



Full wwPDB EM Validation Report ⓘ

Sep 1, 2025 – 03:29 PM EDT

PDB ID : 9B4Z / pdb_00009b4z
EMDB ID : EMD-44192
Title : E. coli 70S ribosome complex (N1-methylated 16S A1408 + arbekacin)
Authors : Mattingly, J.M.; Dey, D.; Zelinskaya, N.; Dunham, C.M.; Conn, G.L.
Deposited on : 2024-03-21
Resolution : 2.20 Å (reported)
Based on initial models : 7K00, 5JTE

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.dev126
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

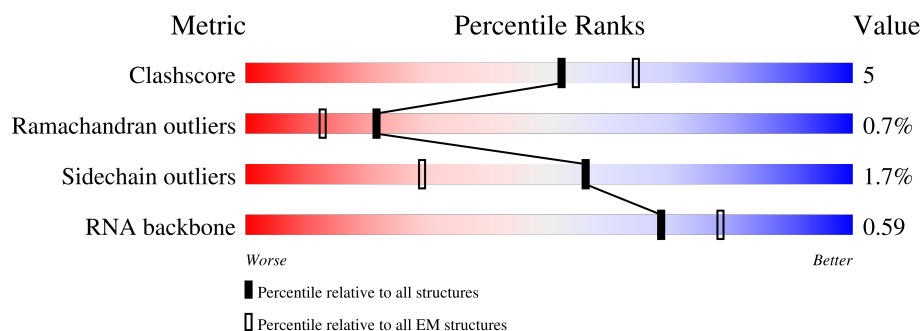
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

























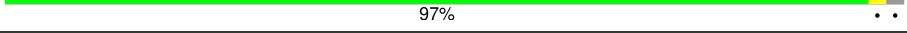


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	AA	1539	
2	AB	240	
3	AC	233	
4	AD	206	
5	AE	167	
6	AF	135	
7	AG	179	














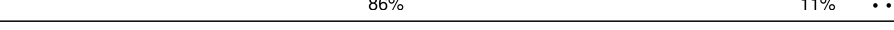
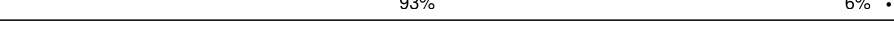






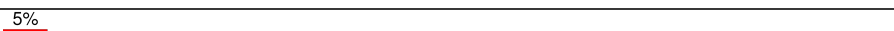


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Mol	Chain	Length	Quality of chain
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	101	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	89	
23	AW	76	
23	AY	76	
24	AX	77	
25	B0	57	
26	B1	55	
27	B2	46	
28	B3	65	
29	B4	38	
30	B5	70	
31	BA	2903	

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Mol	Chain	Length	Quality of chain
32	BB	120	 78% 18% ..
33	BC	273	 88% 11% .
34	BD	209	 91% 9%
35	BE	201	 91% 9%
36	BF	179	 86% 12% ..
37	BG	177	 82% 16% ..
38	BH	149	 5% 23% 7% . 68%
39	BJ	142	 92% 8%
40	BK	123	 85% 13% ..
41	BL	144	 81% 17% ..
42	BM	136	 90% 10%
43	BN	127	 85% 9% 6%
44	BO	117	 86% 11% ..
45	BP	115	 86% 11% ..
46	BQ	118	 93% 6% .
47	BR	103	 88% 12%
48	BS	110	 89% 10% .
49	BT	100	 79% 11% . 7%
50	BU	104	 74% 22% ..
51	BV	94	 90% 10%
52	BW	85	 82% 6% 12%
53	BX	78	 88% 10% .
54	BY	63	 5% 86% 14%
55	BZ	59	 90% 7% ..

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 146493 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
			33016	14726	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 tRNA-Val.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AW	74	Total	C	N	O	P	S	0	0
			1581	707	288	512	73	1		
23	AY	74	Total	C	N	O	P	S	0	0
			1581	707	288	512	73	1		

- Molecule 24 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AX	77	Total	C	N	O	P	0	0
			1643	732	297	537	77		

- Molecule 25 is a protein called 50S ribosomal protein L32.

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

- Molecule 26 is a protein called 50S ribosomal protein L33.

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

- Molecule 27 is a protein called 50S ribosomal protein L34.

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

- Molecule 28 is a protein called 50S ribosomal protein L35.

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

- Molecule 29 is a protein called 50S ribosomal protein L36.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B5	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 31 is a RNA chain called 23S ribosomal RNA.

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

- Molecule 32 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 33 is a protein called 50S ribosomal protein L2.

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

- Molecule 34 is a protein called 50S ribosomal protein L3.

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

- Molecule 35 is a protein called 50S ribosomal protein L4.

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

- Molecule 36 is a protein called 50S ribosomal protein L5.

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

- Molecule 37 is a protein called 50S ribosomal protein L6.

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

- Molecule 38 is a protein called 50S ribosomal protein L9.

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

- Molecule 39 is a protein called 50S ribosomal protein L13.

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

- Molecule 40 is a protein called 50S ribosomal protein L14.

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

- Molecule 41 is a protein called 50S ribosomal protein L15.

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

- Molecule 42 is a protein called 50S ribosomal protein L16.

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

- Molecule 43 is a protein called 50S ribosomal protein L17.

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

- Molecule 44 is a protein called 50S ribosomal protein L18.

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

- Molecule 45 is a protein called 50S ribosomal protein L19.

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

- Molecule 46 is a protein called 50S ribosomal protein L20.

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

- Molecule 47 is a protein called 50S ribosomal protein L21.

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

- Molecule 48 is a protein called 50S ribosomal protein L22.

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

- Molecule 49 is a protein called 50S ribosomal protein L23.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L25.

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

- Molecule 52 is a protein called 50S ribosomal protein L27.

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

- Molecule 53 is a protein called 50S ribosomal protein L28.

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

- Molecule 54 is a protein called 50S ribosomal protein L29.

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

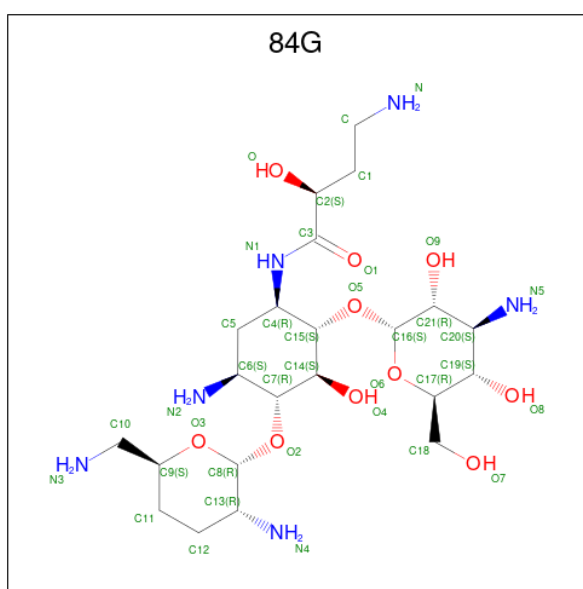
- Molecule 55 is a protein called 50S ribosomal protein L30.

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

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	AA	93	Total	Mg	0
			93	93	
56	B0	1	Total	Mg	0
			1	1	
56	BA	210	Total	Mg	0
			210	210	
56	BB	5	Total	Mg	0
			5	5	

- Molecule 57 is Arbekacin (CCD ID: 84G) (formula: $C_{22}H_{44}N_6O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
57	AA	1	Total	C	N	O	0
			38	22	6	10	
57	AA	1	Total	C	N	O	0
			38	22	6	10	

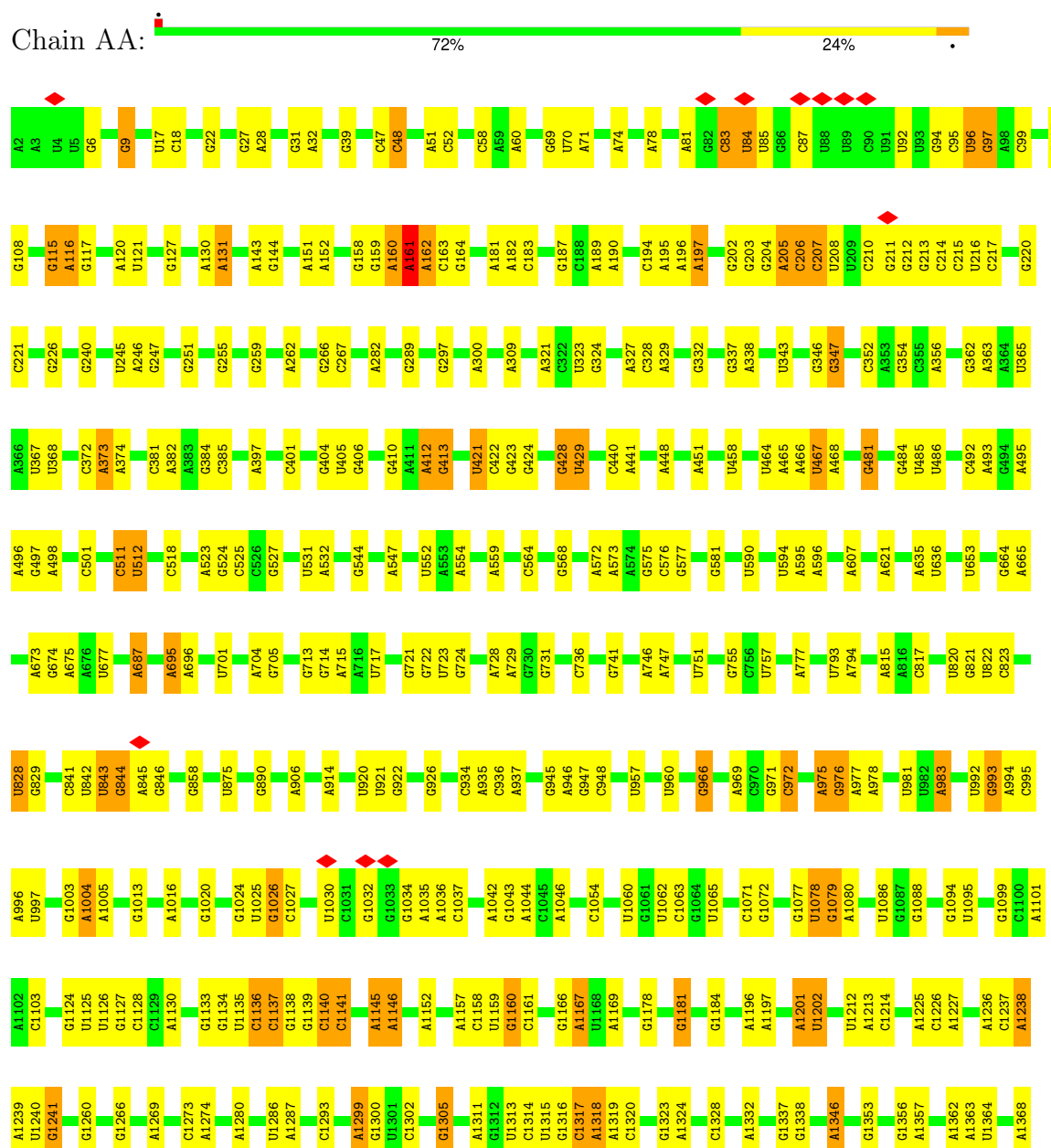
- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	B4	1	Total	Zn	0
			1	1	
58	B5	1	Total	Zn	0
			1	1	

3 Residue-property plots

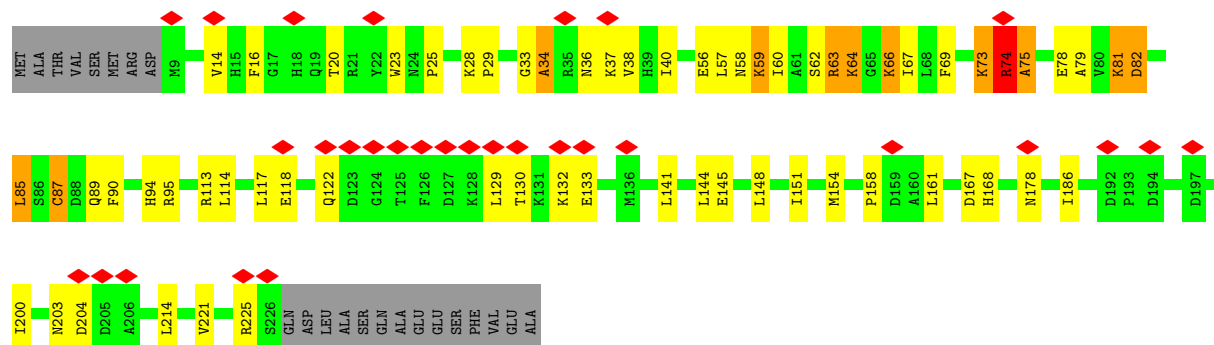
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

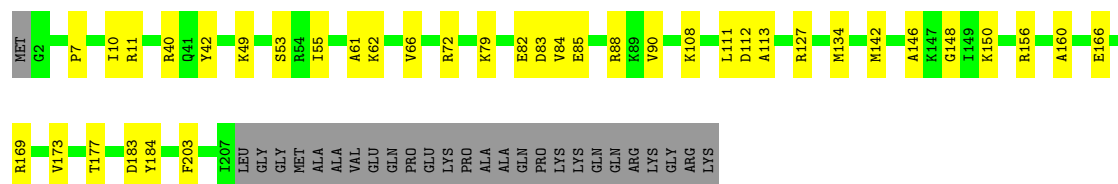




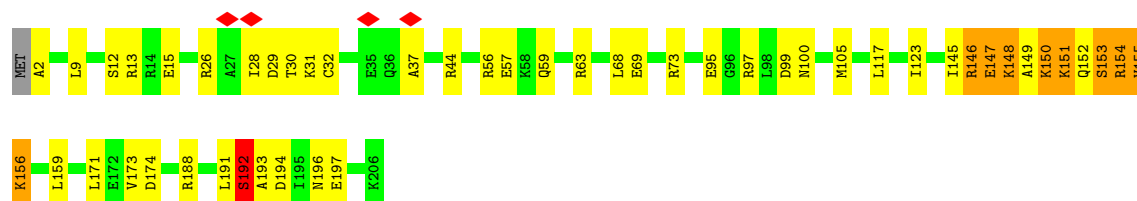
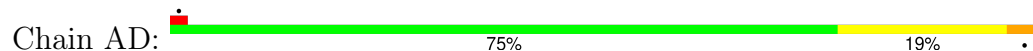
• Molecule 2: 30S ribosomal protein S2



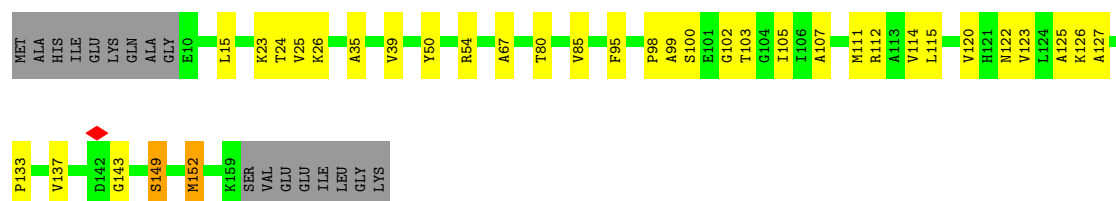
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5



