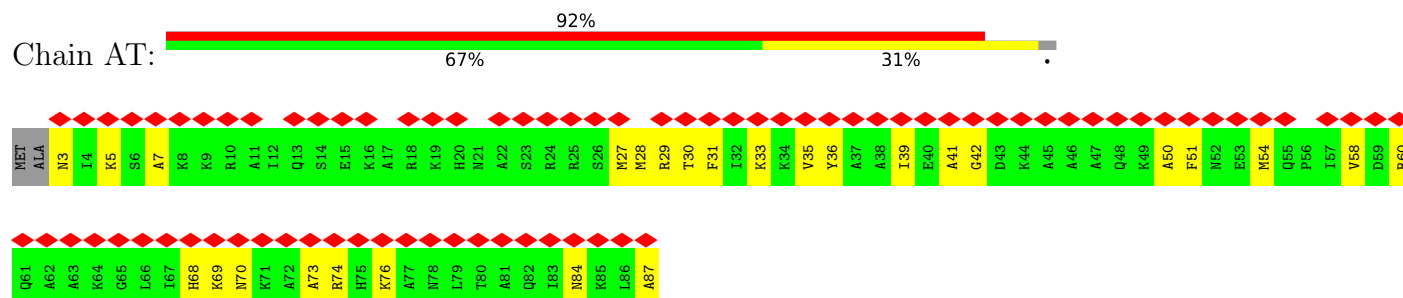


• Molecule 19: 30S ribosomal protein S19



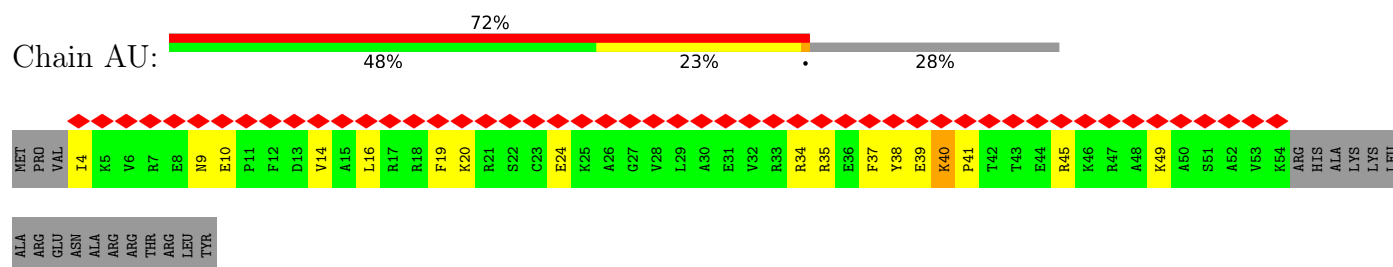
- Molecule 20: 30S ribosomal protein S20

Chain AT:



- Molecule 21: 30S ribosomal protein S21

Chain AU:



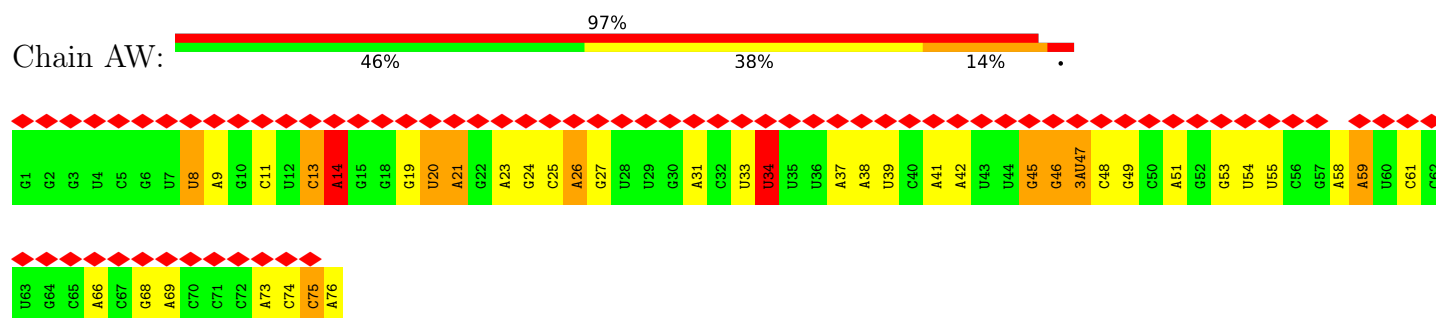
- Molecule 22: mRNA

Chain AV:



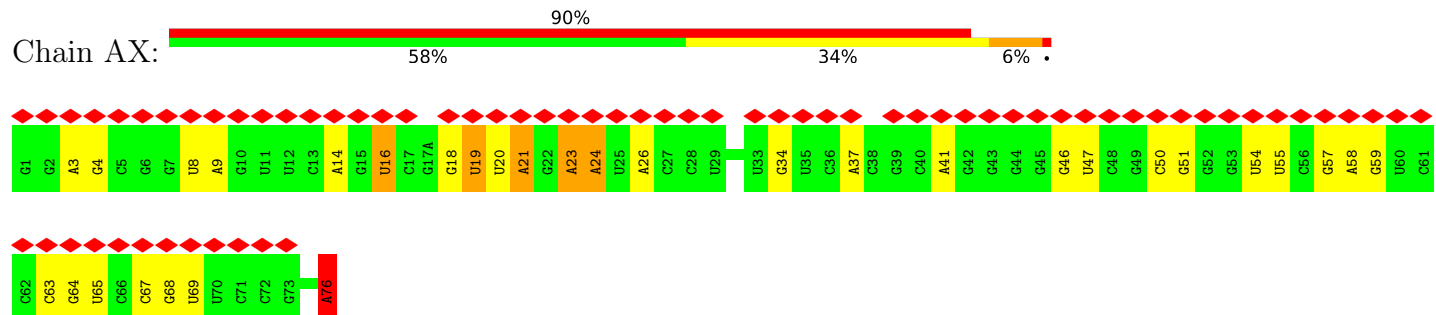
- Molecule 23: A-site Lysine tRNA Lysine

Chain AW:



- Molecule 24: P-site tRNA Aspartate

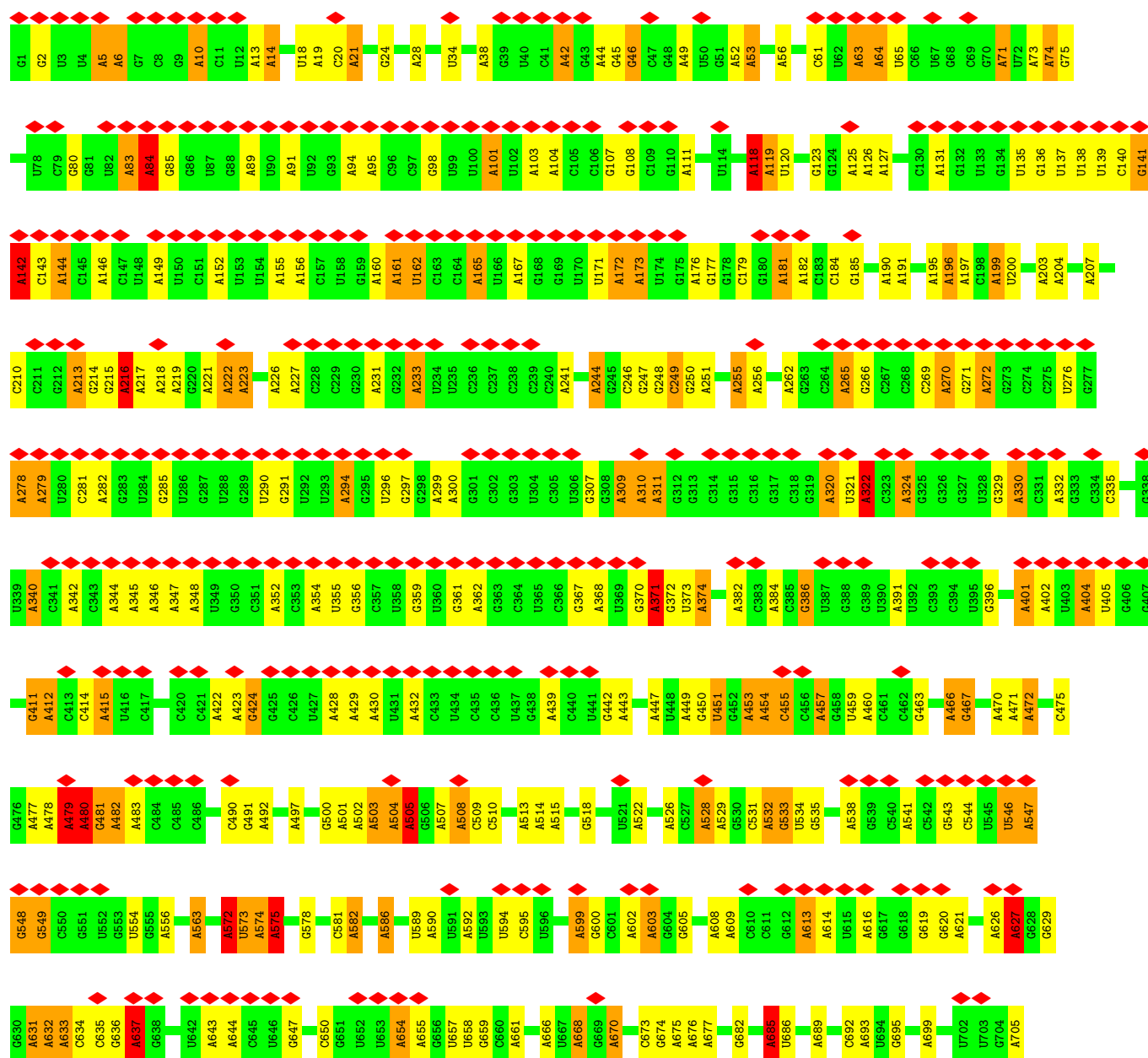
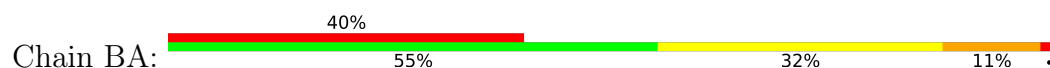
Chain AX:

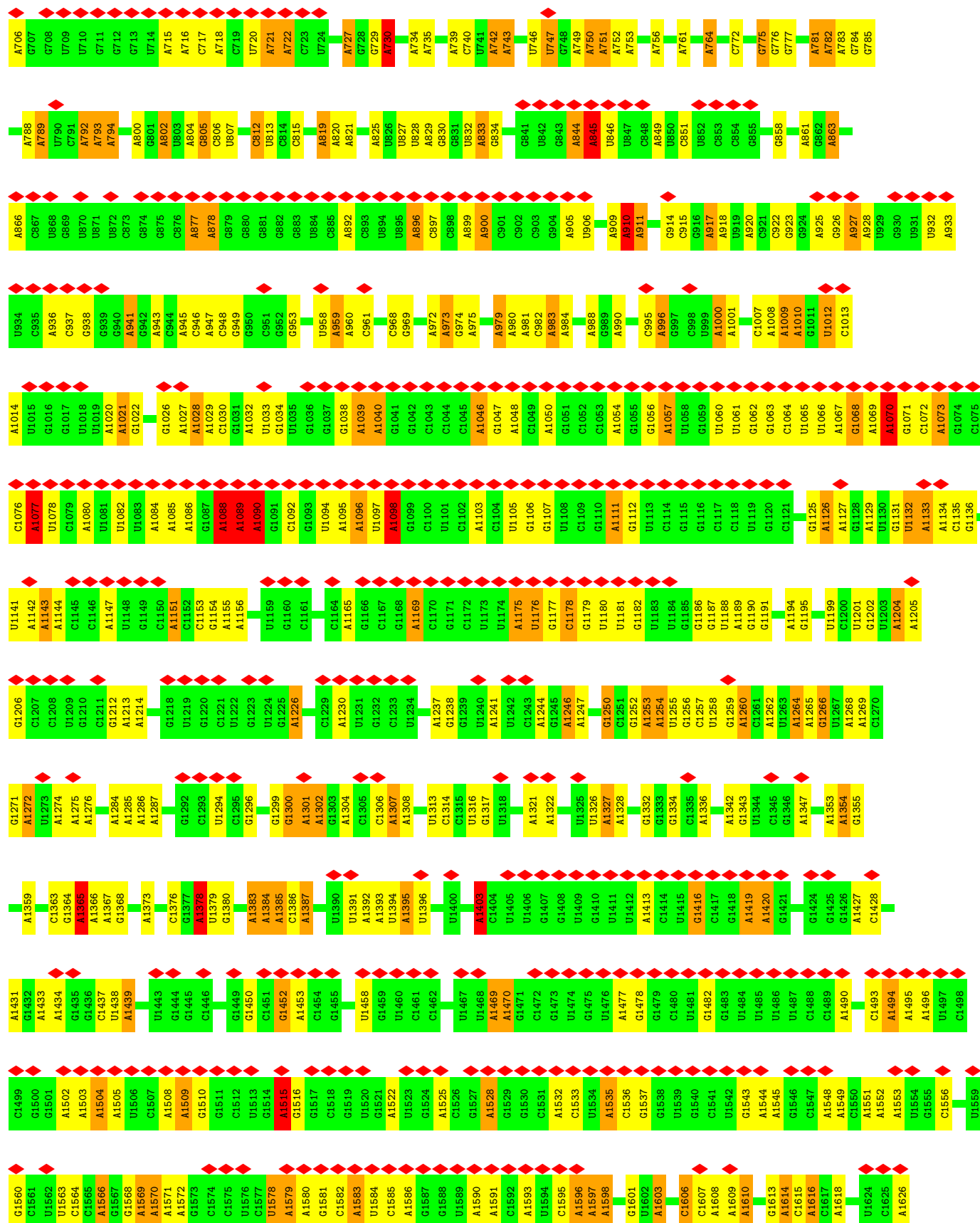


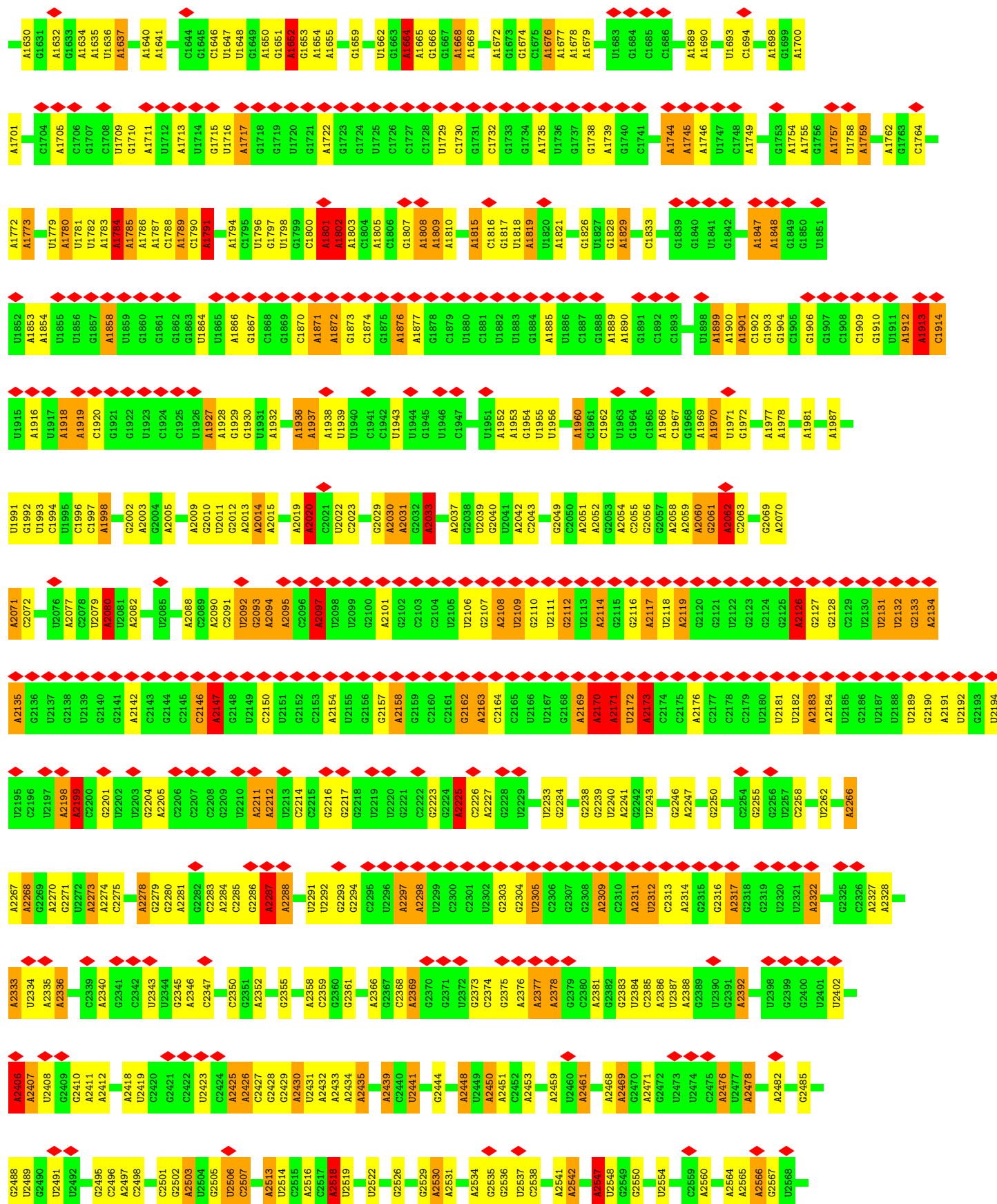
● Molecule 25: E-site tRNA Valine

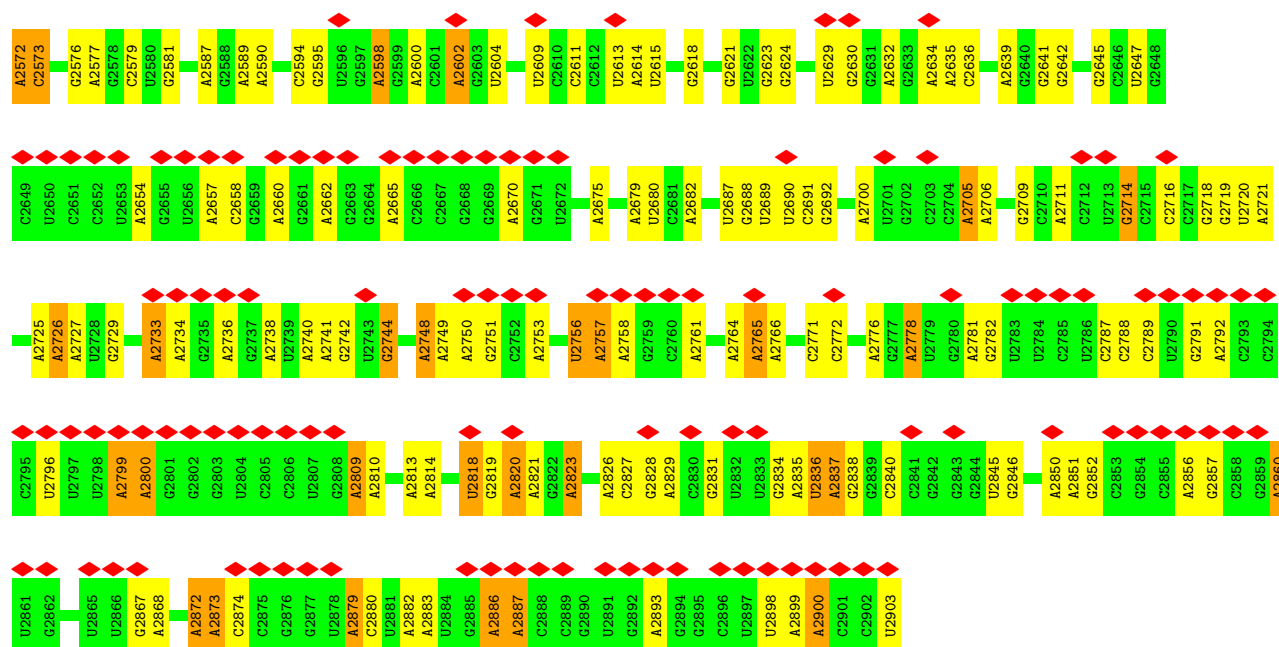


● Molecule 26: 23S ribosomal RNA

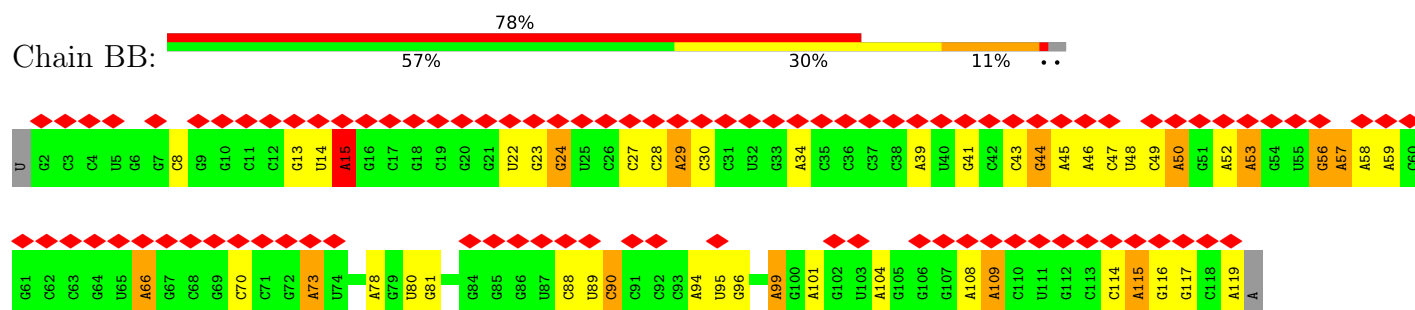




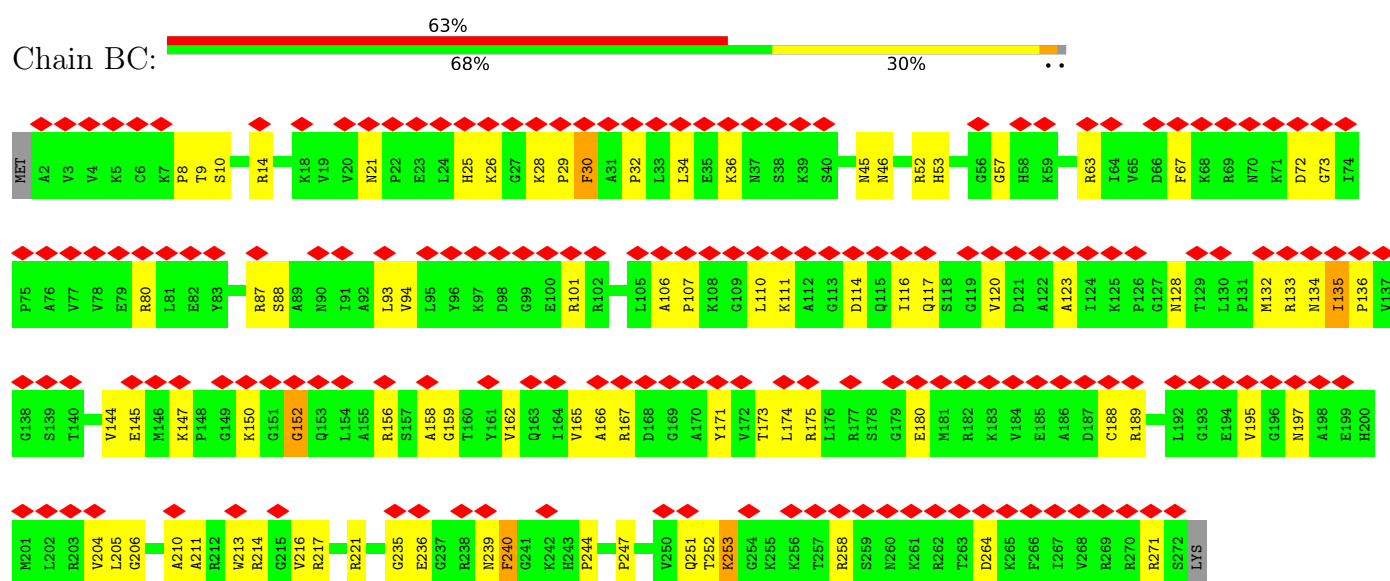




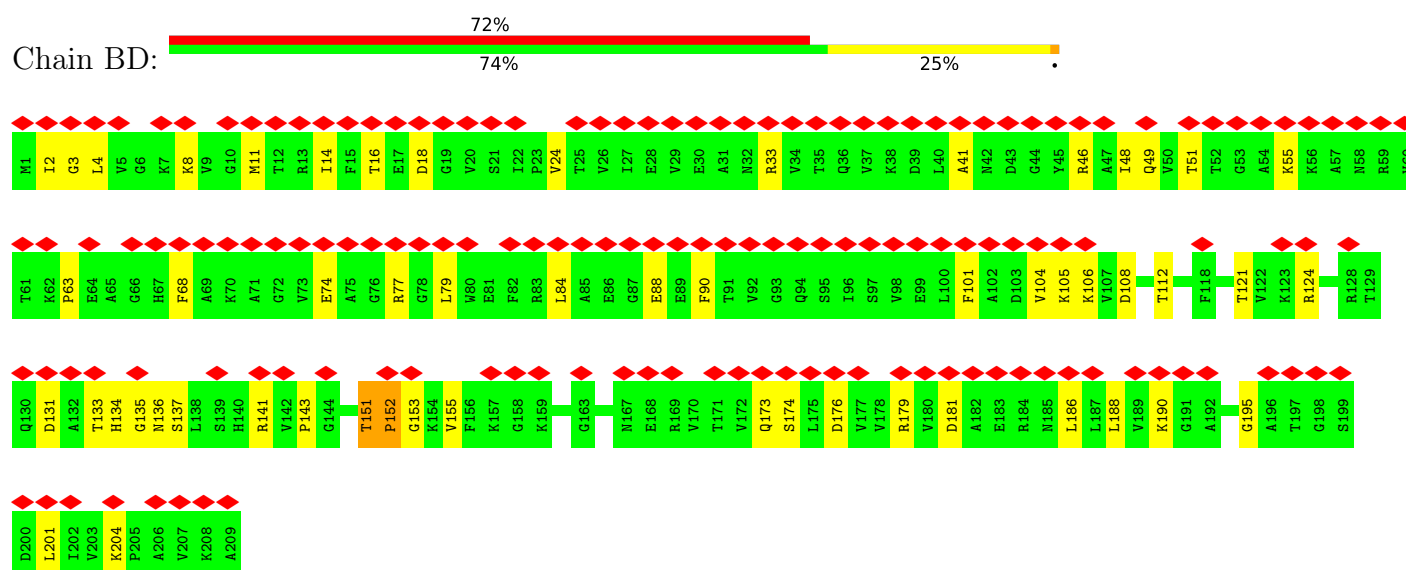
• Molecule 27: 5S ribosomal RNA



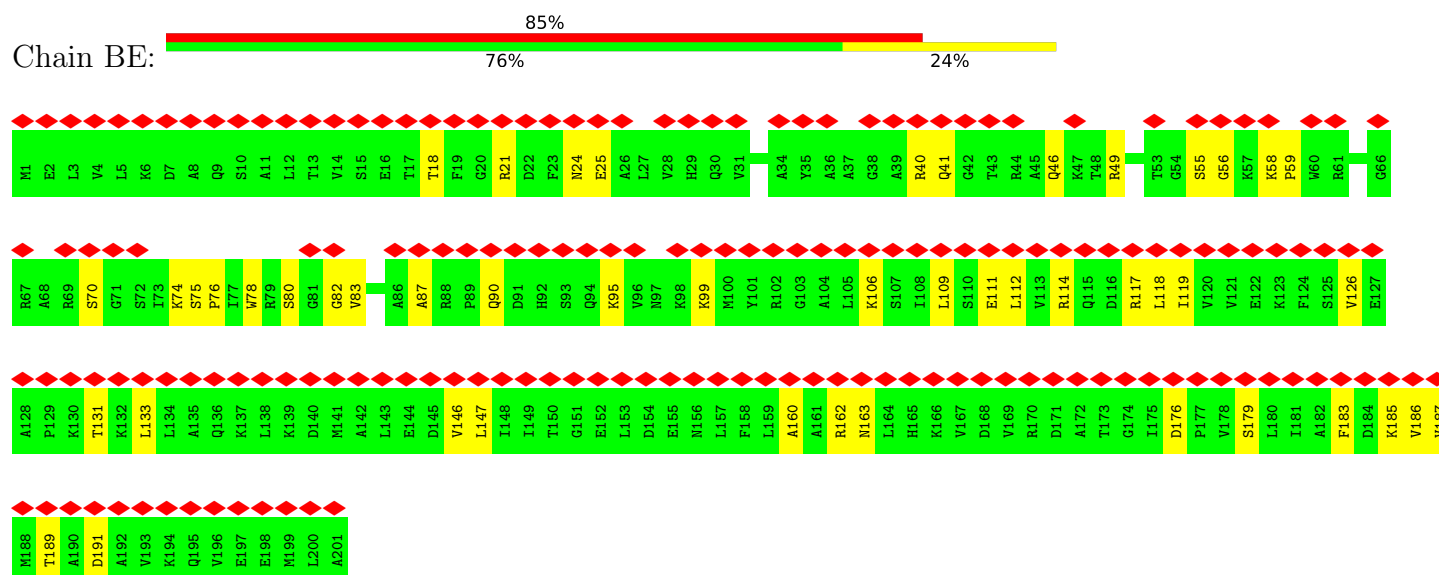
• Molecule 28: 50S ribosomal protein L2



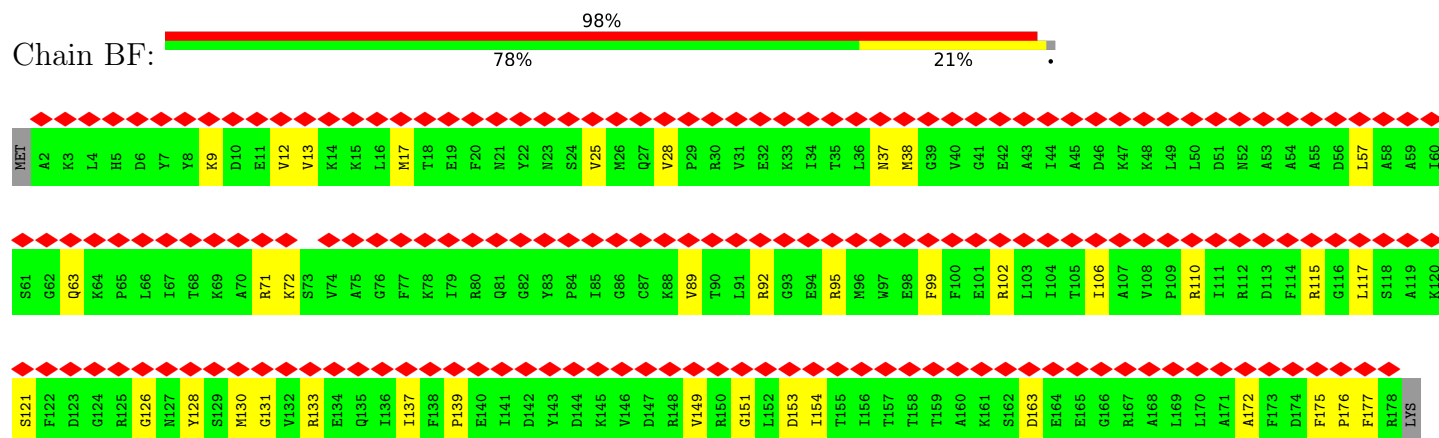
• Molecule 29: 50S ribosomal protein L3



- Molecule 30: 50S ribosomal protein L4



- Molecule 31: 50S ribosomal protein L5



- Molecule 32: 50S ribosomal protein L6

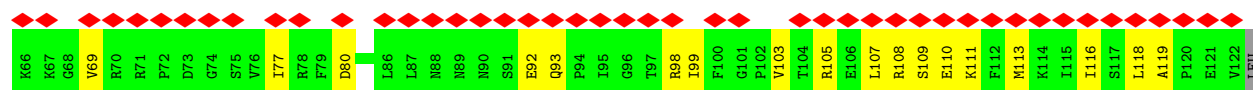
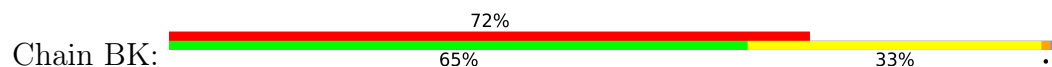
I121	G61	R2
T122	W62	R3
A123	A63	V4
E124	Q64	A5
G125	A65	K6
P126	G66	A7
T127	T67	P8
Q128	A68	V9
T129	R69	V10
E130	A70	V11
I131	L71	P12
V132	L72	A13
L133	N73	G14
K134	S74	V15
G135	M75	D16
A136	V76	V17
D137	T77	K18
K138	G78	I19
Q139	V79	N20
V140	T80	G21
I141	E81	Q22
G142	G82	V23
Q143	F83	T24
V144	T84	T25
A145	K85	L26
A146	K86	K27
D147	L87	G28
L148	Q88	K29
R149	L89	N30
A150	V90	G31
V151	G91	E32
R152	V92	L33
R153	G93	T34
P154	Y94	R35
E155	R95	T36
P156	A96	L37
V157	A97	N38
K158	V98	D39
G159	K99	A40
R160	G100	V41
G161	N101	E42
V162	V102	V43
R163	L103	K44
Y164	A104	H45
A165	L105	A46
D166	S106	D47
V168	L107	N48
V169	G108	T49
R170	F109	L50
T171	S110	T51
K172	H111	F52
K173	P112	G53
E174	V113	P54
A174	D114	R55
K175	H115	D56
K176	Q116	G57
K177	L117	Y58
	P118	A59
	A119	G120
		N60

[illegible][illegible]

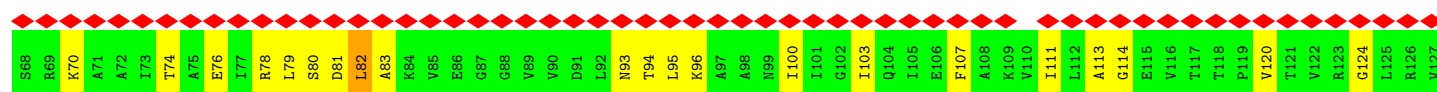
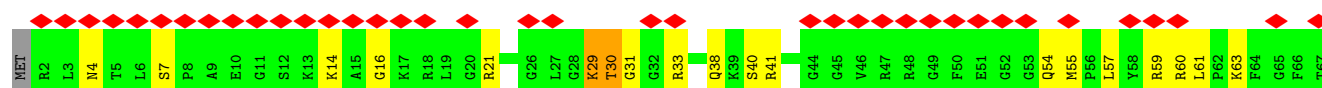
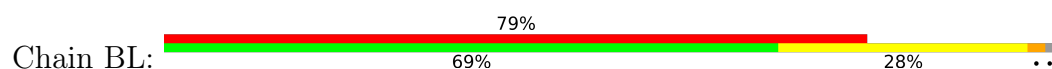
M1	K61
K2	V62
T3	A63
F4	V64
T5	T65
A6	G66
K7	N67
P8	K68
E9	R69
T10	T70
V11	D71
K12	T72
R13	V73
V14	T74
A15	T75
V16	H76
V17	H77
V18	T78
D19	G79
A20	H80
T21	I81
G22	G82
K23	G83
T24	I84
L25	K85
G26	K86
R27	A87
L28	T88
A29	F89
T30	E90
E31	E91
L32	M92
A33	I93
R34	A94
A35	R95
L36	R96
R37	P97
G38	E98
A39	R99
H40	V100
K41	I101
A42	E102
E43	L103
V44	
T45	K106
P46	G107
H47	M108
V48	L109
D49	P110
T50	K111
G51	L114
D52	A117
V53	M118
S54	
V56	F119
L57	R120
N58	K121
A59	L122
	K123



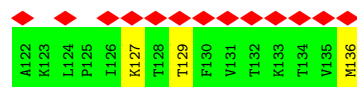
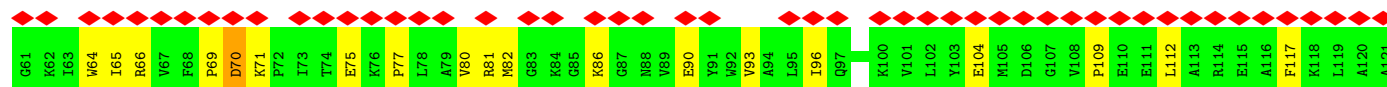
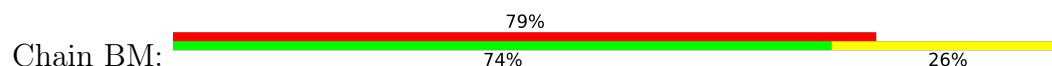
• Molecule 36: 50S ribosomal protein L14



• Molecule 37: 50S ribosomal protein L15

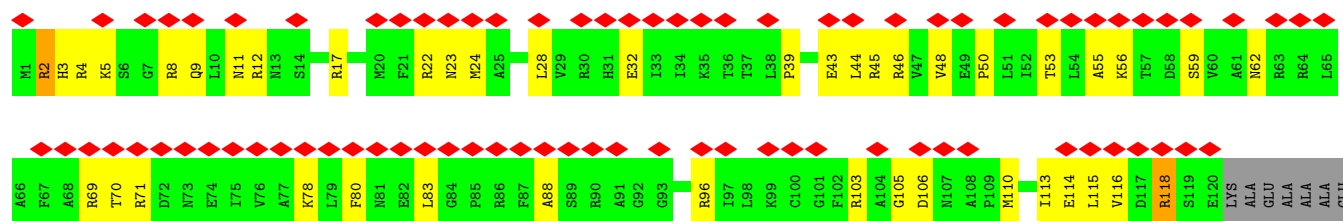


• Molecule 38: 50S ribosomal protein L16



• Molecule 39: 50S ribosomal protein L17





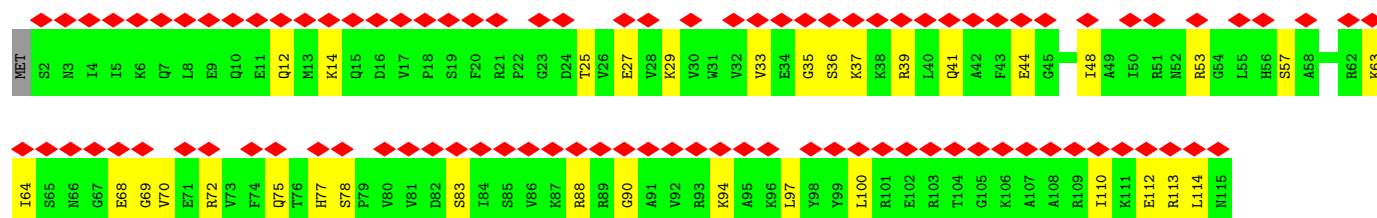
• Molecule 40: 50S ribosomal protein L18

Chain BO: 98%
72% 26%



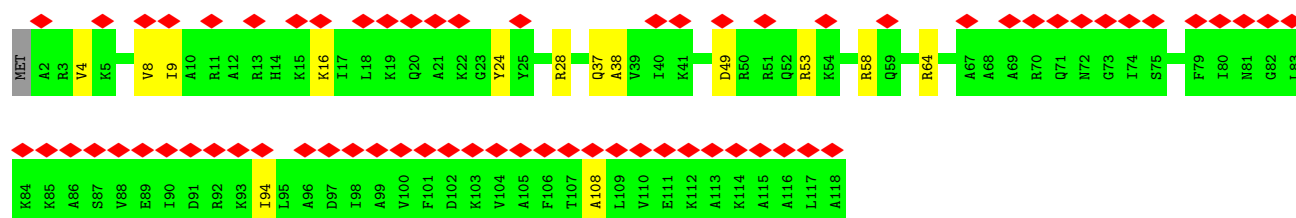
• Molecule 41: 50S ribosomal protein L19

Chain BP: 83%
70% 30%



• Molecule 42: 50S ribosomal protein L20

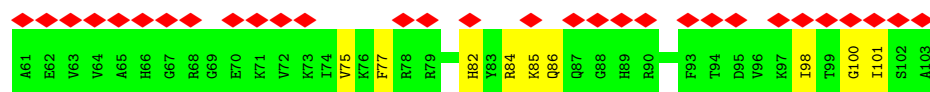
Chain BQ: 57%
87% 12%



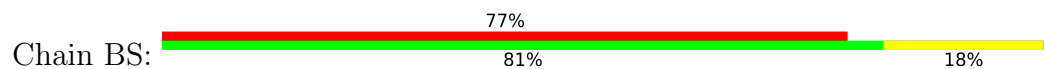
• Molecule 43: 50S ribosomal protein L21

Chain BR: 84%
73% 27%

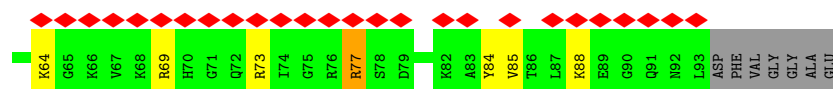
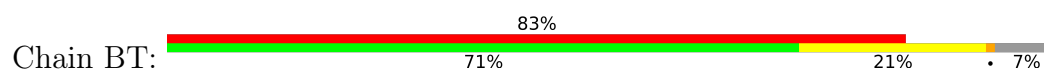




• Molecule 44: 50S ribosomal protein L22



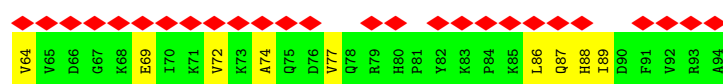
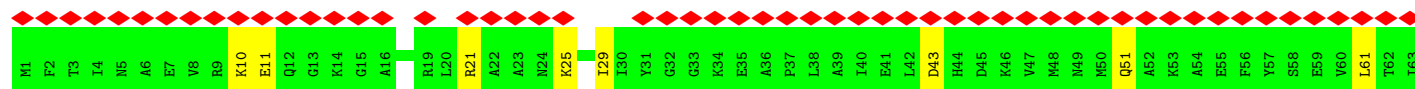
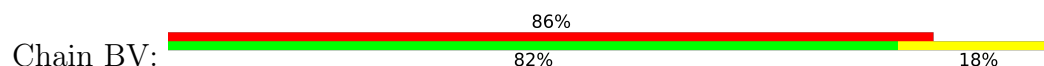
• Molecule 45: 50S ribosomal protein L23



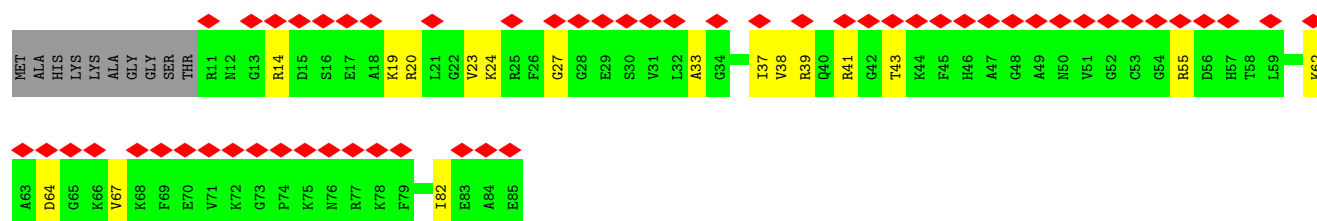
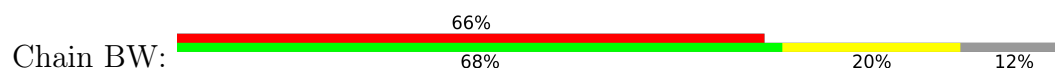
• Molecule 46: 50S ribosomal protein L24