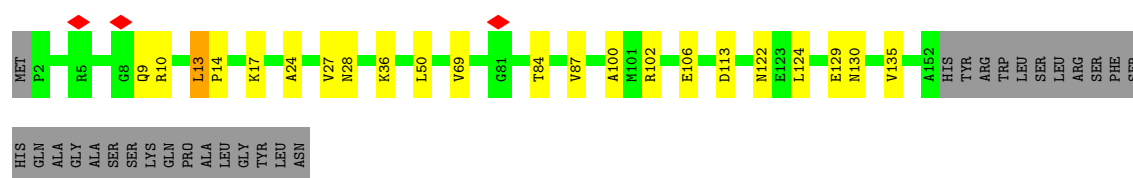
- Molecule 6: 30S ribosomal protein S6

Chain AF: 




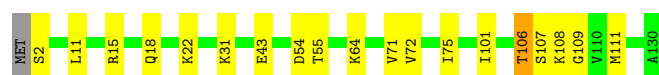
- Molecule 7: 30S ribosomal protein S7

Chain AG: 




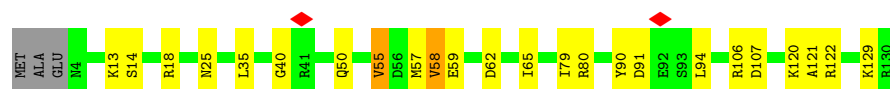
- Molecule 8: 30S ribosomal protein S8

Chain AH: 



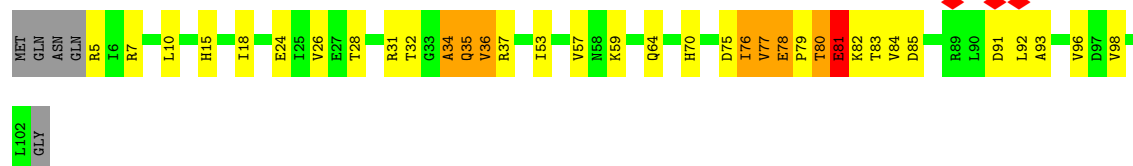
- Molecule 9: 30S ribosomal protein S9

Chain AI: 




- Molecule 10: 30S ribosomal protein S10

Chain AJ: 

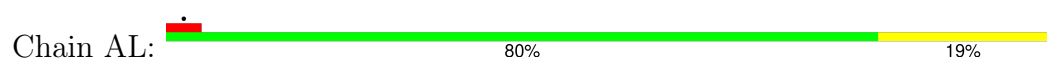


- Molecule 11: 30S ribosomal protein S11

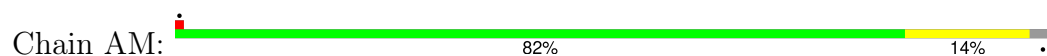
Chain AK: 



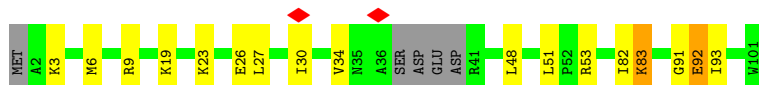
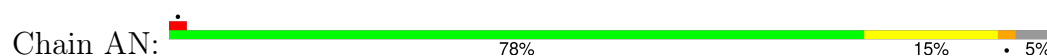
- Molecule 12: 30S ribosomal protein S12



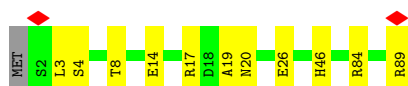
- Molecule 13: 30S ribosomal protein S13



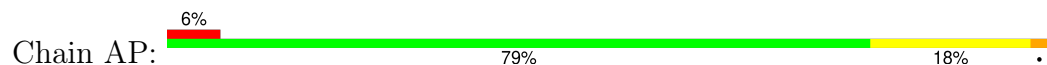
- Molecule 14: 30S ribosomal protein S14



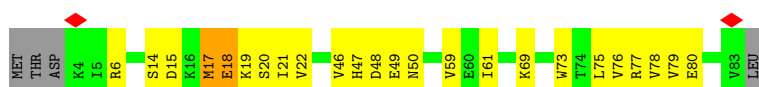
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

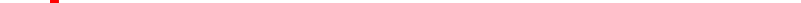


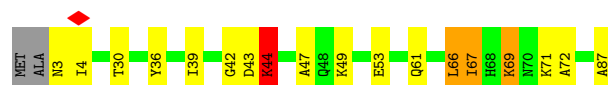
- Molecule 18: 30S ribosomal protein S18

MET	ALA	ARG	TYR	PHE	ARG	ARG	LYS	PHE	CYS	ARG	PHE	THR	ALA	GLU	GLY	VAL	GLN	E20	K24	T34	E35	S36	G37	K38	T47	R48	R61	H74	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

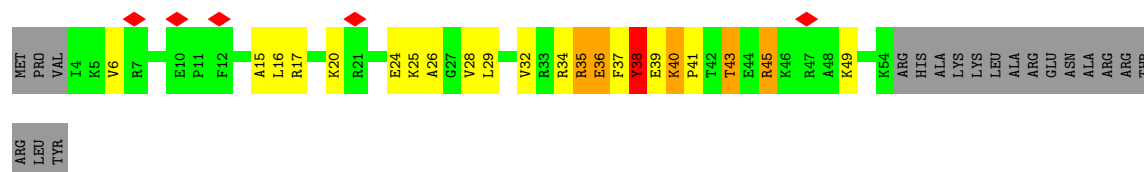
- Chain AS:



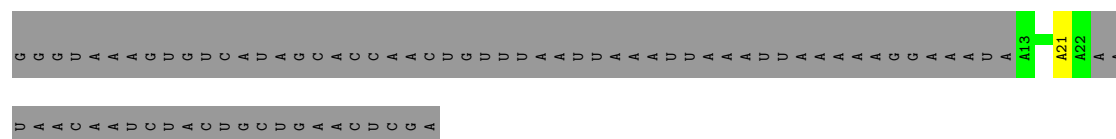
- Chain AT: 



- Chain AU:



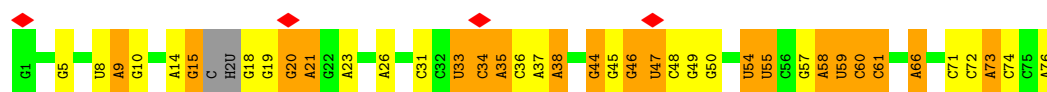
- Chain AV: 10% : 89%



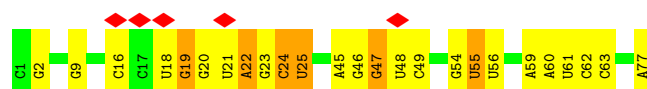
- Chain AW: 59% 24% 14%



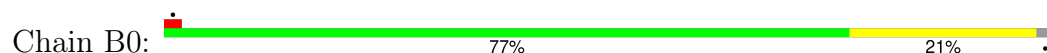
- Chain AY:



- Molecule 24: tRNA-fMet



- Molecule 25: 50S ribosomal protein L32



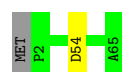
- Molecule 26: 50S ribosomal protein L33



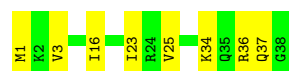
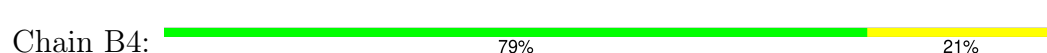
- Molecule 27: 50S ribosomal protein L34



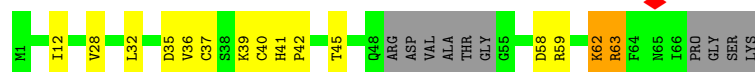
- Molecule 28: 50S ribosomal protein L35



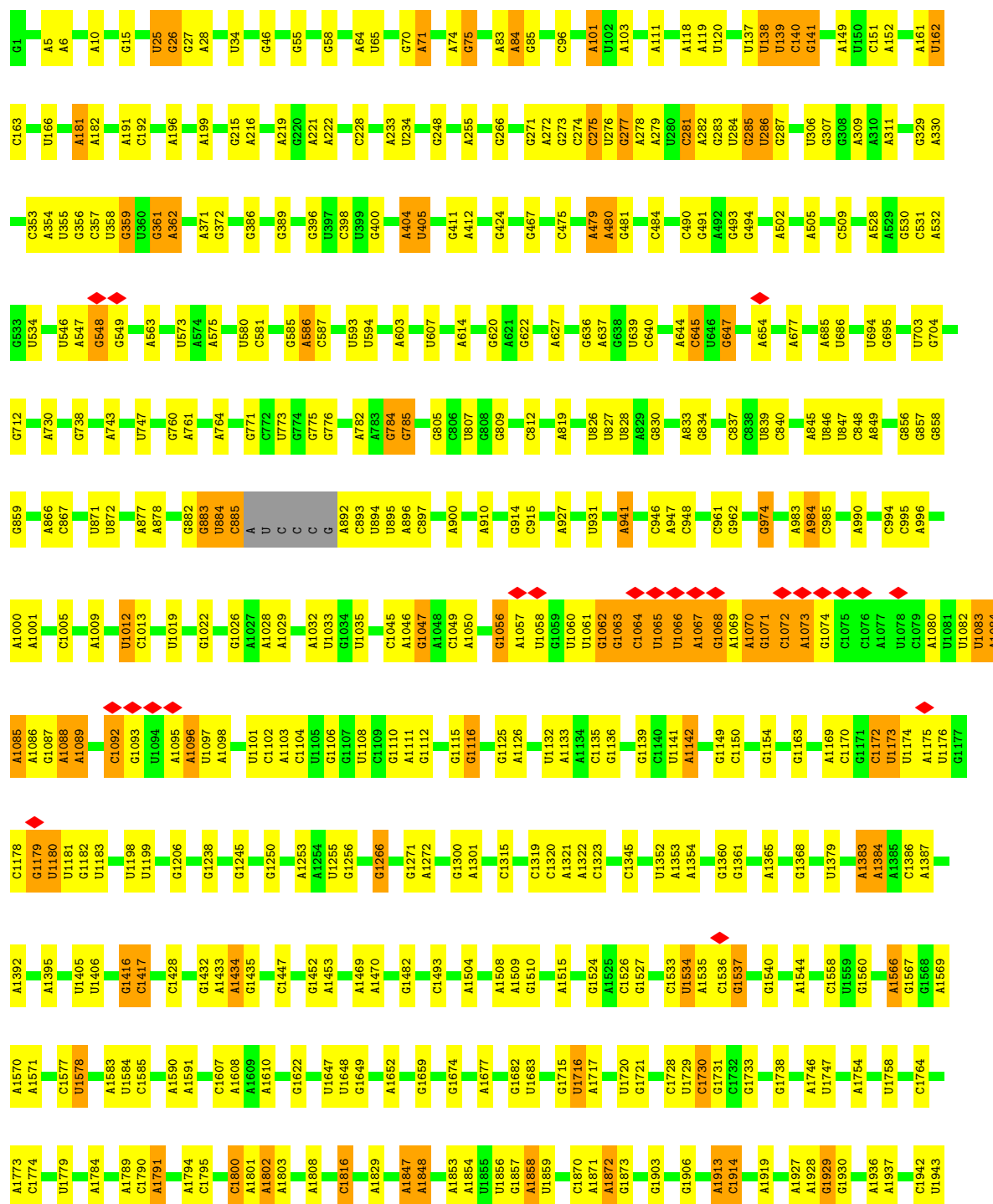
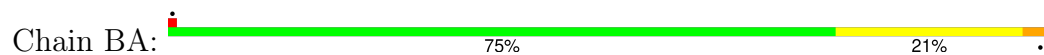
- Molecule 29: 50S ribosomal protein L36

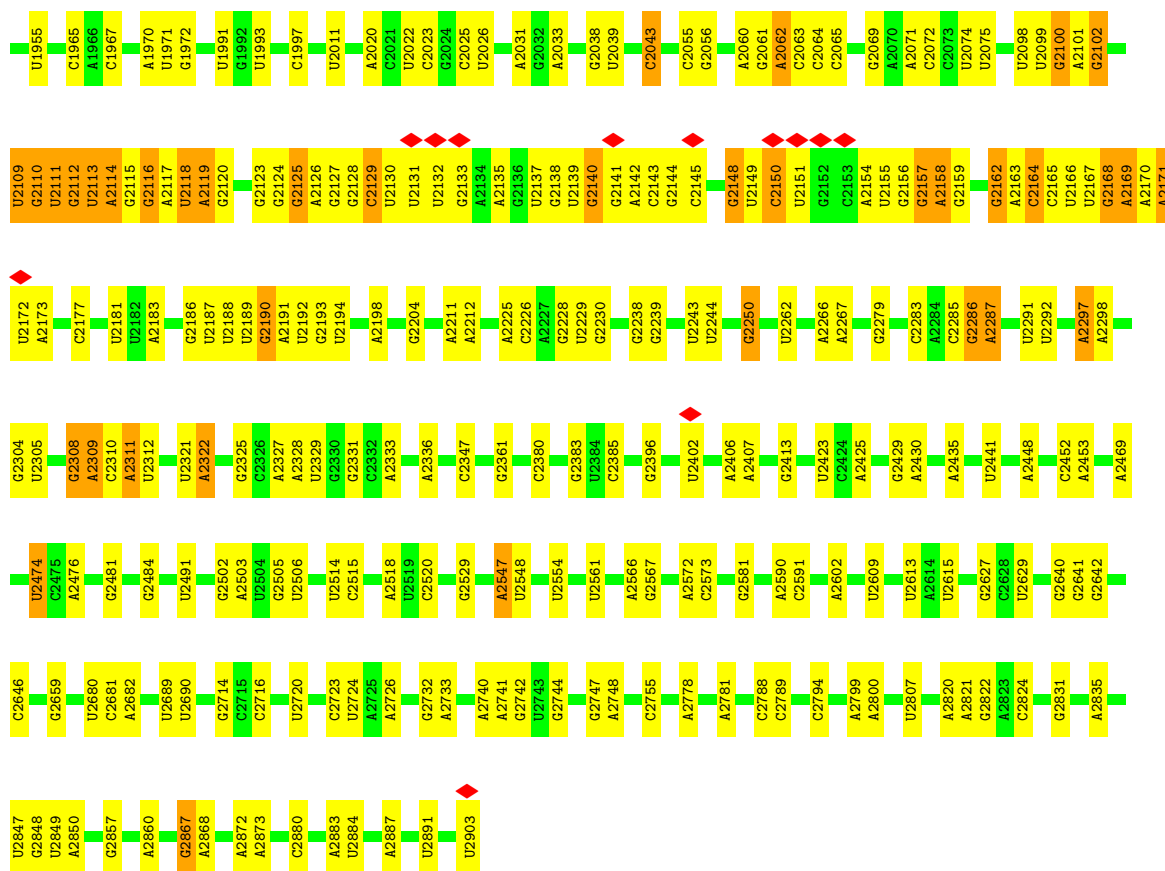


- Molecule 30: 50S ribosomal protein L31



• Molecule 31: 23S ribosomal RNA





- Molecule 32: 5S ribosomal RNA

Chain BB: 78% 18%



- Molecule 33: 50S ribosomal protein L2

Chain BC: 88% 11%



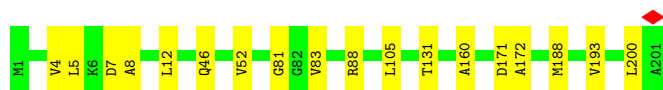
- Molecule 34: 50S ribosomal protein L3

Chain BD: 91% 9%




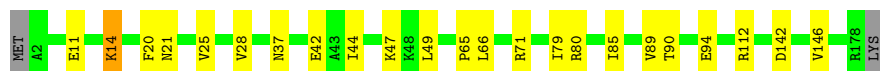
- Molecule 35: 50S ribosomal protein L4

Chain BE:  91% 9%




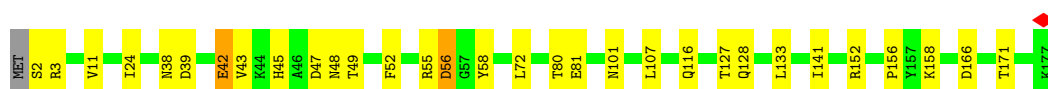
- Molecule 36: 50S ribosomal protein L5

Chain BF:  86% 12% ..



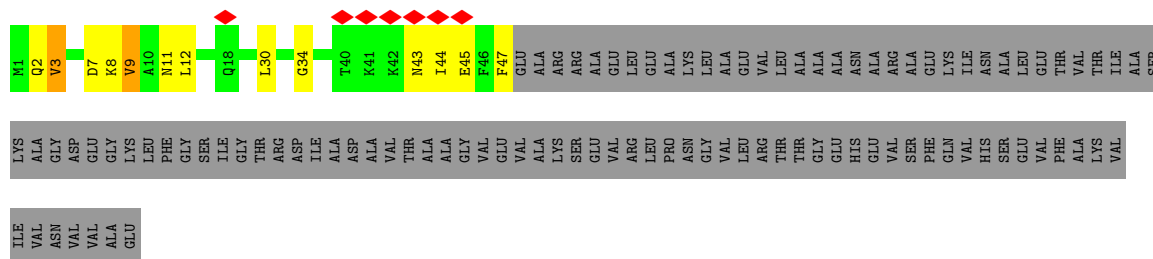
- Molecule 37: 50S ribosomal protein L6

Chain BG:  82% 16% ..



- Molecule 38: 50S ribosomal protein L9

Chain BH:  5% 23% 7% 68%




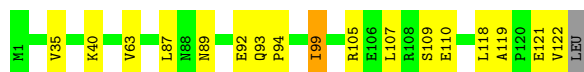
- Molecule 39: 50S ribosomal protein L13

Chain BJ:  92% 8%




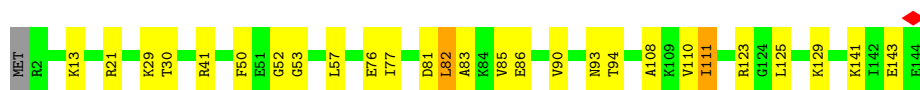
- Molecule 40: 50S ribosomal protein L14

Chain BK:  85% 13% ..



- Molecule 41: 50S ribosomal protein L15

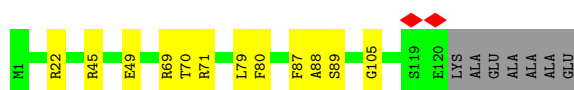
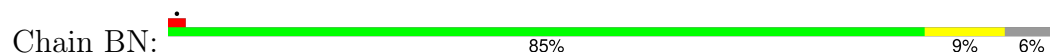
Chain BL:  81% 17% ..



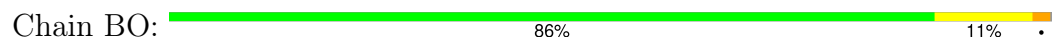
- Molecule 42: 50S ribosomal protein L16



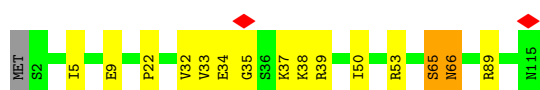
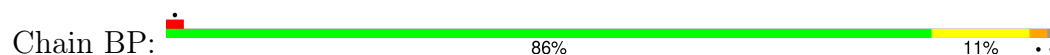
- Molecule 43: 50S ribosomal protein L17



- Molecule 44: 50S ribosomal protein L18



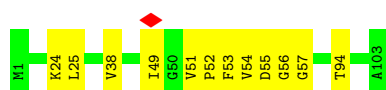
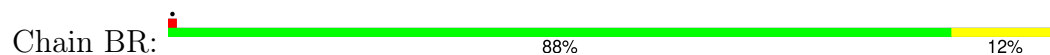
- Molecule 45: 50S ribosomal protein L19



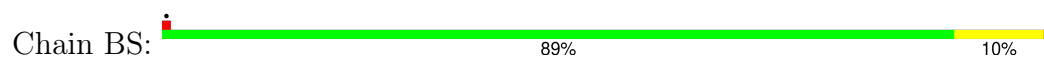
- Molecule 46: 50S ribosomal protein L20



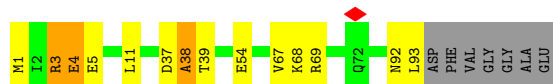
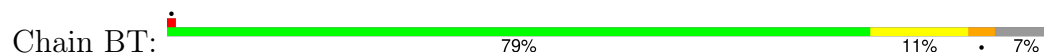
- Molecule 47: 50S ribosomal protein L21



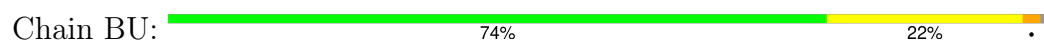
- Molecule 48: 50S ribosomal protein L22



- Molecule 49: 50S ribosomal protein L23



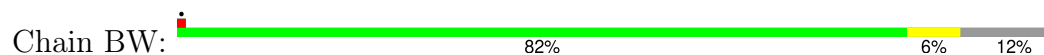
- Molecule 50: 50S ribosomal protein L24



- Molecule 51: 50S ribosomal protein L25



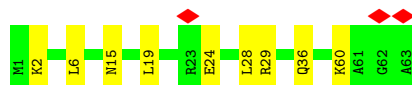
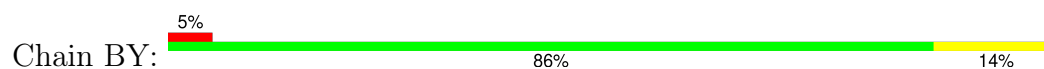
- Molecule 52: 50S ribosomal protein L27



- Molecule 53: 50S ribosomal protein L28

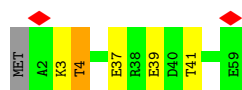


- Molecule 54: 50S ribosomal protein L29



- Molecule 55: 50S ribosomal protein L30

Chain BZ:  90% 7% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	218006	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	29.095	Depositor
Minimum map value	-7.708	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.7	Depositor
Map size (\AA)	416.768, 416.768, 416.768	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.814, 0.814, 0.814	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, PSU, ZN, 4SU, 84G, 7MG, MG, 1MA

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	0.15	0/36941	0.28	1/57627 (0.0%)
2	AB	0.29	0/1735	0.48	2/2338 (0.1%)
3	AC	0.20	0/1651	0.35	0/2225
4	AD	0.37	1/1665 (0.1%)	0.44	2/2227 (0.1%)
5	AE	0.28	0/1118	0.41	0/1504
6	AF	0.35	1/835 (0.1%)	0.46	0/1128
7	AG	0.17	0/1195	0.31	0/1602
8	AH	0.24	0/989	0.38	1/1326 (0.1%)
9	AI	0.24	0/1034	0.37	0/1375
10	AJ	0.35	0/796	0.58	2/1077 (0.2%)
11	AK	0.34	0/893	0.46	1/1205 (0.1%)
12	AL	0.13	0/969	0.35	0/1300
13	AM	0.13	0/892	0.40	0/1193
14	AN	0.33	0/785	0.37	0/1043
15	AO	0.10	0/718	0.23	0/959
16	AP	0.37	0/659	0.53	1/884 (0.1%)
17	AQ	0.37	0/657	0.46	0/881
18	AR	0.12	0/462	0.26	0/621
19	AS	0.37	0/652	0.47	1/877 (0.1%)
20	AT	0.44	0/671	0.62	4/888 (0.5%)
21	AU	0.80	1/430 (0.2%)	0.71	0/570
22	AV	0.12	0/245	0.18	0/380
23	AW	0.22	1/1672 (0.1%)	0.33	0/2604
23	AY	0.24	0/1672	0.38	0/2604
24	AX	0.15	0/1835	0.28	0/2859
25	B0	0.29	0/450	0.39	0/599
26	B1	0.61	1/416 (0.2%)	0.53	0/554
27	B2	0.16	0/380	0.29	0/498
28	B3	0.14	0/513	0.27	0/676
29	B4	0.26	0/303	0.38	0/397
30	B5	0.29	0/488	0.39	0/649
31	BA	0.17	0/69659	0.29	1/108672 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	BB	0.14	0/2828	0.23	0/4410
33	BC	0.14	0/2121	0.33	0/2852
34	BD	0.27	0/1586	0.35	0/2134
35	BE	0.23	0/1571	0.30	0/2113
36	BF	0.28	0/1434	0.32	0/1926
37	BG	0.22	0/1343	0.34	0/1816
38	BH	0.14	0/364	0.36	0/490
39	BJ	0.15	0/1152	0.26	0/1551
40	BK	0.24	0/947	0.38	0/1268
41	BL	0.15	0/1054	0.40	0/1403
42	BM	0.15	0/1093	0.29	0/1460
43	BN	0.31	0/973	0.38	1/1301 (0.1%)
44	BO	0.28	0/902	0.39	1/1209 (0.1%)
45	BP	0.31	0/929	0.38	0/1242
46	BQ	0.13	0/960	0.23	0/1278
47	BR	0.16	0/829	0.34	0/1107
48	BS	0.14	0/864	0.28	0/1156
49	BT	0.32	0/744	0.34	0/994
50	BU	0.26	0/787	0.51	2/1051 (0.2%)
51	BV	0.14	0/766	0.25	0/1025
52	BW	0.13	0/576	0.28	0/762
53	BX	0.15	0/635	0.26	0/848
54	BY	0.37	0/510	0.36	0/677
55	BZ	0.13	0/453	0.25	0/605
All	All	0.20	5/158801 (0.0%)	0.31	20/238020 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AU	45	ARG	C-N	-9.48	1.21	1.33
4	AD	146	ARG	C-N	-8.17	1.24	1.33
26	B1	33	LYS	C-N	6.12	1.41	1.33
6	AF	89	VAL	C-N	5.23	1.41	1.33
23	AW	8	4SU	O3'-P	5.01	1.61	1.56

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AT	43	ASP	N-CA-C	7.77	122.46	110.42
20	AT	44	LYS	N-CA-C	-7.18	104.39	113.43
4	AD	150	LYS	N-CA-C	-6.99	103.66	111.28
31	BA	984	A	C2'-C3'-O3'	-6.94	103.30	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AT	67	ILE	N-CA-C	-6.27	99.68	108.27
10	AJ	77	VAL	N-CA-C	6.21	118.23	111.77
10	AJ	34	ALA	N-CA-C	6.11	116.07	108.19
2	AB	85	LEU	N-CA-C	-5.92	104.52	110.97
19	AS	34	TRP	N-CA-C	-5.79	104.39	113.02
50	BU	54	GLN	CA-C-N	-5.61	114.46	120.47
50	BU	54	GLN	C-N-CA	-5.61	114.46	120.47
2	AB	63	ARG	N-CA-C	-5.59	106.04	112.92
44	BO	33	ARG	N-CA-C	-5.56	101.11	109.95
1	AA	161	A	C4'-C3'-O3'	-5.48	104.78	113.00
20	AT	66	LEU	N-CA-C	-5.48	105.23	113.89
43	BN	105	GLY	N-CA-C	5.45	120.67	114.67
8	AH	109	GLY	N-CA-C	5.29	118.20	111.85
16	AP	20	VAL	N-CA-C	5.22	117.57	108.90
11	AK	42	LEU	N-CA-C	-5.13	107.68	114.04
4	AD	192	SER	N-CA-C	5.02	121.50	110.80

There are no chirality outliers.

There are no planarity outliers.

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	33016	0	16618	226	0
2	AB	1704	0	1732	54	0
3	AC	1624	0	1696	24	0
4	AD	1643	0	1707	39	0
5	AE	1105	0	1148	25	0
6	AF	817	0	808	20	0
7	AG	1181	0	1238	14	0
8	AH	979	0	1031	15	0
9	AI	1022	0	1070	17	0
10	AJ	786	0	828	34	0
11	AK	877	0	887	18	0
12	AL	955	0	1016	19	0
13	AM	883	0	941	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	AN	774	0	824	11	0
15	AO	710	0	728	8	0
16	AP	649	0	666	10	0
17	AQ	648	0	691	22	0
18	AR	455	0	478	8	0
19	AS	637	0	665	11	0
20	AT	665	0	714	10	0
21	AU	425	0	449	33	0
22	AV	218	0	109	1	0
23	AW	1581	0	811	19	0
23	AY	1581	0	811	30	0
24	AX	1643	0	836	9	0
25	B0	444	0	458	12	0
26	B1	409	0	440	12	0
27	B2	377	0	418	5	0
28	B3	504	0	572	1	0
29	B4	302	0	340	8	0
30	B5	480	0	478	11	0
31	BA	62195	0	31280	352	0
32	BB	2529	0	1281	14	0
33	BC	2082	0	2154	21	0
34	BD	1565	0	1616	13	0
35	BE	1552	0	1619	9	0
36	BF	1410	0	1444	17	0
37	BG	1323	0	1371	22	0
38	BH	359	0	381	8	0
39	BJ	1129	0	1162	12	0
40	BK	938	0	1012	16	0
41	BL	1045	0	1116	23	0
42	BM	1074	0	1157	11	0
43	BN	960	0	1000	6	0
44	BO	892	0	923	9	0
45	BP	917	0	962	10	0
46	BQ	947	0	1019	6	0
47	BR	816	0	839	8	0
48	BS	857	0	922	7	0
49	BT	738	0	807	14	0
50	BU	779	0	831	16	0
51	BV	753	0	780	6	0
52	BW	569	0	581	6	0
53	BX	625	0	652	6	0
54	BY	509	0	543	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	BZ	449	0	488	3	0
56	AA	93	0	0	0	0
56	B0	1	0	0	0	0
56	BA	210	0	0	0	0
56	BB	5	0	0	0	0
57	AA	76	0	0	1	0
58	B4	1	0	0	0	0
58	B5	1	0	0	0	0
All	All	146493	0	97148	1226	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 5.