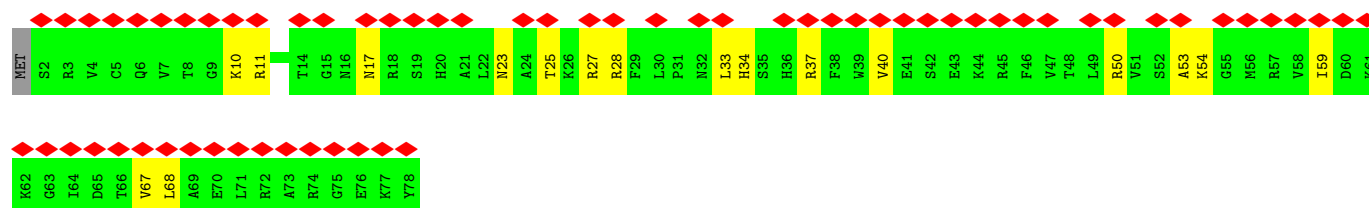
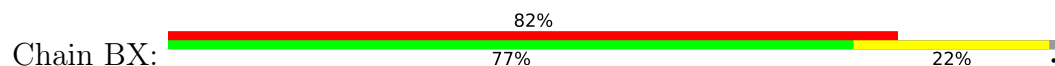
• Molecule 47: 50S ribosomal protein L25



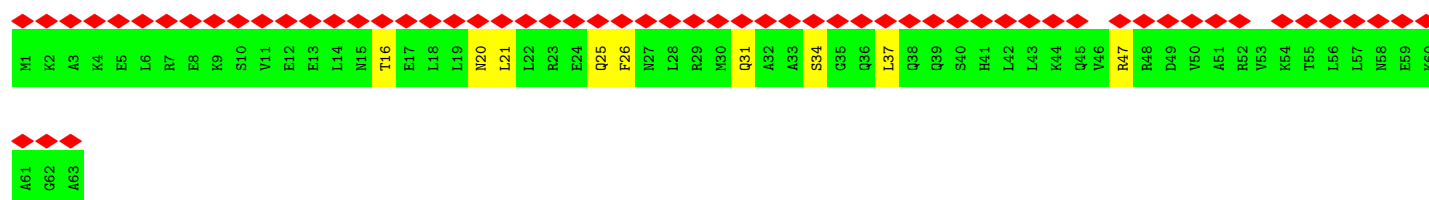
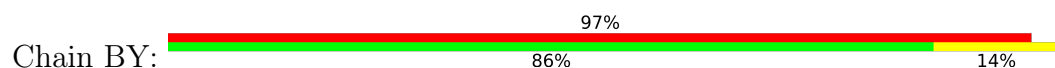
• Molecule 48: 50S ribosomal protein L27



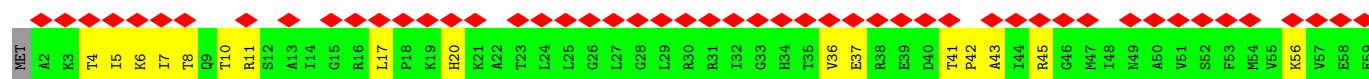
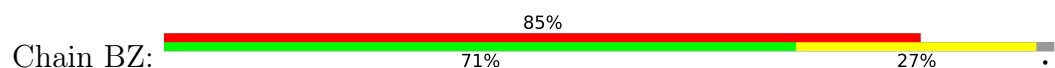
- Molecule 49: 50S ribosomal protein L28



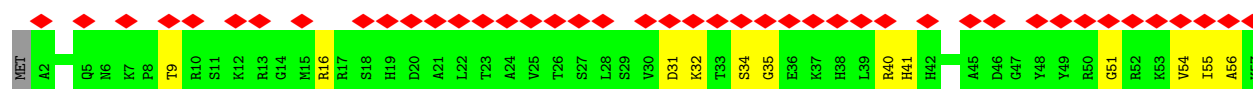
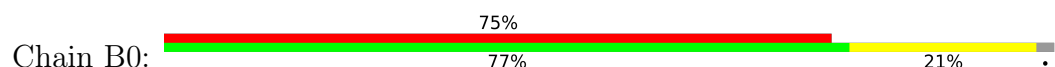
- Molecule 50: 50S ribosomal protein L29



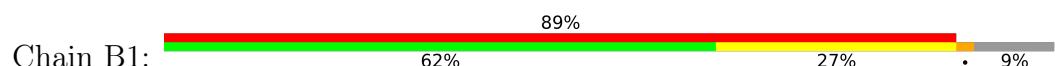
- Molecule 51: 50S ribosomal protein L30



- Molecule 52: 50S ribosomal protein L32

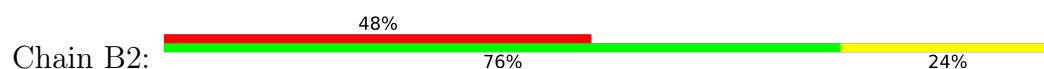


- Molecule 53: 50S ribosomal protein L33

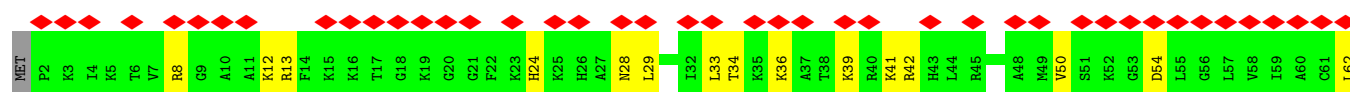
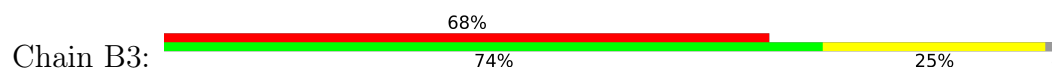




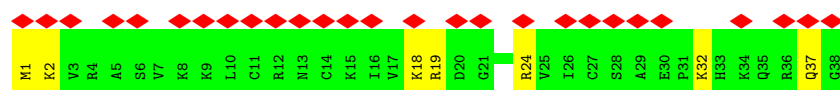
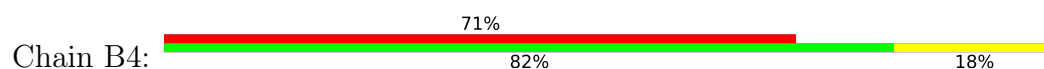
- Molecule 54: 50S ribosomal protein L34



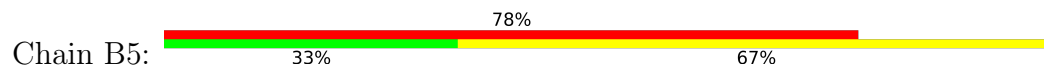
- Molecule 55: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L36



- Molecule 57: ErmBL



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85393	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	4	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.010	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.00194	Depositor
Map size (Å)	407.74402, 407.74402, 407.74402	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.108, 1.108, 1.108	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, QUO, 6MZ, U8U, CM0, T6A, 5MU, 2MA, 7MG, ERY, 3AU, 4SU

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	0.86	387/36965 (1.0%)	0.64	0/57662
2	AB	0.44	0/1735	0.74	1/2338 (0.0%)
3	AC	0.35	0/1651	0.72	0/2225
4	AD	0.37	0/1665	0.76	1/2227 (0.0%)
5	AE	0.34	0/1118	0.78	0/1504
6	AF	0.35	0/835	0.72	0/1128
7	AG	0.33	0/1195	0.70	0/1602
8	AH	0.37	0/989	0.76	3/1326 (0.2%)
9	AI	0.41	1/1034 (0.1%)	0.76	0/1375
10	AJ	0.45	0/796	0.76	0/1077
11	AK	0.36	0/893	0.75	2/1205 (0.2%)
12	AL	0.36	0/969	0.84	5/1300 (0.4%)
13	AM	0.38	0/892	0.75	0/1193
14	AN	0.32	0/785	0.71	0/1043
15	AO	0.37	0/718	0.64	0/959
16	AP	0.36	0/659	0.71	0/884
17	AQ	0.41	0/657	0.82	0/881
18	AR	0.36	0/462	0.67	0/621
19	AS	0.38	0/652	0.73	0/877
20	AT	0.34	0/671	0.70	0/888
21	AU	0.34	0/430	0.77	2/570 (0.4%)
22	AV	1.32	6/245 (2.4%)	0.97	0/380
23	AW	0.94	18/1569 (1.1%)	0.65	0/2437
24	AX	0.86	13/1668 (0.8%)	0.52	0/2593
25	AY	0.78	13/1554 (0.8%)	0.58	0/2416
26	BA	0.88	761/69659 (1.1%)	0.65	0/108672
27	BB	0.76	23/2828 (0.8%)	0.56	0/4410
28	BC	0.36	0/2121	0.77	9/2852 (0.3%)
29	BD	0.38	0/1586	0.74	0/2134
30	BE	0.38	0/1571	0.69	0/2113
31	BF	0.40	0/1434	0.73	0/1926
32	BG	0.39	0/1343	0.74	0/1816

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BH	0.42	0/364	0.75	0/490
34	BI	0.41	0/1046	0.80	4/1410 (0.3%)
35	BJ	0.37	0/1152	0.68	0/1551
36	BK	0.37	0/947	0.77	1/1268 (0.1%)
37	BL	0.35	0/1054	0.74	0/1403
38	BM	0.36	1/1093 (0.1%)	0.69	0/1460
39	BN	0.36	0/973	0.72	0/1301
40	BO	0.35	0/902	0.64	0/1209
41	BP	0.32	0/929	0.72	0/1242
42	BQ	0.31	0/960	0.64	0/1278
43	BR	0.32	0/829	0.67	0/1107
44	BS	0.42	0/864	0.75	1/1156 (0.1%)
45	BT	0.31	0/744	0.68	0/994
46	BU	0.38	0/787	0.74	0/1051
47	BV	0.35	0/766	0.71	0/1025
48	BW	0.33	0/576	0.71	0/762
49	BX	0.30	0/635	0.73	0/848
50	BY	0.28	0/510	0.60	0/677
51	BZ	0.35	0/453	0.72	0/605
52	B0	0.36	0/450	0.69	0/599
53	B1	0.30	0/416	0.66	0/554
54	B2	0.25	0/380	0.65	0/498
55	B3	0.30	0/513	0.66	0/676
56	B4	0.35	0/303	0.73	0/397
57	B5	0.47	0/74	0.84	0/98
All	All	0.77	1223/159069 (0.8%)	0.67	29/238293 (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
29	BD	0	1

All (1223) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	20	U	C5-C6	10.49	1.55	1.34
23	AW	20	U	C5-C6	10.48	1.55	1.34
24	AX	16	U	C5-C6	10.47	1.55	1.34
24	AX	19	U	C5-C6	10.43	1.55	1.34