All (1226) 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)
31:BA:1056:G:H21	31:BA:1103:A:H62	1.07	0.95
34:BD:148:GLN:HB2	34:BD:152:PRO:HG3	1.51	0.93
10:AJ:5:ARG:HG3	10:AJ:79:PRO:HD3	1.54	0.90
31:BA:1115:G:O2'	31:BA:1116:G:O5'	1.91	0.88
31:BA:1096:A:O2'	31:BA:1097:U:O4'	1.92	0.87
10:AJ:26:VAL:HG13	10:AJ:36:VAL:HG11	1.57	0.87
1:AA:1140:C:HO2'	1:AA:1141:C:H6	1.21	0.86
31:BA:2111:U:O2'	31:BA:2112:G:O5'	1.95	0.84
1:AA:204:G:H3'	1:AA:205:A:C8	2.13	0.83
11:AK:123:PRO:HD2	21:AU:35:ARG:HG2	1.62	0.82
8:AH:106:THR:HG23	8:AH:108:LYS:H	1.43	0.82
31:BA:2168:G:H2'	31:BA:2169:A:C8	2.16	0.81
1:AA:195:A:O2'	1:AA:196:A:O4'	1.98	0.80
23:AY:36:C:H3'	23:AY:37:A:H8	1.44	0.80
31:BA:75:G:H22	31:BA:111:A:H2	1.29	0.80
31:BA:1416:G:O2'	31:BA:1417:C:OP2	2.00	0.80
31:BA:1062:G:O2'	31:BA:1063:G:O4'	2.00	0.79
5:AE:115:LEU:HD13	5:AE:123:VAL:HG21	1.63	0.78
23:AY:58:A:H2'	23:AY:60:C:H5	1.49	0.78
31:BA:1056:G:H21	31:BA:1103:A:N6	1.81	0.78
31:BA:1056:G:N2	31:BA:1103:A:H62	1.82	0.77
1:AA:1145:A:O2'	1:AA:1146:A:O5'	2.03	0.76
21:AU:16:LEU:O	21:AU:16:LEU:HD23	1.85	0.76
31:BA:1383:A:O2'	31:BA:1384:A:O5'	2.01	0.76
21:AU:37:PHE:CE1	21:AU:39:GLU:HB2	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BE:52:VAL:HG21	35:BE:81:GLY:HA2	1.68	0.75
21:AU:36:GLU:HG2	21:AU:40:LYS:HE3	1.69	0.75
31:BA:2109:U:O2'	31:BA:2110:G:OP1	2.04	0.75
37:BG:80:THR:OG1	37:BG:81:GLU:OE1	2.04	0.74
31:BA:2308:G:O2'	31:BA:2309:A:OP1	2.04	0.74
1:AA:204:G:H3'	1:AA:205:A:H8	1.48	0.74
21:AU:37:PHE:O	21:AU:41:PRO:HD2	1.88	0.74
1:AA:127:G:O2'	17:AQ:6:ARG:NH2	2.20	0.74
1:AA:255:G:H4'	17:AQ:19:LYS:HD3	1.69	0.74
1:AA:1525:G:H5''	21:AU:38:TYR:HE2	1.52	0.74
31:BA:1064:C:C2	31:BA:1074:G:N2	2.57	0.73
33:BC:29:PRO:HG2	33:BC:34:LEU:HD11	1.71	0.72
1:AA:1525:G:H5''	21:AU:38:TYR:CE2	2.24	0.72
40:BK:121:GLU:HG2	40:BK:122:VAL:HG23	1.70	0.72
1:AA:722:G:O3'	21:AU:49:LYS:NZ	2.22	0.72
31:BA:2112:G:O2'	31:BA:2113:U:OP1	2.06	0.72
23:AY:36:C:H3'	23:AY:37:A:C8	2.25	0.72
48:BS:28:LYS:O	48:BS:30:SER:N	2.22	0.72
31:BA:585:G:N7	46:BQ:6:ARG:NH2	2.37	0.71
22:AV:21:A:H61	23:AW:34:C:H42	1.38	0.71
1:AA:451:A:OP2	16:AP:70:ARG:NH2	2.23	0.71
1:AA:204:G:H2'	1:AA:205:A:H5'	1.72	0.70
4:AD:188:ARG:HH22	4:AD:193:ALA:HA	1.56	0.70
1:AA:363:A:OP2	12:AL:31:ARG:NH1	2.24	0.70
9:AI:57:MET:SD	9:AI:58:VAL:N	2.64	0.70
33:BC:165:VAL:HG21	33:BC:181:MET:HE1	1.73	0.70
36:BF:11:GLU:HA	36:BF:14:LYS:HE3	1.72	0.70
13:AM:11:ASP:OD1	13:AM:12:HIS:N	2.25	0.70
1:AA:501:C:OP1	12:AL:114:ARG:NH2	2.25	0.70
1:AA:405:U:O4	4:AD:2:ALA:N	2.25	0.70
35:BE:171:ASP:OD1	35:BE:172:ALA:N	2.25	0.70
43:BN:87:PHE:O	43:BN:89:SER:N	2.25	0.69
50:BU:45:HIS:HB3	50:BU:58:ILE:HD13	1.74	0.69
49:BT:54:GLU:N	49:BT:54:GLU:OE1	2.25	0.69
7:AG:50:LEU:HD22	7:AG:124:LEU:CD1	2.22	0.69
7:AG:28:ASN:OD1	7:AG:36:LYS:NZ	2.25	0.69
17:AQ:61:ILE:HG22	17:AQ:73:TRP:HE3	1.58	0.69
7:AG:130:ASN:HA	7:AG:135:VAL:HG21	1.74	0.69
35:BE:46:GLN:O	35:BE:88:ARG:NH2	2.26	0.69
31:BA:2304:G:H22	31:BA:2312:U:H3	1.39	0.68
31:BA:1847:A:O2'	31:BA:1848:A:O5'	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BU:46:GLN:N	50:BU:46:GLN:OE1	2.26	0.68
16:AP:18:GLN:HG2	16:AP:35:ARG:HE	1.59	0.68
1:AA:1526:G:P	21:AU:39:GLU:HG2	2.34	0.68
31:BA:2162:G:O2'	31:BA:2164:C:N4	2.27	0.68
12:AL:77:HIS:O	12:AL:78:SER:OG	2.09	0.68
31:BA:1789:A:OP2	33:BC:221:ARG:NH1	2.27	0.68
9:AI:50:GLN:OE1	9:AI:80:ARG:NH1	2.26	0.67
10:AJ:10:LEU:HD22	10:AJ:98:VAL:HG22	1.76	0.67
12:AL:75:GLN:O	12:AL:77:HIS:N	2.26	0.67
31:BA:2130:U:O2'	31:BA:2158:A:N1	2.25	0.67
31:BA:1163:G:OP1	47:BR:24:LYS:NZ	2.24	0.67
37:BG:24:ILE:HD13	37:BG:72:LEU:HD21	1.77	0.67
10:AJ:35:GLN:HB3	10:AJ:77:VAL:HG12	1.75	0.67
49:BT:68:LYS:O	49:BT:69:ARG:NH2	2.28	0.67
23:AW:59:U:O2'	23:AW:60:C:OP1	2.13	0.67
40:BK:89:ASN:HD22	40:BK:89:ASN:C	2.01	0.67
41:BL:108:ALA:HB3	41:BL:125:LEU:HD22	1.77	0.66
27:B2:12:ARG:HE	27:B2:44:VAL:HG21	1.59	0.66
31:BA:1082:U:H2'	31:BA:1083:U:C2	2.31	0.66
6:AF:22:ILE:O	6:AF:26:THR:HG23	1.95	0.66
7:AG:113:ASP:OD2	7:AG:122:ASN:ND2	2.27	0.66
43:BN:69:ARG:O	43:BN:70:THR:OG1	2.12	0.66
31:BA:1534:U:HO2'	31:BA:1537:G:H1	1.43	0.66
1:AA:410:G:OP1	4:AD:26:ARG:NH2	2.28	0.66
37:BG:2:SER:OG	37:BG:3:ARG:N	2.28	0.66
31:BA:994:C:OP2	46:BQ:54:LYS:NZ	2.29	0.65
47:BR:38:VAL:HG21	47:BR:57:GLY:HA3	1.78	0.65
16:AP:4:ILE:HD12	16:AP:21:VAL:HG22	1.77	0.65
23:AW:1:G:N2	23:AW:73:A:H1'	2.11	0.65
31:BA:1064:C:C6	31:BA:1066:U:H1'	2.31	0.65
31:BA:1084:A:H2'	31:BA:1085:A:C2	2.31	0.65
41:BL:77:ILE:CD1	41:BL:108:ALA:HB1	2.26	0.65
1:AA:1311:A:OP1	30:B5:59:ARG:NH1	2.29	0.65
5:AE:102:GLY:O	5:AE:103:THR:OG1	2.10	0.65
10:AJ:35:GLN:HG3	10:AJ:78:GLU:N	2.11	0.65
1:AA:511:C:O2'	1:AA:512:U:OP2	2.10	0.65
10:AJ:32:THR:HG23	10:AJ:83:THR:HG22	1.79	0.65
13:AM:11:ASP:O	13:AM:12:HIS:ND1	2.29	0.65
50:BU:53:ASN:C	50:BU:55:PRO:HD3	2.22	0.65
4:AD:188:ARG:NH2	4:AD:197:GLU:OE2	2.29	0.65
23:AY:47:U:C4	23:AY:50:G:H5''	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BA:1070:A:N7	31:BA:1096:A:O2'	2.30	0.65
34:BD:105:LYS:HA	34:BD:177:VAL:HG12	1.77	0.64
1:AA:995:C:N3	1:AA:1046:A:O2'	2.30	0.64
10:AJ:35:GLN:NE2	10:AJ:78:GLU:HB2	2.12	0.64
15:AO:14:GLU:OE2	15:AO:84:ARG:NH2	2.31	0.64
31:BA:1047:G:HO2'	31:BA:1110:G:H1	1.46	0.64
31:BA:2111:U:HO2'	31:BA:2112:G:P	2.20	0.64
10:AJ:93:ALA:HB1	10:AJ:96:VAL:HG12	1.80	0.64
32:BB:42:C:N3	36:BF:90:THR:HG22	2.13	0.64
3:AC:49:LYS:O	3:AC:72:ARG:NH1	2.30	0.64
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.32	0.63
2:AB:114:LEU:HD13	2:AB:144:LEU:HB3	1.79	0.63
37:BG:38:ASN:OD1	37:BG:39:ASP:N	2.31	0.63
31:BA:894:U:O2'	31:BA:895:U:O4'	2.11	0.63
37:BG:80:THR:HG1	37:BG:81:GLU:CD	2.05	0.63
1:AA:1138:G:H2'	1:AA:1140:C:H5'	1.80	0.63
9:AI:120:LYS:O	9:AI:122:ARG:N	2.31	0.63
41:BL:29:LYS:O	41:BL:30:THR:OG1	2.10	0.63
20:AT:3:ASN:OD1	20:AT:4:ILE:N	2.31	0.63
24:AX:23:G:O2'	24:AX:24:C:OP2	2.16	0.63
31:BA:2114:A:C8	31:BA:2167:U:H4'	2.34	0.63
1:AA:9:G:OP2	5:AE:126:LYS:NZ	2.30	0.63
31:BA:84:A:H62	31:BA:101:A:H2	1.47	0.63
37:BG:11:VAL:HG12	37:BG:48:ASN:O	1.99	0.63
29:B4:16:ILE:HD13	29:B4:25:VAL:HG22	1.79	0.63
1:AA:429:U:H5'	4:AD:9:LEU:HD12	1.81	0.62
15:AO:89:ARG:NH1	31:BA:712:G:OP2	2.32	0.62
31:BA:2155:U:H3'	31:BA:2156:G:C8	2.34	0.62
40:BK:105:ARG:HH21	45:BP:32:VAL:HG21	1.64	0.62
47:BR:25:LEU:HG	47:BR:94:THR:HG21	1.80	0.62
3:AC:11:ARG:NH1	3:AC:177:THR:O	2.32	0.62
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.82	0.62
31:BA:2641:G:H5''	39:BJ:78:THR:HG23	1.81	0.62
1:AA:346:G:OP1	45:BP:39:ARG:NH1	2.31	0.62
2:AB:130:THR:N	2:AB:133:GLU:OE2	2.32	0.62
50:BU:16:GLY:O	50:BU:18:ASP:N	2.33	0.62
2:AB:87:CYS:HB2	2:AB:221:VAL:HG13	1.80	0.62
25:B0:54:VAL:HG23	25:B0:55:ILE:HG12	1.80	0.62
1:AA:828:U:OP1	8:AH:22:LYS:NZ	2.33	0.62
1:AA:673:A:H2'	1:AA:674:G:C8	2.35	0.62
31:BA:1154:G:OP2	46:BQ:58:ARG:NH1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BA:2230:G:H1'	53:BX:32:ASN:HB3	1.81	0.62
9:AI:35:LEU:O	9:AI:40:GLY:N	2.33	0.62
2:AB:20:THR:HB	2:AB:38:VAL:HG12	1.81	0.61
23:AW:44:G:O2'	23:AW:45:G:OP1	2.16	0.61
1:AA:401:C:O2'	1:AA:621:A:N3	2.30	0.61
37:BG:52:PHE:CE2	37:BG:72:LEU:HD22	2.35	0.61
41:BL:81:ASP:O	41:BL:83:ALA:N	2.33	0.61
1:AA:1239:A:H62	1:AA:1299:A:N6	1.98	0.61
1:AA:1527:U:OP2	21:AU:39:GLU:HG3	2.00	0.61
17:AQ:76:VAL:HG12	17:AQ:77:ARG:H	1.65	0.61
31:BA:140:C:H6	31:BA:141:G:H1	1.47	0.61
31:BA:2062:A:N1	31:BA:2503:A:N6	2.48	0.61
40:BK:105:ARG:NH1	40:BK:122:VAL:HG13	2.15	0.61
1:AA:1078:U:O2'	1:AA:1079:G:OP1	2.18	0.61
53:BX:65:ASP:OD1	53:BX:66:THR:N	2.33	0.61
1:AA:1140:C:O2'	1:AA:1141:C:H6	1.84	0.61
33:BC:107:PRO:HG2	33:BC:110:LEU:HD13	1.83	0.61
14:AN:27:LEU:HD11	14:AN:48:LEU:HD23	1.82	0.61
1:AA:842:U:N3	1:AA:843:U:O2'	2.33	0.60
23:AW:59:U:HO2'	23:AW:60:C:P	2.24	0.60
23:AY:72:C:H2'	23:AY:73:A:C8	2.36	0.60
25:B0:54:VAL:O	25:B0:56:ALA:N	2.33	0.60
54:BY:6:LEU:O	54:BY:60:LYS:NZ	2.34	0.60
1:AA:1266:G:N2	1:AA:1269:A:OP2	2.29	0.60
31:BA:2168:G:H2'	31:BA:2169:A:H8	1.63	0.60
31:BA:1062:G:H2'	31:BA:1063:G:C8	2.37	0.60
23:AY:18:G:H4'	23:AY:60:C:C4	2.37	0.60
31:BA:2469:A:N6	31:BA:2481:G:O2'	2.34	0.60
1:AA:823:C:HO2'	8:AH:2:SER:N	2.00	0.60
55:BZ:39:GLU:OE1	55:BZ:41:THR:HG23	2.01	0.60
15:AO:4:SER:O	15:AO:8:THR:HG23	2.01	0.60
1:AA:1025:U:H4'	1:AA:1026:G:H8	1.67	0.60
9:AI:106:ARG:NH1	9:AI:107:ASP:O	2.35	0.60
49:BT:5:GLU:CD	49:BT:5:GLU:H	2.10	0.60
1:AA:1005:A:N6	1:AA:1024:G:O2'	2.35	0.59
2:AB:73:LYS:O	2:AB:74:ARG:C	2.45	0.59
17:AQ:46:VAL:HG11	17:AQ:61:ILE:HD12	1.83	0.59
23:AW:74:C:H3'	23:AW:75:C:C6	2.37	0.59
31:BA:2311:A:N3	36:BF:85:ILE:HD11	2.17	0.59
16:AP:42:ILE:O	16:AP:44:SER:N	2.32	0.59
23:AY:58:A:H2'	23:AY:60:C:C5	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BA:2125:G:O2'	31:BA:2173:A:N6	2.35	0.59
3:AC:40:ARG:NH1	3:AC:55:ILE:O	2.35	0.59
4:AD:188:ARG:NH2	4:AD:193:ALA:HA	2.16	0.59
1:AA:544:G:OP1	4:AD:56:ARG:NH2	2.35	0.59
9:AI:65:ILE:HG21	9:AI:79:ILE:HD12	1.85	0.59
35:BE:188:MET:HE2	35:BE:193:VAL:HA	1.84	0.59
21:AU:37:PHE:HD2	21:AU:40:LYS:HZ3	1.50	0.59
30:B5:35:ASP:OD1	30:B5:36:VAL:N	2.36	0.59
10:AJ:35:GLN:CD	10:AJ:78:GLU:HB2	2.27	0.59
31:BA:27:G:O2'	31:BA:28:A:OP2	2.20	0.59
1:AA:1071:C:OP1	5:AE:54:ARG:NH2	2.36	0.59
4:AD:191:LEU:O	4:AD:193:ALA:N	2.36	0.59
31:BA:389:G:C8	31:BA:2413:G:H4'	2.38	0.58
9:AI:25:ASN:N	9:AI:62:ASP:OD2	2.35	0.58
44:BO:2:ASP:OD1	44:BO:3:LYS:N	2.36	0.58
51:BV:6:ALA:HB1	51:BV:40:ILE:HG23	1.85	0.58
54:BY:2:LYS:HZ3	54:BY:6:LEU:HD22	1.68	0.58
31:BA:1064:C:H2'	31:BA:1065:U:H5	1.68	0.58
36:BF:44:ILE:HD11	36:BF:79:ILE:HG22	1.86	0.58
8:AH:54:ASP:OD1	8:AH:55:THR:N	2.37	0.58
13:AM:90:ARG:HB3	13:AM:97:VAL:HG12	1.86	0.58
31:BA:219:A:N3	31:BA:234:U:O2'	2.36	0.58
31:BA:2190:G:H2'	31:BA:2191:A:O4'	2.04	0.58
24:AX:9:G:H5'	24:AX:47:G:H21	1.69	0.58
37:BG:52:PHE:HE2	37:BG:72:LEU:HD22	1.67	0.58
9:AI:65:ILE:HG21	9:AI:79:ILE:CD1	2.34	0.58
17:AQ:59:VAL:HG12	17:AQ:78:VAL:HG23	1.85	0.58
31:BA:1534:U:O2'	31:BA:1537:G:N1	2.35	0.58
31:BA:2162:G:N2	31:BA:2163:A:N3	2.51	0.58
31:BA:2100:G:C6	31:BA:2190:G:C6	2.92	0.57
33:BC:160:THR:HG23	33:BC:177:ARG:HG3	1.85	0.57
30:B5:39:LYS:O	30:B5:45:THR:HG22	2.02	0.57
8:AH:72:VAL:HG23	8:AH:72:VAL:O	2.03	0.57
17:AQ:47:HIS:NE2	17:AQ:49:GLU:OE2	2.36	0.57
1:AA:843:U:OP1	1:AA:844:G:N2	2.33	0.57
14:AN:26:GLU:HB2	14:AN:30:ILE:HD12	1.85	0.57
1:AA:1532:U:O4	1:AA:1533:C:N4	2.38	0.57
2:AB:130:THR:OG1	2:AB:133:GLU:OE1	2.21	0.57
6:AF:62:MET:HG2	6:AF:64:VAL:HG13	1.87	0.57
13:AM:16:VAL:HG13	13:AM:17:ILE:HG13	1.87	0.57
26:B1:6:ARG:NH1	31:BA:2285:C:OP2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BA:1871:A:O2'	31:BA:1872:A:O5'	2.23	0.57
34:BD:136:ASN:ND2	34:BD:139:SER:O	2.37	0.57
52:BW:11:ARG:O	52:BW:14:ARG:NH2	2.36	0.57
1:AA:751:U:OP1	15:AO:17:ARG:NH2	2.38	0.57
4:AD:57:GLU:OE2	4:AD:196:ASN:N	2.37	0.57
37:BG:55:ARG:HB3	37:BG:58:TYR:HE2	1.70	0.56
42:BM:69:PRO:O	42:BM:70:ASP:OD1	2.23	0.56
1:AA:1145:A:HO2'	1:AA:1146:A:P	2.28	0.56
23:AW:71:C:H2'	23:AW:72:C:O4'	2.06	0.56
27:B2:44:VAL:HG13	27:B2:44:VAL:O	2.05	0.56
31:BA:286:U:H2'	31:BA:287:G:H8	1.69	0.56
6:AF:54:LEU:HD23	6:AF:54:LEU:O	2.04	0.56
31:BA:2286:G:H4'	31:BA:2287:A:O5'	2.05	0.56
42:BM:26:VAL:HG23	42:BM:104:GLU:CD	2.30	0.56
1:AA:70:U:O2'	1:AA:94:G:N7	2.22	0.56
1:AA:362:G:N2	1:AA:365:U:OP2	2.36	0.56
1:AA:1166:G:N1	1:AA:1169:A:OP2	2.38	0.56
3:AC:79:LYS:O	3:AC:82:GLU:OE1	2.23	0.56
29:B4:3:VAL:CG1	29:B4:37:GLN:OE1	2.54	0.56
4:AD:95:GLU:O	4:AD:100:ASN:ND2	2.38	0.56
13:AM:3:ARG:NE	30:B5:35:ASP:OD2	2.37	0.56
27:B2:24:THR:HG23	27:B2:27:GLY:H	1.71	0.56
31:BA:2641:G:O3'	39:BJ:78:THR:HG21	2.06	0.56
1:AA:161:A:H2	1:AA:347:G:H21	1.53	0.56
16:AP:23:ASP:OD1	16:AP:24:SER:N	2.38	0.56
31:BA:1064:C:C5	31:BA:1066:U:H1'	2.41	0.56
37:BG:133:LEU:HB3	37:BG:141:ILE:HD11	1.86	0.56
5:AE:99:ALA:HB3	5:AE:122:ASN:O	2.06	0.56
14:AN:92:GLU:N	14:AN:92:GLU:OE1	2.38	0.56
1:AA:1538:C:N3	1:AA:1539:C:N4	2.54	0.56
5:AE:105:ILE:HD11	5:AE:120:VAL:HG23	1.88	0.56
31:BA:2111:U:O4'	31:BA:2118:U:O2'	2.23	0.56
1:AA:1178:G:N2	1:AA:1181:G:OP2	2.32	0.56
18:AR:38:LYS:NZ	21:AU:24:GLU:OE2	2.33	0.56
31:BA:484:C:OP2	50:BU:47:LYS:NZ	2.34	0.56
49:BT:92:ASN:C	49:BT:93:LEU:HD12	2.30	0.56
1:AA:160:A:H2'	1:AA:161:A:C8	2.40	0.55
31:BA:2572:A:N7	34:BD:150:GLN:HB2	2.21	0.55
37:BG:101:ASN:ND2	37:BG:116:GLN:OE1	2.39	0.55
55:BZ:3:LYS:O	55:BZ:4:THR:OG1	2.13	0.55
1:AA:664:G:H22	1:AA:741:G:H1	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1368:A:OP1	10:AJ:64:GLN:NE2	2.37	0.55
5:AE:149:SER:HB2	5:AE:152:MET:HE3	1.88	0.55
14:AN:34:VAL:O	14:AN:34:VAL:HG13	2.05	0.55
38:BH:7:ASP:OD1	38:BH:8:LYS:N	2.35	0.55
45:BP:33:VAL:HG12	45:BP:35:GLY:H	1.71	0.55
49:BT:67:VAL:CG1	49:BT:69:ARG:HH22	2.20	0.55
1:AA:717:U:H4'	11:AK:119:ASN:HD21	1.70	0.55
5:AE:80:THR:OG1	5:AE:98:PRO:O	2.24	0.55
26:B1:25:LYS:HD3	26:B1:27:LYS:HG3	1.89	0.55
31:BA:398:C:OP1	53:BX:32:ASN:ND2	2.40	0.55
54:BY:2:LYS:NZ	54:BY:6:LEU:HD22	2.21	0.55
2:AB:81:LYS:HG2	2:AB:82:ASP:N	2.20	0.55
31:BA:1012:U:O4	39:BJ:30:THR:HG21	2.07	0.55
31:BA:2298:A:OP1	36:BF:71:ARG:NH1	2.40	0.55
3:AC:111:LEU:CD2	3:AC:146:ALA:HB2	2.36	0.55
46:BQ:86:ALA:O	46:BQ:87:SER:OG	2.21	0.55
14:AN:19:LYS:O	14:AN:23:LYS:NZ	2.39	0.55
25:B0:30:VAL:HG12	25:B0:37:LYS:HD3	1.88	0.55
31:BA:856:G:H2'	31:BA:857:G:C8	2.41	0.55
1:AA:161:A:C4	1:AA:162:A:C2	2.95	0.54
2:AB:66:LYS:HE2	2:AB:158:PRO:HA	1.89	0.54
4:AD:188:ARG:NH1	4:AD:191:LEU:O	2.39	0.54
25:B0:25:VAL:O	25:B0:26:THR:HG22	2.07	0.54
25:B0:16:ARG:NH1	31:BA:1266:G:OP1	2.40	0.54
1:AA:981:U:OP1	14:AN:9:ARG:NH1	2.40	0.54
1:AA:1226:C:OP2	13:AM:90:ARG:NH2	2.40	0.54
23:AY:34:C:H3'	23:AY:35:A:C8	2.41	0.54
26:B1:50:LYS:HG2	26:B1:51:GLU:H	1.70	0.54
31:BA:283:G:H2'	31:BA:284:U:O4'	2.06	0.54
1:AA:160:A:N6	1:AA:343:U:O2'	2.39	0.54
10:AJ:92:LEU:O	10:AJ:92:LEU:HD12	2.07	0.54
31:BA:1045:C:O2	31:BA:1047:G:N1	2.41	0.54
2:AB:74:ARG:O	2:AB:75:ALA:C	2.50	0.54
38:BH:2:GLN:O	38:BH:3:VAL:HG22	2.07	0.54
50:BU:4:LYS:O	50:BU:94:ARG:NH1	2.41	0.54
1:AA:511:C:O3'	4:AD:44:ARG:NH2	2.40	0.54
35:BE:105:LEU:HD23	35:BE:200:LEU:HD21	1.89	0.54
47:BR:55:ASP:OD1	47:BR:56:GLY:N	2.40	0.54
1:AA:202:G:H21	1:AA:466:A:H61	1.55	0.54
1:AA:1137:C:O2	1:AA:1138:G:N2	2.40	0.54
1:AA:1157:A:H4'	1:AA:1158:C:O5'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AJ:35:GLN:CG	10:AJ:78:GLU:HB2	2.38	0.54
1:AA:96:U:O2'	1:AA:97:G:P	2.66	0.54
1:AA:975:A:H8	1:AA:1357:A:HO2'	1.56	0.54
21:AU:40:LYS:HB3	21:AU:41:PRO:HD3	1.89	0.54
50:BU:34:VAL:HG13	50:BU:67:VAL:HG22	1.90	0.54
19:AS:11:ILE:HG13	19:AS:12:ASP:N	2.23	0.54
24:AX:24:C:O2'	24:AX:25:U:OP2	2.21	0.54
1:AA:205:A:N3	1:AA:206:C:N4	2.56	0.54
4:AD:149:ALA:O	4:AD:152:GLN:HB2	2.08	0.54
12:AL:14:ARG:HE	12:AL:15:LYS:H	1.56	0.54
23:AY:72:C:H2'	23:AY:73:A:H8	1.73	0.54
1:AA:6:G:O6	5:AE:100:SER:N	2.40	0.53
1:AA:202:G:N1	1:AA:216:U:N3	2.56	0.53
1:AA:451:A:H61	1:AA:481:G:H5'	1.73	0.53
3:AC:134:MET:HE1	3:AC:166:GLU:O	2.08	0.53
23:AW:72:C:H2'	23:AW:73:A:O4'	2.08	0.53
42:BM:34:LYS:HD2	42:BM:131:VAL:HG11	1.89	0.53
13:AM:13:LYS:O	13:AM:14:HIS:CD2	2.61	0.53
31:BA:807:U:OP2	41:BL:41:ARG:NH2	2.42	0.53
23:AY:71:C:H2'	23:AY:72:C:O4'	2.07	0.53
31:BA:140:C:H1'	31:BA:141:G:C2	2.43	0.53
1:AA:1152:A:OP1	10:AJ:70:HIS:ND1	2.40	0.53
2:AB:151:ILE:HD11	2:AB:154:MET:SD	2.48	0.53
2:AB:167:ASP:OD2	2:AB:168:HIS:N	2.41	0.53
24:AX:20:G:O6	36:BF:80:ARG:NH2	2.42	0.53
31:BA:85:G:OP1	50:BU:7:ARG:N	2.40	0.53
31:BA:2156:G:O5'	31:BA:2156:G:H8	1.90	0.53
36:BF:11:GLU:HG2	36:BF:14:LYS:NZ	2.23	0.53
4:AD:29:ASP:C	4:AD:30:THR:HG1	2.13	0.53
31:BA:974:G:H8	31:BA:990:A:H62	1.56	0.53
2:AB:117:LEU:HB2	2:AB:141:LEU:HD13	1.90	0.53
6:AF:19:PRO:O	6:AF:23:GLU:OE1	2.27	0.53
31:BA:2848:G:O2'	31:BA:2867:G:N2	2.32	0.53
41:BL:141:LYS:NZ	41:BL:143:GLU:OE1	2.41	0.53
1:AA:131:A:O2'	1:AA:262:A:N3	2.36	0.53
31:BA:1847:A:HO2'	31:BA:1848:A:P	2.32	0.53
40:BK:99:ILE:HG23	40:BK:118:LEU:CB	2.38	0.53
1:AA:1026:G:H1	1:AA:1035:A:H61	1.57	0.53
6:AF:49:TYR:HB3	18:AR:74:HIS:HD1	1.72	0.53
21:AU:37:PHE:CD2	21:AU:40:LYS:HB2	2.44	0.53
23:AY:60:C:H5'	23:AY:61:C:H5	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BA:475:C:O2	31:BA:479:A:N6	2.34	0.53
1:AA:160:A:H61	1:AA:343:U:H1'	1.74	0.53
1:AA:722:G:H5''	21:AU:45:ARG:HH21	1.72	0.53
31:BA:1567:G:H2'	33:BC:85:PRO:HG3	1.90	0.53
39:BJ:125:TYR:OH	39:BJ:132:HIS:NE2	2.34	0.53
54:BY:24:GLU:O	54:BY:28:LEU:HD23	2.09	0.53
8:AH:64:LYS:HB3	8:AH:71:VAL:HG21	1.91	0.52
10:AJ:7:ARG:NE	10:AJ:75:ASP:OD1	2.29	0.52