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	454	A	C6-N6	6.88	1.47	1.33
26	BA	1570	A	C6-N6	6.85	1.47	1.33
1	AA	74	A	C6-N6	6.84	1.47	1.33
26	BA	819	A	C6-N6	6.83	1.47	1.33
26	BA	1937	A	C6-N6	6.83	1.47	1.33
1	AA	681	A	C6-N6	6.82	1.47	1.33
1	AA	1227	A	C6-N6	6.82	1.47	1.33
27	BB	34	A	C6-N6	6.82	1.47	1.33
26	BA	479	A	C6-N6	6.82	1.47	1.33
26	BA	1641	A	C6-N6	6.82	1.47	1.33
1	AA	1005	A	C6-N6	6.82	1.47	1.33
1	AA	1374	A	C6-N6	6.82	1.47	1.33
1	AA	411	A	C6-N6	6.82	1.47	1.33
26	BA	2513	A	C6-N6	6.82	1.47	1.33
1	AA	162	A	C6-N6	6.81	1.47	1.33
26	BA	633	A	C6-N6	6.81	1.47	1.33
26	BA	1014	A	C6-N6	6.81	1.47	1.33
1	AA	431	A	C6-N6	6.81	1.47	1.33
26	BA	190	A	C6-N6	6.81	1.47	1.33
26	BA	905	A	C6-N6	6.81	1.47	1.33
26	BA	1165	A	C6-N6	6.81	1.47	1.33
26	BA	2019	A	C6-N6	6.81	1.47	1.33
26	BA	2033	A	C6-N6	6.80	1.47	1.33
26	BA	2378	A	C6-N6	6.80	1.47	1.33
1	AA	873	A	C6-N6	6.80	1.47	1.33
1	AA	1311	A	C6-N6	6.80	1.47	1.33
1	AA	1375	A	C6-N6	6.80	1.47	1.33
1	AA	190	A	C6-N6	6.80	1.47	1.33
1	AA	1225	A	C6-N6	6.80	1.47	1.33
26	BA	556	A	C6-N6	6.80	1.47	1.33
26	BA	1866	A	C6-N6	6.80	1.47	1.33
26	BA	2392	A	C6-N6	6.80	1.47	1.33
1	AA	50	A	C6-N6	6.80	1.47	1.33
1	AA	554	A	C6-N6	6.80	1.47	1.33
26	BA	52	A	C6-N6	6.80	1.47	1.33
26	BA	1469	A	C6-N6	6.80	1.47	1.33
26	BA	1241	A	C6-N6	6.79	1.47	1.33
26	BA	1590	A	C6-N6	6.79	1.47	1.33
26	BA	429	A	C6-N6	6.79	1.47	1.33
26	BA	654	A	C6-N6	6.79	1.47	1.33
26	BA	1040	A	C6-N6	6.79	1.47	1.33
26	BA	2154	A	C6-N6	6.79	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2776	A	C6-N6	6.79	1.47	1.33
1	AA	155	A	C6-N6	6.79	1.47	1.33
26	BA	191	A	C6-N6	6.79	1.47	1.33
26	BA	1194	A	C6-N6	6.79	1.47	1.33
26	BA	2418	A	C6-N6	6.79	1.47	1.33
1	AA	393	A	C6-N6	6.79	1.47	1.33
1	AA	977	A	C6-N6	6.79	1.47	1.33
1	AA	456	A	C6-N6	6.79	1.47	1.33
1	AA	547	A	C6-N6	6.79	1.47	1.33
1	AA	1000	A	C6-N6	6.79	1.47	1.33
26	BA	127	A	C6-N6	6.79	1.47	1.33
26	BA	2176	A	C6-N6	6.79	1.47	1.33
26	BA	2430	A	C6-N6	6.79	1.47	1.33
1	AA	228	A	C6-N6	6.79	1.47	1.33
1	AA	649	A	C6-N6	6.79	1.47	1.33
1	AA	1410	A	C6-N6	6.79	1.47	1.33
1	AA	572	A	C6-N6	6.79	1.47	1.33
1	AA	907	A	C6-N6	6.79	1.47	1.33
1	AA	908	A	C6-N6	6.79	1.47	1.33
1	AA	1248	A	C6-N6	6.79	1.47	1.33
1	AA	1437	A	C6-N6	6.79	1.47	1.33
26	BA	42	A	C6-N6	6.79	1.47	1.33
26	BA	1284	A	C6-N6	6.79	1.47	1.33
26	BA	1969	A	C6-N6	6.79	1.47	1.33
26	BA	2589	A	C6-N6	6.79	1.47	1.33
1	AA	414	A	C6-N6	6.78	1.47	1.33
1	AA	1441	A	C6-N6	6.78	1.47	1.33
1	AA	1500	A	C6-N6	6.78	1.47	1.33
1	AA	1513	A	C6-N6	6.78	1.47	1.33
26	BA	1508	A	C6-N6	6.78	1.47	1.33
26	BA	2297	A	C6-N6	6.78	1.47	1.33
1	AA	1261	A	C6-N6	6.78	1.47	1.33
26	BA	749	A	C6-N6	6.78	1.47	1.33
1	AA	243	A	C6-N6	6.78	1.47	1.33
1	AA	609	A	C6-N6	6.78	1.47	1.33
1	AA	790	A	C6-N6	6.78	1.47	1.33
1	AA	1146	A	C6-N6	6.78	1.47	1.33
1	AA	1418	A	C6-N6	6.78	1.47	1.33
26	BA	38	A	C6-N6	6.78	1.47	1.33
26	BA	352	A	C6-N6	6.78	1.47	1.33
26	BA	668	A	C6-N6	6.78	1.47	1.33
26	BA	792	A	C6-N6	6.78	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1246	A	C6-N6	6.78	1.47	1.33
26	BA	1490	A	C6-N6	6.78	1.47	1.33
26	BA	1981	A	C6-N6	6.78	1.47	1.33
26	BA	2266	A	C6-N6	6.78	1.47	1.33
26	BA	2366	A	C6-N6	6.78	1.47	1.33
26	BA	2665	A	C6-N6	6.78	1.47	1.33
1	AA	901	A	C6-N6	6.78	1.47	1.33
26	BA	401	A	C6-N6	6.78	1.47	1.33
26	BA	1987	A	C6-N6	6.78	1.47	1.33
26	BA	2632	A	C6-N6	6.78	1.47	1.33
26	BA	2781	A	C6-N6	6.78	1.47	1.33
1	AA	59	A	C6-N6	6.78	1.47	1.33
1	AA	860	A	C6-N6	6.78	1.47	1.33
1	AA	1014	A	C6-N6	6.78	1.47	1.33
1	AA	1110	A	C6-N6	6.78	1.47	1.33
1	AA	1319	A	C6-N6	6.78	1.47	1.33
1	AA	1329	A	C6-N6	6.78	1.47	1.33
26	BA	432	A	C6-N6	6.78	1.47	1.33
26	BA	447	A	C6-N6	6.78	1.47	1.33
26	BA	614	A	C6-N6	6.78	1.47	1.33
26	BA	960	A	C6-N6	6.78	1.47	1.33
26	BA	1054	A	C6-N6	6.78	1.47	1.33
26	BA	1336	A	C6-N6	6.78	1.47	1.33
26	BA	1366	A	C6-N6	6.78	1.47	1.33
26	BA	2602	A	C6-N6	6.78	1.47	1.33
26	BA	2748	A	C6-N6	6.78	1.47	1.33
26	BA	2821	A	C6-N6	6.78	1.47	1.33
1	AA	309	A	C6-N6	6.78	1.47	1.33
1	AA	825	A	C6-N6	6.78	1.47	1.33
1	AA	983	A	C6-N6	6.78	1.47	1.33
1	AA	1179	A	C6-N6	6.78	1.47	1.33
1	AA	1483	A	C6-N6	6.78	1.47	1.33
26	BA	310	A	C6-N6	6.78	1.47	1.33
26	BA	340	A	C6-N6	6.78	1.47	1.33
26	BA	439	A	C6-N6	6.78	1.47	1.33
26	BA	945	A	C6-N6	6.78	1.47	1.33
26	BA	984	A	C6-N6	6.78	1.47	1.33
26	BA	1304	A	C6-N6	6.78	1.47	1.33
26	BA	1757	A	C6-N6	6.78	1.47	1.33
26	BA	2205	A	C6-N6	6.78	1.47	1.33
26	BA	2340	A	C6-N6	6.78	1.47	1.33
26	BA	2426	A	C6-N6	6.78	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2435	A	C6-N6	6.78	1.47	1.33
26	BA	2468	A	C6-N6	6.78	1.47	1.33
1	AA	77	A	C6-N6	6.77	1.47	1.33
1	AA	749	A	C6-N6	6.77	1.47	1.33
26	BA	203	A	C6-N6	6.77	1.47	1.33
26	BA	2434	A	C6-N6	6.77	1.47	1.33
26	BA	2736	A	C6-N6	6.77	1.47	1.33
1	AA	60	A	C6-N6	6.77	1.47	1.33
1	AA	994	A	C6-N6	6.77	1.47	1.33
26	BA	1070	A	C6-N6	6.77	1.47	1.33
26	BA	1151	A	C6-N6	6.77	1.47	1.33
26	BA	1205	A	C6-N6	6.77	1.47	1.33
26	BA	1274	A	C6-N6	6.77	1.47	1.33
26	BA	1384	A	C6-N6	6.77	1.47	1.33
26	BA	2042	A	C6-N6	6.77	1.47	1.33
26	BA	2273	A	C6-N6	6.77	1.47	1.33
26	BA	2823	A	C6-N6	6.77	1.47	1.33
26	BA	2893	A	C6-N6	6.77	1.47	1.33
1	AA	900	A	C6-N6	6.77	1.47	1.33
1	AA	1280	A	C6-N6	6.77	1.47	1.33
26	BA	126	A	C6-N6	6.77	1.47	1.33
26	BA	309	A	C6-N6	6.77	1.47	1.33
26	BA	513	A	C6-N6	6.77	1.47	1.33
26	BA	2530	A	C6-N6	6.77	1.47	1.33
27	BB	101	A	C6-N6	6.77	1.47	1.33
1	AA	131	A	C6-N6	6.77	1.47	1.33
1	AA	415	A	C6-N6	6.77	1.47	1.33
1	AA	687	A	C6-N6	6.77	1.47	1.33
1	AA	1274	A	C6-N6	6.77	1.47	1.33
1	AA	1468	A	C6-N6	6.77	1.47	1.33
23	AW	42	A	C6-N6	6.77	1.47	1.33
26	BA	181	A	C6-N6	6.77	1.47	1.33
26	BA	219	A	C6-N6	6.77	1.47	1.33
26	BA	2705	A	C6-N6	6.77	1.47	1.33
26	BA	2860	A	C6-N6	6.77	1.47	1.33
26	BA	2899	A	C6-N6	6.77	1.47	1.33
1	AA	7	A	C6-N6	6.77	1.47	1.33
1	AA	179	A	C6-N6	6.77	1.47	1.33
1	AA	253	A	C6-N6	6.77	1.47	1.33
1	AA	498	A	C6-N6	6.77	1.47	1.33
23	AW	41	A	C6-N6	6.77	1.47	1.33
23	AW	59	A	C6-N6	6.77	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	AY	26	A	C6-N6	6.77	1.47	1.33
26	BA	422	A	C6-N6	6.77	1.47	1.33
26	BA	718	A	C6-N6	6.77	1.47	1.33
26	BA	1021	A	C6-N6	6.77	1.47	1.33
26	BA	1385	A	C6-N6	6.77	1.47	1.33
26	BA	1571	A	C6-N6	6.77	1.47	1.33
26	BA	1711	A	C6-N6	6.77	1.47	1.33
26	BA	1749	A	C6-N6	6.77	1.47	1.33
26	BA	1890	A	C6-N6	6.77	1.47	1.33
26	BA	1998	A	C6-N6	6.77	1.47	1.33
26	BA	2071	A	C6-N6	6.77	1.47	1.33
26	BA	2227	A	C6-N6	6.77	1.47	1.33
26	BA	2670	A	C6-N6	6.77	1.47	1.33
26	BA	2814	A	C6-N6	6.77	1.47	1.33
1	AA	167	A	C6-N6	6.77	1.47	1.33
1	AA	958	A	C6-N6	6.77	1.47	1.33
26	BA	402	A	C6-N6	6.77	1.47	1.33
26	BA	1970	A	C6-N6	6.77	1.47	1.33
26	BA	2309	A	C6-N6	6.77	1.47	1.33
26	BA	2381	A	C6-N6	6.77	1.47	1.33
26	BA	2679	A	C6-N6	6.77	1.47	1.33
1	AA	101	A	C6-N6	6.76	1.47	1.33
1	AA	363	A	C6-N6	6.76	1.47	1.33
1	AA	441	A	C6-N6	6.76	1.47	1.33
1	AA	648	A	C6-N6	6.76	1.47	1.33
1	AA	702	A	C6-N6	6.76	1.47	1.33
1	AA	747	A	C6-N6	6.76	1.47	1.33
1	AA	787	A	C6-N6	6.76	1.47	1.33
1	AA	978	A	C6-N6	6.76	1.47	1.33
1	AA	1036	A	C6-N6	6.76	1.47	1.33
1	AA	1306	A	C6-N6	6.76	1.47	1.33
1	AA	1502	A	C6-N6	6.76	1.47	1.33
1	AA	1531	A	C6-N6	6.76	1.47	1.33
26	BA	195	A	C6-N6	6.76	1.47	1.33
26	BA	751	A	C6-N6	6.76	1.47	1.33
26	BA	1373	A	C6-N6	6.76	1.47	1.33
26	BA	1393	A	C6-N6	6.76	1.47	1.33
26	BA	1593	A	C6-N6	6.76	1.47	1.33
26	BA	1780	A	C6-N6	6.76	1.47	1.33
26	BA	1960	A	C6-N6	6.76	1.47	1.33
26	BA	2009	A	C6-N6	6.76	1.47	1.33
26	BA	2030	A	C6-N6	6.76	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2082	A	C6-N6	6.76	1.47	1.33
26	BA	2117	A	C6-N6	6.76	1.47	1.33
26	BA	2142	A	C6-N6	6.76	1.47	1.33
26	BA	2590	A	C6-N6	6.76	1.47	1.33
26	BA	2634	A	C6-N6	6.76	1.47	1.33
26	BA	2662	A	C6-N6	6.76	1.47	1.33
26	BA	2778	A	C6-N6	6.76	1.47	1.33
27	BB	15	A	C6-N6	6.76	1.47	1.33
27	BB	29	A	C6-N6	6.76	1.47	1.33
1	AA	51	A	C6-N6	6.76	1.47	1.33
1	AA	196	A	C6-N6	6.76	1.47	1.33
1	AA	640	A	C6-N6	6.76	1.47	1.33
1	AA	676	A	C6-N6	6.76	1.47	1.33
1	AA	816	A	C6-N6	6.76	1.47	1.33
1	AA	959	A	C6-N6	6.76	1.47	1.33
1	AA	1080	A	C6-N6	6.76	1.47	1.33
26	BA	14	A	C6-N6	6.76	1.47	1.33
26	BA	347	A	C6-N6	6.76	1.47	1.33
26	BA	480	A	C6-N6	6.76	1.47	1.33
26	BA	631	A	C6-N6	6.76	1.47	1.33
26	BA	727	A	C6-N6	6.76	1.47	1.33
26	BA	1395	A	C6-N6	6.76	1.47	1.33
26	BA	1505	A	C6-N6	6.76	1.47	1.33
26	BA	1580	A	C6-N6	6.76	1.47	1.33
26	BA	1938	A	C6-N6	6.76	1.47	1.33
26	BA	2587	A	C6-N6	6.76	1.47	1.33
1	AA	19	A	C6-N6	6.76	1.47	1.33
1	AA	468	A	C6-N6	6.76	1.47	1.33
1	AA	510	A	C6-N6	6.76	1.47	1.33
1	AA	780	A	C6-N6	6.76	1.47	1.33
1	AA	815	A	C6-N6	6.76	1.47	1.33
1	AA	819	A	C6-N6	6.76	1.47	1.33
1	AA	1408	A	C6-N6	6.76	1.47	1.33
23	AW	66	A	C6-N6	6.76	1.47	1.33
24	AX	14	A	C6-N6	6.76	1.47	1.33
25	AY	69	A	C6-N6	6.76	1.47	1.33
26	BA	111	A	C6-N6	6.76	1.47	1.33
26	BA	156	A	C6-N6	6.76	1.47	1.33
26	BA	213	A	C6-N6	6.76	1.47	1.33
26	BA	507	A	C6-N6	6.76	1.47	1.33
26	BA	699	A	C6-N6	6.76	1.47	1.33
26	BA	849	A	C6-N6	6.76	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	892	A	C6-N6	6.76	1.47	1.33
26	BA	943	A	C6-N6	6.76	1.47	1.33
26	BA	979	A	C6-N6	6.76	1.47	1.33
26	BA	1029	A	C6-N6	6.76	1.47	1.33
26	BA	1077	A	C6-N6	6.76	1.47	1.33
26	BA	1086	A	C6-N6	6.76	1.47	1.33
26	BA	1144	A	C6-N6	6.76	1.47	1.33
26	BA	1237	A	C6-N6	6.76	1.47	1.33
26	BA	1403	A	C6-N6	6.76	1.47	1.33
26	BA	1453	A	C6-N6	6.76	1.47	1.33
26	BA	1744	A	C6-N6	6.76	1.47	1.33
26	BA	1871	A	C6-N6	6.76	1.47	1.33
26	BA	2198	A	C6-N6	6.76	1.47	1.33
26	BA	2887	A	C6-N6	6.76	1.47	1.33
1	AA	44	A	C6-N6	6.76	1.47	1.33
1	AA	72	A	C6-N6	6.76	1.47	1.33
1	AA	181	A	C6-N6	6.76	1.47	1.33
1	AA	349	A	C6-N6	6.76	1.47	1.33
1	AA	559	A	C6-N6	6.76	1.47	1.33
1	AA	704	A	C6-N6	6.76	1.47	1.33
1	AA	743	A	C6-N6	6.76	1.47	1.33
1	AA	935	A	C6-N6	6.76	1.47	1.33
1	AA	1433	A	C6-N6	6.76	1.47	1.33
23	AW	26	A	C6-N6	6.76	1.47	1.33
23	AW	58	A	C6-N6	6.76	1.47	1.33
26	BA	83	A	C6-N6	6.76	1.47	1.33
26	BA	160	A	C6-N6	6.76	1.47	1.33
26	BA	165	A	C6-N6	6.76	1.47	1.33
26	BA	632	A	C6-N6	6.76	1.47	1.33
26	BA	742	A	C6-N6	6.76	1.47	1.33
26	BA	972	A	C6-N6	6.76	1.47	1.33
26	BA	1073	A	C6-N6	6.76	1.47	1.33
26	BA	1126	A	C6-N6	6.76	1.47	1.33
26	BA	1302	A	C6-N6	6.76	1.47	1.33
26	BA	1596	A	C6-N6	6.76	1.47	1.33
26	BA	1746	A	C6-N6	6.76	1.47	1.33
26	BA	2114	A	C6-N6	6.76	1.47	1.33
26	BA	2270	A	C6-N6	6.76	1.47	1.33
26	BA	2322	A	C6-N6	6.76	1.47	1.33
26	BA	2352	A	C6-N6	6.76	1.47	1.33
26	BA	2482	A	C6-N6	6.76	1.47	1.33
1	AA	66	A	C6-N6	6.76	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	831	A	C6-N6	6.76	1.47	1.33
1	AA	1176	A	C6-N6	6.76	1.47	1.33
1	AA	1534	A	C6-N6	6.76	1.47	1.33
23	AW	69	A	C6-N6	6.76	1.47	1.33
26	BA	471	A	C6-N6	6.76	1.47	1.33
26	BA	505	A	C6-N6	6.76	1.47	1.33
26	BA	844	A	C6-N6	6.76	1.47	1.33
26	BA	899	A	C6-N6	6.76	1.47	1.33
26	BA	1597	A	C6-N6	6.76	1.47	1.33
26	BA	1630	A	C6-N6	6.76	1.47	1.33
26	BA	1918	A	C6-N6	6.76	1.47	1.33
26	BA	1952	A	C6-N6	6.76	1.47	1.33
26	BA	2284	A	C6-N6	6.76	1.47	1.33
26	BA	2439	A	C6-N6	6.76	1.47	1.33
1	AA	116	A	C6-N6	6.76	1.47	1.33
1	AA	250	A	C6-N6	6.76	1.47	1.33
1	AA	300	A	C6-N6	6.76	1.47	1.33
1	AA	373	A	C6-N6	6.76	1.47	1.33
1	AA	496	A	C6-N6	6.76	1.47	1.33
1	AA	1019	A	C6-N6	6.76	1.47	1.33
1	AA	1111	A	C6-N6	6.76	1.47	1.33
1	AA	1150	A	C6-N6	6.76	1.47	1.33
1	AA	1346	A	C6-N6	6.76	1.47	1.33
22	AV	17	A	C6-N6	6.76	1.47	1.33
25	AY	58	A	C6-N6	6.76	1.47	1.33
26	BA	63	A	C6-N6	6.76	1.47	1.33
26	BA	64	A	C6-N6	6.76	1.47	1.33
26	BA	89	A	C6-N6	6.76	1.47	1.33
26	BA	103	A	C6-N6	6.76	1.47	1.33
26	BA	590	A	C6-N6	6.76	1.47	1.33
26	BA	603	A	C6-N6	6.76	1.47	1.33
26	BA	693	A	C6-N6	6.76	1.47	1.33
26	BA	959	A	C6-N6	6.76	1.47	1.33
26	BA	1095	A	C6-N6	6.76	1.47	1.33
26	BA	1262	A	C6-N6	6.76	1.47	1.33
26	BA	1367	A	C6-N6	6.76	1.47	1.33
26	BA	1413	A	C6-N6	6.76	1.47	1.33
26	BA	1433	A	C6-N6	6.76	1.47	1.33
26	BA	1495	A	C6-N6	6.76	1.47	1.33
26	BA	1701	A	C6-N6	6.76	1.47	1.33
26	BA	1953	A	C6-N6	6.76	1.47	1.33
26	BA	1966	A	C6-N6	6.76	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2058	A	C6-N6	6.76	1.47	1.33
26	BA	2183	A	C6-N6	6.76	1.47	1.33
26	BA	2753	A	C6-N6	6.76	1.47	1.33
26	BA	2761	A	C6-N6	6.76	1.47	1.33
1	AA	2	A	C6-N6	6.75	1.47	1.33
1	AA	466	A	C6-N6	6.75	1.47	1.33
1	AA	487	A	C6-N6	6.75	1.47	1.33
1	AA	1271	A	C6-N6	6.75	1.47	1.33
1	AA	1287	A	C6-N6	6.75	1.47	1.33
1	AA	1398	A	C6-N6	6.75	1.47	1.33
1	AA	1480	A	C6-N6	6.75	1.47	1.33
22	AV	22	A	C6-N6	6.75	1.47	1.33
23	AW	73	A	C6-N6	6.75	1.47	1.33
24	AX	21	A	C6-N6	6.75	1.47	1.33
26	BA	49	A	C6-N6	6.75	1.47	1.33
26	BA	74	A	C6-N6	6.75	1.47	1.33
26	BA	118	A	C6-N6	6.75	1.47	1.33
26	BA	477	A	C6-N6	6.75	1.47	1.33
26	BA	947	A	C6-N6	6.75	1.47	1.33
26	BA	1503	A	C6-N6	6.75	1.47	1.33
26	BA	1583	A	C6-N6	6.75	1.47	1.33
26	BA	2314	A	C6-N6	6.75	1.47	1.33
27	BB	57	A	C6-N6	6.75	1.47	1.33
1	AA	80	A	C6-N6	6.75	1.47	1.33
1	AA	129	A	C6-N6	6.75	1.47	1.33
1	AA	152	A	C6-N6	6.75	1.47	1.33
1	AA	263	A	C6-N6	6.75	1.47	1.33
1	AA	315	A	C6-N6	6.75	1.47	1.33
1	AA	338	A	C6-N6	6.75	1.47	1.33
1	AA	563	A	C6-N6	6.75	1.47	1.33
1	AA	845	A	C6-N6	6.75	1.47	1.33
1	AA	1004	A	C6-N6	6.75	1.47	1.33
1	AA	1204	A	C6-N6	6.75	1.47	1.33
1	AA	1339	A	C6-N6	6.75	1.47	1.33
1	AA	1507	A	C6-N6	6.75	1.47	1.33
26	BA	28	A	C6-N6	6.75	1.47	1.33
26	BA	104	A	C6-N6	6.75	1.47	1.33
26	BA	282	A	C6-N6	6.75	1.47	1.33
26	BA	478	A	C6-N6	6.75	1.47	1.33
26	BA	497	A	C6-N6	6.75	1.47	1.33
26	BA	609	A	C6-N6	6.75	1.47	1.33
26	BA	734	A	C6-N6	6.75	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	764	A	C6-N6	6.75	1.47	1.33
26	BA	829	A	C6-N6	6.75	1.47	1.33
26	BA	980	A	C6-N6	6.75	1.47	1.33
26	BA	1080	A	C6-N6	6.75	1.47	1.33
26	BA	1147	A	C6-N6	6.75	1.47	1.33
26	BA	1175	A	C6-N6	6.75	1.47	1.33
26	BA	1285	A	C6-N6	6.75	1.47	1.33
26	BA	1365	A	C6-N6	6.75	1.47	1.33
26	BA	1679	A	C6-N6	6.75	1.47	1.33
26	BA	1772	A	C6-N6	6.75	1.47	1.33
26	BA	1927	A	C6-N6	6.75	1.47	1.33
26	BA	1928	A	C6-N6	6.75	1.47	1.33
26	BA	2003	A	C6-N6	6.75	1.47	1.33
26	BA	2013	A	C6-N6	6.75	1.47	1.33
26	BA	2750	A	C6-N6	6.75	1.47	1.33
26	BA	2792	A	C6-N6	6.75	1.47	1.33
26	BA	2809	A	C6-N6	6.75	1.47	1.33
26	BA	2829	A	C6-N6	6.75	1.47	1.33
27	BB	73	A	C6-N6	6.75	1.47	1.33
1	AA	223	A	C6-N6	6.75	1.47	1.33
1	AA	246	A	C6-N6	6.75	1.47	1.33
1	AA	313	A	C6-N6	6.75	1.47	1.33
1	AA	448	A	C6-N6	6.75	1.47	1.33
1	AA	532	A	C6-N6	6.75	1.47	1.33
1	AA	560	A	C6-N6	6.75	1.47	1.33
1	AA	607	A	C6-N6	6.75	1.47	1.33
1	AA	715	A	C6-N6	6.75	1.47	1.33
1	AA	892	A	C6-N6	6.75	1.47	1.33
1	AA	1256	A	C6-N6	6.75	1.47	1.33
1	AA	1413	A	C6-N6	6.75	1.47	1.33
23	AW	51	A	C6-N6	6.75	1.47	1.33
25	AY	35	A	C6-N6	6.75	1.47	1.33
26	BA	91	A	C6-N6	6.75	1.47	1.33
26	BA	125	A	C6-N6	6.75	1.47	1.33
26	BA	155	A	C6-N6	6.75	1.47	1.33
26	BA	322	A	C6-N6	6.75	1.47	1.33
26	BA	344	A	C6-N6	6.75	1.47	1.33
26	BA	453	A	C6-N6	6.75	1.47	1.33
26	BA	781	A	C6-N6	6.75	1.47	1.33
26	BA	917	A	C6-N6	6.75	1.47	1.33
26	BA	1008	A	C6-N6	6.75	1.47	1.33
26	BA	1134	A	C6-N6	6.75	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1204	A	C6-N6	6.75	1.47	1.33
26	BA	1213	A	C6-N6	6.75	1.47	1.33
26	BA	1322	A	C6-N6	6.75	1.47	1.33
26	BA	1535	A	C6-N6	6.75	1.47	1.33
26	BA	1551	A	C6-N6	6.75	1.47	1.33
26	BA	1553	A	C6-N6	6.75	1.47	1.33
26	BA	1810	A	C6-N6	6.75	1.47	1.33
26	BA	1913	A	C6-N6	6.75	1.47	1.33
26	BA	2031	A	C6-N6	6.75	1.47	1.33
26	BA	2171	A	C6-N6	6.75	1.47	1.33
26	BA	2281	A	C6-N6	6.75	1.47	1.33
26	BA	2311	A	C6-N6	6.75	1.47	1.33
26	BA	2476	A	C6-N6	6.75	1.47	1.33
26	BA	2564	A	C6-N6	6.75	1.47	1.33
26	BA	2654	A	C6-N6	6.75	1.47	1.33
26	BA	2721	A	C6-N6	6.75	1.47	1.33
26	BA	2837	A	C6-N6	6.75	1.47	1.33
26	BA	2851	A	C6-N6	6.75	1.47	1.33
26	BA	2872	A	C6-N6	6.75	1.47	1.33
1	AA	282	A	C6-N6	6.75	1.47	1.33
1	AA	1188	A	C6-N6	6.75	1.47	1.33
1	AA	1428	A	C6-N6	6.75	1.47	1.33
26	BA	173	A	C6-N6	6.75	1.47	1.33
26	BA	199	A	C6-N6	6.75	1.47	1.33
26	BA	342	A	C6-N6	6.75	1.47	1.33
26	BA	368	A	C6-N6	6.75	1.47	1.33
26	BA	627	A	C6-N6	6.75	1.47	1.33
26	BA	753	A	C6-N6	6.75	1.47	1.33
26	BA	1010	A	C6-N6	6.75	1.47	1.33
26	BA	2407	A	C6-N6	6.75	1.47	1.33
26	BA	2453	A	C6-N6	6.75	1.47	1.33
26	BA	2758	A	C6-N6	6.75	1.47	1.33
1	AA	71	A	C6-N6	6.75	1.47	1.33
1	AA	78	A	C6-N6	6.75	1.47	1.33
1	AA	694	A	C6-N6	6.75	1.47	1.33
1	AA	767	A	C6-N6	6.75	1.47	1.33
1	AA	1016	A	C6-N6	6.75	1.47	1.33
1	AA	1169	A	C6-N6	6.75	1.47	1.33
1	AA	1257	A	C6-N6	6.75	1.47	1.33
1	AA	1396	A	C6-N6	6.75	1.47	1.33
1	AA	1519	A	C6-N6	6.75	1.47	1.33
22	AV	20	A	C6-N6	6.75	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	76	A	C6-N6	6.75	1.47	1.33
25	AY	66	A	C6-N6	6.75	1.47	1.33
26	BA	19	A	C6-N6	6.75	1.47	1.33
26	BA	217	A	C6-N6	6.75	1.47	1.33
26	BA	231	A	C6-N6	6.75	1.47	1.33
26	BA	345	A	C6-N6	6.75	1.47	1.33
26	BA	430	A	C6-N6	6.75	1.47	1.33
26	BA	528	A	C6-N6	6.75	1.47	1.33
26	BA	833	A	C6-N6	6.75	1.47	1.33
26	BA	1027	A	C6-N6	6.75	1.47	1.33
26	BA	1039	A	C6-N6	6.75	1.47	1.33
26	BA	1129	A	C6-N6	6.75	1.47	1.33
26	BA	1133	A	C6-N6	6.75	1.47	1.33
26	BA	1286	A	C6-N6	6.75	1.47	1.33
26	BA	1672	A	C6-N6	6.75	1.47	1.33
26	BA	1858	A	C6-N6	6.75	1.47	1.33
26	BA	1872	A	C6-N6	6.75	1.47	1.33
26	BA	1932	A	C6-N6	6.75	1.47	1.33
26	BA	2014	A	C6-N6	6.75	1.47	1.33
26	BA	2135	A	C6-N6	6.75	1.47	1.33
26	BA	2274	A	C6-N6	6.75	1.47	1.33
26	BA	2850	A	C6-N6	6.75	1.47	1.33
27	BB	46	A	C6-N6	6.75	1.47	1.33
1	AA	16	A	C6-N6	6.75	1.47	1.33
1	AA	197	A	C6-N6	6.75	1.47	1.33
1	AA	320	A	C6-N6	6.75	1.47	1.33
1	AA	366	A	C6-N6	6.75	1.47	1.33
1	AA	574	A	C6-N6	6.75	1.47	1.33
1	AA	675	A	C6-N6	6.75	1.47	1.33
1	AA	781	A	C6-N6	6.75	1.47	1.33
1	AA	913	A	C6-N6	6.75	1.47	1.33
1	AA	1042	A	C6-N6	6.75	1.47	1.33
1	AA	1093	A	C6-N6	6.75	1.47	1.33
1	AA	1101	A	C6-N6	6.75	1.47	1.33
1	AA	1130	A	C6-N6	6.75	1.47	1.33
1	AA	1318	A	C6-N6	6.75	1.47	1.33
1	AA	1368	A	C6-N6	6.75	1.47	1.33
1	AA	1499	A	C6-N6	6.75	1.47	1.33
25	AY	41	A	C6-N6	6.75	1.47	1.33
26	BA	176	A	C6-N6	6.75	1.47	1.33
26	BA	272	A	C6-N6	6.75	1.47	1.33
26	BA	354	A	C6-N6	6.75	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	470	A	C6-N6	6.75	1.47	1.33
26	BA	482	A	C6-N6	6.75	1.47	1.33
26	BA	504	A	C6-N6	6.75	1.47	1.33
26	BA	666	A	C6-N6	6.75	1.47	1.33
26	BA	1169	A	C6-N6	6.75	1.47	1.33
26	BA	1652	A	C6-N6	6.75	1.47	1.33
26	BA	1754	A	C6-N6	6.75	1.47	1.33
26	BA	1755	A	C6-N6	6.75	1.47	1.33
26	BA	1847	A	C6-N6	6.75	1.47	1.33
26	BA	2051	A	C6-N6	6.75	1.47	1.33
26	BA	2090	A	C6-N6	6.75	1.47	1.33
26	BA	2097	A	C6-N6	6.75	1.47	1.33
26	BA	2191	A	C6-N6	6.75	1.47	1.33
26	BA	2317	A	C6-N6	6.75	1.47	1.33
26	BA	2635	A	C6-N6	6.75	1.47	1.33
26	BA	2813	A	C6-N6	6.75	1.47	1.33
27	BB	104	A	C6-N6	6.75	1.47	1.33
1	AA	192	A	C6-N6	6.75	1.47	1.33
1	AA	329	A	C6-N6	6.75	1.47	1.33
1	AA	1092	A	C6-N6	6.75	1.47	1.33
1	AA	1197	A	C6-N6	6.75	1.47	1.33
1	AA	1246	A	C6-N6	6.75	1.47	1.33
1	AA	1360	A	C6-N6	6.75	1.47	1.33
25	AY	73	A	C6-N6	6.75	1.47	1.33
26	BA	101	A	C6-N6	6.75	1.47	1.33
26	BA	196	A	C6-N6	6.75	1.47	1.33
26	BA	299	A	C6-N6	6.75	1.47	1.33
26	BA	1069	A	C6-N6	6.75	1.47	1.33
26	BA	1090	A	C6-N6	6.75	1.47	1.33
26	BA	1103	A	C6-N6	6.75	1.47	1.33
26	BA	1156	A	C6-N6	6.75	1.47	1.33
26	BA	1287	A	C6-N6	6.75	1.47	1.33
26	BA	1700	A	C6-N6	6.75	1.47	1.33
26	BA	1785	A	C6-N6	6.75	1.47	1.33
26	BA	1802	A	C6-N6	6.75	1.47	1.33
26	BA	1912	A	C6-N6	6.75	1.47	1.33
26	BA	1978	A	C6-N6	6.75	1.47	1.33
26	BA	2060	A	C6-N6	6.75	1.47	1.33
26	BA	2062	A	C6-N6	6.75	1.47	1.33
26	BA	2101	A	C6-N6	6.75	1.47	1.33
26	BA	2108	A	C6-N6	6.75	1.47	1.33
26	BA	2336	A	C6-N6	6.75	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2534	A	C6-N6	6.75	1.47	1.33
1	AA	3	A	C6-N6	6.74	1.47	1.33
1	AA	143	A	C6-N6	6.74	1.47	1.33
1	AA	336	A	C6-N6	6.74	1.47	1.33
1	AA	533	A	C6-N6	6.74	1.47	1.33
1	AA	729	A	C6-N6	6.74	1.47	1.33
1	AA	807	A	C6-N6	6.74	1.47	1.33
1	AA	974	A	C6-N6	6.74	1.47	1.33
1	AA	1362	A	C6-N6	6.74	1.47	1.33
24	AX	9	A	C6-N6	6.74	1.47	1.33
24	AX	26	A	C6-N6	6.74	1.47	1.33
26	BA	161	A	C6-N6	6.74	1.47	1.33
26	BA	223	A	C6-N6	6.74	1.47	1.33
26	BA	256	A	C6-N6	6.74	1.47	1.33
26	BA	300	A	C6-N6	6.74	1.47	1.33
26	BA	348	A	C6-N6	6.74	1.47	1.33
26	BA	443	A	C6-N6	6.74	1.47	1.33
26	BA	466	A	C6-N6	6.74	1.47	1.33
26	BA	592	A	C6-N6	6.74	1.47	1.33
26	BA	825	A	C6-N6	6.74	1.47	1.33
26	BA	878	A	C6-N6	6.74	1.47	1.33
26	BA	925	A	C6-N6	6.74	1.47	1.33
26	BA	1669	A	C6-N6	6.74	1.47	1.33
26	BA	1676	A	C6-N6	6.74	1.47	1.33
26	BA	1885	A	C6-N6	6.74	1.47	1.33
26	BA	1900	A	C6-N6	6.74	1.47	1.33
26	BA	2173	A	C6-N6	6.74	1.47	1.33
26	BA	2376	A	C6-N6	6.74	1.47	1.33
26	BA	2433	A	C6-N6	6.74	1.47	1.33
26	BA	2600	A	C6-N6	6.74	1.47	1.33
26	BA	2660	A	C6-N6	6.74	1.47	1.33
1	AA	32	A	C6-N6	6.74	1.47	1.33
1	AA	149	A	C6-N6	6.74	1.47	1.33
1	AA	236	A	C6-N6	6.74	1.47	1.33
1	AA	579	A	C6-N6	6.74	1.47	1.33
1	AA	878	A	C6-N6	6.74	1.47	1.33
1	AA	914	A	C6-N6	6.74	1.47	1.33
1	AA	1340	A	C6-N6	6.74	1.47	1.33
24	AX	41	A	C6-N6	6.74	1.47	1.33
26	BA	94	A	C6-N6	6.74	1.47	1.33
26	BA	233	A	C6-N6	6.74	1.47	1.33
26	BA	391	A	C6-N6	6.74	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	404	A	C6-N6	6.74	1.47	1.33
26	BA	716	A	C6-N6	6.74	1.47	1.33
26	BA	788	A	C6-N6	6.74	1.47	1.33
26	BA	793	A	C6-N6	6.74	1.47	1.33
26	BA	802	A	C6-N6	6.74	1.47	1.33
26	BA	1383	A	C6-N6	6.74	1.47	1.33
26	BA	1549	A	C6-N6	6.74	1.47	1.33
26	BA	1610	A	C6-N6	6.74	1.47	1.33
26	BA	1632	A	C6-N6	6.74	1.47	1.33
26	BA	1745	A	C6-N6	6.74	1.47	1.33
26	BA	1786	A	C6-N6	6.74	1.47	1.33
26	BA	2448	A	C6-N6	6.74	1.47	1.33
26	BA	2749	A	C6-N6	6.74	1.47	1.33
1	AA	161	A	C6-N6	6.74	1.47	1.33
1	AA	274	A	C6-N6	6.74	1.47	1.33
1	AA	288	A	C6-N6	6.74	1.47	1.33
1	AA	520	A	C6-N6	6.74	1.47	1.33
1	AA	635	A	C6-N6	6.74	1.47	1.33
1	AA	728	A	C6-N6	6.74	1.47	1.33
1	AA	949	A	C6-N6	6.74	1.47	1.33
1	AA	968	A	C6-N6	6.74	1.47	1.33
1	AA	1046	A	C6-N6	6.74	1.47	1.33
1	AA	1251	A	C6-N6	6.74	1.47	1.33
1	AA	1252	A	C6-N6	6.74	1.47	1.33
1	AA	1332	A	C6-N6	6.74	1.47	1.33
1	AA	1446	A	C6-N6	6.74	1.47	1.33
1	AA	1493	A	C6-N6	6.74	1.47	1.33
1	AA	1503	A	C6-N6	6.74	1.47	1.33
22	AV	21	A	C6-N6	6.74	1.47	1.33
23	AW	31	A	C6-N6	6.74	1.47	1.33
24	AX	3	A	C6-N6	6.74	1.47	1.33
25	AY	23	A	C6-N6	6.74	1.47	1.33
26	BA	244	A	C6-N6	6.74	1.47	1.33
26	BA	262	A	C6-N6	6.74	1.47	1.33
26	BA	384	A	C6-N6	6.74	1.47	1.33
26	BA	472	A	C6-N6	6.74	1.47	1.33
26	BA	501	A	C6-N6	6.74	1.47	1.33
26	BA	538	A	C6-N6	6.74	1.47	1.33
26	BA	789	A	C6-N6	6.74	1.47	1.33
26	BA	927	A	C6-N6	6.74	1.47	1.33
26	BA	1020	A	C6-N6	6.74	1.47	1.33
26	BA	1067	A	C6-N6	6.74	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1260	A	C6-N6	6.74	1.47	1.33
26	BA	1347	A	C6-N6	6.74	1.47	1.33
26	BA	1439	A	C6-N6	6.74	1.47	1.33
26	BA	1477	A	C6-N6	6.74	1.47	1.33
26	BA	1525	A	C6-N6	6.74	1.47	1.33
26	BA	1616	A	C6-N6	6.74	1.47	1.33
26	BA	1634	A	C6-N6	6.74	1.47	1.33
26	BA	1677	A	C6-N6	6.74	1.47	1.33
26	BA	1690	A	C6-N6	6.74	1.47	1.33
26	BA	1698	A	C6-N6	6.74	1.47	1.33
26	BA	1717	A	C6-N6	6.74	1.47	1.33
26	BA	1791	A	C6-N6	6.74	1.47	1.33
26	BA	1815	A	C6-N6	6.74	1.47	1.33
26	BA	2119	A	C6-N6	6.74	1.47	1.33
26	BA	2531	A	C6-N6	6.74	1.47	1.33
26	BA	2598	A	C6-N6	6.74	1.47	1.33
26	BA	2738	A	C6-N6	6.74	1.47	1.33
1	AA	279	A	C6-N6	6.74	1.47	1.33
1	AA	461	A	C6-N6	6.74	1.47	1.33
1	AA	523	A	C6-N6	6.74	1.47	1.33
1	AA	918	A	C6-N6	6.74	1.47	1.33
1	AA	1022	A	C6-N6	6.74	1.47	1.33
1	AA	1155	A	C6-N6	6.74	1.47	1.33
1	AA	1236	A	C6-N6	6.74	1.47	1.33
1	AA	1254	A	C6-N6	6.74	1.47	1.33
23	AW	14	A	C6-N6	6.74	1.47	1.33
23	AW	23	A	C6-N6	6.74	1.47	1.33
26	BA	167	A	C6-N6	6.74	1.47	1.33
26	BA	428	A	C6-N6	6.74	1.47	1.33
26	BA	782	A	C6-N6	6.74	1.47	1.33
26	BA	1050	A	C6-N6	6.74	1.47	1.33
26	BA	1254	A	C6-N6	6.74	1.47	1.33
26	BA	1307	A	C6-N6	6.74	1.47	1.33
26	BA	1308	A	C6-N6	6.74	1.47	1.33
26	BA	1470	A	C6-N6	6.74	1.47	1.33
26	BA	1528	A	C6-N6	6.74	1.47	1.33
26	BA	1572	A	C6-N6	6.74	1.47	1.33
26	BA	1598	A	C6-N6	6.74	1.47	1.33
26	BA	1618	A	C6-N6	6.74	1.47	1.33
26	BA	1762	A	C6-N6	6.74	1.47	1.33
26	BA	1794	A	C6-N6	6.74	1.47	1.33
26	BA	2126	A	C6-N6	6.74	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2147	A	C6-N6	6.74	1.47	1.33
26	BA	2288	A	C6-N6	6.74	1.47	1.33
26	BA	2377	A	C6-N6	6.74	1.47	1.33
26	BA	2614	A	C6-N6	6.74	1.47	1.33
26	BA	2868	A	C6-N6	6.74	1.47	1.33
27	BB	109	A	C6-N6	6.74	1.47	1.33
27	BB	119	A	C6-N6	6.74	1.47	1.33
1	AA	1229	A	C6-N6	6.74	1.47	1.33
1	AA	1447	A	C6-N6	6.74	1.47	1.33
23	AW	38	A	C6-N6	6.74	1.47	1.33
26	BA	492	A	C6-N6	6.74	1.47	1.33
26	BA	547	A	C6-N6	6.74	1.47	1.33
26	BA	866	A	C6-N6	6.74	1.47	1.33
26	BA	981	A	C6-N6	6.74	1.47	1.33
26	BA	1046	A	C6-N6	6.74	1.47	1.33
26	BA	1301	A	C6-N6	6.74	1.47	1.33
26	BA	1342	A	C6-N6	6.74	1.47	1.33
26	BA	1502	A	C6-N6	6.74	1.47	1.33
26	BA	1637	A	C6-N6	6.74	1.47	1.33
26	BA	1739	A	C6-N6	6.74	1.47	1.33
26	BA	1819	A	C6-N6	6.74	1.47	1.33
26	BA	2412	A	C6-N6	6.74	1.47	1.33
26	BA	2566	A	C6-N6	6.74	1.47	1.33
1	AA	10	A	C6-N6	6.74	1.47	1.33
1	AA	120	A	C6-N6	6.74	1.47	1.33
1	AA	139	A	C6-N6	6.74	1.47	1.33
1	AA	174	A	C6-N6	6.74	1.47	1.33
1	AA	655	A	C6-N6	6.74	1.47	1.33
1	AA	712	A	C6-N6	6.74	1.47	1.33
1	AA	792	A	C6-N6	6.74	1.47	1.33
1	AA	906	A	C6-N6	6.74	1.47	1.33
1	AA	1055	A	C6-N6	6.74	1.47	1.33
1	AA	1492	A	C6-N6	6.74	1.47	1.33
1	AA	1508	A	C6-N6	6.74	1.47	1.33
23	AW	21	A	C6-N6	6.74	1.47	1.33
25	AY	6	A	C6-N6	6.74	1.47	1.33
26	BA	21	A	C6-N6	6.74	1.47	1.33
26	BA	131	A	C6-N6	6.74	1.47	1.33
26	BA	226	A	C6-N6	6.74	1.47	1.33
26	BA	412	A	C6-N6	6.74	1.47	1.33
26	BA	896	A	C6-N6	6.74	1.47	1.33
26	BA	1321	A	C6-N6	6.74	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1789	A	C6-N6	6.74	1.47	1.33
26	BA	1803	A	C6-N6	6.74	1.47	1.33
26	BA	2170	A	C6-N6	6.74	1.47	1.33
26	BA	2406	A	C6-N6	6.74	1.47	1.33
26	BA	2425	A	C6-N6	6.74	1.47	1.33
26	BA	2886	A	C6-N6	6.74	1.47	1.33
27	BB	58	A	C6-N6	6.74	1.47	1.33
1	AA	189	A	C6-N6	6.73	1.47	1.33
1	AA	509	A	C6-N6	6.73	1.47	1.33
1	AA	673	A	C6-N6	6.73	1.47	1.33
1	AA	1288	A	C6-N6	6.73	1.47	1.33
1	AA	1465	A	C6-N6	6.73	1.47	1.33
25	AY	14	A	C6-N6	6.73	1.47	1.33
26	BA	5	A	C6-N6	6.73	1.47	1.33
26	BA	918	A	C6-N6	6.73	1.47	1.33
26	BA	996	A	C6-N6	6.73	1.47	1.33
26	BA	1057	A	C6-N6	6.73	1.47	1.33
26	BA	1354	A	C6-N6	6.73	1.47	1.33
26	BA	1420	A	C6-N6	6.73	1.47	1.33
26	BA	2020	A	C6-N6	6.73	1.47	1.33
26	BA	2163	A	C6-N6	6.73	1.47	1.33
1	AA	55	A	C6-N6	6.73	1.47	1.33
1	AA	172	A	C6-N6	6.73	1.47	1.33
1	AA	195	A	C6-N6	6.73	1.47	1.33
1	AA	262	A	C6-N6	6.73	1.47	1.33
1	AA	303	A	C6-N6	6.73	1.47	1.33
1	AA	321	A	C6-N6	6.73	1.47	1.33
1	AA	371	A	C6-N6	6.73	1.47	1.33
1	AA	435	A	C6-N6	6.73	1.47	1.33
1	AA	465	A	C6-N6	6.73	1.47	1.33
1	AA	535	A	C6-N6	6.73	1.47	1.33
1	AA	768	A	C6-N6	6.73	1.47	1.33
1	AA	1035	A	C6-N6	6.73	1.47	1.33
1	AA	1363	A	C6-N6	6.73	1.47	1.33
26	BA	152	A	C6-N6	6.73	1.47	1.33
26	BA	216	A	C6-N6	6.73	1.47	1.33
26	BA	221	A	C6-N6	6.73	1.47	1.33
26	BA	371	A	C6-N6	6.73	1.47	1.33
26	BA	382	A	C6-N6	6.73	1.47	1.33
26	BA	616	A	C6-N6	6.73	1.47	1.33
26	BA	670	A	C6-N6	6.73	1.47	1.33
26	BA	743	A	C6-N6	6.73	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	820	A	C6-N6	6.73	1.47	1.33
26	BA	941	A	C6-N6	6.73	1.47	1.33
26	BA	988	A	C6-N6	6.73	1.47	1.33
26	BA	1089	A	C6-N6	6.73	1.47	1.33
26	BA	1635	A	C6-N6	6.73	1.47	1.33
26	BA	1722	A	C6-N6	6.73	1.47	1.33
26	BA	1821	A	C6-N6	6.73	1.47	1.33
26	BA	1919	A	C6-N6	6.73	1.47	1.33
26	BA	2059	A	C6-N6	6.73	1.47	1.33
26	BA	2211	A	C6-N6	6.73	1.47	1.33
26	BA	2411	A	C6-N6	6.73	1.47	1.33
26	BA	2706	A	C6-N6	6.73	1.47	1.33
26	BA	2711	A	C6-N6	6.73	1.47	1.33
26	BA	2734	A	C6-N6	6.73	1.47	1.33
26	BA	2882	A	C6-N6	6.73	1.47	1.33
27	BB	108	A	C6-N6	6.73	1.47	1.33
1	AA	53	A	C6-N6	6.73	1.47	1.33
1	AA	182	A	C6-N6	6.73	1.47	1.33
1	AA	344	A	C6-N6	6.73	1.47	1.33
1	AA	364	A	C6-N6	6.73	1.47	1.33
1	AA	383	A	C6-N6	6.73	1.47	1.33
1	AA	539	A	C6-N6	6.73	1.47	1.33
1	AA	964	A	C6-N6	6.73	1.47	1.33
1	AA	1180	A	C6-N6	6.73	1.47	1.33
26	BA	146	A	C6-N6	6.73	1.47	1.33
26	BA	362	A	C6-N6	6.73	1.47	1.33
26	BA	374	A	C6-N6	6.73	1.47	1.33
26	BA	502	A	C6-N6	6.73	1.47	1.33
26	BA	508	A	C6-N6	6.73	1.47	1.33
26	BA	541	A	C6-N6	6.73	1.47	1.33
26	BA	626	A	C6-N6	6.73	1.47	1.33
26	BA	689	A	C6-N6	6.73	1.47	1.33
26	BA	705	A	C6-N6	6.73	1.47	1.33
26	BA	706	A	C6-N6	6.73	1.47	1.33
26	BA	973	A	C6-N6	6.73	1.47	1.33
26	BA	1048	A	C6-N6	6.73	1.47	1.33
26	BA	1096	A	C6-N6	6.73	1.47	1.33
26	BA	1264	A	C6-N6	6.73	1.47	1.33
26	BA	1504	A	C6-N6	6.73	1.47	1.33
26	BA	1640	A	C6-N6	6.73	1.47	1.33
26	BA	1678	A	C6-N6	6.73	1.47	1.33
26	BA	1853	A	C6-N6	6.73	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2070	A	C6-N6	6.73	1.47	1.33
26	BA	2369	A	C6-N6	6.73	1.47	1.33
26	BA	2503	A	C6-N6	6.73	1.47	1.33
26	BA	2733	A	C6-N6	6.73	1.47	1.33
26	BA	2826	A	C6-N6	6.73	1.47	1.33
26	BA	2883	A	C6-N6	6.73	1.47	1.33
26	BA	2900	A	C6-N6	6.73	1.47	1.33
1	AA	28	A	C6-N6	6.73	1.47	1.33
1	AA	327	A	C6-N6	6.73	1.47	1.33
1	AA	482	A	C6-N6	6.73	1.47	1.33
1	AA	595	A	C6-N6	6.73	1.47	1.33
1	AA	996	A	C6-N6	6.73	1.47	1.33
1	AA	1012	A	C6-N6	6.73	1.47	1.33
22	AV	19	A	C6-N6	6.73	1.47	1.33
26	BA	6	A	C6-N6	6.73	1.47	1.33
26	BA	149	A	C6-N6	6.73	1.47	1.33
26	BA	197	A	C6-N6	6.73	1.47	1.33
26	BA	251	A	C6-N6	6.73	1.47	1.33
26	BA	515	A	C6-N6	6.73	1.47	1.33
26	BA	574	A	C6-N6	6.73	1.47	1.33
26	BA	1085	A	C6-N6	6.73	1.47	1.33
26	BA	1509	A	C6-N6	6.73	1.47	1.33
26	BA	1665	A	C6-N6	6.73	1.47	1.33
26	BA	1916	A	C6-N6	6.73	1.47	1.33
26	BA	2095	A	C6-N6	6.73	1.47	1.33
26	BA	2451	A	C6-N6	6.73	1.47	1.33
1	AA	26	A	C6-N6	6.73	1.47	1.33
1	AA	160	A	C6-N6	6.73	1.47	1.33
1	AA	459	A	C6-N6	6.73	1.47	1.33
1	AA	621	A	C6-N6	6.73	1.47	1.33
1	AA	718	A	C6-N6	6.73	1.47	1.33
1	AA	777	A	C6-N6	6.73	1.47	1.33
1	AA	919	A	C6-N6	6.73	1.47	1.33
1	AA	1216	A	C6-N6	6.73	1.47	1.33
1	AA	1250	A	C6-N6	6.73	1.47	1.33
22	AV	15	A	C6-N6	6.73	1.47	1.33
26	BA	172	A	C6-N6	6.73	1.47	1.33
26	BA	294	A	C6-N6	6.73	1.47	1.33
26	BA	483	A	C6-N6	6.73	1.47	1.33
26	BA	599	A	C6-N6	6.73	1.47	1.33
26	BA	761	A	C6-N6	6.73	1.47	1.33
26	BA	975	A	C6-N6	6.73	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1084	A	C6-N6	6.73	1.47	1.33
26	BA	1253	A	C6-N6	6.73	1.47	1.33
26	BA	1544	A	C6-N6	6.73	1.47	1.33
26	BA	1548	A	C6-N6	6.73	1.47	1.33
26	BA	1569	A	C6-N6	6.73	1.47	1.33
26	BA	1586	A	C6-N6	6.73	1.47	1.33
26	BA	1829	A	C6-N6	6.73	1.47	1.33
26	BA	1854	A	C6-N6	6.73	1.47	1.33
26	BA	1876	A	C6-N6	6.73	1.47	1.33
26	BA	2134	A	C6-N6	6.73	1.47	1.33
26	BA	2241	A	C6-N6	6.73	1.47	1.33
26	BA	2247	A	C6-N6	6.73	1.47	1.33
26	BA	2278	A	C6-N6	6.73	1.47	1.33
26	BA	2727	A	C6-N6	6.73	1.47	1.33
27	BB	39	A	C6-N6	6.73	1.47	1.33
1	AA	583	A	C6-N6	6.73	1.47	1.33
1	AA	938	A	C6-N6	6.73	1.47	1.33
1	AA	1105	A	C6-N6	6.73	1.47	1.33
26	BA	311	A	C6-N6	6.73	1.47	1.33
26	BA	332	A	C6-N6	6.73	1.47	1.33
1	AA	109	A	C6-N6	6.72	1.47	1.33
1	AA	151	A	C6-N6	6.72	1.47	1.33
1	AA	642	A	C6-N6	6.72	1.47	1.33
1	AA	716	A	C6-N6	6.72	1.47	1.33
1	AA	794	A	C6-N6	6.72	1.47	1.33
1	AA	975	A	C6-N6	6.72	1.47	1.33
1	AA	1044	A	C6-N6	6.72	1.47	1.33
26	BA	621	A	C6-N6	6.72	1.47	1.33
26	BA	677	A	C6-N6	6.72	1.47	1.33
26	BA	1088	A	C6-N6	6.72	1.47	1.33
26	BA	1614	A	C6-N6	6.72	1.47	1.33
26	BA	1787	A	C6-N6	6.72	1.47	1.33
26	BA	1977	A	C6-N6	6.72	1.47	1.33
26	BA	2037	A	C6-N6	6.72	1.47	1.33
26	BA	2077	A	C6-N6	6.72	1.47	1.33
26	BA	2199	A	C6-N6	6.72	1.47	1.33
26	BA	2212	A	C6-N6	6.72	1.47	1.33
26	BA	2682	A	C6-N6	6.72	1.47	1.33
26	BA	2799	A	C6-N6	6.72	1.47	1.33
1	AA	8	A	C6-N6	6.72	1.47	1.33
1	AA	33	A	C6-N6	6.72	1.47	1.33
1	AA	238	A	C6-N6	6.72	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	306	A	C6-N6	6.72	1.47	1.33
1	AA	356	A	C6-N6	6.72	1.47	1.33
1	AA	665	A	C6-N6	6.72	1.47	1.33
1	AA	706	A	C6-N6	6.72	1.47	1.33
1	AA	753	A	C6-N6	6.72	1.47	1.33
1	AA	1171	A	C6-N6	6.72	1.47	1.33
1	AA	1269	A	C6-N6	6.72	1.47	1.33
1	AA	1377	A	C6-N6	6.72	1.47	1.33
24	AX	58	A	C6-N6	6.72	1.47	1.33
25	AY	21	A	C6-N6	6.72	1.47	1.33
26	BA	13	A	C6-N6	6.72	1.47	1.33
26	BA	71	A	C6-N6	6.72	1.47	1.33
26	BA	84	A	C6-N6	6.72	1.47	1.33
26	BA	637	A	C6-N6	6.72	1.47	1.33
26	BA	721	A	C6-N6	6.72	1.47	1.33
26	BA	722	A	C6-N6	6.72	1.47	1.33
26	BA	735	A	C6-N6	6.72	1.47	1.33
26	BA	756	A	C6-N6	6.72	1.47	1.33
26	BA	911	A	C6-N6	6.72	1.47	1.33
26	BA	928	A	C6-N6	6.72	1.47	1.33
26	BA	936	A	C6-N6	6.72	1.47	1.33
26	BA	1009	A	C6-N6	6.72	1.47	1.33
26	BA	1032	A	C6-N6	6.72	1.47	1.33
26	BA	1111	A	C6-N6	6.72	1.47	1.33
26	BA	1143	A	C6-N6	6.72	1.47	1.33
26	BA	1230	A	C6-N6	6.72	1.47	1.33
26	BA	1265	A	C6-N6	6.72	1.47	1.33
26	BA	1387	A	C6-N6	6.72	1.47	1.33
26	BA	1608	A	C6-N6	6.72	1.47	1.33
26	BA	2328	A	C6-N6	6.72	1.47	1.33
26	BA	2497	A	C6-N6	6.72	1.47	1.33
26	BA	2541	A	C6-N6	6.72	1.47	1.33
26	BA	2757	A	C6-N6	6.72	1.47	1.33
26	BA	2879	A	C6-N6	6.72	1.47	1.33
27	BB	94	A	C6-N6	6.72	1.47	1.33
27	BB	99	A	C6-N6	6.72	1.47	1.33
27	BB	115	A	C6-N6	6.72	1.47	1.33
1	AA	546	A	C6-N6	6.72	1.47	1.33
1	AA	600	A	C6-N6	6.72	1.47	1.33
1	AA	602	A	C6-N6	6.72	1.47	1.33
1	AA	629	A	C6-N6	6.72	1.47	1.33
1	AA	1394	A	C6-N6	6.72	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	255	A	C6-N6	6.72	1.47	1.33
26	BA	602	A	C6-N6	6.72	1.47	1.33
26	BA	730	A	C6-N6	6.72	1.47	1.33
26	BA	1705	A	C6-N6	6.72	1.47	1.33
26	BA	1889	A	C6-N6	6.72	1.47	1.33
26	BA	1936	A	C6-N6	6.72	1.47	1.33
1	AA	630	A	C6-N6	6.72	1.47	1.33
1	AA	663	A	C6-N6	6.72	1.47	1.33
1	AA	937	A	C6-N6	6.72	1.47	1.33
1	AA	1238	A	C6-N6	6.72	1.47	1.33
1	AA	1299	A	C6-N6	6.72	1.47	1.33
1	AA	1456	A	C6-N6	6.72	1.47	1.33
26	BA	73	A	C6-N6	6.72	1.47	1.33
26	BA	218	A	C6-N6	6.72	1.47	1.33
26	BA	270	A	C6-N6	6.72	1.47	1.33
26	BA	613	A	C6-N6	6.72	1.47	1.33
26	BA	715	A	C6-N6	6.72	1.47	1.33
26	BA	752	A	C6-N6	6.72	1.47	1.33
26	BA	877	A	C6-N6	6.72	1.47	1.33
26	BA	1532	A	C6-N6	6.72	1.47	1.33
26	BA	1609	A	C6-N6	6.72	1.47	1.33
26	BA	1713	A	C6-N6	6.72	1.47	1.33
26	BA	2432	A	C6-N6	6.72	1.47	1.33
26	BA	2461	A	C6-N6	6.72	1.47	1.33
26	BA	2516	A	C6-N6	6.72	1.47	1.33
26	BA	2657	A	C6-N6	6.72	1.47	1.33
26	BA	2765	A	C6-N6	6.72	1.47	1.33
26	BA	2873	A	C6-N6	6.72	1.47	1.33
1	AA	1081	A	C6-N6	6.72	1.47	1.33
1	AA	1082	A	C6-N6	6.72	1.47	1.33
1	AA	1163	A	C6-N6	6.72	1.47	1.33
26	BA	1275	A	C6-N6	6.72	1.47	1.33
26	BA	1579	A	C6-N6	6.72	1.47	1.33
26	BA	1650	A	C6-N6	6.72	1.47	1.33
26	BA	1809	A	C6-N6	6.72	1.47	1.33
26	BA	2471	A	C6-N6	6.72	1.47	1.33
27	BB	45	A	C6-N6	6.72	1.47	1.33
1	AA	573	A	C6-N6	6.72	1.47	1.33
1	AA	696	A	C6-N6	6.72	1.47	1.33
1	AA	909	A	C6-N6	6.72	1.47	1.33
1	AA	969	A	C6-N6	6.72	1.47	1.33
1	AA	1067	A	C6-N6	6.72	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1191	A	C6-N6	6.72	1.47	1.33
1	AA	1196	A	C6-N6	6.72	1.47	1.33
1	AA	1434	A	C6-N6	6.72	1.47	1.33
26	BA	144	A	C6-N6	6.72	1.47	1.33
26	BA	423	A	C6-N6	6.72	1.47	1.33
26	BA	532	A	C6-N6	6.72	1.47	1.33
26	BA	1000	A	C6-N6	6.72	1.47	1.33
26	BA	1127	A	C6-N6	6.72	1.47	1.33
26	BA	1142	A	C6-N6	6.72	1.47	1.33
26	BA	1247	A	C6-N6	6.72	1.47	1.33
26	BA	1654	A	C6-N6	6.72	1.47	1.33
26	BA	2015	A	C6-N6	6.72	1.47	1.33
26	BA	2184	A	C6-N6	6.72	1.47	1.33
26	BA	2268	A	C6-N6	6.72	1.47	1.33
26	BA	2327	A	C6-N6	6.72	1.47	1.33
1	AA	759	A	C6-N6	6.71	1.47	1.33
1	AA	802	A	C6-N6	6.71	1.47	1.33
1	AA	1117	A	C6-N6	6.71	1.47	1.33
1	AA	1201	A	C6-N6	6.71	1.47	1.33
1	AA	1213	A	C6-N6	6.71	1.47	1.33
1	AA	1431	A	C6-N6	6.71	1.47	1.33
24	AX	23	A	C6-N6	6.71	1.47	1.33
26	BA	182	A	C6-N6	6.71	1.47	1.33
26	BA	241	A	C6-N6	6.71	1.47	1.33
26	BA	265	A	C6-N6	6.71	1.47	1.33
26	BA	278	A	C6-N6	6.71	1.47	1.33
26	BA	608	A	C6-N6	6.71	1.47	1.33
26	BA	675	A	C6-N6	6.71	1.47	1.33
26	BA	1098	A	C6-N6	6.71	1.47	1.33
26	BA	1272	A	C6-N6	6.71	1.47	1.33
26	BA	1327	A	C6-N6	6.71	1.47	1.33
26	BA	1427	A	C6-N6	6.71	1.47	1.33
26	BA	1434	A	C6-N6	6.71	1.47	1.33
26	BA	1689	A	C6-N6	6.71	1.47	1.33
26	BA	2298	A	C6-N6	6.71	1.47	1.33
26	BA	2386	A	C6-N6	6.71	1.47	1.33
26	BA	2572	A	C6-N6	6.71	1.47	1.33
26	BA	2726	A	C6-N6	6.71	1.47	1.33
27	BB	66	A	C6-N6	6.71	1.47	1.33
1	AA	408	A	C6-N6	6.71	1.47	1.33
1	AA	782	A	C6-N6	6.71	1.47	1.33
1	AA	946	A	C6-N6	6.71	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1378	A	C6-N6	6.71	1.47	1.33
26	BA	1603	A	C6-N6	6.71	1.47	1.33
26	BA	2542	A	C6-N6	6.71	1.47	1.33
27	BB	52	A	C6-N6	6.71	1.47	1.33
1	AA	65	A	C6-N6	6.71	1.47	1.33
1	AA	130	A	C6-N6	6.71	1.47	1.33
1	AA	298	A	C6-N6	6.71	1.47	1.33
1	AA	325	A	C6-N6	6.71	1.47	1.33
1	AA	889	A	C6-N6	6.71	1.47	1.33
1	AA	1219	A	C6-N6	6.71	1.47	1.33
26	BA	739	A	C6-N6	6.71	1.47	1.33
26	BA	800	A	C6-N6	6.71	1.47	1.33
26	BA	861	A	C6-N6	6.71	1.47	1.33
26	BA	990	A	C6-N6	6.71	1.47	1.33
26	BA	1155	A	C6-N6	6.71	1.47	1.33
26	BA	1359	A	C6-N6	6.71	1.47	1.33
26	BA	1392	A	C6-N6	6.71	1.47	1.33
26	BA	1626	A	C6-N6	6.71	1.47	1.33
26	BA	1735	A	C6-N6	6.71	1.47	1.33
26	BA	1759	A	C6-N6	6.71	1.47	1.33
26	BA	2158	A	C6-N6	6.71	1.47	1.33
1	AA	452	A	C6-N6	6.71	1.47	1.33
1	AA	915	A	C6-N6	6.71	1.47	1.33
1	AA	1289	A	C6-N6	6.71	1.47	1.33
26	BA	95	A	C6-N6	6.71	1.47	1.33
26	BA	222	A	C6-N6	6.71	1.47	1.33
26	BA	346	A	C6-N6	6.71	1.47	1.33
26	BA	460	A	C6-N6	6.71	1.47	1.33
26	BA	1805	A	C6-N6	6.71	1.47	1.33
1	AA	205	A	C6-N6	6.71	1.47	1.33
1	AA	374	A	C6-N6	6.71	1.47	1.33
1	AA	784	A	C6-N6	6.71	1.47	1.33
1	AA	1170	A	C6-N6	6.71	1.47	1.33
1	AA	1324	A	C6-N6	6.71	1.47	1.33
1	AA	1333	A	C6-N6	6.71	1.47	1.33
1	AA	1476	A	C6-N6	6.71	1.47	1.33
25	AY	38	A	C6-N6	6.71	1.47	1.33
26	BA	563	A	C6-N6	6.71	1.47	1.33
26	BA	676	A	C6-N6	6.71	1.47	1.33
26	BA	1494	A	C6-N6	6.71	1.47	1.33
26	BA	1591	A	C6-N6	6.71	1.47	1.33
26	BA	1877	A	C6-N6	6.71	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2088	A	C6-N6	6.71	1.47	1.33
26	BA	2565	A	C6-N6	6.71	1.47	1.33
26	BA	2810	A	C6-N6	6.71	1.47	1.33
1	AA	199	A	C6-N6	6.71	1.47	1.33
1	AA	766	A	C6-N6	6.71	1.47	1.33
1	AA	1021	A	C6-N6	6.71	1.47	1.33
1	AA	1357	A	C6-N6	6.71	1.47	1.33
1	AA	1430	A	C6-N6	6.71	1.47	1.33
26	BA	207	A	C6-N6	6.71	1.47	1.33
26	BA	324	A	C6-N6	6.71	1.47	1.33
26	BA	526	A	C6-N6	6.71	1.47	1.33
26	BA	783	A	C6-N6	6.71	1.47	1.33
26	BA	1269	A	C6-N6	6.71	1.47	1.33
26	BA	2478	A	C6-N6	6.71	1.47	1.33
26	BA	2560	A	C6-N6	6.71	1.47	1.33
26	BA	2835	A	C6-N6	6.71	1.47	1.33
27	BB	53	A	C6-N6	6.71	1.47	1.33
26	BA	522	A	C6-N6	6.71	1.47	1.33
26	BA	920	A	C6-N6	6.71	1.47	1.33
1	AA	382	A	C6-N6	6.70	1.47	1.33
1	AA	460	A	C6-N6	6.70	1.47	1.33
1	AA	814	A	C6-N6	6.70	1.47	1.33
1	AA	1285	A	C6-N6	6.70	1.47	1.33
1	AA	1518	A	C6-N6	6.70	1.47	1.33
26	BA	10	A	C6-N6	6.70	1.47	1.33
26	BA	449	A	C6-N6	6.70	1.47	1.33
26	BA	586	A	C6-N6	6.70	1.47	1.33
26	BA	655	A	C6-N6	6.70	1.47	1.33
26	BA	863	A	C6-N6	6.70	1.47	1.33
26	BA	1268	A	C6-N6	6.70	1.47	1.33
26	BA	1328	A	C6-N6	6.70	1.47	1.33
26	BA	1522	A	C6-N6	6.70	1.47	1.33
26	BA	1552	A	C6-N6	6.70	1.47	1.33
26	BA	1783	A	C6-N6	6.70	1.47	1.33
26	BA	1808	A	C6-N6	6.70	1.47	1.33
26	BA	1848	A	C6-N6	6.70	1.47	1.33
26	BA	1901	A	C6-N6	6.70	1.47	1.33
26	BA	2287	A	C6-N6	6.70	1.47	1.33
26	BA	2820	A	C6-N6	6.70	1.47	1.33
1	AA	451	A	C6-N6	6.70	1.47	1.33
1	AA	1157	A	C6-N6	6.70	1.47	1.33
26	BA	804	A	C6-N6	6.70	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	909	A	C6-N6	6.70	1.47	1.33
26	BA	983	A	C6-N6	6.70	1.47	1.33
26	BA	2094	A	C6-N6	6.70	1.47	1.33
26	BA	2358	A	C6-N6	6.70	1.47	1.33
1	AA	119	A	C6-N6	6.70	1.47	1.33
1	AA	1349	A	C6-N6	6.70	1.47	1.33
1	AA	1429	A	C6-N6	6.70	1.47	1.33
26	BA	821	A	C6-N6	6.70	1.47	1.33
26	BA	2518	A	C6-N6	6.70	1.47	1.33
26	BA	2577	A	C6-N6	6.70	1.47	1.33
26	BA	2764	A	C6-N6	6.70	1.47	1.33
1	AA	493	A	C6-N6	6.70	1.47	1.33
1	AA	499	A	C6-N6	6.70	1.47	1.33
1	AA	695	A	C6-N6	6.70	1.47	1.33
1	AA	746	A	C6-N6	6.70	1.47	1.33
1	AA	872	A	C6-N6	6.70	1.47	1.33
1	AA	923	A	C6-N6	6.70	1.47	1.33
1	AA	1350	A	C6-N6	6.70	1.47	1.33
26	BA	204	A	C6-N6	6.70	1.47	1.33
26	BA	643	A	C6-N6	6.70	1.47	1.33
26	BA	1028	A	C6-N6	6.70	1.47	1.33
26	BA	1664	A	C6-N6	6.70	1.47	1.33
26	BA	2169	A	C6-N6	6.70	1.47	1.33
25	AY	9	A	C6-N6	6.70	1.47	1.33
26	BA	1419	A	C6-N6	6.70	1.47	1.33
26	BA	1801	A	C6-N6	6.70	1.47	1.33
26	BA	2005	A	C6-N6	6.70	1.47	1.33
26	BA	2333	A	C6-N6	6.70	1.47	1.33
26	BA	2725	A	C6-N6	6.70	1.47	1.33
1	AA	1275	A	C6-N6	6.70	1.47	1.33
26	BA	415	A	C6-N6	6.70	1.47	1.33
26	BA	529	A	C6-N6	6.70	1.47	1.33
26	BA	1773	A	C6-N6	6.70	1.47	1.33
1	AA	81	A	C6-N6	6.69	1.47	1.33
1	AA	353	A	C6-N6	6.69	1.47	1.33
26	BA	1353	A	C6-N6	6.69	1.47	1.33
26	BA	320	A	C6-N6	6.69	1.47	1.33
26	BA	661	A	C6-N6	6.69	1.47	1.33
26	BA	750	A	C6-N6	6.69	1.47	1.33
26	BA	910	A	C6-N6	6.69	1.47	1.33
26	BA	1566	A	C6-N6	6.69	1.47	1.33
26	BA	1668	A	C6-N6	6.69	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2700	A	C6-N6	6.69	1.47	1.33
26	BA	2740	A	C6-N6	6.69	1.47	1.33
1	AA	389	A	C6-N6	6.69	1.47	1.33
26	BA	794	A	C6-N6	6.69	1.47	1.33
26	BA	1431	A	C6-N6	6.69	1.47	1.33
26	BA	2225	A	C6-N6	6.69	1.47	1.33
26	BA	2547	A	C6-N6	6.69	1.47	1.33
26	BA	900	A	C6-N6	6.69	1.47	1.33
26	BA	1244	A	C6-N6	6.69	1.47	1.33
26	BA	2346	A	C6-N6	6.69	1.47	1.33
1	AA	98	A	C6-N6	6.69	1.47	1.33
1	AA	865	A	C6-N6	6.69	1.47	1.33
1	AA	1167	A	C6-N6	6.69	1.47	1.33
1	AA	1239	A	C6-N6	6.69	1.47	1.33
24	AX	76	A	C6-N6	6.69	1.47	1.33
26	BA	2267	A	C6-N6	6.69	1.47	1.33
26	BA	2450	A	C6-N6	6.69	1.47	1.33
26	BA	2459	A	C6-N6	6.69	1.47	1.33
26	BA	2766	A	C6-N6	6.69	1.47	1.33
26	BA	2335	A	C6-N6	6.69	1.47	1.33
1	AA	622	A	C6-N6	6.68	1.47	1.33
1	AA	1145	A	C6-N6	6.68	1.47	1.33
1	AA	1152	A	C6-N6	6.68	1.47	1.33
24	AX	24	A	C6-N6	6.68	1.47	1.33
26	BA	1226	A	C6-N6	6.68	1.47	1.33
26	BA	2080	A	C6-N6	6.68	1.47	1.33
27	BB	50	A	C6-N6	6.68	1.47	1.33
27	BB	78	A	C6-N6	6.68	1.47	1.33
26	BA	44	A	C6-N6	6.68	1.47	1.33
26	BA	119	A	C6-N6	6.68	1.47	1.33
26	BA	330	A	C6-N6	6.68	1.47	1.33
26	BA	503	A	C6-N6	6.68	1.47	1.33
26	BA	1655	A	C6-N6	6.68	1.47	1.33
26	BA	2741	A	C6-N6	6.68	1.47	1.33
27	BB	59	A	C6-N6	6.68	1.47	1.33
1	AA	553	A	C6-N6	6.68	1.47	1.33
26	BA	1001	A	C6-N6	6.68	1.47	1.33
26	BA	2052	A	C6-N6	6.68	1.47	1.33
26	BA	2675	A	C6-N6	6.68	1.47	1.33
26	BA	279	A	C6-N6	6.68	1.47	1.33
26	BA	575	A	C6-N6	6.68	1.47	1.33
26	BA	845	A	C6-N6	6.68	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	864	A	C6-N6	6.68	1.47	1.33
23	AW	9	A	C6-N6	6.68	1.47	1.33
26	BA	227	A	C6-N6	6.68	1.47	1.33
1	AA	171	A	C6-N6	6.67	1.47	1.33
1	AA	270	A	C6-N6	6.67	1.47	1.33
1	AA	397	A	C6-N6	6.67	1.47	1.33
1	AA	430	A	C6-N6	6.67	1.47	1.33
1	AA	596	A	C6-N6	6.67	1.47	1.33
26	BA	933	A	C6-N6	6.67	1.47	1.33
26	BA	1189	A	C6-N6	6.67	1.47	1.33
1	AA	502	A	C6-N6	6.67	1.47	1.33
26	BA	1515	A	C6-N6	6.67	1.47	1.33
26	BA	582	A	C6-N6	6.67	1.47	1.33
26	BA	1214	A	C6-N6	6.67	1.47	1.33
26	BA	2388	A	C6-N6	6.67	1.47	1.33
26	BA	2639	A	C6-N6	6.67	1.47	1.33
1	AA	412	A	C6-N6	6.67	1.47	1.33
26	BA	56	A	C6-N6	6.67	1.47	1.33
26	BA	1784	A	C6-N6	6.67	1.47	1.33
26	BA	457	A	C6-N6	6.67	1.47	1.33
26	BA	685	A	C6-N6	6.67	1.47	1.33
26	BA	644	A	C6-N6	6.66	1.47	1.33
26	BA	1276	A	C6-N6	6.66	1.47	1.33
1	AA	1151	A	C6-N6	6.66	1.47	1.33
26	BA	2856	A	C6-N6	6.66	1.47	1.33
1	AA	432	A	C6-N6	6.66	1.47	1.33
26	BA	2054	A	C6-N6	6.66	1.47	1.33
1	AA	478	A	C6-N6	6.66	1.47	1.33
1	AA	608	A	C6-N6	6.65	1.47	1.33
26	BA	1496	A	C6-N6	6.65	1.47	1.33
26	BA	1899	A	C6-N6	6.65	1.47	1.33
26	BA	572	A	C6-N6	6.65	1.47	1.33
26	BA	1545	A	C6-N6	6.65	1.47	1.33
26	BA	142	A	C6-N6	6.64	1.47	1.33
26	BA	2800	A	C6-N6	6.64	1.47	1.33
1	AA	1102	A	C6-N6	6.63	1.47	1.33
26	BA	53	A	C6-N6	6.62	1.47	1.33
26	BA	2469	A	C6-N6	6.62	1.47	1.33
1	AA	495	A	C6-N6	6.58	1.47	1.33
26	BA	514	A	C6-N6	6.56	1.47	1.33
23	AW	75	C	O3'-P	6.47	1.70	1.61
9	AI	91	ASP	N-CA	5.42	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	BM	70	ASP	N-CA	5.25	1.52	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	AL	41	THR	CA-C-N	6.50	126.47	119.78
12	AL	41	THR	C-N-CA	6.50	126.47	119.78
28	BC	135	ILE	CA-C-N	6.18	126.14	119.78
28	BC	135	ILE	C-N-CA	6.18	126.14	119.78
34	BI	73	THR	CA-C-N	6.06	124.08	119.66
34	BI	73	THR	C-N-CA	6.06	124.08	119.66
12	AL	21	VAL	CA-C-N	5.97	125.85	119.28
12	AL	21	VAL	C-N-CA	5.97	125.85	119.28
28	BC	135	ILE	N-CA-C	5.88	113.69	108.63
12	AL	102	LEU	CB-CA-C	-5.75	109.93	116.54
28	BC	106	ALA	CA-C-N	5.72	125.62	119.85
28	BC	106	ALA	C-N-CA	5.72	125.62	119.85
34	BI	25	GLY	CA-C-N	5.67	125.52	119.28
34	BI	25	GLY	C-N-CA	5.67	125.52	119.28
2	AB	129	LEU	CB-CA-C	-5.54	109.20	115.79
28	BC	28	LYS	CA-C-N	5.44	125.34	119.85
28	BC	28	LYS	C-N-CA	5.44	125.34	119.85
21	AU	10	GLU	CA-C-N	-5.37	113.12	119.84
21	AU	10	GLU	C-N-CA	-5.37	113.12	119.84
36	BK	92	GLU	CB-CA-C	-5.32	109.45	115.79
11	AK	90	GLY	CA-C-N	5.30	125.11	119.28
11	AK	90	GLY	C-N-CA	5.30	125.11	119.28
8	AH	51	VAL	N-CA-C	5.13	111.69	106.21
28	BC	21	ASN	CA-C-N	5.10	124.89	119.28
28	BC	21	ASN	C-N-CA	5.10	124.89	119.28
44	BS	64	ALA	CB-CA-C	-5.07	110.33	117.23
4	AD	174	ASP	CB-CA-C	-5.04	110.74	116.54
8	AH	92	LEU	CA-C-N	5.04	124.94	119.85
8	AH	92	LEU	C-N-CA	5.04	124.94	119.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	BD	151	THR	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	33015	0	16618	260	0
2	AB	1704	0	1732	32	0
3	AC	1624	0	1696	36	0
4	AD	1643	0	1707	79	0
5	AE	1105	0	1148	25	0
6	AF	817	0	808	12	0
7	AG	1181	0	1238	22	0
8	AH	979	0	1031	19	0
9	AI	1022	0	1070	25	0
10	AJ	786	0	828	32	0
11	AK	877	0	887	27	0
12	AL	955	0	1016	20	0
13	AM	883	0	941	22	0
14	AN	774	0	824	26	0
15	AO	710	0	728	9	0
16	AP	649	0	666	25	0
17	AQ	648	0	691	19	0
18	AR	455	0	478	7	0
19	AS	637	0	665	15	0
20	AT	665	0	714	20	0
21	AU	425	0	449	7	0
22	AV	218	0	109	3	0
23	AW	1593	0	820	8	0
24	AX	1656	0	849	9	0
25	AY	1525	0	780	10	0
26	BA	62195	0	31280	435	0
27	BB	2529	0	1281	22	0
28	BC	2082	0	2154	53	0
29	BD	1565	0	1616	40	0
30	BE	1552	0	1619	33	0
31	BF	1410	0	1444	23	0
32	BG	1323	0	1371	28	0
33	BH	359	0	381	13	0
34	BI	1032	0	1085	26	0
35	BJ	1129	0	1162	22	0
36	BK	938	0	1012	27	0
37	BL	1045	0	1117	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BM	1074	0	1157	28	0
39	BN	960	0	1000	33	0
40	BO	892	0	923	21	0
41	BP	917	0	962	22	0
42	BQ	947	0	1019	11	0
43	BR	816	0	839	16	0
44	BS	857	0	922	14	0
45	BT	738	0	807	15	0
46	BU	779	0	831	24	0
47	BV	753	0	780	10	0
48	BW	569	0	581	15	0
49	BX	625	0	652	13	0
50	BY	509	0	543	8	0
51	BZ	449	0	488	10	0
52	B0	444	0	458	8	0
53	B1	409	0	440	12	0
54	B2	377	0	418	9	0
55	B3	504	0	572	14	0
56	B4	302	0	343	8	0
57	B5	74	0	74	21	0
58	AW	9	0	12	2	0
59	BA	51	0	67	12	0
All	All	146760	0	97903	1505	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1505) 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)
26:BA:1782:U:N3	57:B5:-4:MET:HE1	1.55	1.21
59:BA:9000:ERY:C27	57:B5:-2:ASN:ND2	2.18	1.07
59:BA:9000:ERY:H271	57:B5:-2:ASN:HD21	1.13	1.06
26:BA:1782:U:C2	57:B5:-4:MET:HE1	1.92	1.04
59:BA:9000:ERY:H271	57:B5:-2:ASN:ND2	1.74	1.01
59:BA:9000:ERY:C27	57:B5:-2:ASN:HD21	1.72	0.98
58:AW:101:LYS:N	24:AX:76:A:HO2'	1.69	0.91
4:AD:11:LEU:HB3	4:AD:63:ARG:HD3	1.62	0.81
26:BA:1782:U:N3	57:B5:-4:MET:CE	2.43	0.80
4:AD:100:ASN:OD1	4:AD:111:ARG:NH1	2.13	0.79
1:AA:664:G:H22	1:AA:741:G:H1	1.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:66:GLU:HG3	13:AM:67:GLY:H	1.49	0.77
26:BA:1782:U:C4	57:B5:-4:MET:HE1	2.20	0.77
54:B2:39:ARG:HG3	54:B2:41:ARG:H	1.50	0.77
40:BO:40:ILE:HG12	40:BO:47:VAL:HG12	1.68	0.76
1:AA:1127:G:H1	1:AA:1145:A:H61	1.35	0.75
30:BE:146:VAL:HG12	30:BE:185:LYS:HB2	1.70	0.74
20:AT:5:LYS:HG3	20:AT:7:ALA:H	1.53	0.74
10:AJ:45:ARG:HB3	10:AJ:69:THR:HB	1.69	0.73
29:BD:151:THR:HG22	29:BD:152:PRO:HD2	1.69	0.73
23:AW:25:C:H42	23:AW:45:G:H22	1.34	0.73
26:BA:1782:U:C4	57:B5:-4:MET:CE	2.72	0.72
10:AJ:49:PHE:HB2	10:AJ:65:TYR:HB2	1.71	0.72
4:AD:95:GLU:HA	4:AD:100:ASN:HD22	1.55	0.72
1:AA:439:U:H4'	4:AD:121:LYS:HD2	1.72	0.72
26:BA:136:G:H1	26:BA:143:C:H42	1.39	0.71
28:BC:107:PRO:HG2	28:BC:110:LEU:HB2	1.73	0.71
30:BE:126:VAL:HG13	30:BE:133:LEU:HD22	1.72	0.71
4:AD:58:LYS:NZ	4:AD:59:GLN:OE1	2.23	0.70
1:AA:1522:U:H5''	11:AK:128:ARG:HH22	1.56	0.70
1:AA:407:U:H2'	1:AA:408:A:H8	1.56	0.70
7:AG:113:ASP:HB2	7:AG:119:ARG:HG2	1.73	0.70
26:BA:1779:U:OP2	26:BA:1784:A:N6	2.24	0.70
3:AC:14:ILE:HG22	3:AC:15:VAL:HG13	1.74	0.70
40:BO:31:THR:O	40:BO:102:ARG:NH1	2.25	0.70
41:BP:33:VAL:HG12	41:BP:35:GLY:H	1.57	0.69
4:AD:95:GLU:OE1	4:AD:100:ASN:ND2	2.25	0.69
35:BJ:118:MET:HA	35:BJ:121:LYS:HE2	1.73	0.69
37:BL:93:ASN:O	37:BL:95:LEU:N	2.24	0.69
1:AA:1359:C:O2'	1:AA:1361:G:N7	2.25	0.69
1:AA:1124:G:O2'	1:AA:1145:A:N6	2.24	0.69
1:AA:438:U:O2'	1:AA:493:A:N6	2.26	0.69
6:AF:91:ARG:HH21	6:AF:93:LYS:HD3	1.58	0.69
10:AJ:57:VAL:HG22	10:AJ:58:ASN:H	1.57	0.69
26:BA:1062:G:H21	34:BI:135:SER:HB3	1.58	0.69
6:AF:90:MET:SD	18:AR:61:ARG:NH1	2.66	0.68
36:BK:21:CYS:HA	36:BK:41:ILE:HG22	1.76	0.68
12:AL:34:CYS:HA	12:AL:55:VAL:HA	1.76	0.68
34:BI:49:ILE:HG13	34:BI:50:GLU:H	1.59	0.68
10:AJ:25:ILE:HD11	10:AJ:87:LEU:HG	1.76	0.68
26:BA:45:G:H5''	26:BA:46:G:H5'	1.77	0.67
26:BA:807:U:OP2	37:BL:41:ARG:NH1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BF:117:LEU:HD13	31:BF:176:PRO:HG2	1.76	0.67
43:BR:6:GLN:HB3	43:BR:37:GLU:HB3	1.76	0.67
48:BW:37:ILE:HG22	48:BW:38:VAL:HG23	1.75	0.67
1:AA:1491:G:H5''	12:AL:43:LYS:HG2	1.76	0.67
1:AA:407:U:H2'	1:AA:408:A:C8	2.30	0.67
36:BK:43:ILE:HD12	36:BK:56:ASP:HB2	1.76	0.67
5:AE:81:LEU:HD13	5:AE:123:VAL:HG11	1.77	0.67
10:AJ:46:LYS:HG2	10:AJ:68:ARG:HG2	1.77	0.67
30:BE:58:LYS:NZ	30:BE:70:SER:O	2.28	0.67
1:AA:570:G:O6	1:AA:865:A:N6	2.28	0.66
14:AN:13:ARG:HE	14:AN:59:ARG:HE	1.43	0.66
51:BZ:10:THR:HG23	51:BZ:11:ARG:HG3	1.77	0.66
20:AT:73:ALA:HA	20:AT:76:LYS:HG2	1.78	0.66
26:BA:1394:U:H4'	26:BA:1603:A:H4'	1.77	0.66
56:B4:19:ARG:HD2	56:B4:24:ARG:HD2	1.77	0.66
2:AB:219:ALA:O	2:AB:222:ARG:NH1	2.29	0.66
31:BF:63:GLN:HE21	31:BF:95:ARG:HH11	1.43	0.66
1:AA:1373:G:H5''	7:AG:36:LYS:HE2	1.78	0.65
3:AC:34:ASP:OD2	14:AN:65:ARG:NH1	2.30	0.65
20:AT:69:LYS:HG3	20:AT:70:ASN:H	1.61	0.65
34:BI:34:ASN:HB3	34:BI:37:GLU:HG2	1.78	0.65
35:BJ:36:LEU:O	35:BJ:121:LYS:NZ	2.24	0.65
45:BT:59:ASN:HB2	45:BT:84:TYR:HB2	1.78	0.65
55:B3:24:HIS:HD2	55:B3:50:VAL:HG22	1.62	0.65
26:BA:1082:U:H5'	34:BI:119:GLY:HA2	1.78	0.65
1:AA:614:C:OP1	4:AD:83:LYS:NZ	2.30	0.65
29:BD:3:GLY:HA3	29:BD:204:LYS:HG2	1.78	0.65
13:AM:101:ARG:NH1	13:AM:104:THR:OG1	2.29	0.65
49:BX:17:ASN:HB2	49:BX:25:THR:HB	1.77	0.65
1:AA:237:G:H4'	17:AQ:27:ARG:HH12	1.61	0.65
26:BA:482:A:H4'	46:BU:45:HIS:HE1	1.62	0.65
57:B5:-8:ALA:O	57:B5:-6:PHE:N	2.24	0.65
26:BA:2495:G:OP1	38:BM:81:ARG:NH1	2.30	0.65
28:BC:67:PHE:HZ	28:BC:87:ARG:HH22	1.42	0.65
14:AN:3:LYS:HD2	14:AN:6:MET:HG2	1.78	0.64
2:AB:130:THR:HG22	2:AB:132:LYS:H	1.62	0.64
26:BA:2062:A:H8	57:B5:-2:ASN:H	1.44	0.64
1:AA:1221:G:H4'	19:AS:77:THR:HG21	1.78	0.64
3:AC:11:ARG:NH1	3:AC:180:ALA:O	2.30	0.64
1:AA:10:A:OP2	5:AE:131:THR:OG1	2.16	0.64
26:BA:682:G:O6	26:BA:794:A:N6	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BC:210:ALA:O	28:BC:214:ARG:NH1	2.31	0.64
23:AW:75:C:O2'	26:BA:2573:C:N4	2.31	0.64
26:BA:1154:G:OP2	42:BQ:58:ARG:NH1	2.31	0.64
38:BM:11:LYS:HD3	38:BM:86:LYS:HD3	1.80	0.64
59:BA:9000:ERY:H273	57:B5:-2:ASN:ND2	2.12	0.63
36:BK:80:ASP:HB2	41:BP:68:GLU:HB2	1.80	0.63
2:AB:166:ALA:HB3	2:AB:191:SER:HB3	1.81	0.63
29:BD:46:ARG:HB3	29:BD:84:LEU:HD12	1.81	0.63
26:BA:1226:A:OP1	42:BQ:16:LYS:NZ	2.32	0.63
1:AA:243:A:H4'	1:AA:244:U:H3'	1.81	0.63
1:AA:405:U:O4	4:AD:2:ALA:N	2.32	0.63
1:AA:717:U:H4'	11:AK:119:ASN:HD22	1.63	0.63
26:BA:335:C:O2	46:BU:68:SER:OG	2.16	0.63
26:BA:863:A:OP1	38:BM:22:GLN:NE2	2.32	0.63
7:AG:71:PRO:O	7:AG:96:ARG:NH1	2.32	0.63
32:BG:164:TYR:HB2	32:BG:167:GLU:HG2	1.79	0.63
1:AA:19:A:OP1	5:AE:135:ASN:ND2	2.32	0.63
1:AA:1072:G:O6	1:AA:1102:A:N6	2.32	0.63
5:AE:77:ASN:HB2	5:AE:82:GLN:HG2	1.81	0.63
1:AA:970:C:OP1	10:AJ:59:LYS:NZ	2.32	0.62
26:BA:1614:A:N6	44:BS:92:ARG:O	2.31	0.62
26:BA:2271:G:H5'	48:BW:20:ARG:HG2	1.81	0.62
40:BO:90:VAL:HG23	40:BO:117:PHE:HB3	1.80	0.62
29:BD:131:ASP:O	29:BD:136:ASN:ND2	2.31	0.62
59:BA:9000:ERY:H212	57:B5:-2:ASN:OD1	1.98	0.62
1:AA:403:C:OP2	4:AD:71:GLN:NE2	2.32	0.62
5:AE:133:PRO:HA	5:AE:136:VAL:HG12	1.80	0.62
26:BA:2312:U:H2'	31:BF:37:ASN:HD21	1.63	0.62
28:BC:133:ARG:O	28:BC:167:ARG:NH1	2.32	0.62
26:BA:877:A:O2'	26:BA:900:A:N6	2.32	0.62
36:BK:105:ARG:NH2	41:BP:41:GLN:OE1	2.33	0.62
17:AQ:70:THR:HG22	17:AQ:71:LYS:H	1.63	0.62
26:BA:1788:C:OP1	28:BC:221:ARG:NH2	2.33	0.62
1:AA:1494:G:HO2'	26:BA:1912:A:HO2'	1.47	0.62
41:BP:27:GLU:HA	41:BP:44:GLU:HA	1.80	0.62
26:BA:2688:G:N1	26:BA:2720:U:OP2	2.32	0.62
34:BI:8:TYR:HB2	34:BI:59:ILE:H	1.63	0.62
37:BL:79:LEU:HD12	37:BL:113:ALA:H	1.64	0.62
1:AA:978:A:OP2	1:AA:1362:A:N6	2.32	0.61
26:BA:2091:C:H3'	26:BA:2092:U:H5''	1.81	0.61
28:BC:73:GLY:O	28:BC:117:GLN:NE2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BJ:56:VAL:HB	35:BJ:124:VAL:HA	1.82	0.61
1:AA:1397:C:H42	22:AV:22:A:H3'	1.65	0.61
3:AC:28:GLU:O	3:AC:32:ASN:ND2	2.31	0.61
10:AJ:40:ILE:HD12	10:AJ:73:LEU:HD22	1.81	0.61
27:BB:8:C:O2'	40:BO:25:ARG:NH1	2.33	0.61
29:BD:33:ARG:NH1	29:BD:74:GLU:O	2.33	0.61
11:AK:124:PRO:HB2	11:AK:126:LYS:HG2	1.82	0.61
13:AM:25:VAL:HG23	13:AM:29:ARG:HB3	1.82	0.61
9:AI:123:ARG:NH1	9:AI:124:ARG:O	2.33	0.61
2:AB:146:ASN:OD1	2:AB:147:SER:N	2.33	0.61
1:AA:255:G:H4'	17:AQ:19:LYS:HE3	1.83	0.61
28:BC:235:GLY:O	28:BC:239:ASN:ND2	2.32	0.61
26:BA:1789:A:OP2	28:BC:221:ARG:NH1	2.33	0.61
31:BF:131:GLY:HA2	31:BF:153:ASP:HA	1.83	0.61
1:AA:69:G:O6	1:AA:98:A:N6	2.33	0.61
26:BA:2581:G:OP2	26:BA:2581:G:N2	2.32	0.61
39:BN:12:ARG:O	39:BN:17:ARG:NH2	2.34	0.61
26:BA:1343:G:O6	26:BA:1403:A:N6	2.34	0.61
26:BA:2199:A:OP1	49:BX:37:ARG:NH1	2.34	0.61
26:BA:2478:A:O2'	26:BA:2536:G:N2	2.34	0.61
6:AF:21:MET:HG2	6:AF:24:ARG:HH21	1.65	0.60
48:BW:23:VAL:HG13	48:BW:38:VAL:HG22	1.83	0.60
26:BA:2298:A:OP1	31:BF:71:ARG:NH2	2.33	0.60
35:BJ:11:VAL:HG11	35:BJ:50:THR:HA	1.83	0.60
26:BA:958:U:OP2	38:BM:14:LYS:NZ	2.30	0.60
28:BC:159:GLY:H	28:BC:195:VAL:HG13	1.67	0.60
51:BZ:8:THR:HB	51:BZ:56:LYS:HB3	1.84	0.60
1:AA:1396:A:O2'	5:AE:29:ARG:NH2	2.35	0.60
7:AG:57:SER:HB3	7:AG:60:GLU:HG2	1.84	0.60
26:BA:2898:U:O2'	35:BJ:134:ALA:O	2.18	0.60
2:AB:68:LEU:HD12	2:AB:154:MET:HE1	1.84	0.60
3:AC:129:MET:SD	3:AC:132:ARG:NH1	2.75	0.60
6:AF:81:ASN:HB3	6:AF:84:VAL:HG12	1.82	0.60
3:AC:185:ASN:OD1	3:AC:186:THR:N	2.35	0.60
26:BA:793:A:OP2	26:BA:2071:A:O2'	2.18	0.60
26:BA:1998:A:OP2	29:BD:141:ARG:NH1	2.35	0.60
1:AA:546:A:H61	4:AD:4:TYR:HA	1.66	0.60
26:BA:1693:U:O2'	28:BC:14:ARG:NH1	2.35	0.60
28:BC:94:VAL:HG11	28:BC:116:ILE:HD11	1.83	0.60
28:BC:252:THR:HG22	28:BC:253:LYS:HG3	1.84	0.60
56:B4:2:LYS:NZ	56:B4:32:LYS:O	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:28:ASN:O	11:AK:57:LYS:NZ	2.35	0.59
26:BA:2279:G:N7	48:BW:14:ARG:NH2	2.50	0.59
28:BC:53:HIS:HA	28:BC:217:ARG:HB2	1.84	0.59
31:BF:106:ILE:HD12	31:BF:139:PRO:HG2	1.84	0.59
53:B1:8:LYS:HG2	53:B1:24:THR:HG22	1.82	0.59
46:BU:74:ASN:ND2	46:BU:77:THR:OG1	2.35	0.59
47:BV:51:GLN:HE22	47:BV:86:LEU:HD21	1.67	0.59
53:B1:50:LYS:HG2	53:B1:51:GLU:H	1.67	0.59
16:AP:20:VAL:HG12	16:AP:35:ARG:HA	1.83	0.59
33:BH:9:VAL:HB	33:BH:13:GLY:HA3	1.82	0.59
1:AA:502:A:H61	1:AA:543:U:H3	1.49	0.59
1:AA:1097:C:OP1	2:AB:139:ARG:NH2	2.31	0.59
27:BB:30:C:H1'	27:BB:57:A:H61	1.67	0.59
26:BA:1226:A:H5'	43:BR:86:GLN:HE22	1.68	0.59
26:BA:1334:G:OP1	45:BT:69:ARG:NH2	2.36	0.59
39:BN:103:ARG:HG2	39:BN:105:GLY:H	1.66	0.59
1:AA:848:C:OP1	2:AB:37:LYS:NZ	2.36	0.59
3:AC:56:VAL:HB	3:AC:67:THR:HB	1.83	0.59
10:AJ:47:GLU:OE1	14:AN:76:LYS:NZ	2.34	0.59
21:AU:4:ILE:HD13	21:AU:19:PHE:HE2	1.68	0.59
26:BA:24:G:O2'	44:BS:78:GLU:O	2.19	0.59
26:BA:2485:G:H5''	38:BM:45:GLN:HE21	1.67	0.59
26:BA:2595:G:N2	26:BA:2598:A:OP2	2.36	0.59
1:AA:926:G:N2	22:AV:16:G:OP1	2.36	0.59
1:AA:1351:U:O4	9:AI:120:LYS:NZ	2.36	0.59
3:AC:157:LEU:O	3:AC:164:ARG:NH2	2.33	0.59
5:AE:154:ALA:HA	5:AE:157:ARG:HB3	1.84	0.59
19:AS:3:ARG:NH2	19:AS:68:GLY:O	2.34	0.59
26:BA:2303:G:O2'	31:BF:121:SER:O	2.21	0.59
28:BC:57:GLY:HA2	28:BC:213:TRP:HA	1.85	0.59
51:BZ:5:ILE:HD13	51:BZ:45:ARG:HH22	1.68	0.59
1:AA:766:A:OP2	1:AA:812:G:N2	2.36	0.58
4:AD:147:GLU:HA	4:AD:150:LYS:HE2	1.85	0.58
26:BA:589:U:O3'	30:BE:90:GLN:NE2	2.36	0.58
1:AA:546:A:OP1	4:AD:70:ARG:N	2.35	0.58
26:BA:463:G:N2	26:BA:466:A:OP2	2.31	0.58
41:BP:90:GLY:O	41:BP:113:ARG:NH1	2.36	0.58
1:AA:436:C:O2	4:AD:154:ARG:NH1	2.36	0.58
2:AB:163:VAL:HG21	2:AB:173:ILE:HD11	1.84	0.58
11:AK:97:ILE:HA	11:AK:100:LEU:HD13	1.86	0.58
31:BF:57:LEU:HD13	31:BF:89:VAL:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:180:ALA:HB1	3:AC:203:PHE:HE1	1.68	0.58
1:AA:408:A:H61	1:AA:434:U:H3	1.52	0.58
7:AG:69:VAL:HG23	7:AG:100:ALA:HB1	1.83	0.58
40:BO:71:ALA:HB1	40:BO:106:LEU:HB2	1.85	0.58
53:B1:37:LYS:HG2	53:B1:48:ILE:HG13	1.84	0.58
1:AA:618:C:O2'	16:AP:14:ARG:NH2	2.36	0.58
1:AA:890:G:O2'	1:AA:906:A:N6	2.36	0.58
20:AT:84:ASN:HA	20:AT:87:ALA:HB3	1.86	0.58
1:AA:375:U:O2	16:AP:28:ARG:NH2	2.37	0.58
46:BU:33:LYS:HB3	46:BU:64:ALA:HB1	1.85	0.58
3:AC:22:TRP:HB3	3:AC:59:ARG:H	1.69	0.58
59:BA:9000:ERY:H271	57:B5:-2:ASN:CG	2.27	0.58
37:BL:81:ASP:O	37:BL:83:ALA:N	2.32	0.58
1:AA:875:U:O2'	8:AH:15:ARG:NH1	2.34	0.58
7:AG:27:VAL:HG12	7:AG:43:VAL:HG21	1.85	0.58
9:AI:92:GLU:OE1	9:AI:95:ARG:NH1	2.37	0.58
26:BA:1601:G:OP1	45:BT:64:LYS:NZ	2.36	0.58
1:AA:544:G:OP2	4:AD:63:ARG:NH2	2.36	0.58
3:AC:59:ARG:HE	3:AC:64:ILE:HD12	1.67	0.58
26:BA:1007:C:OP1	35:BJ:37:ARG:NH2	2.37	0.58
26:BA:1992:G:N2	26:BA:1996:C:O2'	2.37	0.58
49:BX:34:HIS:HD2	49:BX:53:ALA:HB2	1.69	0.58
2:AB:72:THR:HG23	2:AB:95:ARG:HA	1.86	0.57
9:AI:112:GLU:OE2	9:AI:115:LYS:NZ	2.37	0.57
25:AY:18:G:H1	25:AY:55:PSU:H1'	1.69	0.57
1:AA:976:G:N2	1:AA:1362:A:O2'	2.37	0.57
21:AU:14:VAL:HG12	21:AU:16:LEU:H	1.67	0.57
26:BA:2266:A:N6	26:BA:2273:A:OP2	2.36	0.57
45:BT:47:VAL:HG21	45:BT:85:VAL:HG11	1.85	0.57
46:BU:29:LEU:HD12	46:BU:33:LYS:HB2	1.86	0.57
50:BY:16:THR:O	50:BY:20:ASN:ND2	2.37	0.57
2:AB:70:VAL:HB	2:AB:163:VAL:HA	1.86	0.57
4:AD:151:LYS:HA	4:AD:178:MET:HE1	1.85	0.57
23:AW:33:U:O2'	23:AW:34:U8U:N	2.37	0.57
30:BE:76:PRO:HA	30:BE:82:GLY:HA2	1.84	0.57
1:AA:67:C:H2'	1:AA:68:G:C8	2.40	0.57
1:AA:426:U:H4'	4:AD:40:GLN:HA	1.85	0.57
1:AA:1360:A:OP2	14:AN:75:ARG:NH2	2.38	0.57
46:BU:10:GLU:HA	46:BU:24:LYS:HA	1.86	0.57
1:AA:437:U:H5''	4:AD:149:ALA:HB1	1.86	0.57
1:AA:1359:C:H3'	14:AN:75:ARG:HH22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:1568:G:OP2	28:BC:63:ARG:NH1	2.38	0.57
30:BE:117:ARG:NH2	30:BE:183:PHE:O	2.38	0.57
32:BG:3:ARG:HA	32:BG:6:LYS:HE2	1.86	0.57
41:BP:64:ILE:HA	41:BP:69:GLY:HA2	1.85	0.57
8:AH:106:THR:OG1	8:AH:109:GLY:O	2.19	0.57
26:BA:1450:G:N2	26:BA:1452:G:O6	2.37	0.57
33:BH:4:ILE:HD11	33:BH:44:ILE:HG22	1.86	0.57
36:BK:40:LYS:HA	36:BK:59:LYS:HA	1.87	0.57
1:AA:1020:G:H2'	1:AA:1021:A:H8	1.70	0.57
26:BA:1068:G:O6	26:BA:1073:A:N6	2.34	0.57
32:BG:8:PRO:HB2	32:BG:49:THR:HB	1.86	0.57
41:BP:88:ARG:NH2	41:BP:110:ILE:O	2.36	0.57
52:B0:32:LYS:HE2	52:B0:51:GLY:HA3	1.86	0.57
7:AG:135:VAL:HA	7:AG:138:ARG:HG2	1.87	0.57
19:AS:53:ASN:HB3	19:AS:75:ALA:HB1	1.86	0.57
47:BV:77:VAL:HG23	47:BV:89:ILE:HG12	1.87	0.57
1:AA:404:G:O6	4:AD:2:ALA:N	2.38	0.57
1:AA:451:A:H61	1:AA:481:G:H5'	1.70	0.57
3:AC:129:MET:HE1	4:AD:47:ARG:HH21	1.68	0.57
4:AD:14:ARG:HG3	4:AD:56:ARG:HH12	1.69	0.57
7:AG:69:VAL:HG21	7:AG:104:ILE:HD11	1.85	0.57
37:BL:54:GLN:HE21	37:BL:60:ARG:HH12	1.53	0.57
37:BL:74:THR:HG22	37:BL:107:PHE:HB2	1.87	0.57
39:BN:44:LEU:HD23	39:BN:113:ILE:HD13	1.87	0.57
28:BC:244:PRO:O	28:BC:251:GLN:NE2	2.37	0.56
8:AH:18:GLN:HE21	8:AH:70:ALA:HB1	1.70	0.56
26:BA:1266:G:OP2	44:BS:15:GLN:NE2	2.38	0.56
28:BC:52:ARG:HH12	28:BC:247:PRO:HG2	1.70	0.56
28:BC:145:GLU:HB2	28:BC:188:CYS:HB3	1.86	0.56
1:AA:1077:G:N2	1:AA:1080:A:OP2	2.37	0.56
10:AJ:5:ARG:HG3	10:AJ:6:ILE:HG13	1.86	0.56
16:AP:12:LYS:HG2	16:AP:13:LYS:HG2	1.87	0.56
23:AW:53:G:OP1	38:BM:55:ARG:NH1	2.37	0.56
26:BA:600:G:OP1	30:BE:24:ASN:ND2	2.37	0.56
29:BD:46:ARG:NH2	29:BD:88:GLU:O	2.35	0.56
29:BD:121:THR:HG21	29:BD:143:PRO:HB3	1.86	0.56
29:BD:151:THR:O	29:BD:153:GLY:N	2.37	0.56
38:BM:50:ARG:HD3	38:BM:65:ILE:HD11	1.87	0.56
38:BM:109:PRO:HD2	38:BM:112:LEU:HD22	1.86	0.56
46:BU:18:ASP:HB3	46:BU:21:LYS:HD2	1.87	0.56
16:AP:15:PRO:HG2	16:AP:41:PRO:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:2293:G:H5''	40:BO:94:ARG:HH22	1.70	0.56
1:AA:816:A:OP1	1:AA:1526:G:O2'	2.21	0.56
26:BA:411:G:OP2	26:BA:2406:A:O2'	2.22	0.56
1:AA:972:C:H4'	10:AJ:59:LYS:HD3	1.88	0.56
12:AL:57:LEU:HD12	12:AL:61:PHE:HB2	1.86	0.56
20:AT:27:MET:O	20:AT:30:THR:OG1	2.20	0.56
26:BA:750:A:OP1	26:BA:1615:C:N4	2.37	0.56
26:BA:1716:U:H2'	26:BA:1717:A:H8	1.70	0.56
30:BE:46:GLN:HB2	30:BE:87:ALA:H	1.70	0.56
31:BF:99:PHE:HA	31:BF:102:ARG:HE	1.71	0.56
37:BL:63:LYS:HA	55:B3:13:ARG:HG2	1.86	0.56
1:AA:911:U:OP2	12:AL:94:ARG:NH2	2.35	0.56
26:BA:320:A:O2'	26:BA:322:A:OP2	2.16	0.56
26:BA:2313:C:O4'	31:BF:37:ASN:ND2	2.35	0.56
40:BO:26:LEU:N	40:BO:91:SER:O	2.37	0.56
1:AA:689:C:OP2	11:AK:53:ARG:NH2	2.29	0.56
1:AA:859:G:OP2	1:AA:869:G:N1	2.30	0.56
26:BA:479:A:H1'	26:BA:481:G:H5'	1.86	0.56
26:BA:815:C:OP2	43:BR:85:LYS:NZ	2.39	0.56
6:AF:46:GLN:HA	6:AF:56:LYS:HG2	1.87	0.56
12:AL:114:ARG:HG3	12:AL:119:VAL:HB	1.86	0.56
26:BA:135:U:H3	26:BA:144:A:H61	1.53	0.56
26:BA:505:A:O2'	26:BA:509:C:O2'	2.21	0.56
26:BA:2294:G:OP1	40:BO:98:GLN:NE2	2.37	0.56
1:AA:1458:G:H5'	20:AT:27:MET:HB3	1.87	0.55
12:AL:38:TYR:HB2	12:AL:52:VAL:HG13	1.88	0.55
26:BA:845:A:H61	26:BA:932:U:H3	1.52	0.55
32:BG:28:GLY:HA3	32:BG:79:VAL:HB	1.86	0.55
3:AC:150:LYS:HG3	3:AC:169:ARG:HB3	1.88	0.55
26:BA:370:G:O2'	26:BA:424:G:OP1	2.24	0.55
1:AA:59:A:H5''	1:AA:387:U:H5''	1.88	0.55
8:AH:29:SER:HB3	8:AH:57:PRO:HB2	1.88	0.55
26:BA:1326:U:H2'	26:BA:1327:A:H8	1.71	0.55
26:BA:1653:G:OP2	39:BN:8:ARG:NH2	2.39	0.55
26:BA:2262:U:OP1	48:BW:41:ARG:NH2	2.39	0.55
32:BG:105:LEU:HB2	32:BG:113:VAL:HB	1.88	0.55
1:AA:1363:A:O2'	1:AA:1365:G:N7	2.36	0.55
7:AG:78:ARG:HB2	7:AG:85:TYR:HB2	1.87	0.55
26:BA:2336:A:H61	48:BW:43:THR:HG21	1.71	0.55
54:B2:3:ARG:HG3	54:B2:5:PHE:H	1.70	0.55
1:AA:1013:G:N2	1:AA:1016:A:OP2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:754:C:OP1	15:AO:72:ARG:NH2	2.40	0.55
3:AC:19:ASN:OD1	3:AC:54:ARG:NH2	2.39	0.55
10:AJ:8:ILE:HD11	10:AJ:87:LEU:HD11	1.89	0.55
26:BA:61:C:OP2	50:BY:47:ARG:NH1	2.38	0.55
26:BA:2355:G:O2'	48:BW:24:LYS:NZ	2.40	0.55
1:AA:1239:A:H61	1:AA:1296:C:H2'	1.70	0.55
1:AA:1359:C:OP2	14:AN:75:ARG:NH1	2.40	0.55
10:AJ:80:THR:HG22	10:AJ:82:LYS:H	1.72	0.55
11:AK:88:GLY:H	11:AK:114:THR:HG22	1.70	0.55
26:BA:2384:U:OP2	48:BW:55:ARG:NH2	2.40	0.55
38:BM:36:VAL:HG23	38:BM:129:THR:H	1.72	0.55
1:AA:340:U:OP2	36:BK:98:ARG:NH2	2.39	0.55
1:AA:1064:G:O2'	1:AA:1190:G:N2	2.40	0.55
26:BA:2751:G:OP2	32:BG:3:ARG:NH1	2.40	0.55
26:BA:2796:U:H3	26:BA:2799:A:H61	1.54	0.55
39:BN:114:GLU:OE1	39:BN:118:ARG:NH2	2.40	0.55
26:BA:1030:C:OP2	38:BM:127:LYS:NZ	2.38	0.55
26:BA:1515:A:HO2'	26:BA:1556:C:HO2'	1.55	0.55
32:BG:89:LEU:HD23	32:BG:94:TYR:HB3	1.87	0.55
42:BQ:28:ARG:HH21	42:BQ:38:ALA:HB1	1.70	0.55
45:BT:40:LYS:NZ	45:BT:58:VAL:O	2.30	0.55
1:AA:132:C:H5''	20:AT:69:LYS:HE3	1.89	0.55
4:AD:2:ALA:HA	4:AD:68:LEU:HD11	1.89	0.55
26:BA:2092:U:O2	26:BA:2225:A:O2'	2.24	0.55
35:BJ:45:THR:HB	35:BJ:48:VAL:HB	1.88	0.55
36:BK:30:ARG:NH2	36:BK:37:ASP:OD2	2.39	0.55
1:AA:406:G:N3	4:AD:116:GLN:NE2	2.53	0.54
1:AA:440:C:H42	1:AA:497:G:H1	1.54	0.54
26:BA:1125:G:H5''	56:B4:37:GLN:HE21	1.72	0.54
3:AC:156:ARG:NH1	3:AC:160:ALA:O	2.40	0.54
9:AI:57:MET:O	9:AI:59:GLU:N	2.40	0.54
26:BA:1936:A:H2	26:BA:1943:U:H3	1.53	0.54
47:BV:25:LYS:HG2	47:BV:43:ASP:HA	1.89	0.54
4:AD:91:LEU:HD13	4:AD:191:LEU:HD11	1.89	0.54
14:AN:51:LEU:O	14:AN:53:ARG:N	2.41	0.54
26:BA:210:C:OP1	54:B2:29:GLN:NE2	2.30	0.54
45:BT:1:MET:HB3	45:BT:2:ILE:HD12	1.90	0.54
1:AA:310:G:H5''	16:AP:31:ARG:HB2	1.90	0.54
2:AB:73:LYS:O	2:AB:77:SER:OG	2.24	0.54
6:AF:27:ALA:O	6:AF:30:THR:OG1	2.15	0.54
8:AH:50:LYS:HG2	8:AH:52:GLU:HG2	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BC:8:PRO:HB3	28:BC:14:ARG:HG3	1.89	0.54
29:BD:16:THR:OG1	29:BD:18:ASP:OD1	2.18	0.54
1:AA:982:U:H4'	1:AA:983:A:H5'	1.89	0.54
26:BA:1169:A:H61	26:BA:1178:C:H41	1.54	0.54
26:BA:1817:G:H5''	28:BC:87:ARG:HE	1.72	0.54
37:BL:124:GLY:HA2	37:BL:144:GLU:HA	1.89	0.54
26:BA:1801:A:N6	26:BA:2201:G:O2'	2.33	0.54
26:BA:2029:G:N1	26:BA:2033:A:OP2	2.36	0.54
26:BA:2334:U:H5'	40:BO:12:THR:HB	1.90	0.54
26:BA:2771:C:O2'	29:BD:173:GLN:NE2	2.30	0.54
43:BR:11:GLN:HE22	43:BR:39:LEU:HD22	1.72	0.54
16:AP:42:ILE:O	16:AP:44:SER:N	2.39	0.54
24:AX:76:A:H2	26:BA:2450:A:N3	2.05	0.54
26:BA:2461:A:N6	26:BA:2488:G:O6	2.41	0.54
59:BA:9000:ERY:C27	57:B5:-2:ASN:CG	2.80	0.54
30:BE:147:LEU:HB2	30:BE:183:PHE:HD2	1.73	0.54
1:AA:1347:G:N7	9:AI:12:ARG:NH2	2.51	0.54
26:BA:2172:U:H4'	26:BA:2173:A:H5'	1.89	0.54
41:BP:75:GLN:HB2	41:BP:78:SER:HB2	1.89	0.54
50:BY:25:GLN:HE22	50:BY:47:ARG:HG2	1.71	0.54
7:AG:111:ARG:O	7:AG:119:ARG:NH2	2.40	0.54
10:AJ:78:GLU:OE2	10:AJ:80:THR:OG1	2.26	0.54
1:AA:1366:C:O2'	10:AJ:62:ARG:NH1	2.30	0.54
9:AI:116:VAL:HG21	10:AJ:62:ARG:HB2	1.90	0.53
12:AL:22:PRO:O	12:AL:24:LEU:N	2.37	0.53
16:AP:4:ILE:HG13	16:AP:21:VAL:HG22	1.90	0.53
26:BA:632:A:H2'	26:BA:633:A:H8	1.73	0.53
26:BA:2645:G:OP2	26:BA:2645:G:N2	2.32	0.53
39:BN:43:GLU:OE1	39:BN:46:ARG:NH1	2.38	0.53
39:BN:78:LYS:HG2	39:BN:83:LEU:HG	1.89	0.53
1:AA:954:G:H21	1:AA:1227:A:H61	1.56	0.53
1:AA:1307:U:OP1	13:AM:100:GLN:NE2	2.40	0.53
14:AN:16:LEU:HD22	14:AN:20:TYR:CE2	2.43	0.53
24:AX:18:G:O2'	24:AX:57:G:N2	2.41	0.53
26:BA:1365:A:OP1	49:BX:28:ARG:NH2	2.40	0.53
59:BA:9000:ERY:C21	57:B5:-2:ASN:OD1	2.56	0.53
26:BA:2489:U:O2'	26:BA:2518:A:N6	2.41	0.53
27:BB:27:C:OP1	40:BO:34:HIS:NE2	2.41	0.53
38:BM:17:ASN:O	38:BM:38:ARG:NH1	2.42	0.53
49:BX:59:ILE:HG12	49:BX:67:VAL:HG21	1.91	0.53
1:AA:115:G:H4'	1:AA:116:A:O5'	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:500:G:N1	26:BA:503:A:OP2	2.41	0.53
39:BN:24:MET:HE3	39:BN:44:LEU:HD13	1.90	0.53
55:B3:39:LYS:HG3	55:B3:42:ARG:HH12	1.74	0.53
1:AA:1494:G:O2'	26:BA:1912:A:O2'	2.23	0.53
4:AD:15:GLU:HG3	4:AD:19:LEU:HD11	1.91	0.53
26:BA:1365:A:O2'	49:BX:11:ARG:NH1	2.41	0.53
26:BA:2343:U:O2'	26:BA:2373:G:O2'	2.25	0.53
4:AD:124:MET:HE3	4:AD:146:ARG:HG2	1.90	0.53
20:AT:36:TYR:HA	20:AT:39:ILE:HD12	1.90	0.53
26:BA:2108:A:H4'	26:BA:2150:C:H4'	1.89	0.53
9:AI:95:ARG:HA	9:AI:98:LEU:HB3	1.91	0.53
11:AK:35:THR:HA	11:AK:42:LEU:H	1.73	0.53
13:AM:71:ARG:HH11	31:BF:115:ARG:HH11	1.56	0.53
26:BA:415:A:H61	26:BA:2408:U:H3	1.56	0.53
1:AA:1228:C:OP2	13:AM:110:LYS:NZ	2.31	0.53
26:BA:1651:G:N7	39:BN:11:ASN:ND2	2.51	0.53
28:BC:211:ALA:HB1	28:BC:216:VAL:HB	1.91	0.53
36:BK:35:VAL:HG22	36:BK:69:VAL:HG12	1.91	0.53
47:BV:64:VAL:HG22	47:BV:69:GLU:HG2	1.90	0.53
1:AA:1414:U:H2'	1:AA:1415:G:H8	1.74	0.53
26:BA:2250:G:O2'	26:BA:2496:C:OP1	2.26	0.53
26:BA:2377:A:O2'	40:BO:117:PHE:O	2.26	0.53
1:AA:362:G:N2	1:AA:365:U:OP2	2.35	0.53
1:AA:1439:G:OP2	20:AT:33:LYS:NZ	2.37	0.53
2:AB:120:GLN:HG3	2:AB:124:GLY:HA3	1.91	0.53
39:BN:96:ARG:HH12	39:BN:116:VAL:HG23	1.74	0.53
40:BO:29:HIS:HB3	40:BO:36:TYR:HB2	1.91	0.53
42:BQ:49:ASP:O	42:BQ:53:ARG:N	2.41	0.53
4:AD:62:ARG:O	4:AD:66:GLY:N	2.40	0.52
8:AH:77:ARG:NH2	8:AH:79:SER:O	2.42	0.52
14:AN:27:LEU:HA	14:AN:31:ILE:HD13	1.91	0.52
17:AQ:31:HIS:HD2	17:AQ:34:TYR:H	1.57	0.52
26:BA:2258:C:O2'	26:BA:2427:C:OP2	2.25	0.52
26:BA:2316:G:H2'	26:BA:2317:A:H8	1.74	0.52
26:BA:2419:U:OP1	55:B3:41:LYS:NZ	2.41	0.52
27:BB:28:C:H2'	27:BB:29:A:C8	2.44	0.52
28:BC:144:VAL:HG11	28:BC:174:LEU:HD21	1.89	0.52
43:BR:10:LYS:HG3	43:BR:12:HIS:CE1	2.45	0.52
1:AA:405:U:O4	4:AD:3:ARG:N	2.43	0.52
43:BR:98:ILE:HG22	43:BR:100:GLY:H	1.74	0.52
1:AA:409:U:OP2	4:AD:22:LYS:NZ	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:1613:G:O2'	54:B2:3:ARG:NH1	2.42	0.52
26:BA:1652:A:N6	39:BN:11:ASN:OD1	2.39	0.52
26:BA:2439:A:O4'	57:B5:-3:ARG:NH2	2.39	0.52
28:BC:145:GLU:HA	28:BC:152:GLY:HA2	1.91	0.52
26:BA:578:G:OP1	26:BA:1255:U:O2'	2.27	0.52
28:BC:111:LYS:N	28:BC:114:ASP:OD2	2.42	0.52
1:AA:429:U:H5'	4:AD:9:LEU:HB3	1.92	0.52
1:AA:1001:C:H2'	1:AA:1002:G:C8	2.45	0.52
2:AB:128:LYS:HG3	2:AB:129:LEU:HG	1.92	0.52
26:BA:1363:C:H2'	26:BA:1364:G:H8	1.75	0.52
39:BN:69:ARG:O	39:BN:71:ARG:N	2.31	0.52
3:AC:138:VAL:HA	3:AC:149:ILE:HD13	1.90	0.52
26:BA:340:A:O2'	30:BE:162:ARG:NH1	2.42	0.52
44:BS:29:VAL:HG21	44:BS:69:LEU:HG	1.91	0.52
49:BX:33:LEU:HD23	49:BX:50:ARG:HE	1.75	0.52
17:AQ:25:ILE:HB	17:AQ:42:THR:HB	1.92	0.52
26:BA:1028:A:OP2	26:BA:1126:A:N6	2.42	0.52
26:BA:2131:U:H5'	26:BA:2132:U:H5''	1.92	0.52
26:BA:2469:A:O2'	38:BM:55:ARG:NH2	2.36	0.52
28:BC:180:GLU:HB2	28:BC:271:ARG:HB3	1.92	0.52
29:BD:48:ILE:HG23	29:BD:84:LEU:HD21	1.91	0.52
34:BI:12:GLN:HE21	34:BI:55:ILE:H	1.57	0.52
40:BO:20:GLU:OE2	48:BW:62:LYS:NZ	2.41	0.52
40:BO:24:THR:HG22	40:BO:42:PRO:HD3	1.92	0.52
3:AC:19:ASN:ND2	14:AN:90:ARG:O	2.42	0.52
26:BA:1306:C:H41	26:BA:1606:C:H2'	1.75	0.52
26:BA:2857:G:N2	26:BA:2860:A:OP2	2.37	0.52
12:AL:54:ARG:HA	12:AL:64:THR:HA	1.91	0.52
17:AQ:17:MET:HG3	17:AQ:20:SER:HB3	1.92	0.52
26:BA:627:A:O4'	26:BA:637:A:N6	2.42	0.52
26:BA:1296:G:OP1	26:BA:2709:G:O2'	2.20	0.52
28:BC:158:ALA:HB1	28:BC:197:ASN:HB3	1.90	0.52
9:AI:107:ASP:OD1	9:AI:109:ARG:NE	2.43	0.51
26:BA:636:G:N2	37:BL:76:GLU:OE2	2.43	0.51
26:BA:1038:G:H2'	26:BA:1039:A:H8	1.74	0.51
26:BA:1796:U:H2'	26:BA:1797:G:H8	1.75	0.51
36:BK:77:ILE:HG12	41:BP:72:ARG:HG2	1.91	0.51
1:AA:350:G:OP1	20:AT:3:ASN:N	2.43	0.51
12:AL:5:ASN:ND2	17:AQ:36:LYS:HE2	2.25	0.51
26:BA:659:G:OP1	30:BE:95:LYS:NZ	2.39	0.51
26:BA:1515:A:H3'	26:BA:1516:G:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:1902:C:H5''	28:BC:240:PHE:HE2	1.75	0.51
26:BA:2838:G:H1'	39:BN:45:ARG:HH12	1.75	0.51
29:BD:51:THR:HG21	29:BD:68:PHE:HE1	1.75	0.51
31:BF:110:ARG:NH2	31:BF:137:ILE:O	2.43	0.51
1:AA:427:U:OP1	4:AD:13:ARG:NH2	2.43	0.51
3:AC:150:LYS:HB3	3:AC:201:TRP:HB2	1.93	0.51
8:AH:52:GLU:O	8:AH:58:GLU:N	2.42	0.51
20:AT:51:PHE:HA	20:AT:54:MET:HG2	1.92	0.51
23:AW:11:C:H42	23:AW:24:G:H1	1.57	0.51
26:BA:1438:U:H2'	26:BA:1439:A:H8	1.75	0.51
1:AA:563:A:O2'	1:AA:566:G:O3'	2.29	0.51
9:AI:129:LYS:HG3	9:AI:130:ARG:H	1.74	0.51
26:BA:250:G:O5'	37:BL:59:ARG:NH1	2.43	0.51
26:BA:605:G:OP1	30:BE:99:LYS:NZ	2.44	0.51
26:BA:685:A:O2'	26:BA:772:C:N4	2.43	0.51
26:BA:740:C:H5'	26:BA:1784:A:H2'	1.92	0.51
26:BA:1798:U:OP2	28:BC:271:ARG:NH2	2.35	0.51
26:BA:2020:A:H5'	52:B0:9:THR:HG23	1.93	0.51
26:BA:2519:U:O4'	26:BA:2542:A:N6	2.44	0.51
28:BC:123:ALA:O	28:BC:128:ASN:ND2	2.43	0.51
36:BK:2:ILE:HD12	36:BK:8:LEU:HD11	1.93	0.51
41:BP:37:LYS:HE3	41:BP:39:ARG:HB2	1.92	0.51
9:AI:34:SER:OG	9:AI:36:GLU:OE1	2.28	0.51
12:AL:5:ASN:HD21	17:AQ:36:LYS:HE2	1.75	0.51
12:AL:74:LEU:HD21	12:AL:80:ILE:HG21	1.91	0.51
18:AR:57:ARG:HE	18:AR:61:ARG:HH21	1.58	0.51
26:BA:2285:C:H5	53:B1:6:ARG:HH12	1.59	0.51
28:BC:72:ASP:OD2	28:BC:189:ARG:NH1	2.43	0.51
37:BL:57:LEU:HA	37:BL:60:ARG:HG2	1.93	0.51
1:AA:111:G:HO2'	1:AA:389:A:HO2'	1.57	0.51
1:AA:544:G:OP1	4:AD:59:GLN:HG3	2.11	0.51
4:AD:38:PRO:HD2	4:AD:42:GLY:HA3	1.92	0.51
4:AD:50:ASP:O	4:AD:54:GLN:HG2	2.11	0.51
11:AK:94:GLU:OE2	11:AK:98:ARG:NH2	2.44	0.51
26:BA:2080:A:H61	26:BA:2240:U:H3	1.59	0.51
36:BK:15:GLY:HA3	36:BK:50:GLY:HA3	1.93	0.51
1:AA:180:U:O2	1:AA:196:A:N6	2.43	0.51
1:AA:262:A:H5''	20:AT:74:ARG:HH22	1.76	0.51
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.46	0.51
1:AA:380:G:N2	1:AA:383:A:OP2	2.37	0.51
1:AA:954:G:H21	1:AA:1227:A:N6	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:805:G:H5''	37:BL:38:GLN:HG3	1.91	0.51
26:BA:1141:U:OP2	35:BJ:65:THR:OG1	2.26	0.51
26:BA:1653:G:O6	39:BN:11:ASN:N	2.35	0.51
26:BA:2134:A:H8	26:BA:2157:G:H21	1.59	0.51
27:BB:24:G:O2'	27:BB:56:G:N7	2.35	0.51
14:AN:52:PRO:O	14:AN:54:ASP:N	2.37	0.51
26:BA:1781:U:H5	54:B2:1:MET:HE1	1.76	0.51
26:BA:2441:U:OP2	57:B5:-3:ARG:NH2	2.39	0.51
26:BA:2658:C:OP1	32:BG:158:LYS:NZ	2.43	0.51
32:BG:35:ARG:NH1	32:BG:139:GLN:OE1	2.34	0.51
37:BL:61:LEU:O	55:B3:13:ARG:NE	2.43	0.51
1:AA:1266:G:N2	1:AA:1269:A:OP2	2.39	0.50
9:AI:17:ALA:HB2	9:AI:67:VAL:HG23	1.93	0.50
9:AI:26:GLY:H	9:AI:59:GLU:HG3	1.76	0.50
20:AT:29:ARG:O	20:AT:33:LYS:HG2	2.11	0.50
28:BC:29:PRO:HG2	28:BC:34:LEU:HD11	1.93	0.50
41:BP:48:ILE:HA	41:BP:97:LEU:HD12	1.93	0.50
52:B0:40:ARG:HG2	52:B0:41:HIS:ND1	2.27	0.50
8:AH:66:PHE:CD2	8:AH:67:GLN:HG2	2.46	0.50
12:AL:110:ARG:HH21	12:AL:113:ALA:HB3	1.76	0.50
26:BA:1181:U:H2'	26:BA:1182:G:C8	2.46	0.50
26:BA:1826:G:O2'	26:BA:1971:U:OP2	2.22	0.50
44:BS:41:LYS:HG3	44:BS:43:ALA:H	1.77	0.50
1:AA:458:U:H2'	1:AA:459:A:H8	1.76	0.50
1:AA:1020:G:H2'	1:AA:1021:A:C8	2.46	0.50
30:BE:109:LEU:HD12	30:BE:112:LEU:HD12	1.92	0.50
4:AD:19:LEU:HB3	4:AD:64:ILE:HG12	1.93	0.50
4:AD:104:ARG:HB3	4:AD:168:PRO:HG2	1.92	0.50
5:AE:24:THR:HA	5:AE:29:ARG:HA	1.93	0.50
26:BA:200:U:O4	26:BA:250:G:N2	2.44	0.50
26:BA:373:U:H2'	26:BA:374:A:H8	1.77	0.50
26:BA:1664:A:H61	26:BA:1996:C:H42	1.58	0.50
27:BB:14:U:OP2	27:BB:70:C:O2'	2.24	0.50
30:BE:119:ILE:HB	30:BE:187:VAL:HG22	1.93	0.50
1:AA:922:G:H4'	5:AE:25:VAL:HA	1.93	0.50
1:AA:959:A:HO2'	1:AA:984:C:HO2'	1.58	0.50
25:AY:19:G:N1	26:BA:2112:G:O2'	2.44	0.50
26:BA:851:C:O2'	51:BZ:43:ALA:O	2.26	0.50
26:BA:2011:U:OP2	44:BS:16:LYS:NZ	2.41	0.50
29:BD:179:ARG:HB2	29:BD:188:LEU:HD12	1.93	0.50
1:AA:689:C:HO2'	1:AA:705:G:HO2'	1.56	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1125:U:H4'	10:AJ:7:ARG:HH12	1.77	0.50
4:AD:167:LYS:HD2	4:AD:173:VAL:HG11	1.92	0.50
13:AM:17:ILE:O	13:AM:20:THR:OG1	2.23	0.50
26:BA:85:G:OP1	46:BU:7:ARG:N	2.42	0.50
26:BA:2744:G:H21	32:BG:143:GLN:HE22	1.59	0.50
30:BE:111:GLU:OE2	30:BE:114:ARG:NH2	2.45	0.50
46:BU:45:HIS:HB3	46:BU:58:ILE:HA	1.94	0.50
55:B3:28:ASN:HB3	55:B3:36:LYS:HE2	1.94	0.50
1:AA:309:A:H2'	1:AA:310:G:H8	1.76	0.50
26:BA:137:U:H3	26:BA:142:A:H61	1.59	0.50
33:BH:40:THR:O	33:BH:42:LYS:N	2.41	0.50
34:BI:122:ILE:HA	34:BI:125:MET:HE3	1.94	0.50
45:BT:7:LEU:HD21	45:BT:46:ALA:HA	1.94	0.50
4:AD:71:GLN:HA	4:AD:74:ASN:HD22	1.76	0.50
13:AM:71:ARG:HA	13:AM:74:SER:HB3	1.93	0.50
26:BA:1564:C:OP2	28:BC:26:LYS:NZ	2.45	0.50
29:BD:181:ASP:HB3	29:BD:186:LEU:HB2	1.94	0.50
50:BY:21:LEU:HA	50:BY:25:GLN:HB2	1.92	0.50
1:AA:765:G:N1	1:AA:812:G:O2'	2.42	0.50
8:AH:103:VAL:HG12	8:AH:126:ILE:HD13	1.93	0.50
10:AJ:27:GLU:HA	10:AJ:30:LYS:HE3	1.93	0.50
26:BA:1034:G:O4'	56:B4:18:LYS:NZ	2.45	0.50
26:BA:1246:A:O2'	30:BE:40:ARG:NH1	2.39	0.50
26:BA:2387:U:O2'	48:BW:19:LYS:NZ	2.45	0.50
37:BL:14:LYS:HG3	37:BL:16:GLY:H	1.76	0.50
39:BN:56:LYS:NZ	39:BN:88:ALA:O	2.38	0.50
2:AB:66:LYS:NZ	2:AB:154:MET:O	2.39	0.49
26:BA:1038:G:H2'	26:BA:1039:A:C8	2.47	0.49
26:BA:1864:U:OP1	26:BA:2410:G:O2'	2.25	0.49
39:BN:28:LEU:HD23	39:BN:48:VAL:HG21	1.93	0.49
4:AD:75:TYR:OH	4:AD:97:ARG:NH1	2.43	0.49
27:BB:13:G:O2'	27:BB:15:A:OP2	2.26	0.49
32:BG:24:ILE:HD11	32:BG:43:VAL:HG11	1.94	0.49
32:BG:38:ASN:HB3	32:BG:41:VAL:HG23	1.94	0.49
35:BJ:31:GLU:HG2	35:BJ:142:ILE:HG12	1.93	0.49
35:BJ:40:HIS:CE1	35:BJ:41:LYS:HG3	2.48	0.49
1:AA:809:G:OP2	15:AO:48:LYS:NZ	2.44	0.49
4:AD:29:ASP:O	4:AD:31:LYS:N	2.45	0.49
9:AI:113:ARG:NH1	14:AN:101:TRP:OXT	2.44	0.49
16:AP:71:VAL:O	16:AP:75:ILE:HD12	2.12	0.49
26:BA:1380:G:H21	26:BA:1570:A:H2	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:2787:C:H1'	29:BD:63:PRO:HG3	1.94	0.49
34:BI:53:LEU:HD21	34:BI:82:LYS:HE2	1.93	0.49
51:BZ:8:THR:O	51:BZ:56:LYS:N	2.43	0.49
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.76	0.49
17:AQ:24:ALA:HA	17:AQ:43:LYS:HA	1.93	0.49
26:BA:414:C:H2'	26:BA:415:A:C8	2.47	0.49
51:BZ:17:LEU:HB2	51:BZ:20:HIS:HD2	1.77	0.49
9:AI:36:GLU:HA	9:AI:40:GLY:HA3	1.95	0.49
12:AL:3:THR:HG22	12:AL:5:ASN:H	1.77	0.49
32:BG:7:ALA:O	32:BG:69:ARG:NE	2.30	0.49
42:BQ:8:VAL:HG13	42:BQ:9:ILE:HG23	1.95	0.49
44:BS:28:LYS:O	44:BS:30:SER:N	2.46	0.49
1:AA:1105:A:H2'	1:AA:1106:G:H8	1.77	0.49
17:AQ:64:CYS:SG	17:AQ:74:THR:OG1	2.64	0.49
26:BA:107:G:H2'	26:BA:108:G:H8	1.78	0.49
26:BA:1662:U:O2'	26:BA:2687:U:OP1	2.31	0.49
26:BA:1817:G:P	28:BC:87:ARG:HH21	2.35	0.49
26:BA:2374:C:N4	26:BA:2375:G:O6	2.45	0.49
26:BA:2845:U:O3'	41:BP:53:ARG:NH1	2.46	0.49
41:BP:25:THR:HB	41:BP:88:ARG:HB3	1.94	0.49
50:BY:31:GLN:HG2	50:BY:37:LEU:HB2	1.94	0.49
26:BA:290:U:H2'	26:BA:291:G:H8	1.77	0.49
26:BA:1996:C:N4	36:BK:32:TYR:OH	2.33	0.49
26:BA:2233:U:H2'	26:BA:2234:G:C8	2.48	0.49
5:AE:25:VAL:HG23	5:AE:27:GLY:H	1.78	0.49
8:AH:9:ASP:O	8:AH:13:ARG:HG2	2.13	0.49
24:AX:76:A:C2	26:BA:2450:A:N3	2.80	0.49
26:BA:2133:G:H2'	26:BA:2157:G:H22	1.78	0.49
28:BC:204:VAL:O	28:BC:206:GLY:N	2.46	0.49
1:AA:707:U:OP1	11:AK:87:LYS:NZ	2.40	0.49
19:AS:28:LYS:HG3	19:AS:29:LYS:H	1.78	0.49
26:BA:1068:G:N2	26:BA:1096:A:OP1	2.45	0.49
26:BA:1131:G:N2	26:BA:1132:U:O4	2.37	0.49
26:BA:1264:A:H5''	52:B0:16:ARG:HH22	1.77	0.49
26:BA:1313:U:H4'	26:BA:1332:G:H4'	1.93	0.49
26:BA:2109:U:O2	26:BA:2181:U:N3	2.45	0.49
51:BZ:17:LEU:HB2	51:BZ:20:HIS:CD2	2.48	0.49
1:AA:735:C:H5'	18:AR:60:LYS:HD3	1.95	0.49
1:AA:1313:U:H3	1:AA:1324:A:H61	1.61	0.49
26:BA:246:C:H41	55:B3:8:ARG:HG2	1.78	0.49
26:BA:309:A:H5'	46:BU:17:LYS:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:2134:A:OP2	26:BA:2157:G:N2	2.44	0.49
30:BE:189:THR:HG22	30:BE:191:ASP:H	1.78	0.49
52:B0:31:ASP:HB3	52:B0:35:GLY:H	1.77	0.49
1:AA:321:A:H61	1:AA:332:G:H1	1.61	0.48
1:AA:780:A:N6	1:AA:801:U:OP2	2.42	0.48
25:AY:9:A:N6	25:AY:22:G:N7	2.61	0.48
26:BA:142:A:H1'	45:BT:1:MET:HE3	1.94	0.48
35:BJ:24:THR:HB	35:BJ:27:ARG:HB2	1.95	0.48
42:BQ:94:ILE:HG21	43:BR:4:VAL:HG21	1.94	0.48
1:AA:427:U:O2'	1:AA:541:G:OP1	2.32	0.48
1:AA:458:U:H2'	1:AA:459:A:C8	2.49	0.48
26:BA:1666:G:H1	26:BA:1994:C:H42	1.60	0.48
27:BB:116:G:H2'	27:BB:117:G:H8	1.77	0.48
32:BG:71:LEU:O	32:BG:74:SER:OG	2.28	0.48
34:BI:62:TYR:HD2	34:BI:67:PHE:HA	1.78	0.48
53:B1:38:LYS:HB2	53:B1:49:TYR:CE2	2.48	0.48
1:AA:450:G:H4'	16:AP:41:PRO:HB2	1.94	0.48
1:AA:1317:C:N3	14:AN:53:ARG:NH1	2.61	0.48
7:AG:37:SER:HA	7:AG:40:GLU:HG2	1.95	0.48
11:AK:36:ASP:OD1	11:AK:40:ASN:N	2.46	0.48
17:AQ:64:CYS:HG	17:AQ:74:THR:HG1	1.61	0.48
26:BA:65:U:O3'	45:BT:73:ARG:NH1	2.44	0.48
26:BA:450:G:N1	26:BA:454:A:OP2	2.45	0.48
27:BB:49:C:H2'	27:BB:50:A:H8	1.78	0.48
27:BB:90:C:O3'	38:BM:38:ARG:NH2	2.46	0.48
30:BE:18:THR:HA	30:BE:106:LYS:HD2	1.95	0.48
2:AB:20:THR:OG1	2:AB:37:LYS:O	2.26	0.48
25:AY:12:U:H3	25:AY:23:A:H61	1.62	0.48
26:BA:1416:G:H1	26:BA:1582:C:H42	1.60	0.48
34:BI:33:VAL:HG13	34:BI:67:PHE:HE2	1.77	0.48
1:AA:512:U:H2'	1:AA:513:C:C6	2.49	0.48
4:AD:9:LEU:HD12	4:AD:12:SER:HB2	1.96	0.48
26:BA:2079:U:O2'	49:BX:23:ASN:OD1	2.26	0.48
26:BA:2316:G:H2'	26:BA:2317:A:C8	2.49	0.48
34:BI:109:ILE:O	34:BI:112:THR:OG1	2.28	0.48
49:BX:17:ASN:ND2	49:BX:27:ARG:HD2	2.28	0.48
1:AA:1121:U:H3	1:AA:1152:A:H61	1.62	0.48
1:AA:1124:G:HO2'	1:AA:1145:A:H62	1.58	0.48
7:AG:116:MET:HA	7:AG:119:ARG:HD3	1.94	0.48