31:BA:1068:G:H2'	31:BA:1069:A:O4'	2.09	0.52
31:BA:1084:A:H2'	31:BA:1085:A:N3	2.24	0.52
31:BA:2154:A:N6	31:BA:2156:G:H22	2.06	0.52
1:AA:1539:C:O2'	1:AA:1540:U:O4'	2.15	0.52
12:AL:68:GLY:O	12:AL:99:ARG:NH1	2.39	0.52
31:BA:1068:G:O5'	31:BA:1068:G:H8	1.92	0.52
31:BA:1942:C:OP2	31:BA:1943:U:O2'	2.09	0.52
2:AB:16:PHE:O	2:AB:40:ILE:HG22	2.09	0.52
2:AB:78:GLU:HG3	2:AB:81:LYS:NZ	2.24	0.52
14:AN:3:LYS:O	14:AN:6:MET:N	2.37	0.52
23:AY:58:A:H2'	23:AY:58:A:N3	2.24	0.52
1:AA:115:G:H4'	1:AA:116:A:O5'	2.10	0.52
1:AA:890:G:O2'	1:AA:906:A:N6	2.42	0.52
3:AC:148:GLY:O	3:AC:173:VAL:HG22	2.09	0.52
31:BA:1141:U:H4'	31:BA:1142:A:O4'	2.09	0.52
2:AB:64:LYS:HE2	2:AB:225:ARG:HG3	1.92	0.52
31:BA:277:G:H2'	31:BA:361:G:C6	2.45	0.52
1:AA:1138:G:C2'	1:AA:1140:C:H5'	2.40	0.52
36:BF:25:VAL:O	36:BF:28:VAL:HG12	2.09	0.52
1:AA:323:U:H2'	1:AA:324:G:O4'	2.09	0.52
1:AA:1078:U:HO2'	1:AA:1079:G:P	2.33	0.52
3:AC:156:ARG:NE	3:AC:160:ALA:O	2.43	0.52
26:B1:50:LYS:HG2	26:B1:51:GLU:N	2.24	0.52
1:AA:568:G:O6	12:AL:2:ALA:HB2	2.10	0.52
1:AA:207:C:H4'	1:AA:207:C:OP1	2.09	0.52
11:AK:118:HIS:O	11:AK:119:ASN:OD1	2.28	0.52
16:AP:39:PHE:CD1	16:AP:50:THR:HG22	2.45	0.52
31:BA:286:U:H2'	31:BA:287:G:C8	2.45	0.52
31:BA:883:G:H5''	31:BA:884:U:H5	1.75	0.52
1:AA:1328:C:H5''	13:AM:28:THR:HG21	1.92	0.51
1:AA:187:G:N2	1:AA:190:A:OP2	2.43	0.51
1:AA:205:A:H2'	1:AA:206:C:C5	2.44	0.51
4:AD:151:LYS:O	4:AD:152:GLN:C	2.52	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BA:1178:C:O2'	31:BA:1179:G:H5'	2.10	0.51
31:BA:2857:G:N2	31:BA:2860:A:OP2	2.30	0.51
33:BC:204:VAL:O	33:BC:206:GLY:N	2.43	0.51
15:AO:26:GLU:OE1	15:AO:26:GLU:N	2.39	0.51
31:BA:161:A:H3'	31:BA:162:U:H5''	1.91	0.51
31:BA:1802:A:H2'	31:BA:1803:A:C8	2.45	0.51
31:BA:2646:C:OP2	31:BA:2732:G:O2'	2.27	0.51
39:BJ:9:GLU:HG2	39:BJ:10:THR:HG23	1.93	0.51
41:BL:93:ASN:O	41:BL:94:THR:OG1	2.22	0.51
1:AA:875:U:O2'	8:AH:15:ARG:NH1	2.41	0.51
31:BA:784:G:O2'	31:BA:785:G:P	2.69	0.51
31:BA:1028:A:N6	31:BA:1125:G:H2'	2.26	0.51
17:AQ:14:SER:HB3	17:AQ:22:VAL:CG1	2.41	0.51
31:BA:1064:C:O2	31:BA:1074:G:C2	2.63	0.51
31:BA:2331:G:O2'	52:BW:43:THR:HG22	2.10	0.51
1:AA:204:G:H1'	1:AA:465:A:C2	2.45	0.51
21:AU:37:PHE:CZ	21:AU:39:GLU:HB2	2.44	0.51
31:BA:547:A:H3'	31:BA:548:G:C5'	2.40	0.51
31:BA:2167:U:C2	31:BA:2169:A:H5'	2.46	0.51
36:BF:142:ASP:O	36:BF:146:VAL:HG13	2.09	0.51
37:BG:42:GLU:HA	37:BG:55:ARG:NH2	2.26	0.51
31:BA:883:G:H3'	31:BA:884:U:H6	1.76	0.51
31:BA:2169:A:C8	31:BA:2169:A:H5''	2.46	0.51
1:AA:161:A:C5	1:AA:162:A:C2	2.98	0.51
1:AA:421:U:O2	3:AC:127:ARG:NH2	2.44	0.51
1:AA:1356:G:H2'	1:AA:1357:A:H8	1.74	0.51
26:B1:5:ILE:HG22	26:B1:5:ILE:O	2.10	0.51
31:BA:2156:G:H2'	31:BA:2157:G:N3	2.25	0.51
1:AA:713:G:H2'	1:AA:714:G:C8	2.46	0.51
20:AT:49:LYS:O	20:AT:53:GLU:OE1	2.28	0.51
23:AW:73:A:H2'	23:AW:74:C:O4'	2.11	0.51
31:BA:140:C:H4'	31:BA:140:C:OP1	2.11	0.51
31:BA:1800:C:OP2	33:BC:182:ARG:NH2	2.44	0.51
31:BA:2125:G:C2'	31:BA:2173:A:H61	2.23	0.51
1:AA:206:C:H3'	1:AA:206:C:H6	1.75	0.50
1:AA:1086:U:H3	1:AA:1099:G:H22	1.59	0.50
1:AA:246:A:C2	1:AA:282:A:C5	2.99	0.50
1:AA:464:U:N3	1:AA:467:U:OP2	2.39	0.50
1:AA:1077:G:N2	1:AA:1080:A:OP2	2.40	0.50
2:AB:66:LYS:HA	2:AB:89:GLN:OE1	2.11	0.50
3:AC:85:GLU:OE2	3:AC:88:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AJ:80:THR:HB	10:AJ:83:THR:OG1	2.11	0.50
51:BV:6:ALA:HB1	51:BV:40:ILE:CG2	2.41	0.50
1:AA:1201:A:H1'	1:AA:1202:U:OP2	2.11	0.50
2:AB:64:LYS:HB2	2:AB:225:ARG:NH2	2.26	0.50
31:BA:2328:A:H2'	31:BA:2329:U:C6	2.47	0.50
31:BA:2642:G:P	39:BJ:78:THR:HG21	2.52	0.50
1:AA:1013:G:N2	1:AA:1016:A:OP2	2.41	0.50
2:AB:64:LYS:HB2	2:AB:225:ARG:CZ	2.42	0.50
11:AK:110:ILE:HG21	21:AU:17:ARG:HD3	1.93	0.50
16:AP:51:ARG:O	16:AP:52:LEU:HD12	2.11	0.50
31:BA:593:U:H2'	31:BA:594:U:C6	2.46	0.50
35:BE:4:VAL:HG13	35:BE:4:VAL:O	2.10	0.50
1:AA:714:G:H2'	1:AA:715:A:C8	2.47	0.50
7:AG:69:VAL:HG23	7:AG:100:ALA:HB1	1.92	0.50
11:AK:85:MET:CE	11:AK:113:VAL:HG11	2.42	0.50
21:AU:28:VAL:HG13	21:AU:29:LEU:HD22	1.94	0.50
26:B1:26:ASN:C	26:B1:26:ASN:HD22	2.18	0.50
30:B5:28:VAL:HG11	30:B5:32:LEU:HD11	1.94	0.50
31:BA:1315:C:O2'	31:BA:1392:A:N3	2.44	0.50
1:AA:757:U:OP1	1:AA:822:U:O2'	2.29	0.50
1:AA:1004:A:H2'	1:AA:1005:A:O4'	2.12	0.50
1:AA:1305:G:H21	1:AA:1332:A:H2	1.58	0.50
23:AY:57:G:C5	23:AY:58:A:H1'	2.46	0.50
31:BA:306:U:H2'	31:BA:307:G:O4'	2.12	0.50
1:AA:1003:G:N2	1:AA:1004:A:O2'	2.45	0.50
31:BA:2119:A:C6	31:BA:2169:A:C5	2.99	0.50
3:AC:83:ASP:OD1	3:AC:84:VAL:N	2.45	0.50
5:AE:25:VAL:HG22	5:AE:26:LYS:H	1.75	0.50
9:AI:57:MET:O	9:AI:59:GLU:N	2.44	0.50
23:AY:35:A:H2'	23:AY:36:C:O4'	2.11	0.50
1:AA:1088:G:H21	1:AA:1167:A:N6	2.09	0.50
21:AU:17:ARG:HE	21:AU:20:LYS:HE3	1.77	0.50
41:BL:81:ASP:OD1	41:BL:82:LEU:N	2.41	0.50
48:BS:29:VAL:HG13	48:BS:55:ILE:HD11	1.93	0.50
50:BU:51:ALA:O	50:BU:52:LEU:HB2	2.11	0.50
4:AD:15:GLU:OE2	4:AD:63:ARG:NH1	2.46	0.49
31:BA:948:C:O2	31:BA:984:A:O2'	2.28	0.49
31:BA:1816:C:N4	33:BC:35:GLU:OE2	2.31	0.49
1:AA:161:A:C2	1:AA:162:A:H2	2.29	0.49
4:AD:13:ARG:NH2	4:AD:37:ALA:O	2.45	0.49
23:AY:34:C:H3'	23:AY:35:A:H8	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AY:37:A:H2'	23:AY:38:A:C8	2.48	0.49
31:BA:2581:G:OP2	31:BA:2581:G:N2	2.45	0.49
1:AA:204:G:H5''	1:AA:205:A:N7	2.26	0.49
2:AB:79:ALA:O	2:AB:214:LEU:HD13	2.11	0.49
19:AS:5:LEU:HB3	19:AS:7:LYS:HG2	1.94	0.49
23:AY:55:PSU:N3	23:AY:58:A:N7	2.60	0.49
31:BA:282:A:N6	31:BA:359:G:O6	2.45	0.49
31:BA:877:A:O2'	31:BA:900:A:N6	2.46	0.49
1:AA:373:A:C2	1:AA:374:A:C8	3.00	0.49
6:AF:5:GLU:OE1	18:AR:24:LYS:NZ	2.39	0.49
31:BA:404:A:H1'	31:BA:405:U:OP2	2.12	0.49
44:BO:33:ARG:O	44:BO:34:HIS:HB2	2.11	0.49
4:AD:97:ARG:NH1	4:AD:99:ASP:OD2	2.45	0.49
12:AL:33:VAL:HG12	12:AL:33:VAL:O	2.11	0.49
31:BA:1125:G:OP2	31:BA:1126:A:O2'	2.27	0.49
1:AA:412:A:O2'	1:AA:413:G:H4'	2.12	0.49
2:AB:36:ASN:O	2:AB:38:VAL:HG13	2.12	0.49
4:AD:148:LYS:O	4:AD:149:ALA:HB3	2.12	0.49
31:BA:1009:A:OP1	39:BJ:39:LYS:NZ	2.45	0.49
31:BA:1080:A:H61	31:BA:1087:G:H5''	1.77	0.49
31:BA:2112:G:HO2'	31:BA:2113:U:P	2.33	0.49
31:BA:2262:U:OP2	52:BW:16:SER:OG	2.24	0.49
32:BB:51:G:OP1	44:BO:63:LYS:NZ	2.46	0.49
1:AA:544:G:OP1	4:AD:59:GLN:NE2	2.46	0.49
4:AD:9:LEU:HB3	4:AD:32:CYS:SG	2.53	0.49
11:AK:52:PHE:O	11:AK:52:PHE:CD2	2.66	0.49
25:B0:52:ARG:NH1	25:B0:54:VAL:HG12	2.28	0.49
31:BA:1180:U:H3'	31:BA:1181:U:C6	2.48	0.49
1:AA:945:G:C2	1:AA:946:A:C8	3.00	0.49
6:AF:29:ILE:HD13	6:AF:64:VAL:HG11	1.94	0.49
31:BA:883:G:H3'	31:BA:884:U:C6	2.48	0.49
31:BA:1028:A:H2'	31:BA:1029:A:C8	2.48	0.49
31:BA:2142:A:H2'	31:BA:2143:C:C6	2.47	0.49
39:BJ:88:THR:HG22	39:BJ:91:GLU:CD	2.37	0.49
5:AE:111:MET:CE	5:AE:125:ALA:HB1	2.42	0.49
31:BA:2640:G:OP1	39:BJ:95:ARG:NH1	2.46	0.49
1:AA:203:G:N2	1:AA:204:G:O6	2.45	0.49
1:AA:259:G:OP1	20:AT:36:TYR:OH	2.28	0.49
2:AB:118:GLU:O	2:AB:122:GLN:NE2	2.46	0.49
31:BA:636:G:OP1	41:BL:129:LYS:NZ	2.40	0.49
31:BA:1754:A:N1	31:BA:2716:C:O2'	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BA:2291:U:H2'	31:BA:2292:U:C6	2.47	0.49
44:BO:56:LYS:O	44:BO:60:GLU:OE1	2.30	0.49
1:AA:161:A:C2	1:AA:162:A:C2	3.01	0.48
1:AA:736:C:OP1	18:AR:61:ARG:NH2	2.41	0.48
23:AY:14:A:H61	23:AY:21:A:H1'	1.78	0.48
31:BA:140:C:H1'	31:BA:141:G:N1	2.28	0.48
31:BA:2071:A:H2'	31:BA:2072:C:C6	2.48	0.48
31:BA:2720:U:OP1	45:BP:53:ARG:NH2	2.46	0.48
1:AA:84:U:O2'	1:AA:85:U:O4'	2.29	0.48
28:B3:54:ASP:HB3	41:BL:57:LEU:HD22	1.94	0.48
31:BA:2148:G:O2'	31:BA:2149:U:O4'	2.21	0.48
34:BD:104:VAL:O	34:BD:105:LYS:HG2	2.13	0.48
5:AE:85:VAL:HG21	5:AE:143:GLY:O	2.13	0.48
8:AH:18:GLN:HE21	8:AH:72:VAL:HG22	1.78	0.48
10:AJ:93:ALA:HB1	10:AJ:96:VAL:CG1	2.44	0.48
31:BA:1092:C:H2'	31:BA:1093:G:O4'	2.13	0.48
31:BA:1853:A:H2'	31:BA:1854:A:C8	2.49	0.48
36:BF:42:GLU:OE2	36:BF:49:LEU:HD13	2.13	0.48
1:AA:746:A:H2'	1:AA:747:A:C8	2.49	0.48
2:AB:20:THR:OG1	2:AB:37:LYS:O	2.25	0.48
2:AB:56:GLU:O	2:AB:57:LEU:C	2.56	0.48
17:AQ:76:VAL:HG12	17:AQ:77:ARG:N	2.26	0.48
23:AW:44:G:HO2'	23:AW:45:G:P	2.35	0.48
31:BA:2140:G:H22	31:BA:2151:U:H2'	1.79	0.48
31:BA:2171:A:O2'	31:BA:2173:A:OP1	2.31	0.48
4:AD:146:ARG:O	4:AD:147:GLU:C	2.55	0.48
31:BA:137:U:O2'	31:BA:138:U:O4'	2.30	0.48
31:BA:703:U:H2'	31:BA:704:G:O4'	2.14	0.48