26:BA:1078:U:O2'	26:BA:1088:A:OP1	2.25	0.48
26:BA:1105:U:H2'	26:BA:1106:G:C8	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:1939:U:OP1	26:BA:2604:U:O2'	2.30	0.48
26:BA:2304:G:H4'	31:BF:130:MET:HA	1.96	0.48
26:BA:2359:C:O2'	55:B3:54:ASP:OD2	2.30	0.48
26:BA:2514:U:H5''	35:BJ:81:ILE:HD11	1.96	0.48
27:BB:22:U:H2'	27:BB:23:G:C8	2.48	0.48
27:BB:43:C:O2	31:BF:92:ARG:NH2	2.38	0.48
31:BF:12:VAL:HG22	31:BF:172:ALA:HB1	1.96	0.48
32:BG:89:LEU:N	32:BG:129:THR:O	2.43	0.48
9:AI:84:THR:HG21	9:AI:103:PHE:HB3	1.95	0.48
15:AO:22:THR:HA	15:AO:27:VAL:HG11	1.94	0.48
20:AT:35:VAL:HG21	20:AT:54:MET:SD	2.54	0.48
26:BA:1077:A:N6	26:BA:1089:A:OP1	2.40	0.48
26:BA:1089:A:H2	26:BA:1090:A:H62	1.62	0.48
26:BA:1187:G:N2	26:BA:1188:U:O4	2.46	0.48
26:BA:1918:A:O2'	26:BA:1920:C:N4	2.47	0.48
1:AA:219:U:H2'	1:AA:220:G:H8	1.79	0.48
4:AD:95:GLU:HG2	4:AD:186:PRO:HG3	1.94	0.48
11:AK:35:THR:OG1	11:AK:41:ALA:N	2.46	0.48
26:BA:832:U:H2'	26:BA:833:A:C8	2.49	0.48
26:BA:1791:A:N6	26:BA:1828:G:O2'	2.44	0.48
34:BI:34:ASN:OD1	34:BI:35:ILE:N	2.47	0.48
34:BI:79:LEU:HD21	34:BI:109:ILE:HD13	1.94	0.48
1:AA:299:G:N2	1:AA:565:U:O2	2.47	0.48
25:AY:32:C:N4	25:AY:33:U:O4	2.47	0.48
26:BA:177:G:OP2	26:BA:177:G:N2	2.29	0.48
26:BA:1570:A:H5'	28:BC:36:LYS:HB2	1.95	0.48
26:BA:2506:U:O2'	26:BA:2507:C:OP1	2.28	0.48
59:BA:9000:ERY:H312	59:BA:9000:ERY:H2	1.66	0.48
31:BF:128:TYR:OH	31:BF:130:MET:SD	2.67	0.48
33:BH:3:VAL:HG12	33:BH:38:PRO:HA	1.96	0.48
37:BL:79:LEU:HD12	37:BL:114:GLY:H	1.79	0.48
1:AA:429:U:O2'	4:AD:22:LYS:HE2	2.14	0.48
11:AK:26:SER:OG	11:AK:29:ASN:O	2.22	0.48
26:BA:673:C:OP1	30:BE:49:ARG:NH2	2.47	0.48
26:BA:1063:G:N2	26:BA:1076:C:O2	2.47	0.48
26:BA:1385:A:O2'	26:BA:1396:U:O2	2.29	0.48
52:B0:31:ASP:OD2	52:B0:34:SER:N	2.45	0.48
1:AA:202:G:H1	1:AA:215:C:H42	1.61	0.47
1:AA:236:A:H5''	17:AQ:44:LEU:HD21	1.96	0.47
1:AA:512:U:H1'	4:AD:41:HIS:HE1	1.79	0.47
1:AA:1201:A:H4'	1:AA:1202:U:O5'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:16:VAL:HG23	13:AM:17:ILE:HG13	1.96	0.47
13:AM:101:ARG:NH2	13:AM:103:LYS:HD2	2.29	0.47
14:AN:21:PHE:O	14:AN:23:LYS:N	2.47	0.47
37:BL:33:ARG:NH2	37:BL:40:SER:O	2.39	0.47
4:AD:170:TRP:CD1	4:AD:171:LEU:HG	2.49	0.47
9:AI:118:LEU:HG	9:AI:124:ARG:HA	1.96	0.47
32:BG:38:ASN:OD1	32:BG:39:ASP:N	2.47	0.47
32:BG:101:ASN:ND2	32:BG:116:GLN:HE22	2.12	0.47
1:AA:186:C:H5'	20:AT:73:ALA:HB1	1.96	0.47
1:AA:954:G:H1	1:AA:1226:C:H42	1.62	0.47
5:AE:36:LEU:HD11	5:AE:137:VAL:HG11	1.96	0.47
28:BC:93:LEU:HD11	28:BC:101:ARG:HB3	1.95	0.47
32:BG:35:ARG:HH21	32:BG:71:LEU:HD13	1.79	0.47
39:BN:2:ARG:HA	39:BN:5:LYS:HD2	1.95	0.47
51:BZ:7:ILE:N	51:BZ:36:VAL:O	2.46	0.47
1:AA:34:C:N4	1:AA:35:G:O6	2.47	0.47
1:AA:970:C:N4	9:AI:128:SER:OG	2.47	0.47
4:AD:102:VAL:HG13	4:AD:107:PHE:HB2	1.95	0.47
5:AE:88:VAL:HG12	5:AE:93:ARG:HG2	1.96	0.47
26:BA:917:A:H5''	26:BA:2268:A:H61	1.79	0.47
26:BA:2526:G:N3	56:B4:1:MET:N	2.58	0.47
26:BA:2756:U:OP2	56:B4:19:ARG:NE	2.39	0.47
29:BD:151:THR:HG22	29:BD:152:PRO:CD	2.40	0.47
1:AA:178:C:OP2	20:AT:60:ARG:NH2	2.48	0.47
1:AA:1397:C:P	5:AE:29:ARG:HH22	2.37	0.47
3:AC:11:ARG:NH2	3:AC:177:THR:O	2.47	0.47
3:AC:29:PHE:HZ	14:AN:93:ILE:HG23	1.79	0.47
3:AC:189:ALA:HB3	3:AC:196:ILE:HB	1.97	0.47
26:BA:1294:U:O2'	39:BN:23:ASN:OD1	2.27	0.47
29:BD:14:ILE:HG12	29:BD:24:VAL:HG21	1.97	0.47
32:BG:12:PRO:HG2	32:BG:15:VAL:HG21	1.96	0.47
39:BN:50:PRO:O	39:BN:53:THR:OG1	2.25	0.47
1:AA:1265:C:N4	1:AA:1266:G:O6	2.47	0.47
1:AA:1484:C:HO2'	26:BA:1960:A:HO2'	1.61	0.47
9:AI:99:ARG:NH1	9:AI:105:THR:OG1	2.46	0.47
11:AK:22:HIS:NE2	11:AK:85:MET:SD	2.88	0.47
15:AO:26:GLU:OE2	15:AO:77:ARG:NH2	2.47	0.47
26:BA:442:G:O4'	30:BE:41:GLN:NE2	2.48	0.47
26:BA:475:C:H4'	26:BA:510:C:H5'	1.96	0.47
26:BA:1064:C:H5'	34:BI:90:SER:H	1.79	0.47
44:BS:69:LEU:HA	44:BS:109:ASP:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BT:6:ARG:NH2	45:BT:37:ASP:OD2	2.47	0.47
55:B3:62:LEU:HB3	55:B3:65:ALA:HB2	1.96	0.47
1:AA:28:A:O2'	1:AA:296:U:OP1	2.26	0.47
10:AJ:19:ASP:HA	10:AJ:22:THR:HG22	1.97	0.47
19:AS:31:LEU:H	19:AS:49:ILE:HA	1.79	0.47
26:BA:18:U:O2'	26:BA:554:U:OP1	2.30	0.47
26:BA:968:C:H2'	26:BA:969:G:C8	2.49	0.47
26:BA:1790:C:H2'	26:BA:1791:A:C5	2.50	0.47
26:BA:1796:U:H2'	26:BA:1797:G:C8	2.50	0.47
26:BA:2097:A:H61	26:BA:2192:U:H3	1.62	0.47
37:BL:79:LEU:H	37:BL:113:ALA:HB3	1.79	0.47
38:BM:109:PRO:HB2	38:BM:112:LEU:HD13	1.96	0.47
41:BP:53:ARG:N	41:BP:57:SER:OG	2.41	0.47
43:BR:1:MET:HE2	43:BR:101:ILE:HB	1.95	0.47
1:AA:1217:C:OP2	14:AN:9:ARG:NH2	2.47	0.47
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.49	0.47
2:AB:166:ALA:HB2	2:AB:187:VAL:HG12	1.96	0.47
3:AC:191:THR:OG1	3:AC:194:GLY:O	2.32	0.47
26:BA:1201:U:H2'	26:BA:1202:G:H8	1.80	0.47
26:BA:2623:G:H2'	26:BA:2624:G:H8	1.79	0.47
28:BC:132:MET:HA	28:BC:135:ILE:HD12	1.96	0.47
29:BD:51:THR:HB	29:BD:79:LEU:HD23	1.97	0.47
46:BU:6:ARG:HG2	46:BU:94:ARG:NH2	2.30	0.47
49:BX:34:HIS:CD2	49:BX:53:ALA:HB2	2.48	0.47
1:AA:1279:G:OP1	10:AJ:9:ARG:NH2	2.48	0.47
3:AC:20:SER:HB3	3:AC:22:TRP:CD1	2.49	0.47
7:AG:25:LYS:O	7:AG:29:ILE:HG12	2.15	0.47
8:AH:13:ARG:HB3	8:AH:25:VAL:HG11	1.97	0.47
9:AI:18:ARG:HH21	9:AI:20:PHE:HZ	1.62	0.47
26:BA:657:U:H2'	26:BA:658:U:C6	2.50	0.47
26:BA:1176:U:H2'	26:BA:1177:G:C8	2.50	0.47
26:BA:2063:C:N4	26:BA:2501:C:O2	2.46	0.47
30:BE:25:GLU:OE2	37:BL:7:SER:N	2.47	0.47
38:BM:64:TRP:HB2	38:BM:104:GLU:HB2	1.96	0.47
41:BP:112:GLU:HG2	41:BP:114:LEU:H	1.80	0.47
47:BV:86:LEU:HD13	47:BV:89:ILE:HD11	1.96	0.47
26:BA:1088:A:N6	34:BI:135:SER:OG	2.47	0.47
26:BA:1578:U:H2'	26:BA:1579:A:H8	1.79	0.47
26:BA:1936:A:OP2	26:BA:1962:C:N4	2.40	0.47
29:BD:2:ILE:HD13	29:BD:90:PHE:HE2	1.80	0.47
29:BD:101:PHE:O	29:BD:104:VAL:HG22	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BG:85:LYS:HG2	32:BG:141:ILE:HD12	1.97	0.47
37:BL:82:LEU:HD13	37:BL:120:VAL:HG21	1.97	0.47
45:BT:11:LEU:HB2	50:BY:26:PHE:HE1	1.80	0.47
1:AA:676:A:H4'	11:AK:115:PRO:HB3	1.96	0.46
1:AA:979:C:H1'	1:AA:1317:C:H41	1.80	0.46
1:AA:1503:A:H5'	1:AA:1531:A:H1'	1.97	0.46
1:AA:56:U:H2'	1:AA:57:G:C8	2.51	0.46
1:AA:950:U:H2'	1:AA:951:G:C8	2.49	0.46
10:AJ:27:GLU:HA	10:AJ:30:LYS:HG2	1.97	0.46
26:BA:1105:U:H2'	26:BA:1106:G:H8	1.80	0.46
26:BA:2286:G:H4'	26:BA:2287:A:C4	2.49	0.46
1:AA:51:A:H61	1:AA:314:C:H1'	1.81	0.46
1:AA:376:G:H4'	16:AP:5:ARG:HD2	1.98	0.46
1:AA:406:G:H2'	1:AA:407:U:C6	2.50	0.46
4:AD:188:ARG:NH2	4:AD:197:GLU:OE1	2.48	0.46
10:AJ:10:LEU:HD22	10:AJ:22:THR:HB	1.97	0.46
14:AN:9:ARG:HG2	14:AN:13:ARG:HH12	1.79	0.46
36:BK:98:ARG:HA	36:BK:118:LEU:HD13	1.97	0.46
41:BP:90:GLY:HA2	41:BP:113:ARG:H	1.80	0.46
54:B2:24:THR:HG23	54:B2:27:GLY:H	1.79	0.46
1:AA:335:C:H2'	1:AA:336:A:C8	2.50	0.46
4:AD:145:ILE:HD13	4:AD:178:MET:HB3	1.97	0.46
18:AR:55:LEU:O	18:AR:59:ILE:HG12	2.15	0.46
26:BA:482:A:H4'	46:BU:45:HIS:CE1	2.47	0.46
26:BA:573:U:O2'	26:BA:575:A:OP1	2.27	0.46
26:BA:2216:G:H2'	26:BA:2217:G:H8	1.80	0.46
1:AA:376:G:H5''	16:AP:5:ARG:HB2	1.98	0.46
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.51	0.46
8:AH:39:VAL:HG21	8:AH:110:VAL:HG12	1.97	0.46
26:BA:1257:C:H4'	30:BE:78:TRP:CD1	2.51	0.46
26:BA:1365:A:P	49:BX:28:ARG:HH22	2.38	0.46
26:BA:2010:G:H5''	44:BS:42:LYS:HB2	1.98	0.46
26:BA:2106:U:H2'	26:BA:2107:G:C8	2.51	0.46
39:BN:2:ARG:HG3	39:BN:5:LYS:HB2	1.97	0.46
53:B1:13:SER:HA	53:B1:49:TYR:CD1	2.50	0.46
1:AA:501:C:H2'	1:AA:502:A:C8	2.51	0.46
1:AA:539:A:H2'	1:AA:540:G:C8	2.50	0.46
1:AA:675:A:H1'	11:AK:118:HIS:CE1	2.50	0.46
4:AD:83:LYS:O	4:AD:89:ASN:ND2	2.38	0.46
5:AE:45:ARG:HB3	5:AE:71:MET:SD	2.56	0.46
22:AV:15:A:N6	25:AY:34:CM0:O4	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:184:C:H2'	26:BA:185:G:H8	1.81	0.46
26:BA:1818:U:H2'	28:BC:156:ARG:HB2	1.98	0.46
33:BH:41:LYS:O	33:BH:44:ILE:HG12	2.16	0.46
45:BT:19:LYS:O	45:BT:22:THR:OG1	2.28	0.46
45:BT:23:ALA:O	45:BT:28:ASN:N	2.48	0.46
46:BU:45:HIS:O	46:BU:45:HIS:ND1	2.47	0.46
47:BV:21:ARG:NE	47:BV:87:GLN:OE1	2.47	0.46
53:B1:8:LYS:HD2	55:B3:34:THR:HG21	1.98	0.46
20:AT:35:VAL:HG22	20:AT:50:ALA:HB1	1.96	0.46
26:BA:500:G:OP1	46:BU:43:LYS:NZ	2.45	0.46
26:BA:518:G:O5'	44:BS:18:ARG:NH1	2.49	0.46
26:BA:2744:G:N2	32:BG:143:GLN:HE22	2.13	0.46
29:BD:55:LYS:HB2	29:BD:77:ARG:HA	1.97	0.46
29:BD:112:THR:O	29:BD:195:GLY:HA2	2.15	0.46
34:BI:12:GLN:NE2	34:BI:55:ILE:O	2.49	0.46
43:BR:5:PHE:HB3	43:BR:38:VAL:HG12	1.97	0.46
49:BX:40:VAL:HG11	49:BX:68:LEU:HD11	1.97	0.46
1:AA:408:A:H4'	4:AD:109:ALA:HB3	1.98	0.46
1:AA:927:G:OP1	1:AA:1505:G:N2	2.40	0.46
4:AD:14:ARG:HG3	4:AD:56:ARG:NH1	2.30	0.46
14:AN:13:ARG:HE	14:AN:59:ARG:NE	2.12	0.46
26:BA:6:A:HO2'	35:BJ:132:HIS:HD1	1.64	0.46
26:BA:247:G:O2'	26:BA:250:G:O6	2.34	0.46
26:BA:674:G:H1	26:BA:806:C:H42	1.64	0.46
26:BA:806:C:O2	26:BA:2444:G:O2'	2.34	0.46
26:BA:1363:C:H2'	26:BA:1364:G:C8	2.51	0.46
28:BC:120:VAL:HG13	28:BC:134:ASN:HD21	1.79	0.46
29:BD:133:THR:OG1	29:BD:134:HIS:N	2.45	0.46
36:BK:25:LEU:O	36:BK:30:ARG:NH1	2.49	0.46
43:BR:14:VAL:HG22	43:BR:15:SER:O	2.16	0.46
49:BX:10:LYS:HE3	49:BX:54:LYS:HD3	1.98	0.46
1:AA:830:G:H2'	1:AA:831:A:H8	1.81	0.46
1:AA:1342:C:H2'	1:AA:1343:G:C8	2.51	0.46
10:AJ:11:LYS:HB2	10:AJ:97:ASP:HB3	1.97	0.46
12:AL:38:TYR:OH	12:AL:54:ARG:NH1	2.48	0.46
26:BA:1802:A:OP2	26:BA:1815:A:N6	2.46	0.46
26:BA:2576:G:O2'	26:BA:2579:C:OP2	2.33	0.46
40:BO:94:ARG:HG3	40:BO:96:GLY:H	1.81	0.46
1:AA:126:G:OP1	1:AA:605:U:O2'	2.29	0.46
13:AM:64:VAL:O	13:AM:69:LEU:HB2	2.16	0.46
26:BA:281:C:H42	26:BA:359:G:H1	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:505:A:HO2'	26:BA:509:C:HO2'	1.60	0.46
26:BA:1199:U:H1'	42:BQ:4:VAL:HG22	1.97	0.46
26:BA:2485:G:H5''	38:BM:45:GLN:NE2	2.30	0.46
59:BA:9000:ERY:H352	59:BA:9000:ERY:H4	1.98	0.46
29:BD:4:LEU:HB2	29:BD:101:PHE:CZ	2.51	0.46
37:BL:78:ARG:NH2	37:BL:80:SER:OG	2.49	0.46
1:AA:219:U:H2'	1:AA:220:G:C8	2.52	0.45
5:AE:150:PRO:HA	5:AE:153:VAL:HG22	1.98	0.45
13:AM:4:ILE:HD11	13:AM:10:PRO:HD2	1.98	0.45
25:AY:65:C:H2'	25:AY:66:A:C8	2.51	0.45
26:BA:2742:G:OP2	56:B4:24:ARG:NH1	2.48	0.45
26:BA:2788:C:H2'	26:BA:2789:C:C6	2.51	0.45
31:BF:13:VAL:O	31:BF:17:MET:HG2	2.17	0.45
1:AA:8:A:H62	4:AD:205:SER:HB2	1.80	0.45
1:AA:971:G:O2'	1:AA:1365:G:O2'	2.30	0.45
1:AA:1152:A:OP1	10:AJ:70:HIS:ND1	2.49	0.45
1:AA:1414:U:H2'	1:AA:1415:G:C8	2.51	0.45
7:AG:105:VAL:O	7:AG:109:ARG:HG2	2.17	0.45
8:AH:29:SER:HB2	8:AH:59:LEU:HB2	1.97	0.45
15:AO:36:ILE:O	15:AO:40:GLN:HG2	2.16	0.45
26:BA:1259:G:H2'	26:BA:1260:A:C8	2.51	0.45
26:BA:1913:A:H4'	26:BA:1914:C:O5'	2.15	0.45
26:BA:2291:U:H2'	26:BA:2292:U:C6	2.52	0.45
48:BW:37:ILE:HD11	48:BW:82:ILE:HD11	1.99	0.45
1:AA:1058:G:OP1	3:AC:199:LYS:NZ	2.46	0.45
2:AB:203:ASN:OD1	2:AB:204:ASP:N	2.50	0.45
3:AC:20:SER:HB3	3:AC:22:TRP:NE1	2.31	0.45
13:AM:31:LYS:NZ	13:AM:41:GLU:OE1	2.49	0.45
26:BA:123:G:H4'	26:BA:1376:C:H5'	1.97	0.45
26:BA:475:C:O2	26:BA:479:A:N6	2.49	0.45
30:BE:75:SER:HB3	30:BE:78:TRP:CE3	2.51	0.45
34:BI:54:PRO:HG2	34:BI:78:VAL:HG21	1.99	0.45
36:BK:64:ARG:NE	41:BP:68:GLU:OE2	2.48	0.45
1:AA:8:A:C6	4:AD:206:LYS:HB3	2.51	0.45
1:AA:263:A:OP1	20:AT:74:ARG:NH1	2.49	0.45
1:AA:1317:C:O2'	14:AN:49:GLN:NE2	2.27	0.45
2:AB:205:ASP:OD1	2:AB:206:ALA:N	2.49	0.45
5:AE:96:MET:HE1	5:AE:140:THR:HG23	1.97	0.45
26:BA:1653:G:C6	39:BN:9:GLN:HB3	2.51	0.45
26:BA:2106:U:H2'	26:BA:2107:G:H8	1.81	0.45
1:AA:12:U:O2'	1:AA:914:A:OP2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:79:LYS:O	3:AC:81:GLY:N	2.48	0.45
4:AD:58:LYS:HD3	4:AD:203:LEU:HD23	1.98	0.45
26:BA:1000:A:OP2	26:BA:1154:G:N1	2.37	0.45
26:BA:2530:A:OP2	26:BA:2535:G:N2	2.50	0.45
28:BC:9:THR:O	28:BC:10:SER:OG	2.28	0.45
33:BH:5:LEU:HD13	33:BH:9:VAL:HG21	1.99	0.45
35:BJ:4:PHE:O	42:BQ:64:ARG:NH2	2.38	0.45
47:BV:10:LYS:HG3	47:BV:11:GLU:HG3	1.99	0.45
1:AA:1320:C:N4	19:AS:37:ARG:HG2	2.32	0.45
5:AE:137:VAL:O	5:AE:138:ARG:HB2	2.16	0.45
26:BA:1010:A:H1'	26:BA:1153:C:H1'	1.99	0.45
26:BA:2223:G:OP1	28:BC:171:TYR:OH	2.24	0.45
26:BA:2772:C:H5'	29:BD:173:GLN:HE21	1.82	0.45
28:BC:162:VAL:HG11	28:BC:174:LEU:HD23	1.98	0.45
36:BK:103:VAL:HB	36:BK:107:LEU:HD22	1.98	0.45
38:BM:136:MET:HE1	47:BV:74:ALA:HB1	1.98	0.45
39:BN:32:GLU:HG2	39:BN:115:LEU:HD12	1.97	0.45
39:BN:118:ARG:HH22	52:B0:55:ILE:H	1.63	0.45
41:BP:97:LEU:HB3	41:BP:100:LEU:HD12	1.98	0.45
47:BV:61:LEU:HB2	47:BV:72:VAL:HG23	1.99	0.45
16:AP:52:LEU:HD21	16:AP:57:ILE:HD12	1.99	0.45
26:BA:1326:U:H2'	26:BA:1327:A:C8	2.50	0.45
27:BB:116:G:H2'	27:BB:117:G:C8	2.51	0.45
29:BD:108:ASP:N	29:BD:204:LYS:O	2.31	0.45
1:AA:136:C:O2'	16:AP:64:GLY:O	2.34	0.45
1:AA:939:G:OP1	7:AG:95:ARG:NH2	2.50	0.45
6:AF:5:GLU:OE2	18:AR:23:TYR:OH	2.28	0.45
24:AX:4:G:H1	24:AX:69:U:H3	1.65	0.45
26:BA:250:G:O6	26:BA:386:G:N1	2.38	0.45
26:BA:1597:A:H5''	26:BA:1598:A:H5'	1.98	0.45
26:BA:2719:G:H4'	26:BA:2846:G:H4'	1.98	0.45
26:BA:2840:C:H5''	39:BN:53:THR:HG21	1.98	0.45
27:BB:48:U:P	40:BO:30:ARG:HH22	2.40	0.45
27:BB:95:U:H2'	27:BB:96:G:C8	2.52	0.45
28:BC:166:ALA:HB3	28:BC:173:THR:HB	1.98	0.45
29:BD:4:LEU:HB2	29:BD:101:PHE:HZ	1.81	0.45
36:BK:99:ILE:HD12	36:BK:118:LEU:HD12	1.99	0.45
1:AA:944:G:N1	1:AA:1338:G:OP2	2.32	0.45
3:AC:172:ARG:HG2	3:AC:174:PRO:HD3	1.99	0.45
25:AY:68:C:H2'	25:AY:69:A:H8	1.81	0.45
26:BA:459:U:OP2	54:B2:39:ARG:NH1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:743:A:O2'	26:BA:1659:G:OP1	2.30	0.45
26:BA:1258:U:H2'	26:BA:1259:G:C8	2.51	0.45
26:BA:1313:U:H2'	26:BA:1313:U:O2	2.16	0.45
26:BA:1651:G:H4'	39:BN:39:PRO:HG2	1.98	0.45
26:BA:2691:C:H2'	26:BA:2692:G:C8	2.52	0.45
34:BI:11:LEU:HD12	34:BI:11:LEU:O	2.16	0.45
1:AA:1217:C:P	14:AN:9:ARG:HH21	2.40	0.45
14:AN:99:ALA:HB1	14:AN:101:TRP:HZ3	1.81	0.45
26:BA:813:U:OP1	43:BR:84:ARG:NH1	2.49	0.45
26:BA:1306:C:H2'	26:BA:1307:A:H8	1.82	0.45
26:BA:2392:A:C2	37:BL:55:MET:HE3	2.52	0.45
1:AA:1031:C:H4'	1:AA:1032:G:C2	2.52	0.44
1:AA:1060:U:H5''	10:AJ:53:ILE:HG12	1.99	0.44
7:AG:130:ASN:C	7:AG:135:VAL:HG21	2.42	0.44
11:AK:61:PHE:HA	11:AK:64:GLN:HG2	1.97	0.44
14:AN:61:ARG:HE	14:AN:70:PRO:HB2	1.83	0.44
17:AQ:46:VAL:HG13	17:AQ:74:THR:HA	1.99	0.44
26:BA:451:U:O2	26:BA:453:A:N6	2.50	0.44
26:BA:1801:A:OP2	28:BC:150:LYS:NZ	2.38	0.44
26:BA:2170:A:H1'	26:BA:2171:A:C8	2.52	0.44
26:BA:2827:C:H2'	26:BA:2828:G:H8	1.82	0.44
28:BC:147:LYS:HB2	28:BC:150:LYS:HB2	1.97	0.44
1:AA:254:G:O2'	17:AQ:18:GLU:O	2.35	0.44
1:AA:300:A:O2'	1:AA:564:C:N3	2.48	0.44
1:AA:408:A:H5''	4:AD:110:THR:HG23	1.98	0.44
5:AE:151:GLU:HG3	5:AE:152:MET:HG2	1.99	0.44
10:AJ:9:ARG:NH2	10:AJ:99:GLN:OE1	2.50	0.44
11:AK:112:ASP:OD1	11:AK:114:THR:HG23	2.16	0.44
26:BA:581:C:H2'	26:BA:582:A:C8	2.52	0.44
26:BA:2039:U:H2'	26:BA:2040:G:C8	2.52	0.44
31:BF:37:ASN:OD1	31:BF:38:MET:N	2.50	0.44
33:BH:30:LEU:HB3	33:BH:36:ALA:HB3	1.99	0.44
1:AA:227:G:O2'	16:AP:63:GLN:NE2	2.49	0.44
1:AA:1437:A:H2'	1:AA:1438:G:H8	1.82	0.44
3:AC:8:ASN:HD22	14:AN:90:ARG:HA	1.83	0.44
4:AD:118:VAL:HG11	4:AD:133:ALA:HA	1.98	0.44
11:AK:126:LYS:O	11:AK:127:ARG:HB2	2.18	0.44
17:AQ:27:ARG:HH21	17:AQ:40:ARG:HG2	1.82	0.44
17:AQ:31:HIS:CD2	17:AQ:34:TYR:H	2.34	0.44
26:BA:2298:A:H5''	31:BF:72:LYS:NZ	2.32	0.44
1:AA:830:G:H2'	1:AA:831:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:28:ILE:HG22	4:AD:30:THR:H	1.83	0.44
13:AM:114:LYS:H	13:AM:115:PRO:HD2	1.82	0.44
17:AQ:60:GLU:OE2	17:AQ:77:ARG:NH2	2.50	0.44
26:BA:619:G:H3'	26:BA:620:G:H21	1.82	0.44
26:BA:1070:A:N6	26:BA:1096:A:O2'	2.51	0.44
26:BA:2874:C:OP1	39:BN:4:ARG:NH2	2.51	0.44
29:BD:104:VAL:O	29:BD:106:LYS:N	2.49	0.44
34:BI:19:ASN:HB2	34:BI:39:CYS:HB3	1.99	0.44
38:BM:33:LEU:HD13	38:BM:117:PHE:HB3	1.98	0.44
2:AB:217:VAL:O	2:AB:221:VAL:HG23	2.18	0.44
13:AM:27:LYS:O	13:AM:31:LYS:HG2	2.17	0.44
23:AW:26:A:H2'	23:AW:27:G:C8	2.53	0.44
30:BE:58:LYS:HA	30:BE:59:PRO:HD3	1.85	0.44
34:BI:61:VAL:HA	34:BI:67:PHE:HB3	1.98	0.44
37:BL:29:LYS:O	37:BL:31:GLY:N	2.51	0.44
43:BR:77:PHE:HD1	43:BR:84:ARG:HB3	1.83	0.44
1:AA:402:G:H2'	1:AA:403:C:C6	2.52	0.44
1:AA:1512:U:H2'	1:AA:1513:A:C8	2.51	0.44
4:AD:162:ALA:O	4:AD:167:LYS:HE3	2.17	0.44
26:BA:2:G:O6	26:BA:2900:A:N6	2.51	0.44
26:BA:599:A:H2'	26:BA:600:G:C8	2.52	0.44
26:BA:812:C:H5	37:BL:21:ARG:HB3	1.83	0.44
26:BA:979:A:H2'	26:BA:982:C:H42	1.83	0.44
28:BC:165:VAL:HG11	28:BC:175:ARG:HH21	1.83	0.44
34:BI:94:ASN:ND2	34:BI:137:GLY:HA2	2.32	0.44
37:BL:29:LYS:C	37:BL:30:THR:HG1	2.24	0.44
46:BU:41:LEU:HB3	46:BU:60:GLU:HG2	1.99	0.44
1:AA:1268:G:N3	1:AA:1326:U:O2'	2.47	0.44
4:AD:101:VAL:HG21	4:AD:137:VAL:HG21	1.99	0.44
7:AG:73:VAL:HG12	7:AG:90:GLU:HG3	1.99	0.44
24:AX:23:A:H2'	24:AX:24:A:C8	2.53	0.44
26:BA:355:U:H2'	26:BA:356:G:H8	1.83	0.44
26:BA:2621:G:OP1	29:BD:124:ARG:NH2	2.46	0.44
26:BA:2709:G:H5'	39:BN:22:ARG:HH22	1.82	0.44
1:AA:745:G:OP1	1:AA:851:G:O2'	2.36	0.44
2:AB:67:ILE:HD12	2:AB:160:ALA:HB3	2.00	0.44
6:AF:3:HIS:CD2	6:AF:94:HIS:HA	2.53	0.44
9:AI:28:ILE:HG23	9:AI:63:LEU:HD11	1.99	0.44
20:AT:28:MET:HA	20:AT:31:PHE:HD2	1.82	0.44
24:AX:63:C:H2'	24:AX:64:G:C8	2.52	0.44
26:BA:161:A:H3'	26:BA:162:U:H5''	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:910:A:H2'	26:BA:911:A:C8	2.53	0.44
26:BA:926:G:H2'	26:BA:927:A:C8	2.52	0.44
26:BA:1106:G:H2'	26:BA:1107:G:H8	1.83	0.44
26:BA:1867:G:H1	26:BA:1874:C:H42	1.66	0.44
26:BA:2368:C:H2'	26:BA:2369:A:C8	2.52	0.44
26:BA:2594:C:N4	26:BA:2595:G:O6	2.51	0.44
30:BE:21:ARG:HH21	30:BE:106:LYS:HE3	1.82	0.44
40:BO:43:ASN:OD1	40:BO:44:GLY:N	2.51	0.44
32:BG:64:GLN:O	32:BG:67:THR:OG1	2.35	0.44
1:AA:373:A:H61	1:AA:391:G:H1'	1.82	0.43
1:AA:392:C:H2'	1:AA:393:A:C8	2.53	0.43
1:AA:875:U:O3'	8:AH:15:ARG:NH1	2.51	0.43
1:AA:1151:A:O2'	1:AA:1152:A:H5''	2.18	0.43
1:AA:1191:A:H5''	3:AC:4:LYS:HE3	2.00	0.43
3:AC:168:TYR:OH	5:AE:55:GLU:OE2	2.29	0.43
8:AH:95:VAL:HG23	8:AH:102:ALA:HB2	2.00	0.43
21:AU:40:LYS:HB3	21:AU:41:PRO:HD3	1.99	0.43
26:BA:1779:U:H5''	26:BA:1780:A:H5''	2.00	0.43
26:BA:2377:A:H2'	26:BA:2378:A:C8	2.53	0.43
38:BM:75:GLU:HB2	38:BM:90:GLU:HG3	1.99	0.43
2:AB:114:LEU:HD13	2:AB:144:LEU:HB2	2.00	0.43
8:AH:22:LYS:O	8:AH:65:TYR:OH	2.30	0.43
26:BA:467:G:OP2	54:B2:34:ARG:HD3	2.17	0.43
26:BA:692:C:HO2'	26:BA:1354:A:HO2'	1.66	0.43
30:BE:147:LEU:HB3	30:BE:186:VAL:HG22	2.01	0.43
39:BN:59:SER:OG	39:BN:62:ASN:OD1	2.35	0.43
4:AD:124:MET:HA	4:AD:129:VAL:HA	1.98	0.43
25:AY:19:G:N2	25:AY:56:C:N3	2.67	0.43
26:BA:215:G:H4'	26:BA:216:A:H4'	2.00	0.43
27:BB:95:U:H2'	27:BB:96:G:H8	1.83	0.43
28:BC:25:HIS:CG	28:BC:80:ARG:HD2	2.53	0.43
28:BC:88:SER:O	28:BC:197:ASN:ND2	2.51	0.43
36:BK:109:SER:O	36:BK:111:LYS:N	2.51	0.43
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.53	0.43
6:AF:10:VAL:HB	6:AF:58:HIS:HB3	2.01	0.43
8:AH:75:ILE:HD12	8:AH:128:TYR:O	2.18	0.43
10:AJ:19:ASP:OD1	10:AJ:20:GLN:N	2.49	0.43
11:AK:23:ILE:HD11	11:AK:86:VAL:HG22	2.00	0.43
11:AK:93:ARG:HH21	21:AU:20:LYS:HG3	1.84	0.43
19:AS:40:ILE:HD13	19:AS:66:MET:HB3	2.00	0.43
26:BA:973:A:H5'	26:BA:1188:U:H1'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:1076:C:H2'	26:BA:1077:A:O4'	2.18	0.43
26:BA:1744:A:H3'	26:BA:1745:A:H8	1.84	0.43
26:BA:1807:G:O2'	26:BA:1809:A:N6	2.51	0.43
26:BA:2279:G:O6	48:BW:14:ARG:NE	2.50	0.43
32:BG:97:ALA:H	32:BG:104:ASN:HB3	1.83	0.43
35:BJ:23:LYS:NZ	35:BJ:142:ILE:OXT	2.51	0.43
53:B1:39:PHE:HA	53:B1:46:HIS:HA	2.00	0.43
1:AA:64:G:H4'	1:AA:65:A:H5''	2.00	0.43
1:AA:960:U:H2'	1:AA:1225:A:H62	1.83	0.43
11:AK:13:ARG:O	11:AK:15:GLN:N	2.46	0.43
12:AL:114:ARG:HH22	12:AL:121:ARG:HH11	1.66	0.43
58:AW:101:LYS:HB3	26:BA:2506:U:O2	2.19	0.43
26:BA:1250:G:OP2	37:BL:21:ARG:NH2	2.52	0.43
26:BA:2548:U:O2	36:BK:23:LYS:NZ	2.50	0.43
34:BI:21:SER:HB3	34:BI:22:PRO:HD3	1.99	0.43
50:BY:21:LEU:HD23	50:BY:25:GLN:HG3	1.99	0.43
55:B3:29:LEU:HA	55:B3:33:LEU:HD21	1.99	0.43
1:AA:403:C:H5'	4:AD:132:ILE:HG23	2.00	0.43
8:AH:92:LEU:HD21	8:AH:113:ASP:HB2	2.01	0.43
32:BG:54:PRO:HG3	32:BG:62:TRP:CD2	2.54	0.43
33:BH:8:LYS:HD3	33:BH:15:LEU:HG	2.00	0.43
46:BU:89:ASP:CG	46:BU:90:GLY:H	2.25	0.43
52:B0:54:VAL:O	52:B0:56:ALA:N	2.49	0.43
1:AA:739:C:O2'	15:AO:42:HIS:ND1	2.50	0.43
1:AA:1329:A:H5''	13:AM:26:GLY:H	1.84	0.43
3:AC:152:GLU:HG2	3:AC:167:TRP:HB3	2.00	0.43
11:AK:127:ARG:HB2	21:AU:34:ARG:HE	1.83	0.43
13:AM:11:ASP:OD1	13:AM:12:HIS:N	2.51	0.43
18:AR:29:LEU:HD23	18:AR:59:ILE:HD13	2.00	0.43
26:BA:213:A:H2'	26:BA:214:G:C8	2.54	0.43
26:BA:548:G:O2'	26:BA:549:G:N7	2.51	0.43
26:BA:1954:G:O2'	26:BA:1956:U:O4	2.29	0.43
26:BA:2093:G:H2'	26:BA:2094:A:H8	1.84	0.43
26:BA:2146:C:O2'	26:BA:2147:A:O5'	2.23	0.43
35:BJ:32:LEU:HD22	35:BJ:54:ILE:HG21	2.00	0.43
44:BS:69:LEU:C	44:BS:70:LYS:HD2	2.43	0.43
51:BZ:6:LYS:HA	51:BZ:37:GLU:HA	1.99	0.43
55:B3:33:LEU:HB3	55:B3:41:LYS:HD3	2.01	0.43
1:AA:252:U:O4	1:AA:253:A:N6	2.46	0.43
2:AB:199:VAL:HG22	2:AB:201:PRO:HD3	2.01	0.43
3:AC:84:VAL:HG13	3:AC:101:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:50:PRO:HG3	6:AF:55:HIS:CE1	2.53	0.43
23:AW:13:C:H4'	23:AW:14:A:OP1	2.18	0.43
26:BA:53:A:H2	26:BA:179:C:H4'	1.83	0.43
26:BA:572:A:H61	26:BA:2029:G:H21	1.67	0.43
26:BA:632:A:H2'	26:BA:633:A:C8	2.53	0.43
26:BA:720:U:H2'	26:BA:721:A:C8	2.54	0.43
27:BB:24:G:N2	27:BB:28:C:O2	2.51	0.43
30:BE:131:THR:HG22	30:BE:160:ALA:HA	2.00	0.43
30:BE:176:ASP:OD1	30:BE:179:SER:OG	2.33	0.43
35:BJ:77:HIS:HD1	35:BJ:79:GLY:H	1.67	0.43
35:BJ:117:ALA:HA	35:BJ:120:ARG:HH21	1.84	0.43
41:BP:29:LYS:HD2	41:BP:83:SER:HB2	2.01	0.43
53:B1:50:LYS:HG2	53:B1:51:GLU:N	2.33	0.43
1:AA:407:U:O2'	4:AD:113:GLU:HB2	2.19	0.43
2:AB:106:THR:O	2:AB:109:GLN:NE2	2.52	0.43
5:AE:80:THR:HB	5:AE:122:ASN:HD21	1.83	0.43
19:AS:8:GLY:HA2	19:AS:9:PRO:HD3	1.90	0.43
26:BA:1254:A:H5''	26:BA:1255:U:H5''	2.01	0.43
26:BA:1266:G:O2'	26:BA:2012:G:O6	2.33	0.43
26:BA:1636:U:H2'	26:BA:1637:A:C8	2.54	0.43
30:BE:55:SER:O	30:BE:74:LYS:NZ	2.52	0.43
44:BS:62:ASP:OD1	44:BS:62:ASP:N	2.51	0.43
2:AB:138:THR:HA	2:AB:141:LEU:HD13	2.01	0.43
4:AD:154:ARG:O	4:AD:158:ALA:N	2.47	0.43
8:AH:104:VAL:HA	8:AH:125:ILE:HA	2.01	0.43
12:AL:38:TYR:N	12:AL:52:VAL:O	2.52	0.43
12:AL:83:ARG:HB2	12:AL:98:VAL:HG23	2.01	0.43
24:AX:16:U:H5'	24:AX:59:G:H1	1.84	0.43
26:BA:296:U:H2'	26:BA:297:G:C8	2.54	0.43
26:BA:1190:G:H2'	26:BA:1191:G:H8	1.84	0.43
26:BA:2680:U:O2'	29:BD:11:MET:SD	2.77	0.43
27:BB:114:C:H2'	27:BB:115:A:C8	2.53	0.43
31:BF:126:GLY:HA2	31:BF:163:ASP:HA	2.01	0.43
34:BI:33:VAL:HG13	34:BI:67:PHE:CE2	2.54	0.43
43:BR:82:HIS:O	43:BR:82:HIS:ND1	2.52	0.43
1:AA:96:U:H2'	1:AA:97:G:C8	2.54	0.42
1:AA:337:G:H2'	1:AA:338:A:C8	2.54	0.42
1:AA:403:C:OP1	4:AD:134:SER:HB3	2.18	0.42
1:AA:413:G:H1'	1:AA:428:G:N2	2.34	0.42
1:AA:497:G:H2'	1:AA:498:A:C8	2.54	0.42
1:AA:1227:A:H5'	13:AM:110:LYS:NZ	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1251:A:H2'	1:AA:1252:A:C8	2.54	0.42
5:AE:105:ILE:HD13	5:AE:121:HIS:HA	2.00	0.42
7:AG:151:PHE:CE2	11:AK:56:ARG:HG2	2.54	0.42
16:AP:57:ILE:O	16:AP:61:VAL:HG23	2.19	0.42
16:AP:72:ALA:O	16:AP:76:LYS:HG2	2.19	0.42
26:BA:634:C:H2'	26:BA:635:C:C6	2.54	0.42
26:BA:2002:G:H5''	39:BN:9:GLN:HE21	1.84	0.42
26:BA:2818:U:H2'	26:BA:2819:G:C8	2.53	0.42
29:BD:14:ILE:HA	41:BP:12:GLN:HE22	1.83	0.42
32:BG:83:PHE:HB3	32:BG:141:ILE:HD13	1.99	0.42
38:BM:77:PRO:HB2	38:BM:80:VAL:HG21	2.00	0.42
39:BN:28:LEU:HD22	39:BN:44:LEU:HD21	2.00	0.42
1:AA:408:A:H5''	4:AD:110:THR:CG2	2.49	0.42
26:BA:742:A:H2'	26:BA:743:A:C8	2.54	0.42
26:BA:1469:A:H2'	26:BA:1470:A:C8	2.54	0.42
26:BA:1709:U:H2'	26:BA:1710:G:C8	2.53	0.42
26:BA:1909:C:H2'	26:BA:1910:G:C8	2.54	0.42
26:BA:2537:U:H2'	26:BA:2538:C:C6	2.54	0.42
32:BG:85:LYS:HB2	32:BG:133:LEU:HD11	2.00	0.42
33:BH:8:LYS:HA	33:BH:15:LEU:H	1.83	0.42
41:BP:14:LYS:HE3	41:BP:77:HIS:HA	2.01	0.42
45:BT:37:ASP:OD1	45:BT:37:ASP:N	2.52	0.42
50:BY:31:GLN:O	50:BY:34:SER:OG	2.32	0.42
4:AD:8:LYS:HB3	4:AD:21:LEU:HD13	2.00	0.42
16:AP:18:GLN:HA	16:AP:38:PHE:HA	2.01	0.42
19:AS:36:ARG:NH2	19:AS:72:GLY:O	2.52	0.42
21:AU:37:PHE:O	21:AU:39:GLU:N	2.51	0.42
23:AW:13:C:O2'	23:AW:14:A:O5'	2.35	0.42
26:BA:629:G:H5''	26:BA:650:C:O2'	2.18	0.42
1:AA:21:G:H2'	1:AA:22:G:C8	2.54	0.42
1:AA:542:G:H2'	1:AA:543:U:C6	2.55	0.42
1:AA:674:G:N2	1:AA:717:U:O2	2.52	0.42
10:AJ:81:GLU:HA	10:AJ:84:VAL:HG12	2.02	0.42
26:BA:269:C:H2'	26:BA:270:A:H8	1.84	0.42
26:BA:322:A:P	30:BE:163:ASN:HD21	2.41	0.42
26:BA:2126:A:O2'	26:BA:2162:G:O6	2.30	0.42
26:BA:2522:U:O2'	26:BA:2647:U:OP1	2.26	0.42
30:BE:112:LEU:HB3	30:BE:118:LEU:HB2	2.00	0.42
35:BJ:8:PRO:HB3	35:BJ:48:VAL:HG13	2.02	0.42
53:B1:9:ILE:HG21	53:B1:25:LYS:HE2	2.01	0.42
1:AA:495:A:N6	4:AD:116:GLN:HE21	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:675:A:OP1	18:AR:74:HIS:NE2	2.53	0.42
1:AA:1238:A:H5'	1:AA:1336:C:H41	1.83	0.42
15:AO:46:HIS:C	15:AO:48:LYS:H	2.26	0.42
17:AQ:15:ASP:HB2	17:AQ:55:ILE:HB	2.01	0.42
26:BA:729:G:H5''	26:BA:730:A:H5''	2.01	0.42
26:BA:747:U:O2	26:BA:2014:A:O2'	2.29	0.42
26:BA:2837:A:H2'	26:BA:2838:G:C8	2.55	0.42
29:BD:105:LYS:HG2	29:BD:106:LYS:HG3	2.02	0.42
29:BD:176:ASP:HB2	29:BD:190:LYS:HE2	2.01	0.42
1:AA:1522:U:H2'	1:AA:1523:G:H8	1.85	0.42
13:AM:4:ILE:HD12	13:AM:22:ILE:HD11	2.01	0.42
16:AP:35:ARG:HH21	16:AP:38:PHE:HB3	1.84	0.42
26:BA:922:C:H2'	26:BA:923:G:H8	1.84	0.42
26:BA:1595:C:H2'	26:BA:1596:A:C8	2.55	0.42
26:BA:1782:U:C2	57:B5:-4:MET:CE	2.84	0.42
26:BA:2097:A:OP2	26:BA:2097:A:H8	2.01	0.42
38:BM:41:LEU:HG	38:BM:96:ILE:HG13	2.01	0.42
46:BU:4:LYS:HB3	46:BU:83:VAL:HG21	2.01	0.42
1:AA:52:C:H2'	1:AA:53:A:C8	2.55	0.42
1:AA:587:G:N2	1:AA:754:C:OP2	2.43	0.42
26:BA:84:A:OP2	46:BU:6:ARG:NH1	2.53	0.42
26:BA:371:A:H61	26:BA:401:A:H3'	1.85	0.42
26:BA:1097:U:C4	26:BA:1098:A:H1'	2.55	0.42
26:BA:1899:A:H4'	26:BA:1901:A:H5''	2.01	0.42
2:AB:47:VAL:HB	2:AB:48:PRO:HD3	2.01	0.42
4:AD:168:PRO:HB3	4:AD:170:TRP:CH2	2.55	0.42
5:AE:12:GLN:HB3	5:AE:40:GLY:O	2.19	0.42
7:AG:72:THR:HA	7:AG:96:ARG:HH12	1.83	0.42
26:BA:171:U:H2'	26:BA:172:A:C8	2.55	0.42
26:BA:906:U:O2'	38:BM:66:ARG:NH2	2.41	0.42
26:BA:906:U:HO2'	38:BM:66:ARG:HH21	1.63	0.42
26:BA:1903:G:H2'	26:BA:1904:G:H8	1.83	0.42
26:BA:2831:G:OP1	26:BA:2834:G:O2'	2.34	0.42
35:BJ:16:TYR:HE1	35:BJ:138:GLN:HE21	1.68	0.42
43:BR:75:VAL:HG12	43:BR:77:PHE:H	1.85	0.42
1:AA:106:C:H2'	1:AA:107:G:C8	2.54	0.42
1:AA:439:U:H2'	1:AA:440:C:C6	2.55	0.42
1:AA:545:C:H5'	4:AD:69:GLU:CB	2.49	0.42
1:AA:950:U:H2'	1:AA:951:G:H8	1.85	0.42
4:AD:121:LYS:HB3	4:AD:129:VAL:CG2	2.50	0.42
13:AM:5:ALA:H	13:AM:57:ARG:NH1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:2495:G:H4'	38:BM:82:MET:HE3	2.01	0.42
27:BB:49:C:H2'	27:BB:50:A:C8	2.54	0.42
1:AA:73:C:O2'	1:AA:74:A:H8	2.02	0.42
1:AA:1105:A:H2'	1:AA:1106:G:C8	2.54	0.42
19:AS:41:PHE:HB2	19:AS:44:MET:HG3	2.01	0.42
26:BA:1028:A:N6	26:BA:1125:G:H2'	2.34	0.42
26:BA:1178:C:H2'	26:BA:1179:G:H8	1.85	0.42
26:BA:1438:U:H2'	26:BA:1439:A:C8	2.54	0.42
36:BK:15:GLY:O	36:BK:47:ILE:HG13	2.19	0.42
39:BN:103:ARG:HB2	39:BN:110:MET:HE3	2.02	0.42
42:BQ:108:ALA:HB1	43:BR:48:LYS:NZ	2.35	0.42
1:AA:995:C:N3	1:AA:1046:A:O2'	2.46	0.41
1:AA:1227:A:H5'	13:AM:110:LYS:HZ2	1.85	0.41
10:AJ:12:ALA:HB3	10:AJ:18:ILE:HB	2.02	0.41
11:AK:31:ILE:HG13	11:AK:46:THR:HG22	2.02	0.41
11:AK:86:VAL:HB	11:AK:112:ASP:HA	2.02	0.41
14:AN:7:LYS:O	14:AN:11:VAL:HG23	2.20	0.41
16:AP:43:ALA:HB1	16:AP:49:GLY:HA2	2.02	0.41
16:AP:46:LYS:HG3	16:AP:47:GLU:HG2	2.02	0.41
17:AQ:61:ILE:HD11	17:AQ:73:TRP:HB3	2.01	0.41
19:AS:11:ILE:HG22	19:AS:39:THR:H	1.84	0.41
20:AT:28:MET:HE3	20:AT:58:VAL:HG13	2.02	0.41
26:BA:141:G:OP2	26:BA:142:A:N6	2.53	0.41
26:BA:244:A:OP2	55:B3:8:ARG:NH1	2.51	0.41
26:BA:290:U:H2'	26:BA:291:G:C8	2.55	0.41
26:BA:2355:G:H1'	48:BW:39:ARG:HH21	1.84	0.41
26:BA:2836:U:H2'	26:BA:2837:A:C8	2.55	0.41
29:BD:108:ASP:OD1	29:BD:174:SER:N	2.41	0.41
1:AA:408:A:N6	1:AA:434:U:H3	2.15	0.41
1:AA:891:U:H2'	1:AA:892:A:H8	1.84	0.41
7:AG:73:VAL:HG12	7:AG:90:GLU:HA	2.01	0.41
7:AG:97:ASN:OD1	7:AG:98:ALA:N	2.53	0.41
9:AI:6:TYR:CE1	9:AI:89:GLU:HG2	2.56	0.41
10:AJ:6:ILE:HG22	10:AJ:8:ILE:HG13	2.02	0.41
19:AS:63:THR:HB	19:AS:66:MET:HG2	2.02	0.41
26:BA:546:U:O2	26:BA:546:U:H2'	2.19	0.41
26:BA:594:U:H2'	26:BA:595:C:C6	2.55	0.41
26:BA:958:U:H5'	38:BM:14:LYS:HE2	2.03	0.41
26:BA:1252:G:H1	42:BQ:37:GLN:HE21	1.67	0.41
26:BA:1668:A:H61	26:BA:1676:A:H61	1.67	0.41
26:BA:2623:G:H2'	26:BA:2624:G:C8	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:BA:9000:ERY:H151	59:BA:9000:ERY:H202	1.84	0.41
27:BB:80:U:H2'	27:BB:81:G:H8	1.85	0.41
36:BK:30:ARG:HH22	36:BK:37:ASP:CG	2.29	0.41
44:BS:44:ALA:HA	44:BS:47:VAL:HG12	2.02	0.41
1:AA:626:G:OP1	16:AP:35:ARG:NH2	2.48	0.41
1:AA:662:U:O2'	1:AA:836:G:OP1	2.23	0.41
1:AA:1222:G:OP2	1:AA:1322:C:N4	2.53	0.41
1:AA:1316:G:N2	1:AA:1319:A:OP2	2.53	0.41
2:AB:68:LEU:O	2:AB:162:PHE:HB3	2.19	0.41
3:AC:35:SER:OG	3:AC:59:ARG:NH2	2.45	0.41
9:AI:7:TYR:HD1	9:AI:20:PHE:HE1	1.67	0.41
11:AK:23:ILE:HG22	11:AK:32:VAL:HG22	2.01	0.41
26:BA:307:G:N1	26:BA:310:A:OP2	2.50	0.41
28:BC:45:ASN:OD1	28:BC:46:ASN:N	2.53	0.41
28:BC:135:ILE:HA	28:BC:136:PRO:HD3	1.89	0.41
34:BI:5:VAL:HA	34:BI:8:TYR:HE2	1.86	0.41
34:BI:90:SER:HB3	34:BI:93:PRO:HG3	2.03	0.41
1:AA:495:A:N6	4:AD:120:HIS:HE1	2.18	0.41
1:AA:837:U:H2'	1:AA:838:G:H8	1.85	0.41
4:AD:88:GLU:HG2	4:AD:188:ARG:HD3	2.01	0.41
26:BA:249:C:O2	55:B3:12:LYS:NZ	2.54	0.41
26:BA:1012:U:O4	35:BJ:30:THR:HG21	2.20	0.41
26:BA:2286:G:H1	53:B1:23:THR:HG21	1.85	0.41
26:BA:2705:A:O2'	26:BA:2852:G:OP1	2.34	0.41
33:BH:26:ALA:HA	33:BH:30:LEU:HB2	2.01	0.41
36:BK:10:VAL:HG12	36:BK:12:ASP:H	1.85	0.41
36:BK:47:ILE:HA	36:BK:48:PRO:HD3	1.90	0.41
46:BU:74:ASN:HB2	46:BU:79:LYS:O	2.21	0.41
46:BU:86:ARG:H	46:BU:95:PHE:HE2	1.68	0.41
51:BZ:41:THR:OG1	51:BZ:42:PRO:HD2	2.19	0.41
1:AA:235:C:H2'	1:AA:236:A:C8	2.55	0.41
1:AA:409:U:O5'	4:AD:24:GLY:HA3	2.21	0.41
1:AA:658:C:H1'	15:AO:22:THR:HG21	2.03	0.41
4:AD:48:LEU:HD21	4:AD:52:GLY:C	2.46	0.41
7:AG:69:VAL:HA	7:AG:138:ARG:HD3	2.02	0.41
9:AI:83:ILE:O	9:AI:87:LEU:HG	2.20	0.41
14:AN:80:SER:O	14:AN:84:VAL:HG23	2.20	0.41
24:AX:50:C:H2'	24:AX:51:G:C8	2.55	0.41
26:BA:534:U:H2'	26:BA:535:G:C8	2.55	0.41
26:BA:1190:G:H2'	26:BA:1191:G:C8	2.56	0.41
26:BA:1759:A:O2'	26:BA:2714:G:O2'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:2428:G:N2	37:BL:60:ARG:HH22	2.19	0.41
38:BM:13:HIS:O	38:BM:71:LYS:NZ	2.53	0.41
38:BM:42:THR:HA	38:BM:93:VAL:HG12	2.01	0.41
1:AA:426:U:P	4:AD:33:LYS:HD3	2.61	0.41
1:AA:603:U:H2'	1:AA:604:G:C8	2.56	0.41
6:AF:62:MET:HG2	6:AF:64:VAL:HG23	2.03	0.41
26:BA:64:A:H5''	45:BT:77:ARG:HA	2.03	0.41
26:BA:833:A:H2'	26:BA:834:G:C8	2.55	0.41
26:BA:937:C:H2'	26:BA:938:G:C8	2.56	0.41
26:BA:1316:U:H2'	26:BA:1317:G:C8	2.55	0.41
26:BA:1668:A:N6	26:BA:1676:A:H61	2.19	0.41
26:BA:2061:G:H2'	26:BA:2501:C:O2'	2.21	0.41
26:BA:2092:U:P	33:BH:28:ASN:HD21	2.43	0.41
26:BA:2216:G:H2'	26:BA:2217:G:C8	2.55	0.41
30:BE:56:GLY:HA2	30:BE:74:LYS:HZ1	1.85	0.41
32:BG:88:GLN:HA	32:BG:130:GLU:HA	2.02	0.41
34:BI:93:PRO:HB2	34:BI:94:ASN:H	1.66	0.41
36:BK:113:MET:SD	36:BK:116:ILE:HD11	2.60	0.41
41:BP:63:LYS:O	41:BP:70:VAL:N	2.41	0.41
46:BU:82:ARG:O	46:BU:97:LYS:HG2	2.20	0.41
47:BV:29:ILE:HG22	47:BV:88:HIS:CE1	2.56	0.41
1:AA:309:A:H2'	1:AA:310:G:C8	2.56	0.41
2:AB:69:PHE:HB2	2:AB:91:PHE:HB3	2.03	0.41
2:AB:210:VAL:O	2:AB:214:LEU:HB2	2.20	0.41
5:AE:113:ALA:HA	5:AE:116:GLU:HG2	2.03	0.41
15:AO:24:SER:HB3	15:AO:27:VAL:HG23	2.02	0.41
16:AP:12:LYS:C	16:AP:14:ARG:H	2.28	0.41
26:BA:5:A:H2'	26:BA:6:A:C8	2.55	0.41
26:BA:118:A:OP1	54:B2:22:MET:HE2	2.20	0.41
26:BA:668:A:H2'	26:BA:670:A:H62	1.85	0.41
26:BA:1299:G:H5''	26:BA:1300:G:H5''	2.02	0.41
26:BA:1563:U:H2'	26:BA:1564:C:C6	2.56	0.41
26:BA:2478:A:OP2	56:B4:2:LYS:HD3	2.21	0.41
26:BA:2547:A:H4'	36:BK:29:HIS:HE1	1.86	0.41
28:BC:30:PHE:CE2	28:BC:32:PRO:HG2	2.55	0.41
29:BD:136:ASN:OD1	29:BD:137:SER:N	2.53	0.41
33:BH:27:ARG:NH1	33:BH:38:PRO:HB3	2.36	0.41
48:BW:27:GLY:HA2	48:BW:67:VAL:HB	2.02	0.41
1:AA:99:C:H2'	1:AA:100:G:C8	2.55	0.41
1:AA:110:C:O2'	16:AP:25:ARG:O	2.36	0.41
1:AA:216:U:H2'	1:AA:217:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:96:TRP:CZ3	2:AB:98:GLY:HA2	2.56	0.41
3:AC:23:PHE:CZ	10:AJ:11:LYS:HE2	2.56	0.41
21:AU:45:ARG:O	21:AU:49:LYS:HG2	2.20	0.41
26:BA:1902:C:H5''	28:BC:240:PHE:CE2	2.55	0.41
26:BA:2062:A:C8	57:B5:-3:ARG:HA	2.56	0.41
29:BD:49:GLN:NE2	29:BD:79:LEU:HD13	2.36	0.41
36:BK:9:ASN:OD1	36:BK:18:ARG:NH1	2.53	0.41
37:BL:135:ILE:HG22	37:BL:140:GLY:HA3	2.03	0.41
44:BS:2:GLU:HA	44:BS:108:SER:HB3	2.02	0.41
1:AA:8:A:N6	4:AD:202:GLU:O	2.54	0.41
1:AA:728:A:H2'	1:AA:729:A:C8	2.55	0.41
1:AA:784:A:H2'	1:AA:785:G:C8	2.56	0.41
1:AA:1075:U:H2'	1:AA:1076:U:C6	2.56	0.41
3:AC:47:LEU:HB3	3:AC:50:ALA:HB3	2.01	0.41
4:AD:34:ILE:O	4:AD:36:GLN:N	2.47	0.41
4:AD:102:VAL:HB	4:AD:114:ALA:HB1	2.03	0.41
4:AD:109:ALA:HB1	4:AD:161:LEU:HD21	2.03	0.41
12:AL:44:LYS:N	12:AL:45:PRO:HD2	2.35	0.41
19:AS:52:HIS:CE1	19:AS:54:GLY:H	2.39	0.41
25:AY:53:G:H1	25:AY:61:C:H42	1.69	0.41
26:BA:45:G:H2'	26:BA:215:G:C5	2.55	0.41
26:BA:172:A:H2'	26:BA:173:A:C8	2.56	0.41
26:BA:355:U:H2'	26:BA:356:G:C8	2.55	0.41
26:BA:948:C:H2'	26:BA:949:G:C8	2.56	0.41
26:BA:968:C:H2'	26:BA:969:G:H8	1.86	0.41
26:BA:1378:A:O2'	26:BA:1380:G:OP2	2.25	0.41
26:BA:1528:A:N6	26:BA:1543:G:O2'	2.53	0.41
26:BA:1782:U:C4	57:B5:-4:MET:SD	3.14	0.41
26:BA:2182:U:H2'	26:BA:2183:A:C8	2.56	0.41
26:BA:2255:G:H1	26:BA:2275:C:H42	1.69	0.41
26:BA:2641:G:H2'	26:BA:2642:G:H8	1.85	0.41
28:BC:258:ARG:NH2	28:BC:264:ASP:OD1	2.47	0.41
29:BD:8:LYS:HB2	29:BD:201:LEU:HD11	2.03	0.41
31:BF:130:MET:O	31:BF:154:ILE:N	2.48	0.41
32:BG:133:LEU:HD21	32:BG:145:ALA:HB2	2.03	0.41
35:BJ:96:ARG:HH21	35:BJ:99:ARG:HG2	1.85	0.41
40:BO:27:VAL:HA	40:BO:93:ASP:HB3	2.02	0.41
40:BO:74:VAL:O	40:BO:78:VAL:HG23	2.21	0.41
1:AA:374:A:H5''	1:AA:452:A:N1	2.36	0.41
1:AA:1073:U:H3	1:AA:1102:A:H61	1.69	0.41
1:AA:1163:A:H2'	1:AA:1164:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1538:C:H2'	1:AA:1539:C:C6	2.55	0.41
9:AI:92:GLU:HB3	9:AI:95:ARG:HH12	1.86	0.41
26:BA:480:A:H5''	46:BU:44:LYS:HD2	2.02	0.41
33:BH:27:ARG:HH12	33:BH:38:PRO:HB3	1.85	0.41
1:AA:147:G:H2'	1:AA:148:G:C8	2.56	0.40
1:AA:591:U:H2'	1:AA:592:G:C8	2.56	0.40
2:AB:151:ILE:HA	2:AB:154:MET:HB2	2.02	0.40
3:AC:6:HIS:HA	3:AC:7:PRO:HD3	1.88	0.40
16:AP:6:LEU:HA	16:AP:19:VAL:HA	2.02	0.40
26:BA:721:A:H2'	26:BA:722:A:C8	2.56	0.40
26:BA:1595:C:H2'	26:BA:1596:A:H8	1.86	0.40
1:AA:19:A:H2'	1:AA:20:U:C6	2.57	0.40
1:AA:392:C:H2'	1:AA:393:A:H8	1.86	0.40
1:AA:512:U:H1'	4:AD:41:HIS:CE1	2.56	0.40
1:AA:540:G:H2'	1:AA:541:G:O4'	2.21	0.40
1:AA:1318:A:O2'	19:AS:37:ARG:HD3	2.21	0.40
1:AA:1515:G:H2'	1:AA:1516:G:C8	2.56	0.40
5:AE:149:SER:O	5:AE:153:VAL:HG13	2.22	0.40
6:AF:51:ILE:HG13	6:AF:51:ILE:O	2.22	0.40
10:AJ:78:GLU:HG3	10:AJ:80:THR:H	1.86	0.40
19:AS:50:ALA:HA	19:AS:59:PRO:HA	2.04	0.40
26:BA:948:C:H2'	26:BA:949:G:H8	1.86	0.40
26:BA:2618:G:H21	29:BD:155:VAL:HG21	1.86	0.40
30:BE:18:THR:HG23	30:BE:106:LYS:HG2	2.03	0.40
39:BN:55:ALA:HA	39:BN:80:PHE:CE1	2.56	0.40
1:AA:454:G:H1	1:AA:478:A:H61	1.69	0.40
1:AA:912:C:H5''	12:AL:43:LYS:NZ	2.36	0.40
2:AB:157:LEU:HA	2:AB:158:PRO:HD3	1.90	0.40
5:AE:107:ALA:H	5:AE:112:ARG:NH2	2.19	0.40
26:BA:20:C:H2'	26:BA:21:A:C8	2.57	0.40
26:BA:1437:C:H2'	26:BA:1438:U:C6	2.57	0.40
26:BA:2547:A:H4'	36:BK:29:HIS:CE1	2.56	0.40
27:BB:44:G:H1'	27:BB:47:C:H42	1.85	0.40
31:BF:25:VAL:O	31:BF:28:VAL:HG12	2.22	0.40
37:BL:96:LYS:HD3	37:BL:103:ILE:HA	2.03	0.40
46:BU:32:GLY:O	46:BU:67:VAL:HG23	2.21	0.40
46:BU:72:ILE:HD13	46:BU:83:VAL:HG22	2.03	0.40
53:B1:12:VAL:HG22	53:B1:51:GLU:HB3	2.03	0.40
26:BA:307:G:N2	26:BA:309:A:H3'	2.37	0.40
26:BA:455:C:N3	26:BA:472:A:H2'	2.37	0.40
26:BA:775:G:OP1	26:BA:777:G:O2'	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:1056:G:H5''	26:BA:1057:A:O4'	2.21	0.40
26:BA:2305:U:C2	31:BF:151:GLY:HA3	2.56	0.40
27:BB:115:A:H2'	27:BB:116:G:C8	2.56	0.40
40:BO:66:GLY:HA2	40:BO:102:ARG:HH22	1.86	0.40
48:BW:33:ALA:N	48:BW:64:ASP:OD1	2.52	0.40
1:AA:709:U:H2'	1:AA:710:G:H8	1.87	0.40
2:AB:193:PRO:HB2	2:AB:194:ASP:H	1.61	0.40
10:AJ:12:ALA:HB2	10:AJ:96:VAL:HG22	2.03	0.40
12:AL:30:LYS:O	12:AL:82:ILE:HG22	2.21	0.40
13:AM:8:ASN:ND2	13:AM:21:SER:HB3	2.37	0.40
26:BA:533:G:H5'	42:BQ:24:TYR:CD1	2.56	0.40
26:BA:743:A:OP1	29:BD:135:GLY:HA2	2.22	0.40
26:BA:746:U:O2'	26:BA:2611:C:O2'	2.32	0.40
26:BA:2799:A:O2'	26:BA:2800:A:H5''	2.22	0.40
38:BM:42:THR:HG22	38:BM:93:VAL:HG12	2.04	0.40
39:BN:69:ARG:C	39:BN:71:ARG:H	2.23	0.40
40:BO:92:PHE:HB2	40:BO:117:PHE:CD1	2.57	0.40
43:BR:49:ILE:HB	43:BR:51:VAL:O	2.22	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	216/240 (90%)	190 (88%)	19 (9%)	7 (3%)	3	24
3	AC	204/233 (88%)	180 (88%)	20 (10%)	4 (2%)	6	32
4	AD	203/206 (98%)	188 (93%)	8 (4%)	7 (3%)	3	23
5	AE	148/167 (89%)	124 (84%)	17 (12%)	7 (5%)	2	17
6	AF	98/135 (73%)	85 (87%)	8 (8%)	5 (5%)	1	15
7	AG	149/179 (83%)	140 (94%)	8 (5%)	1 (1%)	18	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	AH	127/130 (98%)	116 (91%)	10 (8%)	1 (1%)	16	49
9	AI	125/130 (96%)	113 (90%)	6 (5%)	6 (5%)	2	16
10	AJ	96/103 (93%)	82 (85%)	8 (8%)	6 (6%)	1	12
11	AK	115/129 (89%)	99 (86%)	13 (11%)	3 (3%)	4	27
12	AL	121/124 (98%)	108 (89%)	6 (5%)	7 (6%)	1	13
13	AM	112/118 (95%)	104 (93%)	7 (6%)	1 (1%)	14	46
14	AN	92/101 (91%)	79 (86%)	8 (9%)	5 (5%)	1	14
15	AO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
16	AP	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	4	28
17	AQ	78/84 (93%)	64 (82%)	11 (14%)	3 (4%)	2	21
18	AR	53/75 (71%)	51 (96%)	2 (4%)	0	100	100
19	AS	77/92 (84%)	71 (92%)	5 (6%)	1 (1%)	9	39
20	AT	83/87 (95%)	76 (92%)	4 (5%)	3 (4%)	2	22
21	AU	49/71 (69%)	36 (74%)	8 (16%)	5 (10%)	0	5
28	BC	269/273 (98%)	247 (92%)	16 (6%)	6 (2%)	5	30
29	BD	207/209 (99%)	190 (92%)	15 (7%)	2 (1%)	12	45
30	BE	199/201 (99%)	188 (94%)	9 (4%)	2 (1%)	12	45
31	BF	175/179 (98%)	154 (88%)	16 (9%)	5 (3%)	3	26
32	BG	174/177 (98%)	161 (92%)	10 (6%)	3 (2%)	7	35
33	BH	45/149 (30%)	37 (82%)	4 (9%)	4 (9%)	0	7
34	BI	139/142 (98%)	116 (84%)	15 (11%)	8 (6%)	1	13
35	BJ	140/142 (99%)	131 (94%)	8 (6%)	1 (1%)	18	51
36	BK	120/123 (98%)	106 (88%)	9 (8%)	5 (4%)	2	19
37	BL	141/144 (98%)	117 (83%)	16 (11%)	8 (6%)	1	13
38	BM	134/136 (98%)	124 (92%)	7 (5%)	3 (2%)	5	30
39	BN	118/127 (93%)	104 (88%)	9 (8%)	5 (4%)	2	19
40	BO	114/117 (97%)	104 (91%)	7 (6%)	3 (3%)	4	27
41	BP	112/115 (97%)	105 (94%)	5 (4%)	2 (2%)	6	34
42	BQ	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
43	BR	101/103 (98%)	91 (90%)	6 (6%)	4 (4%)	2	20
44	BS	108/110 (98%)	97 (90%)	9 (8%)	2 (2%)	6	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BT	91/100 (91%)	80 (88%)	9 (10%)	2 (2%)	5	30
46	BU	100/104 (96%)	82 (82%)	13 (13%)	5 (5%)	1	16
47	BV	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
48	BW	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
49	BX	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
50	BY	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
51	BZ	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	6	34
52	B0	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
53	B1	48/55 (87%)	45 (94%)	2 (4%)	1 (2%)	5	31
54	B2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	5	30
55	B3	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
56	B4	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
57	B5	7/9 (78%)	3 (43%)	3 (43%)	1 (14%)	0	3
All	All	5522/5993 (92%)	4968 (90%)	406 (7%)	148 (3%)	6	27