31:BA:2484:G:OP1	42:BM:44:ARG:NH1	2.42	0.48
34:BD:150:GLN:O	34:BD:151:THR:C	2.57	0.48
49:BT:37:ASP:O	49:BT:38:ALA:O	2.31	0.48
1:AA:31:G:O2'	1:AA:48:C:N4	2.46	0.48
13:AM:3:ARG:NH2	13:AM:7:ILE:HG22	2.29	0.48
1:AA:17:U:H2'	1:AA:18:C:C6	2.49	0.48
1:AA:160:A:N6	1:AA:161:A:N1	2.62	0.48
2:AB:60:ILE:HD13	2:AB:63:ARG:HH21	1.78	0.48
9:AI:55:VAL:HG11	9:AI:94:LEU:HD22	1.95	0.48
31:BA:1066:U:N3	31:BA:1069:A:OP2	2.41	0.48
31:BA:1086:A:H1'	31:BA:1103:A:H61	1.78	0.48
1:AA:1458:G:OP1	20:AT:30:THR:OG1	2.32	0.48
1:AA:1516:G:N2	1:AA:1519:A:OP2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AW:72:C:H2'	23:AW:73:A:C8	2.48	0.48
27:B2:34:ARG:HD3	31:BA:467:G:OP2	2.14	0.48
31:BA:282:A:H2'	31:BA:283:G:C8	2.49	0.48
1:AA:158:G:C6	1:AA:159:G:C5	3.02	0.48
2:AB:33:GLY:O	2:AB:34:ALA:HB2	2.14	0.48
11:AK:52:PHE:HE2	11:AK:62:ALA:HB1	1.79	0.48
11:AK:56:ARG:HG3	11:AK:56:ARG:HH11	1.78	0.48
30:B5:37:CYS:N	30:B5:40:CYS:SG	2.81	0.48
40:BK:87:LEU:HB3	40:BK:92:GLU:HA	1.94	0.48
50:BU:7:ARG:HG3	50:BU:8:ASP:N	2.29	0.48
50:BU:54:GLN:N	50:BU:55:PRO:HD3	2.29	0.48
1:AA:206:C:H42	1:AA:214:C:H1'	1.78	0.48
35:BE:5:LEU:HD23	35:BE:12:LEU:HD11	1.95	0.48
37:BG:55:ARG:HB3	37:BG:58:TYR:CE2	2.48	0.48
40:BK:63:VAL:HG12	40:BK:107:LEU:HD11	1.96	0.48
50:BU:99:ASN:CG	50:BU:101:GLU:OE1	2.57	0.48
19:AS:10:PHE:O	19:AS:39:THR:HG22	2.13	0.47
31:BA:882:G:C4	31:BA:883:G:C8	3.02	0.47
31:BA:2452:C:H2'	31:BA:2453:A:C8	2.49	0.47
31:BA:2561:U:O3'	40:BK:40:LYS:HE3	2.14	0.47
49:BT:3:ARG:NH2	49:BT:5:GLU:HB2	2.29	0.47
1:AA:687:A:C2	1:AA:704:A:C5	3.02	0.47
8:AH:43:GLU:HG3	8:AH:101:ILE:HD13	1.96	0.47
31:BA:1180:U:H3'	31:BA:1181:U:H6	1.79	0.47
2:AB:67:ILE:O	2:AB:161:LEU:HA	2.13	0.47
4:AD:146:ARG:HB3	4:AD:148:LYS:HD3	1.96	0.47
23:AY:33:U:H3'	23:AY:34:C:H5''	1.96	0.47
26:B1:52:ALA:O	26:B1:53:LYS:C	2.58	0.47
31:BA:1066:U:H2'	31:BA:1069:A:N7	2.29	0.47
31:BA:1720:U:H2'	31:BA:1721:G:O4'	2.14	0.47
31:BA:2186:G:N3	31:BA:2186:G:H2'	2.28	0.47
55:BZ:4:THR:HB	55:BZ:37:GLU:OE2	2.13	0.47
21:AU:28:VAL:O	21:AU:32:VAL:HG22	2.14	0.47
23:AW:49:G:O6	23:AW:66:A:N6	2.47	0.47
31:BA:275:C:H2'	31:BA:362:A:N6	2.30	0.47
31:BA:2191:A:H2'	31:BA:2192:U:O4'	2.14	0.47
44:BO:35:ILE:H	44:BO:53:THR:HG22	1.79	0.47
1:AA:127:G:HO2'	17:AQ:6:ARG:HH22	1.58	0.47
1:AA:404:G:O2'	1:AA:498:A:N1	2.47	0.47
1:AA:957:U:H4'	19:AS:79:THR:HG23	1.97	0.47
1:AA:1078:U:O2'	1:AA:1079:G:P	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:62:MET:HG2	6:AF:64:VAL:CG1	2.44	0.47
10:AJ:79:PRO:O	10:AJ:80:THR:C	2.57	0.47
11:AK:63:ALA:HB1	11:AK:96:THR:HG23	1.97	0.47
12:AL:34:CYS:HA	12:AL:55:VAL:HG22	1.95	0.47
25:B0:17:ARG:NE	31:BA:1266:G:OP2	2.47	0.47
31:BA:25:U:O2'	31:BA:26:G:OP1	2.32	0.47
31:BA:1179:G:H3'	31:BA:1180:U:H5''	1.96	0.47
31:BA:2168:G:H8	31:BA:2168:G:OP1	1.98	0.47
31:BA:2169:A:H8	31:BA:2169:A:H5''	1.78	0.47
2:AB:81:LYS:HE3	2:AB:81:LYS:HB3	1.64	0.47
4:AD:148:LYS:HE2	4:AD:148:LYS:HB2	1.55	0.47
31:BA:140:C:H1'	31:BA:141:G:N2	2.30	0.47
31:BA:285:G:C6	31:BA:286:U:C4	3.01	0.47
31:BA:826:U:O2'	41:BL:53:GLY:HA3	2.15	0.47
31:BA:2286:G:H5''	31:BA:2287:A:OP1	2.15	0.47
29:B4:23:ILE:HD13	31:BA:1032:A:H1'	1.97	0.47
31:BA:947:A:O2'	31:BA:984:A:H2	1.98	0.47
31:BA:2114:A:N9	31:BA:2167:U:H4'	2.29	0.47
31:BA:2189:U:N3	31:BA:2190:G:N7	2.63	0.47
31:BA:2266:A:H4'	31:BA:2267:A:N3	2.29	0.47
1:AA:820:U:H4'	1:AA:821:G:OP2	2.15	0.47
5:AE:105:ILE:HG23	5:AE:105:ILE:O	2.14	0.47
31:BA:25:U:HO2'	31:BA:26:G:P	2.38	0.47
40:BK:109:SER:O	40:BK:110:GLU:HG3	2.14	0.47
40:BK:118:LEU:O	40:BK:119:ALA:HB3	2.15	0.47
49:BT:38:ALA:O	49:BT:39:THR:HG23	2.14	0.47
1:AA:81:A:N7	1:AA:83:C:N4	2.62	0.47
1:AA:492:C:H2'	1:AA:493:A:C8	2.50	0.47
2:AB:67:ILE:HD11	2:AB:69:PHE:CE2	2.50	0.47
2:AB:117:LEU:CB	2:AB:141:LEU:HD13	2.44	0.47
10:AJ:34:ALA:C	10:AJ:35:GLN:HG2	2.40	0.47
19:AS:26:GLY:O	19:AS:28:LYS:NZ	2.42	0.47
31:BA:644:A:H2'	31:BA:645:C:O4'	2.15	0.47
31:BA:2110:G:O2'	31:BA:2120:G:OP2	2.30	0.47
2:AB:62:SER:O	2:AB:225:ARG:HG2	2.15	0.47
4:AD:105:MET:HG3	4:AD:171:LEU:HD13	1.96	0.47
13:AM:13:LYS:O	13:AM:14:HIS:CG	2.68	0.47
17:AQ:79:VAL:HG23	17:AQ:80:GLU:OE1	2.15	0.47
31:BA:2129:C:H2'	31:BA:2130:U:O4'	2.15	0.47
32:BB:37:C:O2	44:BO:100:HIS:NE2	2.44	0.47
1:AA:27:G:H2'	1:AA:28:A:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:160:A:C5	1:AA:161:A:C5	3.03	0.46
1:AA:181:A:O2'	1:AA:194:C:N4	2.40	0.46
1:AA:1317:C:HO2'	1:AA:1318:A:P	2.38	0.46
10:AJ:85:ASP:OD2	10:AJ:85:ASP:N	2.46	0.46
1:AA:206:C:N4	1:AA:214:C:O2	2.43	0.46
31:BA:25:U:O2'	31:BA:26:G:P	2.73	0.46
31:BA:1779:U:H5	31:BA:1784:A:N7	2.12	0.46
6:AF:32:ALA:O	6:AF:33:GLU:HG3	2.15	0.46
23:AW:19:G:H4'	23:AW:20:G:OP2	2.13	0.46
31:BA:1071:G:N7	31:BA:1072:C:N4	2.63	0.46
31:BA:2659:G:OP2	37:BG:158:LYS:NZ	2.47	0.46
41:BL:85:VAL:HG21	41:BL:90:VAL:HG12	1.98	0.46
1:AA:1399:C:O2	1:AA:1502:A:N6	2.48	0.46
31:BA:848:C:H2'	31:BA:849:A:H8	1.79	0.46
31:BA:2291:U:OP1	31:BA:2380:C:O2'	2.33	0.46
36:BF:65:PRO:HA	36:BF:89:VAL:HG22	1.98	0.46
37:BG:24:ILE:CD1	37:BG:72:LEU:HD21	2.44	0.46
2:AB:129:LEU:HB3	2:AB:133:GLU:OE2	2.15	0.46
10:AJ:28:THR:O	10:AJ:32:THR:HG22	2.16	0.46
11:AK:123:PRO:HD2	21:AU:35:ARG:CG	2.41	0.46
23:AY:73:A:H3'	23:AY:74:C:C6	2.51	0.46
31:BA:286:U:C2	31:BA:287:G:C8	3.04	0.46
31:BA:1080:A:N6	31:BA:1088:A:OP2	2.48	0.46
31:BA:2119:A:N6	31:BA:2169:A:N7	2.63	0.46
33:BC:260:ASN:C	33:BC:260:ASN:HD22	2.23	0.46
34:BD:108:ASP:OD1	34:BD:173:GLN:HA	2.15	0.46
37:BG:11:VAL:O	37:BG:11:VAL:HG13	2.15	0.46
45:BP:65:SER:O	45:BP:66:ASN:C	2.58	0.46
51:BV:76:ASP:OD1	51:BV:77:VAL:N	2.48	0.46
1:AA:993:G:O2'	1:AA:994:A:N7	2.47	0.46
1:AA:1319:A:O2'	1:AA:1323:G:N7	2.44	0.46
7:AG:9:GLN:OE1	7:AG:10:ARG:N	2.49	0.46
11:AK:126:LYS:HA	21:AU:34:ARG:HD2	1.98	0.46
17:AQ:15:ASP:OD2	17:AQ:15:ASP:C	2.58	0.46
18:AR:34:THR:HG1	18:AR:36:SER:HG	1.61	0.46
31:BA:587:C:OP2	41:BL:21:ARG:NH1	2.45	0.46
31:BA:2308:G:HO2'	31:BA:2309:A:P	2.34	0.46
33:BC:161:TYR:HB3	33:BC:194:GLU:HB3	1.96	0.46
1:AA:440:C:C2	1:AA:441:A:C8	3.04	0.46
2:AB:117:LEU:HD22	2:AB:141:LEU:HB2	1.98	0.46
3:AC:108:LYS:HD3	3:AC:111:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AJ:83:THR:O	10:AJ:84:VAL:C	2.58	0.46
21:AU:24:GLU:HB3	21:AU:28:VAL:HG12	1.97	0.46
31:BA:1068:G:H21	31:BA:1096:A:C5'	2.27	0.46
31:BA:2166:U:H3'	31:BA:2167:U:C6	2.51	0.46
37:BG:107:LEU:O	37:BG:152:ARG:NH1	2.49	0.46
41:BL:81:ASP:C	41:BL:83:ALA:N	2.74	0.46
49:BT:11:LEU:O	54:BY:29:ARG:NH1	2.38	0.46
1:AA:1136:C:O2	1:AA:1136:C:O4'	2.34	0.46
31:BA:534:U:O2'	46:BQ:49:ASP:OD2	2.34	0.46
31:BA:1064:C:C2	31:BA:1074:G:C2	3.03	0.46
52:BW:15:ASP:OD1	52:BW:16:SER:N	2.46	0.46
1:AA:161:A:C6	1:AA:162:A:C2	3.04	0.46
8:AH:11:LEU:HD22	8:AH:75:ILE:HD11	1.96	0.46
31:BA:283:G:N2	31:BA:358:U:O2	2.49	0.46
31:BA:1068:G:H21	31:BA:1096:A:H5''	1.81	0.46
39:BJ:1:MET:SD	39:BJ:2:LYS:O	2.74	0.46
1:AA:677:U:H3	1:AA:713:G:H22	1.63	0.46
2:AB:14:VAL:HG23	2:AB:14:VAL:O	2.16	0.46
2:AB:73:LYS:H	2:AB:73:LYS:HG2	1.46	0.46
2:AB:114:LEU:HD11	2:AB:145:GLU:OE2	2.16	0.46
6:AF:90:MET:HE1	18:AR:61:ARG:CZ	2.46	0.46
7:AG:102:ARG:O	7:AG:106:GLU:HG3	2.16	0.46
12:AL:108:LYS:O	12:AL:109:ASP:OD2	2.34	0.46
16:AP:4:ILE:CD1	16:AP:21:VAL:HG22	2.44	0.46
31:BA:2101:A:C4	31:BA:2102:G:H1'	2.51	0.46
1:AA:159:G:N2	1:AA:161:A:H3'	2.31	0.45
1:AA:160:A:C6	1:AA:161:A:C2	3.04	0.45
1:AA:554:A:H5'	12:AL:26:ALA:HB1	1.98	0.45
19:AS:13:LEU:O	19:AS:14:HIS:C	2.57	0.45
20:AT:44:LYS:CE	20:AT:87:ALA:OXT	2.63	0.45
31:BA:645:C:H2'	31:BA:647:G:C8	2.51	0.45
31:BA:1047:G:O2'	31:BA:1110:G:N1	2.33	0.45
52:BW:43:THR:O	52:BW:43:THR:HG23	2.16	0.45
54:BY:15:ASN:O	54:BY:19:LEU:HD23	2.15	0.45
1:AA:160:A:N6	1:AA:343:U:HO2'	2.13	0.45
1:AA:324:G:N1	1:AA:327:A:OP2	2.49	0.45
31:BA:1942:C:C5	31:BA:1943:U:C4	3.05	0.45
48:BS:92:ARG:NH2	48:BS:94:ASP:OD2	2.49	0.45
4:AD:117:LEU:HB3	4:AD:123:ILE:HD11	1.97	0.45
29:B4:1:MET:HE2	29:B4:34:LYS:HD3	1.99	0.45
31:BA:75:G:N3	31:BA:75:G:H2'	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BA:1064:C:C2'	31:BA:1065:U:H5	2.30	0.45
31:BA:1774:C:H2'	31:BA:1774:C:O2	2.17	0.45
31:BA:1913:A:H4'	31:BA:1914:C:O5'	2.17	0.45
31:BA:2188:U:H2'	31:BA:2189:U:O4'	2.16	0.45
31:BA:2321:U:H5'	31:BA:2322:A:OP2	2.16	0.45