All (148) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AE	105	ILE
9	AI	55	VAL
11	AK	127	ARG
12	AL	23	ALA
17	AQ	17	MET
17	AQ	51	ASN
21	AU	40	LYS
29	BD	152	PRO
33	BH	3	VAL
33	BH	9	VAL
33	BH	10	ALA
34	BI	93	PRO
37	BL	94	THR
57	B5	-7	VAL
2	AB	193	PRO
4	AD	28	ILE
4	AD	30	THR
5	AE	12	GLN
5	AE	158	GLY

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Mol	Chain	Res	Type
9	AI	13	LYS
9	AI	58	VAL
9	AI	91	ASP
9	AI	129	LYS
10	AJ	57	VAL
10	AJ	101	SER
11	AK	89	PRO
12	AL	34	CYS
12	AL	43	LYS
14	AN	22	ALA
14	AN	52	PRO
14	AN	92	GLU
21	AU	9	ASN
21	AU	24	GLU
31	BF	133	ARG
32	BG	175	LYS
34	BI	13	VAL
34	BI	65	ARG
36	BK	108	ARG
37	BL	29	LYS
37	BL	111	ILE
39	BN	70	THR
39	BN	106	ASP
40	BO	57	ALA
45	BT	77	ARG
46	BU	7	ARG
46	BU	17	LYS
46	BU	76	ALA
2	AB	34	ALA
2	AB	68	LEU
2	AB	82	ASP
3	AC	166	GLU
3	AC	206	GLU
4	AD	175	ALA
5	AE	24	THR
5	AE	101	GLU
6	AF	54	LEU
6	AF	86	ARG
6	AF	94	HIS
7	AG	114	LYS
8	AH	88	ARG
9	AI	9	THR

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Mol	Chain	Res	Type
12	AL	24	LEU
12	AL	76	GLU
12	AL	78	SER
13	AM	114	LYS
14	AN	3	LYS
14	AN	21	PHE
16	AP	43	ALA
16	AP	47	GLU
19	AS	5	LEU
20	AT	41	ALA
21	AU	35	ARG
21	AU	38	TYR
28	BC	240	PHE
32	BG	45	HIS
32	BG	46	ALA
34	BI	88	SER
35	BJ	82	GLY
37	BL	30	THR
37	BL	82	LEU
39	BN	3	HIS
41	BP	36	SER
44	BS	12	SER
51	BZ	4	THR
54	B2	45	SER
2	AB	19	GLN
4	AD	165	ARG
4	AD	192	SER
5	AE	122	ASN
6	AF	63	ASN
10	AJ	95	GLY
12	AL	17	ALA
17	AQ	76	VAL
20	AT	42	GLY
20	AT	68	HIS
28	BC	30	PHE
28	BC	152	GLY
28	BC	253	LYS
29	BD	41	ALA
31	BF	9	LYS
34	BI	31	GLN
36	BK	93	GLN
36	BK	110	GLU

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Mol	Chain	Res	Type
37	BL	70	LYS
38	BM	70	ASP
40	BO	100	HIS
41	BP	94	LYS
43	BR	43	ASN
43	BR	53	PHE
46	BU	55	PRO
46	BU	99	ASN
53	B1	51	GLU
2	AB	75	ALA
6	AF	92	THR
10	AJ	36	VAL
28	BC	205	LEU
28	BC	236	GLU
30	BE	80	SER
30	BE	83	VAL
33	BH	41	LYS
34	BI	21	SER
36	BK	119	ALA
37	BL	100	ILE
38	BM	69	PRO
39	BN	2	ARG
39	BN	118	ARG
40	BO	66	GLY
2	AB	86	SER
4	AD	25	VAL
4	AD	167	LYS
31	BF	175	PHE
31	BF	177	PHE
36	BK	35	VAL
37	BL	4	ASN
38	BM	24	THR
43	BR	7	SER
45	BT	88	LYS
10	AJ	42	LEU
43	BR	58	VAL
44	BS	29	VAL
3	AC	66	VAL
3	AC	81	GLY
10	AJ	41	PRO
5	AE	143	GLY
11	AK	92	GLY

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Mol	Chain	Res	Type
31	BF	149	VAL
34	BI	85	GLY
34	BI	89	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/198 (91%)	180 (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	113/126 (90%)	113 (100%)	0	100	100
6	AF	87/116 (75%)	87 (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
10	AJ	86/90 (96%)	86 (100%)	0	100	100
11	AK	90/99 (91%)	90 (100%)	0	100	100
12	AL	103/104 (99%)	103 (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	75/77 (97%)	75 (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	70/79 (89%)	70 (100%)	0	100	100
20	AT	65/66 (98%)	65 (100%)	0	100	100
21	AU	44/61 (72%)	44 (100%)	0	100	100
28	BC	216/218 (99%)	216 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	BD	164/164 (100%)	164 (100%)	0	100	100
30	BE	165/165 (100%)	165 (100%)	0	100	100
31	BF	148/150 (99%)	148 (100%)	0	100	100
32	BG	137/138 (99%)	137 (100%)	0	100	100
33	BH	38/114 (33%)	38 (100%)	0	100	100
34	BI	109/110 (99%)	109 (100%)	0	100	100
35	BJ	116/116 (100%)	116 (100%)	0	100	100
36	BK	103/104 (99%)	103 (100%)	0	100	100
37	BL	102/103 (99%)	102 (100%)	0	100	100
38	BM	109/109 (100%)	109 (100%)	0	100	100
39	BN	100/103 (97%)	100 (100%)	0	100	100
40	BO	86/87 (99%)	86 (100%)	0	100	100
41	BP	99/100 (99%)	99 (100%)	0	100	100
42	BQ	89/90 (99%)	89 (100%)	0	100	100
43	BR	84/84 (100%)	84 (100%)	0	100	100
44	BS	93/93 (100%)	93 (100%)	0	100	100
45	BT	80/84 (95%)	80 (100%)	0	100	100
46	BU	83/85 (98%)	83 (100%)	0	100	100
47	BV	78/78 (100%)	78 (100%)	0	100	100
48	BW	56/63 (89%)	56 (100%)	0	100	100
49	BX	67/68 (98%)	67 (100%)	0	100	100
50	BY	55/55 (100%)	55 (100%)	0	100	100
51	BZ	48/49 (98%)	48 (100%)	0	100	100
52	B0	47/48 (98%)	47 (100%)	0	100	100
53	B1	45/49 (92%)	45 (100%)	0	100	100
54	B2	38/38 (100%)	38 (100%)	0	100	100
55	B3	51/52 (98%)	51 (100%)	0	100	100
56	B4	34/34 (100%)	34 (100%)	0	100	100
57	B5	8/8 (100%)	8 (100%)	0	100	100
All	All	4594/4885 (94%)	4594 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	15	HIS
3	AC	8	ASN
3	AC	102	ASN
4	AD	41	HIS
4	AD	74	ASN
4	AD	120	HIS
4	AD	152	GLN
4	AD	196	ASN
5	AE	73	ASN
5	AE	89	HIS
6	AF	3	HIS
6	AF	37	HIS
6	AF	55	HIS
6	AF	63	ASN
7	AG	28	ASN
7	AG	86	GLN
7	AG	148	ASN
8	AH	4	GLN
8	AH	76	GLN
10	AJ	58	ASN
11	AK	118	HIS
11	AK	119	ASN
12	AL	5	ASN
12	AL	77	HIS
13	AM	100	GLN
14	AN	49	GLN
15	AO	50	HIS
16	AP	63	GLN
17	AQ	31	HIS
19	AS	52	HIS
19	AS	57	HIS
19	AS	69	HIS
20	AT	20	HIS
20	AT	48	GLN
20	AT	75	HIS
28	BC	46	ASN
28	BC	90	ASN
28	BC	243	HIS
29	BD	150	GLN
30	BE	41	GLN
30	BE	92	HIS

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Mol	Chain	Res	Type
30	BE	163	ASN
30	BE	195	GLN
31	BF	63	GLN
32	BG	22	GLN
32	BG	116	GLN
32	BG	143	GLN
33	BH	43	ASN
34	BI	12	GLN
34	BI	43	ASN
35	BJ	80	HIS
36	BK	93	GLN
37	BL	35	HIS
37	BL	54	GLN
38	BM	22	GLN
39	BN	9	GLN
39	BN	31	HIS
40	BO	29	HIS
42	BQ	20	GLN
42	BQ	37	GLN
43	BR	11	GLN
43	BR	86	GLN
44	BS	7	HIS
44	BS	9	HIS
46	BU	66	GLN
46	BU	74	ASN
47	BV	49	ASN
47	BV	51	GLN
50	BY	25	GLN
51	BZ	20	HIS
53	B1	19	HIS
54	B2	13	ASN
55	B3	24	HIS
56	B4	13	ASN
56	B4	37	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	218 (14%)	4 (0%)
22	AV	9/10 (90%)	0	0
23	AW	72/74 (97%)	15 (20%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	AX	76/77 (98%)	6 (7%)	0
25	AY	69/71 (97%)	13 (18%)	1 (1%)
26	BA	2895/2897 (99%)	425 (14%)	10 (0%)
27	BB	117/120 (97%)	13 (11%)	0
All	All	4775/4788 (99%)	690 (14%)	16 (0%)

All (690) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	7	A
1	AA	8	A
1	AA	9	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	51	A
1	AA	70	U
1	AA	74	A
1	AA	81	A
1	AA	83	C
1	AA	85	U
1	AA	87	C
1	AA	88	U
1	AA	95	C
1	AA	97	G
1	AA	108	G
1	AA	116	A
1	AA	120	A
1	AA	121	U
1	AA	130	A
1	AA	131	A
1	AA	149	A
1	AA	182	A
1	AA	204	G
1	AA	207	C
1	AA	208	U
1	AA	210	C
1	AA	211	G
1	AA	212	G
1	AA	247	G

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Mol	Chain	Res	Type
1	AA	251	G
1	AA	266	G
1	AA	267	C
1	AA	279	A
1	AA	280	C
1	AA	289	G
1	AA	298	A
1	AA	321	A
1	AA	328	C
1	AA	329	A
1	AA	330	C
1	AA	332	G
1	AA	347	G
1	AA	352	C
1	AA	354	G
1	AA	356	A
1	AA	367	U
1	AA	372	C
1	AA	378	G
1	AA	397	A
1	AA	406	G
1	AA	409	U
1	AA	411	A
1	AA	412	A
1	AA	413	G
1	AA	421	U
1	AA	422	C
1	AA	424	G
1	AA	429	U
1	AA	436	C
1	AA	437	U
1	AA	451	A
1	AA	452	A
1	AA	459	A
1	AA	467	U
1	AA	468	A
1	AA	478	A
1	AA	479	U
1	AA	482	A
1	AA	485	U
1	AA	486	U
1	AA	496	A

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Mol	Chain	Res	Type
1	AA	497	G
1	AA	509	A
1	AA	511	C
1	AA	518	C
1	AA	527	G
1	AA	532	A
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	568	G
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	596	A
1	AA	633	G
1	AA	642	A
1	AA	650	G
1	AA	665	A
1	AA	675	A
1	AA	687	A
1	AA	702	A
1	AA	703	G
1	AA	721	G
1	AA	723	U
1	AA	731	G
1	AA	747	A
1	AA	755	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	814	A
1	AA	815	A
1	AA	817	C
1	AA	821	G
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	844	G

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Mol	Chain	Res	Type
1	AA	845	A
1	AA	846	G
1	AA	873	A
1	AA	885	G
1	AA	914	A
1	AA	934	C
1	AA	935	A
1	AA	960	U
1	AA	969	A
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	983	A
1	AA	993	G
1	AA	1004	A
1	AA	1008	U
1	AA	1026	G
1	AA	1027	C
1	AA	1030	U
1	AA	1031	C
1	AA	1032	G
1	AA	1033	G
1	AA	1034	G
1	AA	1036	A
1	AA	1043	G
1	AA	1044	A
1	AA	1050	G
1	AA	1054	C
1	AA	1065	U
1	AA	1073	U
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1104	G
1	AA	1125	U
1	AA	1133	G
1	AA	1134	G
1	AA	1136	C
1	AA	1137	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C

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Mol	Chain	Res	Type
1	AA	1142	G
1	AA	1145	A
1	AA	1146	A
1	AA	1157	A
1	AA	1159	U
1	AA	1160	G
1	AA	1161	C
1	AA	1196	A
1	AA	1197	A
1	AA	1201	A
1	AA	1202	U
1	AA	1212	U
1	AA	1213	A
1	AA	1236	A
1	AA	1238	A
1	AA	1240	U
1	AA	1241	G
1	AA	1253	G
1	AA	1256	A
1	AA	1257	A
1	AA	1261	A
1	AA	1275	A
1	AA	1280	A
1	AA	1285	A
1	AA	1286	U
1	AA	1287	A
1	AA	1299	A
1	AA	1300	G
1	AA	1305	G
1	AA	1317	C
1	AA	1318	A
1	AA	1322	C
1	AA	1337	G
1	AA	1346	A
1	AA	1347	G
1	AA	1363	A
1	AA	1364	U
1	AA	1377	A
1	AA	1379	G
1	AA	1394	A
1	AA	1398	A
1	AA	1413	A

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Mol	Chain	Res	Type
1	AA	1429	A
1	AA	1441	A
1	AA	1446	A
1	AA	1452	C
1	AA	1492	A
1	AA	1494	G
1	AA	1497	G
1	AA	1499	A
1	AA	1503	A
1	AA	1505	G
1	AA	1507	A
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1533	C
1	AA	1535	C
1	AA	1536	C
23	AW	8	4SU
23	AW	14	A
23	AW	19	G
23	AW	20	U
23	AW	21	A
23	AW	34	U8U
23	AW	45	G
23	AW	46	7MG
23	AW	47	3AU
23	AW	48	C
23	AW	49	G
23	AW	59	A
23	AW	61	C
23	AW	68	G
23	AW	74	C
24	AX	19	U
24	AX	21	A
24	AX	47	U
24	AX	67	C
24	AX	68	G
24	AX	76	A
25	AY	5	G
25	AY	14	A
25	AY	19	G
25	AY	20	G

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Mol	Chain	Res	Type
25	AY	21	A
25	AY	23	A
25	AY	45	G
25	AY	46	7MG
25	AY	47	U
25	AY	48	C
25	AY	54	5MU
25	AY	59	U
25	AY	60	C
26	BA	10	A
26	BA	14	A
26	BA	34	U
26	BA	42	A
26	BA	46	G
26	BA	63	A
26	BA	71	A
26	BA	74	A
26	BA	75	G
26	BA	80	G
26	BA	83	A
26	BA	84	A
26	BA	98	G
26	BA	101	A
26	BA	118	A
26	BA	119	A
26	BA	120	U
26	BA	138	U
26	BA	139	U
26	BA	140	C
26	BA	141	G
26	BA	142	A
26	BA	162	U
26	BA	165	A
26	BA	181	A
26	BA	196	A
26	BA	199	A
26	BA	216	A
26	BA	222	A
26	BA	223	A
26	BA	233	A
26	BA	248	G
26	BA	249	C

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Mol	Chain	Res	Type
26	BA	255	A
26	BA	265	A
26	BA	266	G
26	BA	271	G
26	BA	272	A
26	BA	276	U
26	BA	278	A
26	BA	279	A
26	BA	285	G
26	BA	294	A
26	BA	311	A
26	BA	321	U
26	BA	322	A
26	BA	324	A
26	BA	329	G
26	BA	330	A
26	BA	361	G
26	BA	367	G
26	BA	371	A
26	BA	372	G
26	BA	386	G
26	BA	396	G
26	BA	404	A
26	BA	405	U
26	BA	411	G
26	BA	412	A
26	BA	424	G
26	BA	451	U
26	BA	455	C
26	BA	457	A
26	BA	467	G
26	BA	479	A
26	BA	480	A
26	BA	481	G
26	BA	490	C
26	BA	491	G
26	BA	504	A
26	BA	505	A
26	BA	508	A
26	BA	528	A
26	BA	531	C
26	BA	532	A

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Mol	Chain	Res	Type
26	BA	533	G
26	BA	543	G
26	BA	544	C
26	BA	546	U
26	BA	547	A
26	BA	548	G
26	BA	549	G
26	BA	563	A
26	BA	572	A
26	BA	573	U
26	BA	574	A
26	BA	575	A
26	BA	586	A
26	BA	603	A
26	BA	613	A
26	BA	627	A
26	BA	631	A
26	BA	637	A
26	BA	647	G
26	BA	654	A
26	BA	685	A
26	BA	686	U
26	BA	695	G
26	BA	717	C
26	BA	727	A
26	BA	730	A
26	BA	747	U
26	BA	751	A
26	BA	764	A
26	BA	775	G
26	BA	776	G
26	BA	781	A
26	BA	782	A
26	BA	784	G
26	BA	785	G
26	BA	789	A
26	BA	792	A
26	BA	802	A
26	BA	805	G
26	BA	812	C
26	BA	819	A
26	BA	827	U

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Mol	Chain	Res	Type
26	BA	828	U
26	BA	830	G
26	BA	844	A
26	BA	845	A
26	BA	846	U
26	BA	858	G
26	BA	878	A
26	BA	896	A
26	BA	897	C
26	BA	910	A
26	BA	914	G
26	BA	915	C
26	BA	941	A
26	BA	946	C
26	BA	953	G
26	BA	959	A
26	BA	961	C
26	BA	974	G
26	BA	983	A
26	BA	995	C
26	BA	996	A
26	BA	1009	A
26	BA	1012	U
26	BA	1013	C
26	BA	1021	A
26	BA	1022	G
26	BA	1026	G
26	BA	1033	U
26	BA	1040	A
26	BA	1046	A
26	BA	1047	G
26	BA	1060	U
26	BA	1061	U
26	BA	1065	U
26	BA	1066	U
26	BA	1068	G
26	BA	1070	A
26	BA	1071	G
26	BA	1072	C
26	BA	1077	A
26	BA	1088	A
26	BA	1089	A

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Mol	Chain	Res	Type
26	BA	1090	A
26	BA	1092	C
26	BA	1094	U
26	BA	1098	A
26	BA	1111	A
26	BA	1112	G
26	BA	1132	U
26	BA	1133	A
26	BA	1135	C
26	BA	1136	G
26	BA	1143	A
26	BA	1151	A
26	BA	1175	A
26	BA	1176	U
26	BA	1178	C
26	BA	1180	U
26	BA	1186	G
26	BA	1195	G
26	BA	1204	A
26	BA	1206	G
26	BA	1212	G
26	BA	1238	G
26	BA	1250	G
26	BA	1253	A
26	BA	1256	G
26	BA	1266	G
26	BA	1271	G
26	BA	1272	A
26	BA	1300	G
26	BA	1301	A
26	BA	1302	A
26	BA	1314	C
26	BA	1355	G
26	BA	1365	A
26	BA	1368	G
26	BA	1378	A
26	BA	1379	U
26	BA	1383	A
26	BA	1384	A
26	BA	1386	C
26	BA	1387	A
26	BA	1391	U

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Mol	Chain	Res	Type
26	BA	1395	A
26	BA	1403	A
26	BA	1416	G
26	BA	1419	A
26	BA	1420	A
26	BA	1428	C
26	BA	1452	G
26	BA	1458	U
26	BA	1478	G
26	BA	1482	G
26	BA	1493	C
26	BA	1494	A
26	BA	1504	A
26	BA	1509	A
26	BA	1510	G
26	BA	1515	A
26	BA	1533	C
26	BA	1535	A
26	BA	1536	C
26	BA	1537	G
26	BA	1560	G
26	BA	1566	A
26	BA	1569	A
26	BA	1578	U
26	BA	1581	G
26	BA	1583	A
26	BA	1584	U
26	BA	1585	C
26	BA	1607	C
26	BA	1610	A
26	BA	1616	A
26	BA	1646	C
26	BA	1647	U
26	BA	1648	U
26	BA	1652	A
26	BA	1664	A
26	BA	1674	G
26	BA	1694	C
26	BA	1715	G
26	BA	1729	U
26	BA	1730	C
26	BA	1732	C

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Mol	Chain	Res	Type
26	BA	1738	G
26	BA	1757	A
26	BA	1758	U
26	BA	1764	C
26	BA	1773	A
26	BA	1784	A
26	BA	1785	A
26	BA	1791	A
26	BA	1800	C
26	BA	1801	A
26	BA	1802	A
26	BA	1808	A
26	BA	1816	C
26	BA	1819	A
26	BA	1829	A
26	BA	1833	C
26	BA	1847	A
26	BA	1848	A
26	BA	1858	A
26	BA	1870	C
26	BA	1871	A
26	BA	1872	A
26	BA	1873	G
26	BA	1876	A
26	BA	1906	G
26	BA	1913	A
26	BA	1914	C
26	BA	1919	A
26	BA	1927	A
26	BA	1929	G
26	BA	1930	G
26	BA	1937	A
26	BA	1955	U
26	BA	1967	C
26	BA	1970	A
26	BA	1972	G
26	BA	1991	U
26	BA	1993	U
26	BA	1997	C
26	BA	2020	A
26	BA	2022	U
26	BA	2023	C

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Mol	Chain	Res	Type
26	BA	2030	A
26	BA	2031	A
26	BA	2033	A
26	BA	2043	C
26	BA	2049	G
26	BA	2055	C
26	BA	2056	G
26	BA	2060	A
26	BA	2061	G
26	BA	2062	A
26	BA	2069	G
26	BA	2072	C
26	BA	2080	A
26	BA	2092	U
26	BA	2093	G
26	BA	2095	A
26	BA	2097	A
26	BA	2110	G
26	BA	2111	U
26	BA	2112	G
26	BA	2114	A
26	BA	2116	G
26	BA	2117	A
26	BA	2118	U
26	BA	2119	A
26	BA	2126	A
26	BA	2127	G
26	BA	2128	G
26	BA	2131	U
26	BA	2132	U
26	BA	2133	G
26	BA	2135	A
26	BA	2147	A
26	BA	2158	A
26	BA	2162	G
26	BA	2163	A
26	BA	2164	C
26	BA	2169	A
26	BA	2170	A
26	BA	2171	A
26	BA	2172	U
26	BA	2173	A

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Mol	Chain	Res	Type
26	BA	2189	U
26	BA	2190	G
26	BA	2194	U
26	BA	2198	A
26	BA	2199	A
26	BA	2204	G
26	BA	2211	A
26	BA	2212	A
26	BA	2214	C
26	BA	2225	A
26	BA	2226	C
26	BA	2238	G
26	BA	2239	G
26	BA	2243	U
26	BA	2246	G
26	BA	2278	A
26	BA	2280	G
26	BA	2283	C
26	BA	2287	A
26	BA	2288	A
26	BA	2297	A
26	BA	2305	U
26	BA	2309	A
26	BA	2311	A
26	BA	2312	U
26	BA	2322	A
26	BA	2333	A
26	BA	2345	G
26	BA	2347	C
26	BA	2350	C
26	BA	2361	G
26	BA	2383	G
26	BA	2385	C
26	BA	2402	U
26	BA	2406	A
26	BA	2407	A
26	BA	2423	U
26	BA	2425	A
26	BA	2426	A
26	BA	2429	G
26	BA	2430	A
26	BA	2431	U

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Mol	Chain	Res	Type
26	BA	2435	A
26	BA	2441	U
26	BA	2448	A
26	BA	2476	A
26	BA	2491	U
26	BA	2498	C
26	BA	2502	G
26	BA	2503	A
26	BA	2505	G
26	BA	2506	U
26	BA	2507	C
26	BA	2513	A
26	BA	2518	A
26	BA	2529	G
26	BA	2547	A
26	BA	2550	G
26	BA	2554	U
26	BA	2566	A
26	BA	2567	G
26	BA	2572	A
26	BA	2573	C
26	BA	2602	A
26	BA	2609	U
26	BA	2613	U
26	BA	2615	U
26	BA	2629	U
26	BA	2630	G
26	BA	2636	C
26	BA	2689	U
26	BA	2690	U
26	BA	2714	G
26	BA	2716	C
26	BA	2718	G
26	BA	2726	A
26	BA	2729	G
26	BA	2733	A
26	BA	2744	G
26	BA	2748	A
26	BA	2757	A
26	BA	2765	A
26	BA	2778	A
26	BA	2782	G

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Mol	Chain	Res	Type
26	BA	2791	G
26	BA	2809	A
26	BA	2818	U
26	BA	2820	A
26	BA	2823	A
26	BA	2836	U
26	BA	2867	G
26	BA	2872	A
26	BA	2873	A
26	BA	2879	A
26	BA	2880	C
26	BA	2886	A
26	BA	2887	A
26	BA	2903	U
27	BB	15	A
27	BB	24	G
27	BB	41	G
27	BB	44	G
27	BB	53	A
27	BB	56	G
27	BB	66	A
27	BB	73	A
27	BB	88	C
27	BB	89	U
27	BB	90	C
27	BB	99	A
27	BB	109	A

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	96	U
1	AA	115	G
1	AA	1201	A
1	AA	1211	U
23	AW	13	C
25	AY	58	A
26	BA	271	G
26	BA	404	A
26	BA	479	A
26	BA	1606	C
26	BA	1913	A

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Mol	Chain	Res	Type
26	BA	2109	U
26	BA	2146	C
26	BA	2225	A
26	BA	2506	U
26	BA	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PSU	AW	55	23	18,21,22	1.30	3 (16%)	22,30,33	1.63	4 (18%)
25	4SU	AY	8	25	18,21,22	1.08	2 (11%)	26,30,33	0.83	2 (7%)
24	5MU	AX	54	24	19,22,23	0.92	2 (10%)	28,32,35	1.13	2 (7%)
24	7MG	AX	46	24	22,26,27	2.05	3 (13%)	29,39,42	1.22	4 (13%)
24	2MA	AX	37	24	22,25,26	2.13	4 (18%)	33,37,40	1.59	4 (12%)
24	QUO	AX	34	24,22	31,35,36	1.12	4 (12%)	39,52,55	1.46	6 (15%)
23	4SU	AW	8	23	18,21,22	1.08	2 (11%)	26,30,33	0.82	2 (7%)
24	PSU	AX	55	24	18,21,22	1.30	3 (16%)	22,30,33	1.61	4 (18%)
25	5MU	AY	54	25	19,22,23	0.94	2 (10%)	28,32,35	1.14	2 (7%)
25	6MZ	AY	37	25	22,25,26	1.66	5 (22%)	30,36,39	1.25	3 (10%)
24	PSU	AX	65	24	18,21,22	1.26	3 (16%)	22,30,33	1.55	5 (22%)
23	3AU	AW	47	23	25,28,29	1.08	1 (4%)	32,40,43	0.93	2 (6%)
23	U8U	AW	34	22,23	19,24,25	0.88	1 (5%)	23,34,37	1.23	4 (17%)
23	7MG	AW	46	23	22,26,27	2.01	3 (13%)	29,39,42	1.22	4 (13%)
25	PSU	AY	55	25	18,21,22	1.29	3 (16%)	22,30,33	1.62	4 (18%)
23	T6A	AW	37	23	31,34,35	1.23	4 (12%)	44,49,52	1.21	2 (4%)
25	7MG	AY	46	25	22,26,27	2.05	3 (13%)	29,39,42	1.22	4 (13%)
23	PSU	AW	39	23	18,21,22	1.30	3 (16%)	22,30,33	1.62	4 (18%)
25	CM0	AY	34	25	22,26,27	0.96	1 (4%)	28,37,40	1.27	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	5MU	AW	54	23	19,22,23	0.92	2 (10%)	28,32,35	1.13	2 (7%)
24	4SU	AX	8	24	18,21,22	1.09	2 (11%)	26,30,33	0.82	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
25	4SU	AY	8	25	-	0/7/25/26	0/2/2/2
24	5MU	AX	54	24	-	0/7/25/26	0/2/2/2
24	7MG	AX	46	24	-	0/7/37/38	0/3/3/3
24	2MA	AX	37	24	-	0/7/25/26	0/3/3/3
24	QUO	AX	34	24,22	-	3/12/43/44	0/4/4/4
23	4SU	AW	8	23	-	0/7/25/26	0/2/2/2
24	PSU	AX	55	24	-	0/7/25/26	0/2/2/2
25	5MU	AY	54	25	-	2/7/25/26	0/2/2/2
25	6MZ	AY	37	25	-	1/9/27/28	0/3/3/3
24	PSU	AX	65	24	-	4/7/25/26	0/2/2/2
23	3AU	AW	47	23	-	6/16/34/35	0/2/2/2
23	U8U	AW	34	22,23	-	2/9/28/29	0/2/2/2
23	7MG	AW	46	23	-	3/7/37/38	0/3/3/3
25	PSU	AY	55	25	-	0/7/25/26	0/2/2/2
23	T6A	AW	37	23	-	0/23/41/42	0/3/3/3
25	7MG	AY	46	25	-	2/7/37/38	0/3/3/3
23	PSU	AW	39	23	-	0/7/25/26	0/2/2/2
25	CM0	AY	34	25	-	3/12/30/31	0/2/2/2
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/7/25/26	0/2/2/2

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	37	2MA	C6-N1	6.94	1.45	1.35
24	AX	46	7MG	C8-N9	6.25	1.49	1.46
25	AY	46	7MG	C8-N9	6.23	1.49	1.46
23	AW	46	7MG	C8-N9	6.03	1.49	1.46
25	AY	46	7MG	C5-N7	5.84	1.42	1.35
24	AX	46	7MG	C5-N7	5.74	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	46	7MG	C5-N7	5.70	1.42	1.35
25	AY	37	6MZ	C6-N6	4.38	1.38	1.34
24	AX	37	2MA	C4-N3	4.22	1.39	1.34
24	AX	37	2MA	C2-N1	3.80	1.40	1.34
23	AW	47	3AU	C2-N1	3.58	1.43	1.38
25	AY	37	6MZ	C5-C4	3.48	1.45	1.39
24	AX	55	PSU	C2-N1	3.46	1.41	1.36
23	AW	55	PSU	C2-N1	3.44	1.41	1.36
25	AY	55	PSU	C2-N1	3.43	1.41	1.36
23	AW	39	PSU	C2-N1	3.41	1.41	1.36
24	AX	8	4SU	C4-S4	-3.22	1.62	1.68
23	AW	8	4SU	C4-S4	-3.20	1.62	1.68
23	AW	37	T6A	C10-N6	3.19	1.44	1.37
25	AY	8	4SU	C4-S4	-3.16	1.62	1.68
24	AX	65	PSU	C2-N1	3.06	1.40	1.36
24	AX	65	PSU	C4-N3	2.69	1.43	1.38
24	AX	34	QUO	C6-N1	2.67	1.43	1.38
25	AY	54	5MU	C2-N1	2.61	1.42	1.38
23	AW	55	PSU	C4-N3	2.60	1.43	1.38
23	AW	39	PSU	C4-N3	2.58	1.43	1.38
25	AY	55	PSU	C4-N3	2.54	1.43	1.38
24	AX	55	PSU	C4-N3	2.54	1.43	1.38
24	AX	46	7MG	C6-N1	2.54	1.43	1.38
23	AW	37	T6A	C8-N9	2.49	1.41	1.37
25	AY	46	7MG	C6-N1	2.49	1.43	1.38
23	AW	46	7MG	C6-N1	2.47	1.43	1.38
23	AW	34	U8U	C4-N3	2.47	1.43	1.38
23	AW	54	5MU	C2-N1	2.44	1.42	1.38
24	AX	54	5MU	C2-N1	2.43	1.42	1.38
24	AX	34	QUO	C4-N3	2.40	1.40	1.34
25	AY	37	6MZ	C8-N7	2.39	1.36	1.31
24	AX	37	2MA	C8-N7	2.37	1.36	1.31
25	AY	34	CM0	C4-N3	2.36	1.43	1.38
25	AY	8	4SU	C2-N3	2.32	1.42	1.38
25	AY	37	6MZ	C2-N1	2.31	1.38	1.33
24	AX	55	PSU	C6-N1	2.29	1.40	1.36
24	AX	8	4SU	C2-N3	2.29	1.42	1.38
23	AW	55	PSU	C6-N1	2.28	1.40	1.36
23	AW	37	T6A	C12-C13	2.28	1.56	1.52
23	AW	8	4SU	C2-N3	2.25	1.42	1.38
23	AW	39	PSU	C6-N1	2.24	1.39	1.36
24	AX	34	QUO	C2-N2	2.23	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	54	5MU	C2-N3	2.22	1.41	1.38
23	AW	54	5MU	C2-N3	2.22	1.41	1.38
25	AY	54	5MU	C2-N3	2.20	1.41	1.38
25	AY	55	PSU	C6-N1	2.20	1.39	1.36
25	AY	37	6MZ	C5-N7	2.16	1.43	1.39
24	AX	65	PSU	C6-N1	2.13	1.39	1.36
24	AX	34	QUO	C13-C12	2.08	1.55	1.53
23	AW	37	T6A	C5-C4	2.05	1.42	1.39

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AX	37	2MA	N6-C6-N1	5.51	124.82	117.03
24	AX	34	QUO	C7-C5-C4	-5.10	106.75	112.66
23	AW	55	PSU	C6-C5-C4	5.07	121.74	118.20
24	AX	55	PSU	C6-C5-C4	4.99	121.69	118.20
23	AW	39	PSU	C6-C5-C4	4.96	121.67	118.20
25	AY	55	PSU	C6-C5-C4	4.94	121.65	118.20
24	AX	37	2MA	C5-C6-N1	-4.52	111.21	119.01
23	AW	37	T6A	C12-N11-C10	-4.44	114.53	121.94
24	AX	65	PSU	C6-C5-C4	4.18	121.12	118.20
25	AY	34	CM0	C7-O5-C5	-4.15	112.14	117.58
25	AY	37	6MZ	C4-N9-C8	3.98	110.04	105.73
23	AW	34	U8U	C1'-N1-C6	-3.35	115.55	121.12
24	AX	54	5MU	C4-N3-C2	-3.15	123.27	127.35
23	AW	54	5MU	C4-N3-C2	-3.12	123.31	127.35
25	AY	54	5MU	C4-N3-C2	-3.12	123.31	127.35
25	AY	54	5MU	C6-C5-C4	2.97	120.51	118.03
24	AX	37	2MA	C6-C5-C4	2.94	121.14	117.18
23	AW	54	5MU	C6-C5-C4	2.94	120.49	118.03
24	AX	54	5MU	C6-C5-C4	2.93	120.48	118.03
24	AX	34	QUO	C7-C8-N9	-2.90	108.22	111.06
24	AX	46	7MG	C5-C4-N9	2.85	110.04	106.35
25	AY	46	7MG	C5-C4-N9	2.83	110.02	106.35
23	AW	46	7MG	C5-C4-N9	2.78	109.96	106.35
24	AX	65	PSU	O2-C2-N1	-2.73	119.79	122.79
25	AY	55	PSU	O2-C2-N1	-2.72	119.79	122.79
24	AX	34	QUO	C10-N11-C12	-2.72	109.26	114.89
25	AY	8	4SU	C4-N3-C2	-2.71	124.71	127.34
25	AY	37	6MZ	C6-C5-N7	2.70	135.32	132.39
23	AW	39	PSU	O2-C2-N1	-2.70	119.82	122.79
25	AY	34	CM0	C4-N3-C2	-2.69	123.87	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AW	8	4SU	C4-N3-C2	-2.65	124.76	127.34
23	AW	55	PSU	O2-C2-N1	-2.65	119.87	122.79
24	AX	8	4SU	C4-N3-C2	-2.65	124.77	127.34
24	AX	55	PSU	O2-C2-N1	-2.62	119.90	122.79
24	AX	37	2MA	C2-N1-C6	2.58	122.11	118.08
25	AY	37	6MZ	N9-C8-N7	-2.57	110.39	113.91
23	AW	47	3AU	C1'-N1-C2	2.57	121.33	116.99
24	AX	34	QUO	C16-C12-C13	2.46	106.83	103.18
24	AX	34	QUO	O13-C13-C12	-2.44	106.39	112.92
24	AX	65	PSU	O4-C4-N3	-2.38	115.55	120.12
24	AX	46	7MG	C2-N1-C6	-2.34	120.84	125.10
23	AW	46	7MG	C2-N1-C6	-2.32	120.87	125.10
23	AW	46	7MG	C4-C5-N7	2.30	108.72	105.53
24	AX	46	7MG	O6-C6-N1	-2.28	115.75	120.12
23	AW	37	T6A	O14-C14-C12	2.28	113.70	109.13
25	AY	46	7MG	C2-N1-C6	-2.27	120.96	125.10
25	AY	46	7MG	C4-C5-N7	2.26	108.67	105.53
23	AW	46	7MG	O6-C6-N1	-2.24	115.82	120.12
24	AX	46	7MG	C4-C5-N7	2.24	108.64	105.53
25	AY	46	7MG	O6-C6-N1	-2.23	115.85	120.12
24	AX	65	PSU	O4-C4-C5	2.14	129.66	124.05
25	AY	8	4SU	C6-C5-C4	2.12	121.79	119.95
24	AX	34	QUO	C2-N1-C6	-2.11	121.26	125.10
23	AW	47	3AU	C4-N3-C2	-2.09	122.00	124.63
24	AX	8	4SU	C6-C5-C4	2.08	121.75	119.95
23	AW	34	U8U	C5-C6-N1	-2.06	120.14	122.91
23	AW	8	4SU	C6-C5-C4	2.06	121.73	119.95
23	AW	55	PSU	N1-C2-N3	2.05	117.45	115.13
25	AY	55	PSU	N1-C2-N3	2.05	117.45	115.13
23	AW	34	U8U	O4-C4-C5	2.04	128.00	124.96
23	AW	34	U8U	C6-C5-C4	2.04	122.36	118.46
23	AW	39	PSU	N1-C2-N3	2.04	117.44	115.13
24	AX	65	PSU	N1-C2-N3	2.03	117.43	115.13
25	AY	34	CM0	O4-C4-N3	-2.03	116.23	120.12
24	AX	55	PSU	O4-C4-N3	-2.02	116.24	120.12
23	AW	39	PSU	O4-C4-N3	-2.02	116.25	120.12
25	AY	55	PSU	O4-C4-N3	-2.01	116.26	120.12
24	AX	55	PSU	N1-C2-N3	2.01	117.41	115.13
23	AW	55	PSU	O4-C4-N3	-2.01	116.27	120.12

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	AW	34	U8U	C3'-C4'-C5'-O5'
23	AW	34	U8U	O4'-C4'-C5'-O5'
23	AW	46	7MG	C3'-C4'-C5'-O5'
23	AW	47	3AU	C10-C11-C12-N40
24	AX	34	QUO	C13-C12-N11-C10
24	AX	34	QUO	C16-C12-N11-C10
24	AX	65	PSU	C2'-C1'-C5-C4
24	AX	65	PSU	O4'-C1'-C5-C4
24	AX	65	PSU	O4'-C1'-C5-C6
25	AY	46	7MG	C4'-C5'-O5'-P
25	AY	46	7MG	C2'-C1'-N9-C8
25	AY	54	5MU	C3'-C4'-C5'-O5'
25	AY	54	5MU	O4'-C4'-C5'-O5'
25	AY	34	CM0	O5-C7-C8-O8
23	AW	46	7MG	O4'-C4'-C5'-O5'
23	AW	47	3AU	O4'-C4'-C5'-O5'
24	AX	65	PSU	C4'-C5'-O5'-P
23	AW	47	3AU	N40-C12-C13-O31
25	AY	34	CM0	O5-C7-C8-O9
23	AW	46	7MG	C4'-C5'-O5'-P
23	AW	47	3AU	C3'-C4'-C5'-O5'
23	AW	47	3AU	N40-C12-C13-O30
23	AW	47	3AU	C10-C11-C12-C13
24	AX	34	QUO	N11-C10-C7-C8
25	AY	37	6MZ	C3'-C4'-C5'-O5'
25	AY	34	CM0	C6-C5-O5-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	34	U8U	1	0
25	AY	55	PSU	1	0
25	AY	34	CM0	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
58	LYS	AW	101	23	7,8,9	0.81	0	3,8,10	0.76	0
59	ERY	BA	9000	-	53,53,53	1.16	5 (9%)	82,82,82	1.69	23 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	LYS	AW	101	23	-	1/6/7/9	-
59	ERY	BA	9000	-	-	13/72/107/107	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	BA	9000	ERY	O13-C12	-2.82	1.39	1.44
59	BA	9000	ERY	O9-C26	-2.77	1.39	1.44
59	BA	9000	ERY	O10-C6	-2.64	1.40	1.44
59	BA	9000	ERY	O2-C13	-2.53	1.42	1.46
59	BA	9000	ERY	C23-C24	2.09	1.58	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	BA	9000	ERY	C36-C13-C12	-3.91	107.79	115.20
59	BA	9000	ERY	C34-C10-C11	-3.82	109.62	114.38
59	BA	9000	ERY	C12-C11-C10	-3.39	112.18	116.43
59	BA	9000	ERY	O13-C12-C13	3.29	112.56	107.28
59	BA	9000	ERY	O2-C1-C2	3.26	118.70	111.56
59	BA	9000	ERY	C16-C15-C14	-3.12	109.66	115.07
59	BA	9000	ERY	C20-O5-C16	-3.02	111.25	117.55
59	BA	9000	ERY	O2-C1-O1	-2.86	118.60	123.94
59	BA	9000	ERY	C22-O9-C26	-2.83	108.42	112.91
59	BA	9000	ERY	C35-C12-C13	-2.58	107.67	111.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	BA	9000	ERY	O5-C16-C17	2.54	107.58	103.81
59	BA	9000	ERY	O6-C17-C16	-2.50	106.45	111.12
59	BA	9000	ERY	O3-C3-C2	2.43	115.37	111.14
59	BA	9000	ERY	C27-C26-C25	-2.42	109.60	113.40
59	BA	9000	ERY	C6-C5-C4	-2.37	110.70	114.05
59	BA	9000	ERY	C7-C6-C5	-2.37	105.86	110.48
59	BA	9000	ERY	C22-O7-C5	-2.31	112.25	116.25
59	BA	9000	ERY	O8-C23-C24	-2.30	105.67	109.77
59	BA	9000	ERY	O5-C16-C15	-2.15	109.51	112.96
59	BA	9000	ERY	O7-C22-O9	-2.09	104.82	110.67
59	BA	9000	ERY	O4-C18-C21	2.08	111.20	106.70
59	BA	9000	ERY	C15-C16-C17	2.07	111.38	107.67
59	BA	9000	ERY	C25-C24-N1	-2.02	109.96	115.67

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	AW	101	LYS	O-C-CA-CB
59	BA	9000	ERY	C34-C10-C11-C12
59	BA	9000	ERY	O13-C12-C13-O2
59	BA	9000	ERY	O13-C12-C13-C36
59	BA	9000	ERY	C35-C12-C13-O2
59	BA	9000	ERY	C35-C12-C13-C36
59	BA	9000	ERY	C11-C12-C13-O2
59	BA	9000	ERY	C11-C12-C13-C36
59	BA	9000	ERY	C34-C10-C11-O12
59	BA	9000	ERY	O2-C13-C36-C37
59	BA	9000	ERY	C9-C10-C11-O12
59	BA	9000	ERY	C9-C10-C11-C12
59	BA	9000	ERY	C25-C24-N1-C29
59	BA	9000	ERY	C12-C13-C36-C37

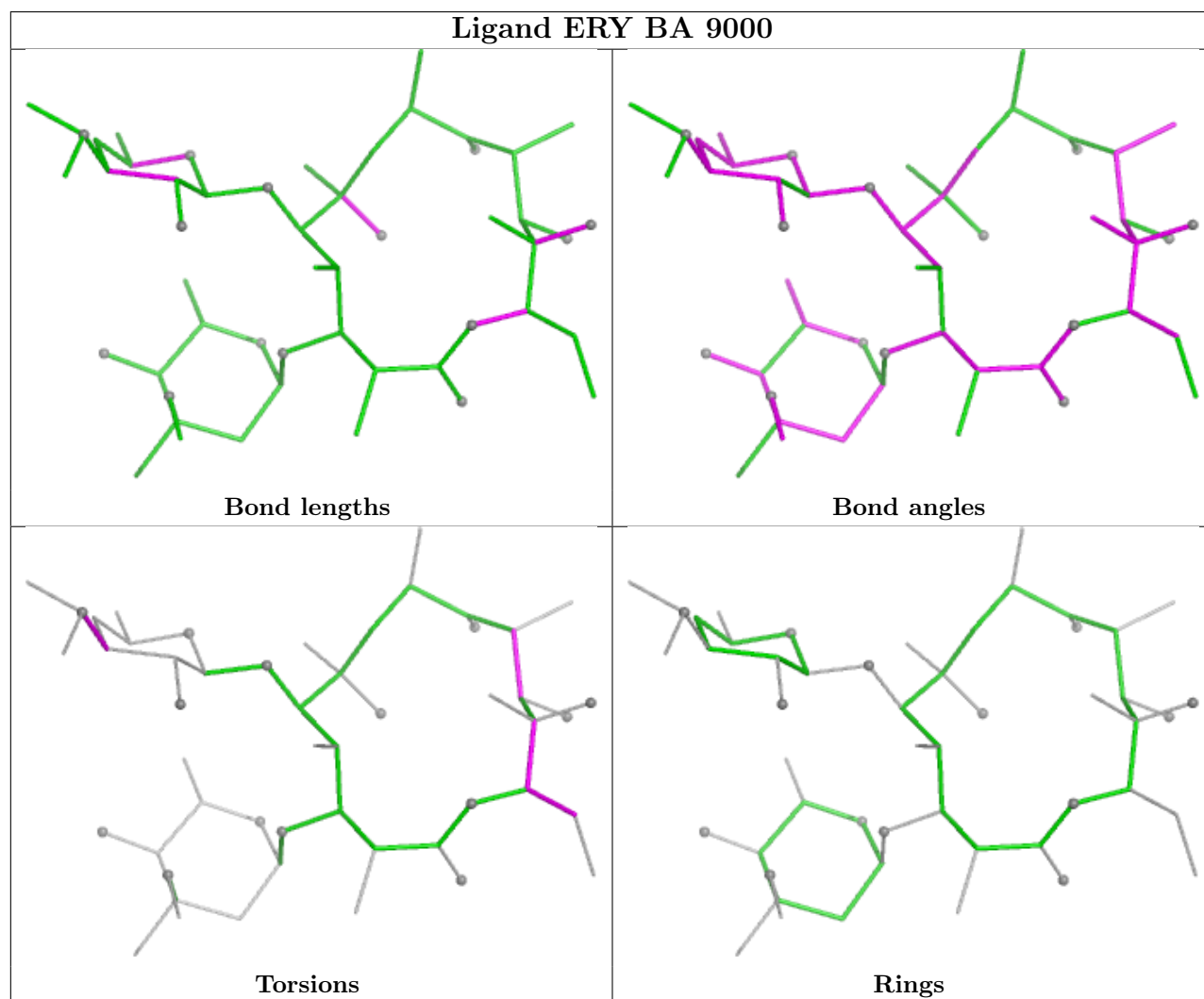
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	AW	101	LYS	2	0
59	BA	9000	ERY	12	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
26	BA	1
23	AW	1
25	AY	1
1	AA	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	13.72
1	AW	15:G	O3'	18:G	P	9.77
1	AY	15:G	O3'	18:G	P	6.82
1	AA	99:C	O3'	100:G	P	4.17

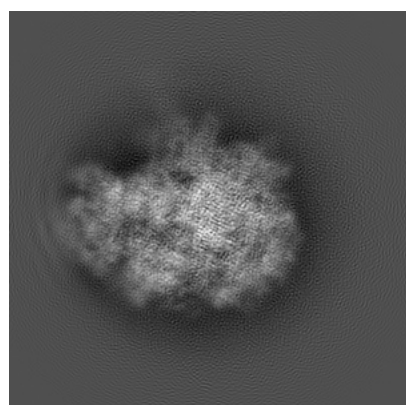
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8175. These allow visual inspection of the internal detail of the map and identification of artifacts.

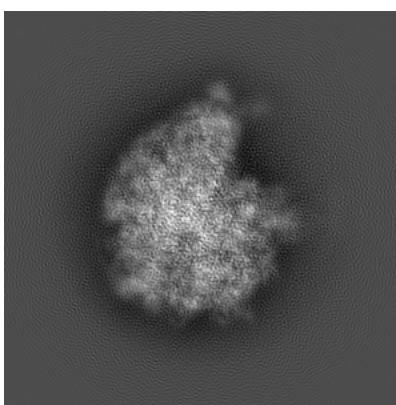
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

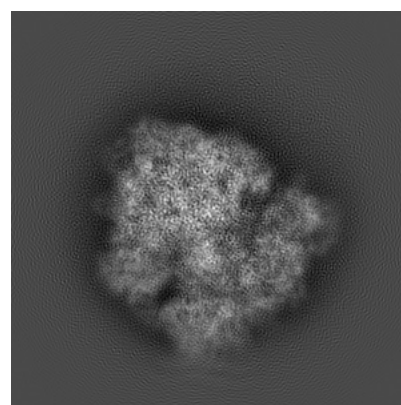
6.1.1 Primary map



X



Y

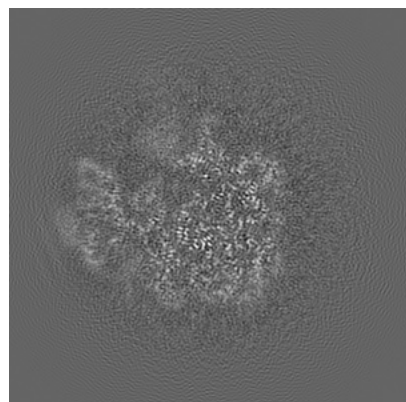


Z

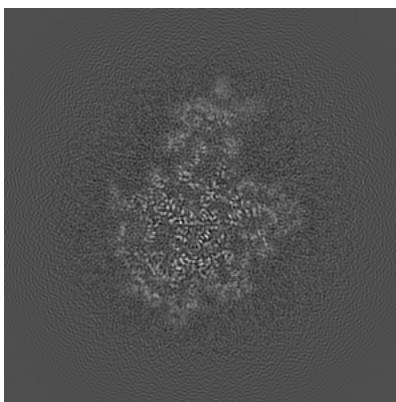
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

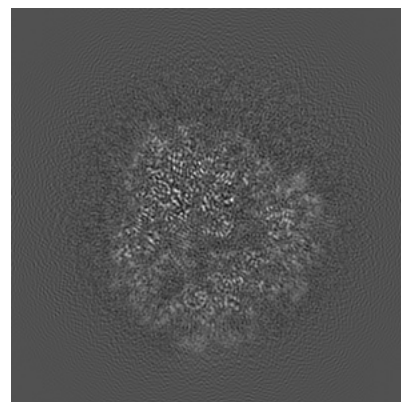
6.2.1 Primary map



X Index: 184



Y Index: 184

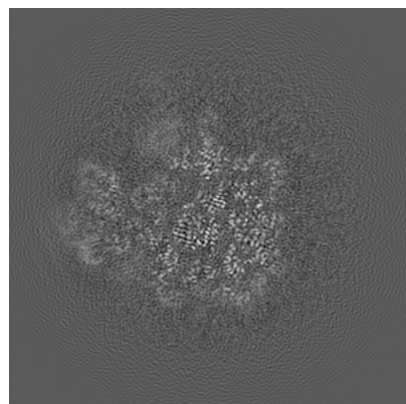


Z Index: 184

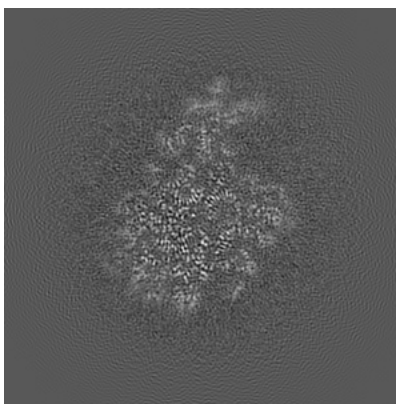
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

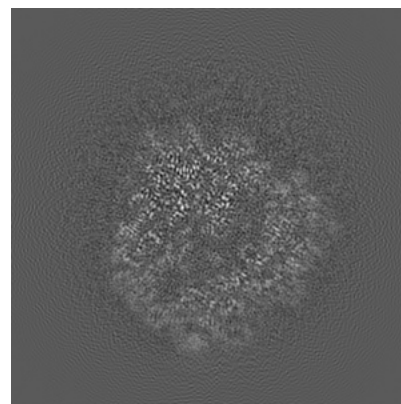
6.3.1 Primary map



X Index: 181



Y Index: 177

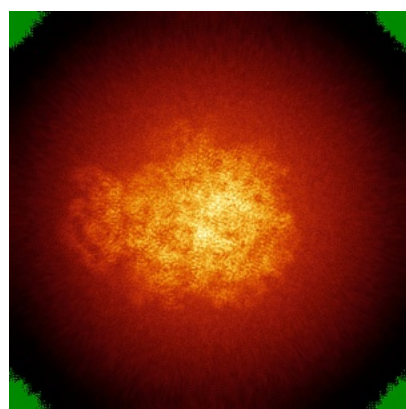


Z Index: 186

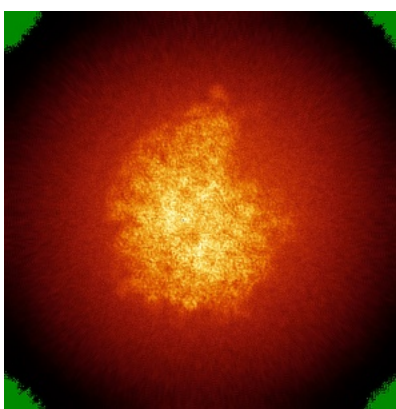
The images above show the largest variance slices of the map in three orthogonal directions.

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

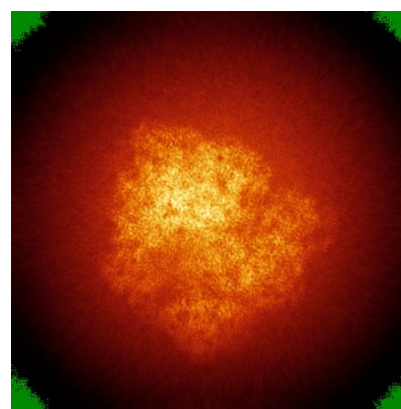
6.4.1 Primary map



X



Y

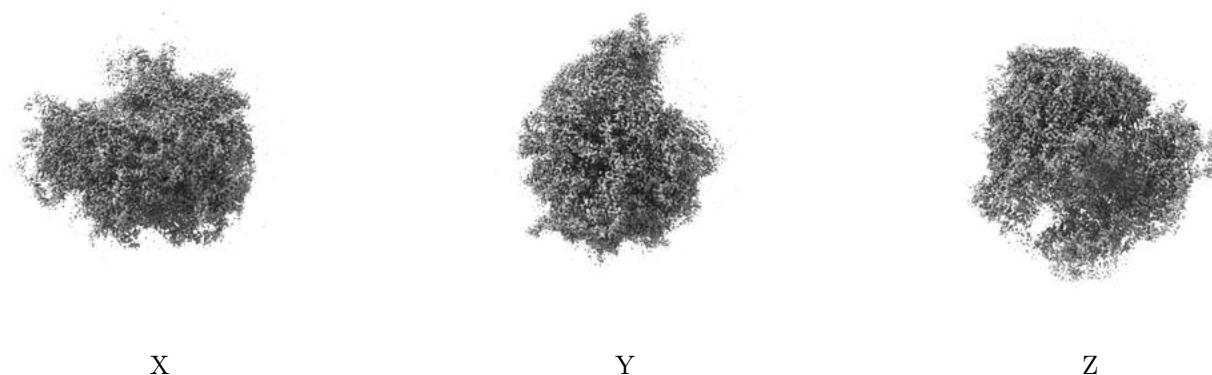


Z

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 0.00194. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

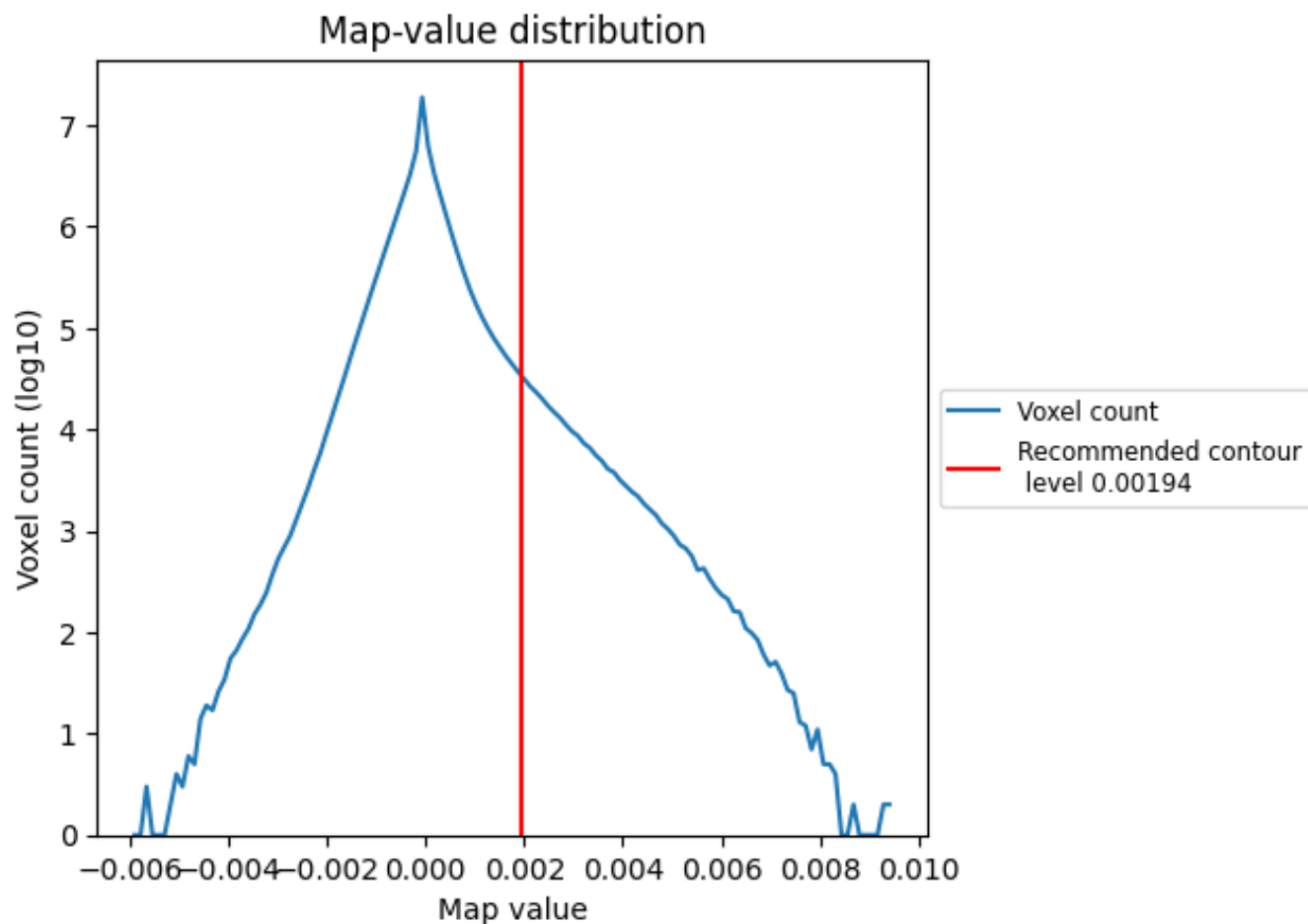
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

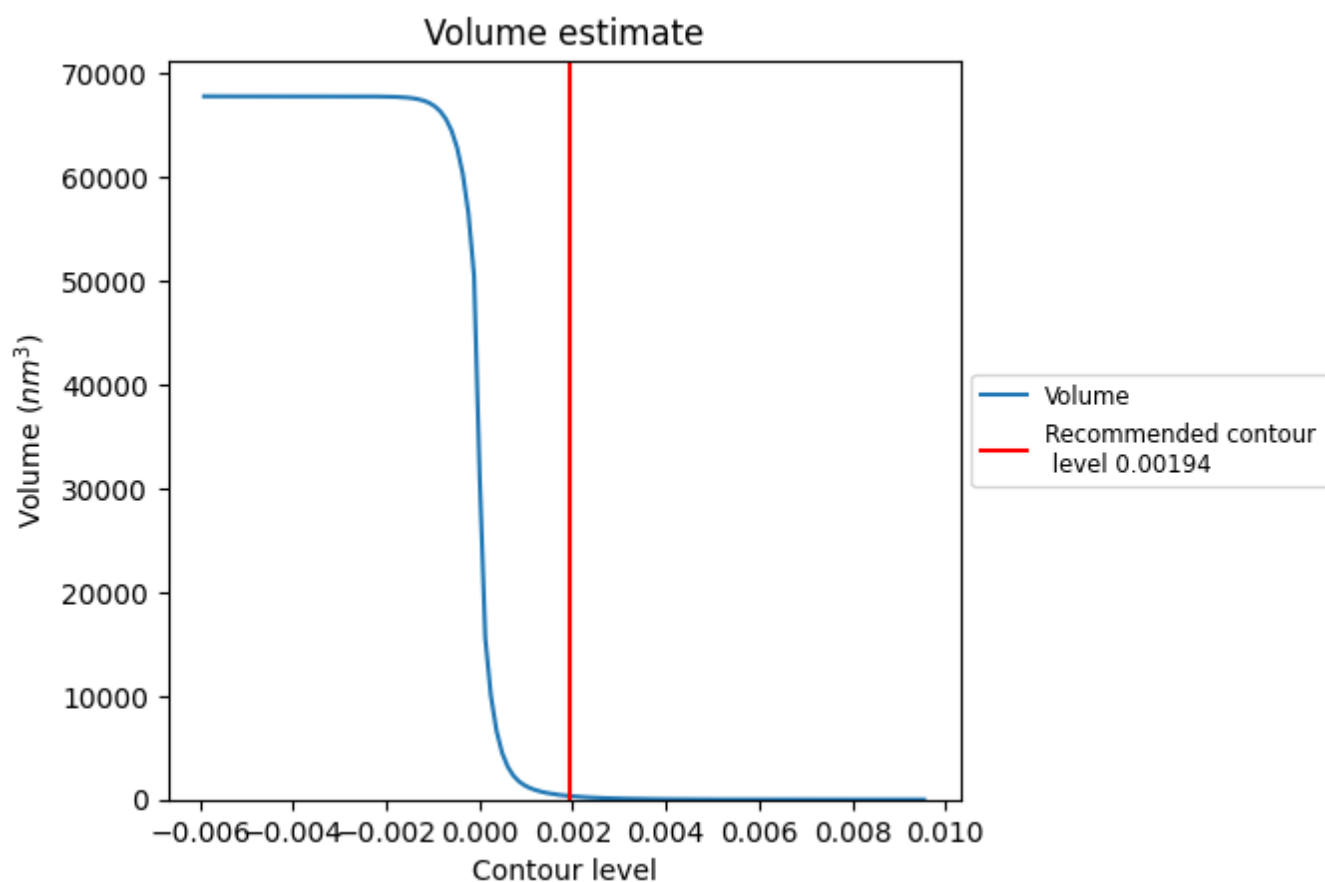
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

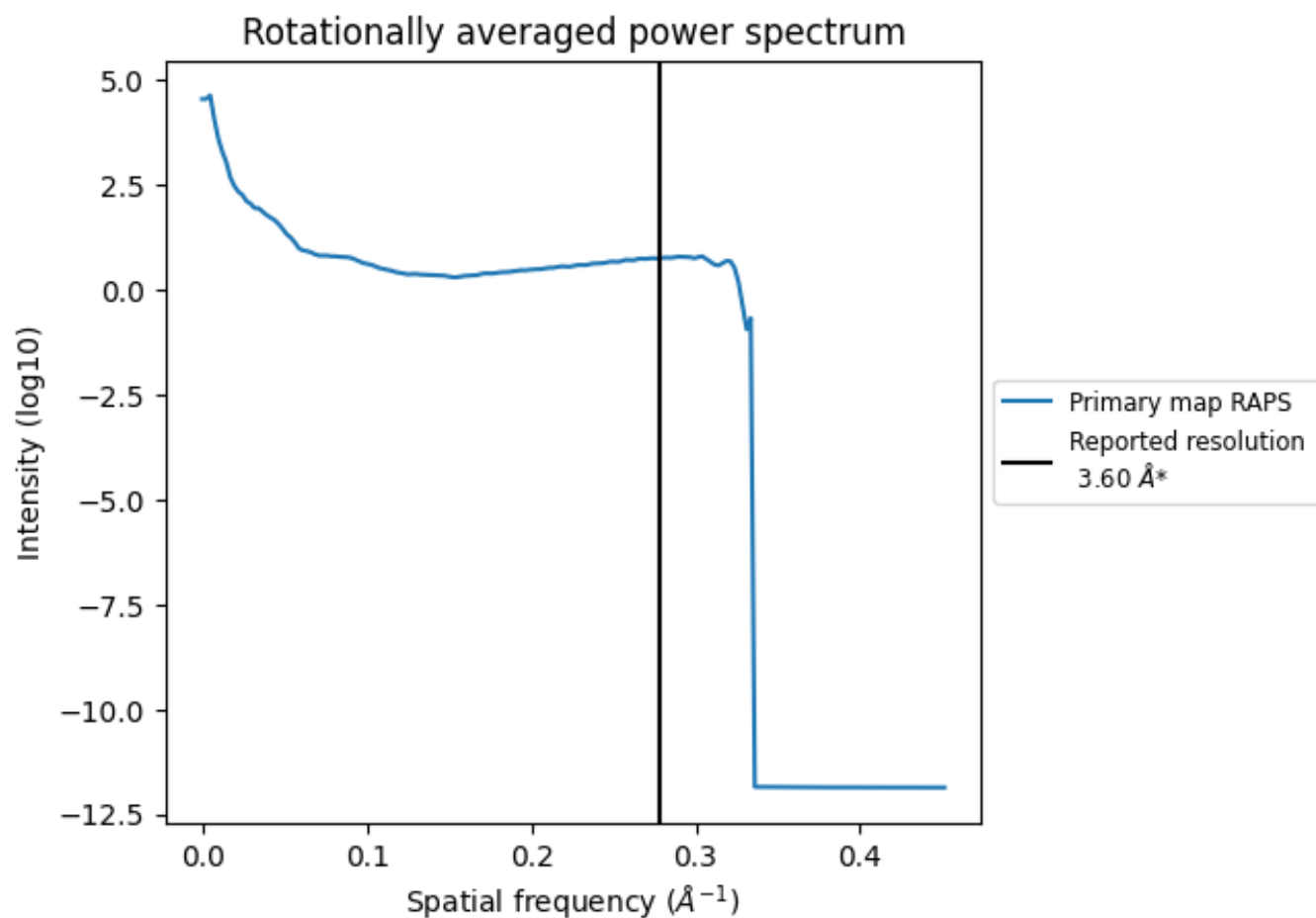
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 337 nm³; this corresponds to an approximate mass of 305 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 0.278 Å⁻¹

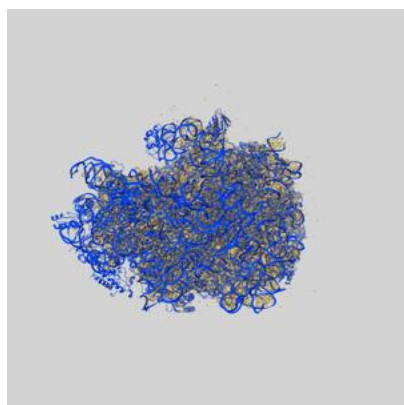
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

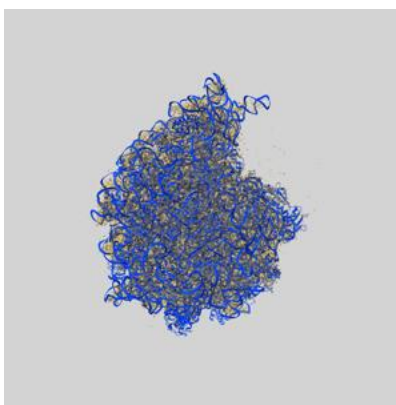
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8175 and PDB model 5JTE. Per-residue inclusion information can be found in section 3 on page 16.

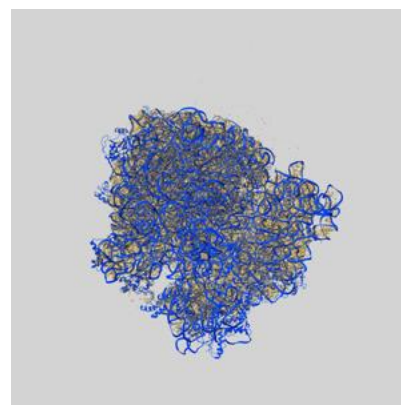
9.1 Map-model overlay [i](#)



X



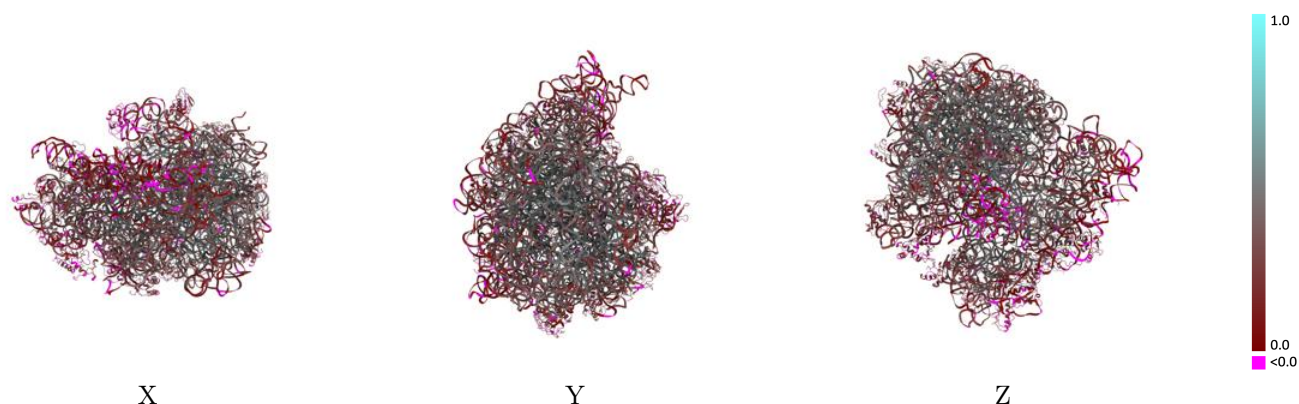
Y



Z

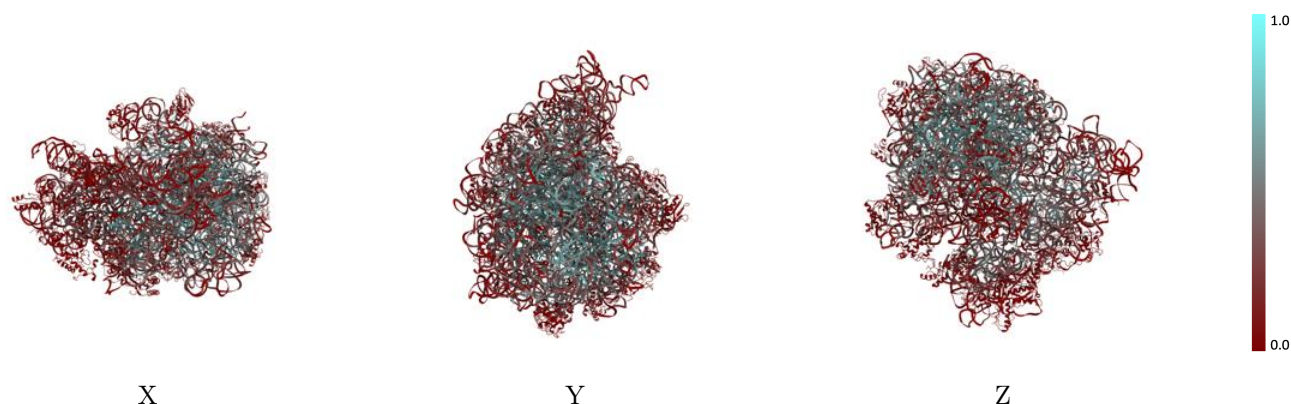
The images above show the 3D surface view of the map at the recommended contour level 0.00194 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



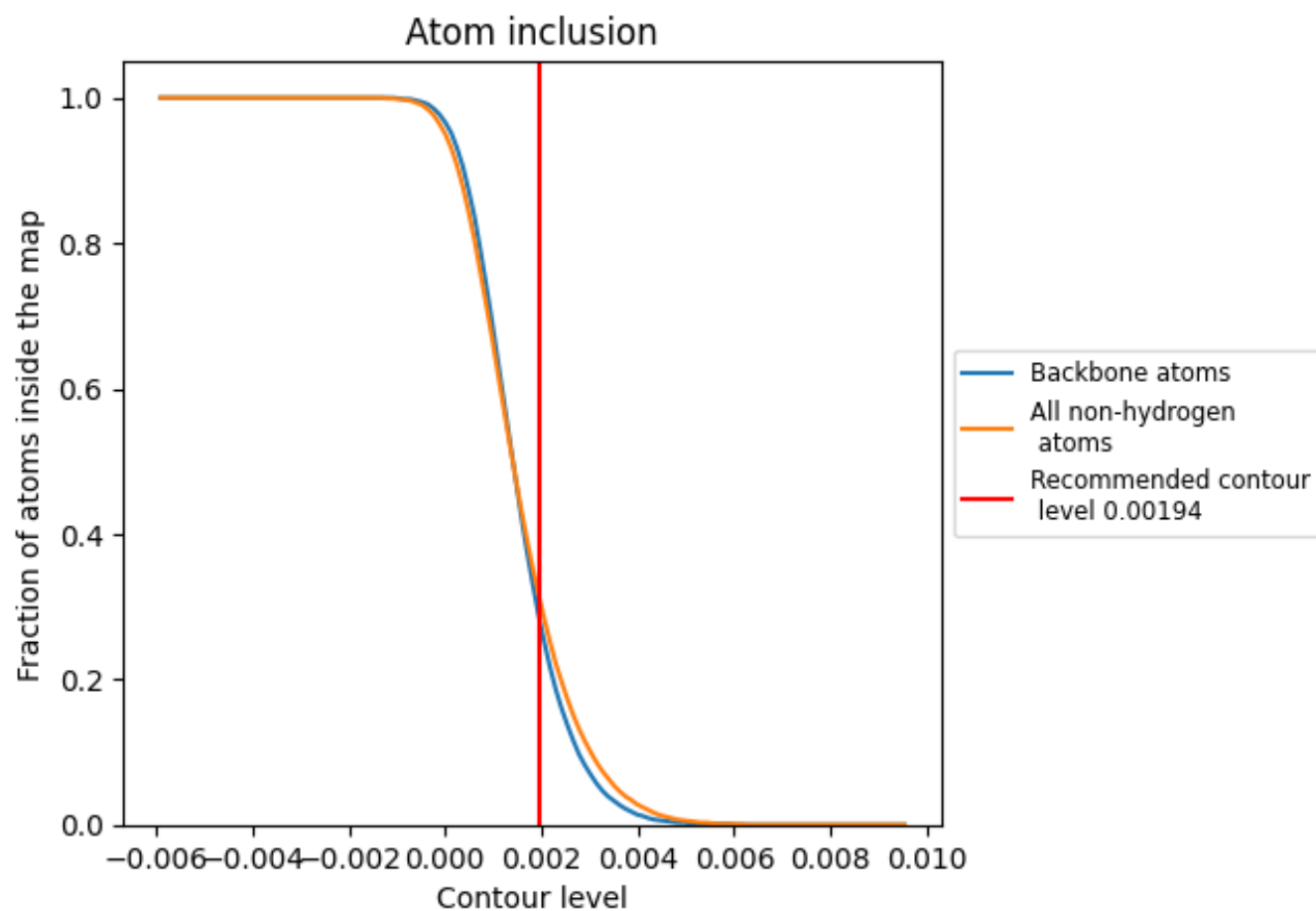
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00194).

9.4 Atom inclusion [i](#)



At the recommended contour level, 29% of all backbone atoms, 32% 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 (0.00194) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3160	 0.3150
AA	 0.3040	 0.2960
AB	 0.0040	 0.1140
AC	 0.0530	 0.2080
AD	 0.0500	 0.1960
AE	 0.1160	 0.2570
AF	 0.0740	 0.1890
AG	 0.0360	 0.2010
AH	 0.1090	 0.2610
AI	 0.0220	 0.1760
AJ	 0.0250	 0.1550
AK	 0.1040	 0.2310
AL	 0.1980	 0.2820
AM	 0.0610	 0.1920
AN	 0.0830	 0.2330
AO	 0.1870	 0.3100
AP	 0.0810	 0.1500
AQ	 0.1550	 0.2000
AR	 0.1380	 0.2600
AS	 0.0720	 0.2110
AT	 0.1460	 0.2250
AU	 0.0220	 0.1370
AV	 0.4450	 0.4210
AW	 0.1270	 0.1380
AX	 0.2450	 0.3190
AY	 0.0810	 0.1960
B0	 0.2730	 0.3400
B1	 0.1020	 0.3010
B2	 0.3970	 0.3760
B3	 0.3280	 0.3790
B4	 0.2740	 0.3260
B5	 0.2360	 0.3650
BA	 0.4520	 0.3820
BB	 0.2720	 0.2950
BC	 0.3220	 0.3360



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Chain	Atom inclusion	Q-score
BD	 0.2710	 0.3410
BE	 0.1500	 0.2550
BF	 0.0500	 0.1400
BG	 0.0820	 0.1870
BH	 0.0110	 0.0990
BI	 0.0010	 0.0330
BJ	 0.2380	 0.3250
BK	 0.2660	 0.3370
BL	 0.2090	 0.2950
BM	 0.2700	 0.3220
BN	 0.3290	 0.3430
BO	 0.0580	 0.2200
BP	 0.2120	 0.2850
BQ	 0.3720	 0.3620
BR	 0.1820	 0.2870
BS	 0.2420	 0.3220
BT	 0.1540	 0.2370
BU	 0.0850	 0.2060
BV	 0.1560	 0.2680
BW	 0.2850	 0.3480
BX	 0.2260	 0.3140
BY	 0.1030	 0.1930
BZ	 0.2130	 0.3060