33:BC:235:GLY:O	33:BC:239:ASN:ND2	2.49	0.45
47:BR:51:VAL:HG13	47:BR:52:PRO:HD2	1.97	0.45
1:AA:1130:A:OP1	9:AI:18:ARG:NH2	2.49	0.45
4:AD:153:SER:O	4:AD:156:LYS:HG2	2.16	0.45
12:AL:35:THR:N	12:AL:54:ARG:O	2.50	0.45
31:BA:2336:A:H61	52:BW:43:THR:HG21	1.81	0.45
38:BH:2:GLN:O	38:BH:3:VAL:O	2.35	0.45
51:BV:35:GLU:OE2	51:BV:93:ARG:NE	2.49	0.45
1:AA:1103:C:OP1	2:AB:95:ARG:NH2	2.49	0.45
3:AC:150:LYS:HD3	3:AC:169:ARG:HE	1.81	0.45
10:AJ:35:GLN:NE2	10:AJ:77:VAL:HG13	2.31	0.45
17:AQ:78:VAL:HG22	17:AQ:79:VAL:N	2.32	0.45
31:BA:400:G:N7	53:BX:57:ARG:NH2	2.65	0.45
31:BA:2850:A:N7	31:BA:2868:A:O2'	2.41	0.45
40:BK:99:ILE:HG23	40:BK:118:LEU:HB3	1.99	0.45
1:AA:220:G:C2	1:AA:221:C:C6	3.05	0.45
6:AF:49:TYR:HB3	18:AR:74:HIS:ND1	2.30	0.45
6:AF:99:ALA:O	6:AF:100:SER:OG	2.27	0.45
11:AK:37:ARG:HB3	11:AK:37:ARG:CZ	2.46	0.45
12:AL:108:LYS:C	12:AL:109:ASP:OD2	2.60	0.45
14:AN:91:GLY:O	14:AN:93:ILE:N	2.49	0.45
30:B5:12:ILE:HD13	30:B5:28:VAL:HG12	1.99	0.45
31:BA:1068:G:O6	31:BA:1073:A:N6	2.50	0.45
31:BA:2064:C:H2'	31:BA:2065:C:C6	2.52	0.45
32:BB:74:U:O2	51:BV:29:ILE:HD13	2.16	0.45
1:AA:96:U:HO2'	1:AA:97:G:P	2.39	0.45
1:AA:337:G:H2'	1:AA:338:A:C8	2.52	0.45
1:AA:1088:G:H21	1:AA:1167:A:H62	1.64	0.45
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.52	0.45
2:AB:114:LEU:HB2	2:AB:144:LEU:HD23	1.99	0.45
3:AC:111:LEU:HD22	3:AC:146:ALA:HB2	1.97	0.45
29:B4:36:ARG:HD3	31:BA:2742:G:OP1	2.16	0.45
31:BA:639:U:H2'	31:BA:640:C:C6	2.52	0.45
32:BB:106:G:H2'	32:BB:107:G:O4'	2.17	0.45
34:BD:177:VAL:HG13	34:BD:177:VAL:O	2.17	0.45
13:AM:52:GLN:O	13:AM:55:THR:OG1	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AY:37:A:H3'	23:AY:38:A:C8	2.52	0.45
31:BA:871:U:H2'	31:BA:872:U:C6	2.52	0.45
31:BA:1049:C:C2	31:BA:1050:A:C8	3.05	0.45
31:BA:1913:A:H1'	31:BA:1914:C:OP2	2.17	0.45
33:BC:204:VAL:O	33:BC:204:VAL:HG12	2.16	0.45
17:AQ:20:SER:N	17:AQ:48:ASP:OD1	2.50	0.45
31:BA:1071:G:OP1	31:BA:1089:A:N6	2.50	0.45
31:BA:1085:A:H3'	31:BA:1085:A:H8	1.82	0.45
31:BA:1527:G:N1	31:BA:1544:A:OP2	2.39	0.45
31:BA:2847:U:H2'	31:BA:2848:G:O4'	2.17	0.45
1:AA:151:A:C2	1:AA:152:A:H1'	2.52	0.45
11:AK:85:MET:HE2	11:AK:113:VAL:HG11	1.99	0.45
17:AQ:19:LYS:C	17:AQ:48:ASP:OD1	2.60	0.45
31:BA:1716:U:H2'	31:BA:1717:A:H8	1.82	0.45
31:BA:2011:U:OP1	48:BS:42:LYS:NZ	2.44	0.45
32:BB:15:A:O4'	32:BB:109:A:C8	2.70	0.45
42:BM:57:VAL:HG13	42:BM:58:LYS:O	2.16	0.45
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.53	0.44
1:AA:1486:G:H2'	1:AA:1487:G:O4'	2.17	0.44
7:AG:129:GLU:O	7:AG:130:ASN:OD1	2.35	0.44
10:AJ:24:GLU:O	10:AJ:28:THR:HG22	2.17	0.44
12:AL:114:ARG:HB2	12:AL:119:VAL:HB	1.99	0.44
23:AY:23:A:C8	23:AY:23:A:H5''	2.52	0.44
31:BA:2243:U:H2'	31:BA:2244:U:C6	2.51	0.44
31:BA:2547:A:H2'	31:BA:2548:U:C6	2.53	0.44
33:BC:237:GLY:O	33:BC:238:ARG:HB2	2.16	0.44
48:BS:63:GLY:O	48:BS:64:ALA:HB3	2.17	0.44
1:AA:71:A:N1	1:AA:99:C:O2'	2.48	0.44
1:AA:1145:A:O2'	1:AA:1146:A:P	2.74	0.44
2:AB:113:ARG:O	2:AB:117:LEU:HD12	2.17	0.44
2:AB:186:ILE:HD13	2:AB:200:ILE:HB	1.98	0.44
7:AG:50:LEU:HD22	7:AG:124:LEU:HD13	1.97	0.44
31:BA:1093:G:N1	31:BA:1097:U:OP1	2.50	0.44
31:BA:2266:A:H4'	31:BA:2267:A:O5'	2.17	0.44
37:BG:127:THR:HG22	37:BG:128:GLN:N	2.32	0.44
1:AA:78:A:N6	1:AA:92:U:O4	2.50	0.44
1:AA:204:G:C8	1:AA:205:A:C8	3.05	0.44
5:AE:133:PRO:O	5:AE:137:VAL:HG12	2.18	0.44
6:AF:51:ILE:O	6:AF:51:ILE:HG13	2.17	0.44
9:AI:13:LYS:O	9:AI:13:LYS:HG3	2.17	0.44
20:AT:61:GLN:OE1	20:AT:66:LEU:HD21	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BA:743:A:O2'	31:BA:1659:G:OP1	2.35	0.44
31:BA:1066:U:O2'	31:BA:1074:G:N2	2.51	0.44
31:BA:1198:U:H2'	31:BA:1199:U:C6	2.52	0.44
31:BA:1469:A:H2'	31:BA:1470:A:C8	2.52	0.44
43:BN:70:THR:O	43:BN:71:ARG:C	2.61	0.44
47:BR:49:ILE:HB	47:BR:52:PRO:HA	2.00	0.44
48:BS:72:THR:HG21	48:BS:108:SER:OG	2.17	0.44
2:AB:178:ASN:OD1	2:AB:178:ASN:C	2.60	0.44
4:AD:146:ARG:O	4:AD:150:LYS:HG3	2.16	0.44
31:BA:479:A:H4'	31:BA:480:A:OP1	2.17	0.44
31:BA:1022:G:N2	31:BA:1142:A:C2	2.84	0.44
42:BM:135:VAL:O	42:BM:135:VAL:HG13	2.17	0.44
1:AA:1202:U:C2	14:AN:82:ILE:HD11	2.53	0.44
3:AC:42:TYR:CZ	3:AC:90:VAL:HG11	2.53	0.44
17:AQ:17:MET:HE3	17:AQ:17:MET:HB2	1.65	0.44
21:AU:24:GLU:HB3	21:AU:28:VAL:CG1	2.47	0.44
31:BA:1856:U:H2'	31:BA:1857:G:O4'	2.18	0.44
36:BF:20:PHE:O	36:BF:21:ASN:OD1	2.35	0.44
1:AA:936:C:C2	1:AA:937:A:C8	3.06	0.44
24:AX:45:A:H2'	24:AX:46:G:C8	2.53	0.44
31:BA:1067:A:H2'	31:BA:1068:G:C8	2.52	0.44
42:BM:34:LYS:CD	42:BM:131:VAL:HG11	2.48	0.44
44:BO:24:THR:HG22	44:BO:42:PRO:HD3	2.00	0.44
1:AA:197:A:N1	1:AA:220:G:O2'	2.49	0.44
1:AA:381:C:H2'	1:AA:382:A:O4'	2.18	0.44
1:AA:966:G:O2'	9:AI:129:LYS:O	2.36	0.44
23:AW:65:C:N4	23:AW:66:A:H62	2.16	0.44
31:BA:1067:A:C5	31:BA:1068:G:C5	3.06	0.44
1:AA:60:A:N1	1:AA:107:G:O2'	2.44	0.44
1:AA:356:A:N3	1:AA:368:U:O2'	2.38	0.44
1:AA:674:G:H2'	1:AA:675:A:H8	1.82	0.44
1:AA:1314:C:H2'	1:AA:1315:U:C6	2.53	0.44
2:AB:74:ARG:CZ	2:AB:74:ARG:HB2	2.45	0.44
4:AD:173:VAL:HG13	4:AD:174:ASP:N	2.33	0.44
6:AF:67:PRO:O	6:AF:70:VAL:HG12	2.17	0.44
31:BA:893:C:H2'	31:BA:893:C:O2	2.18	0.44
31:BA:1065:U:C4	31:BA:1069:A:N6	2.86	0.44
31:BA:1319:C:O2'	31:BA:1320:C:H5'	2.17	0.44
31:BA:2140:G:N1	31:BA:2151:U:C2	2.86	0.44
38:BH:9:VAL:HG11	38:BH:12:LEU:HD21	2.00	0.44
1:AA:946:A:H2'	1:AA:947:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1157:A:C2	1:AA:1181:G:C4	3.05	0.44
1:AA:1160:G:OP1	2:AB:132:LYS:NZ	2.51	0.44
1:AA:1225:A:H2'	1:AA:1226:C:C5	2.53	0.44
16:AP:39:PHE:HD1	16:AP:50:THR:HG22	1.83	0.44
19:AS:5:LEU:O	19:AS:6:LYS:HB3	2.18	0.44
31:BA:1405:U:H2'	31:BA:1406:U:C6	2.53	0.44
32:BB:42:C:C5	36:BF:66:LEU:HD22	2.53	0.44
33:BC:9:THR:O	33:BC:10:SER:OG	2.30	0.44
10:AJ:78:GLU:C	10:AJ:80:THR:N	2.74	0.43
15:AO:3:LEU:HD23	15:AO:8:THR:HG22	2.00	0.43
20:AT:71:LYS:O	20:AT:72:ALA:C	2.58	0.43
30:B5:12:ILE:HD12	30:B5:32:LEU:CD1	2.48	0.43
31:BA:64:A:H2'	31:BA:65:U:C6	2.53	0.43
31:BA:883:G:H2'	31:BA:883:G:N3	2.33	0.43
31:BA:1065:U:C6	31:BA:1066:U:H4'	2.53	0.43
31:BA:2101:A:N3	31:BA:2102:G:H1'	2.32	0.43
31:BA:2788:C:H2'	31:BA:2789:C:C6	2.53	0.43
45:BP:22:PRO:HD3	45:BP:50:ILE:HD12	1.99	0.43
51:BV:2:PHE:HB2	51:BV:61:LEU:HD13	2.00	0.43
25:B0:28:LEU:HD13	25:B0:37:LYS:HB3	1.99	0.43
31:BA:580:U:O3'	46:BQ:31:VAL:HG13	2.19	0.43
41:BL:50:PHE:CZ	41:BL:52:GLY:O	2.70	0.43
49:BT:3:ARG:CZ	49:BT:3:ARG:HB2	2.43	0.43
1:AA:216:U:H2'	1:AA:217:C:C6	2.54	0.43
3:AC:53:SER:HB2	3:AC:112:ASP:OD2	2.18	0.43
8:AH:106:THR:HG22	8:AH:111:MET:HE1	2.00	0.43
10:AJ:35:GLN:HB2	10:AJ:76:ILE:HD12	2.00	0.43
16:AP:79:ASN:ND2	16:AP:82:ALA:O	2.48	0.43
23:AW:47:U:H3'	23:AW:48:C:H5'	2.00	0.43
23:AY:47:U:C5	23:AY:50:G:H5''	2.53	0.43
31:BA:1085:A:N7	31:BA:1086:A:N6	2.66	0.43
6:AF:9:MET:HE3	6:AF:86:ARG:HB3	1.99	0.43
15:AO:19:ALA:O	15:AO:20:ASN:OD1	2.37	0.43
31:BA:285:G:C6	31:BA:355:U:O2	2.72	0.43
31:BA:586:A:N1	31:BA:809:G:O2'	2.48	0.43
31:BA:1019:U:OP1	31:BA:1035:U:O2'	2.26	0.43
31:BA:1566:A:O4'	33:BC:213:TRP:CD1	2.71	0.43
41:BL:77:ILE:O	41:BL:110:VAL:O	2.36	0.43
43:BN:79:LEU:O	43:BN:80:PHE:HB2	2.17	0.43
1:AA:160:A:N6	1:AA:343:U:H1'	2.33	0.43
1:AA:202:G:N2	1:AA:466:A:H61	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1226:C:H2'	13:AM:102:THR:HG22	2.01	0.43
4:AD:145:ILE:HD13	4:AD:155:VAL:HG11	2.01	0.43
5:AE:25:VAL:HG22	5:AE:26:LYS:N	2.33	0.43
10:AJ:91:ASP:N	10:AJ:91:ASP:OD1	2.51	0.43
30:B5:58:ASP:OD1	30:B5:59:ARG:N	2.52	0.43
31:BA:1000:A:H2'	31:BA:1001:A:C8	2.53	0.43
31:BA:1069:A:H4'	31:BA:1070:A:C8	2.53	0.43
31:BA:1172:C:H2'	31:BA:1173:U:C6	2.54	0.43
21:AU:20:LYS:HD3	21:AU:20:LYS:N	2.34	0.43
25:B0:9:THR:CG2	31:BA:2020:A:H5'	2.49	0.43
31:BA:1083:U:C2	31:BA:1085:A:N7	2.87	0.43
31:BA:1434:A:H2'	31:BA:1435:G:C8	2.53	0.43
37:BG:45:HIS:ND1	37:BG:47:ASP:O	2.51	0.43
1:AA:552:U:O2'	12:AL:83:ARG:O	2.34	0.43
5:AE:39:VAL:HG22	5:AE:67:ALA:HB1	2.01	0.43
6:AF:93:LYS:HE2	6:AF:93:LYS:HB3	1.65	0.43
10:AJ:81:GLU:C	10:AJ:83:THR:H	2.25	0.43
31:BA:191:A:H2'	31:BA:192:C:C6	2.54	0.43
31:BA:1182:G:H2'	31:BA:1183:U:O4'	2.18	0.43
31:BA:2167:U:N3	31:BA:2169:A:H5'	2.34	0.43
31:BA:2474:U:H2'	31:BA:2474:U:O2	2.18	0.43
35:BE:131:THR:HG22	35:BE:160:ALA:O	2.19	0.43
1:AA:206:C:H3'	1:AA:206:C:C6	2.54	0.43
1:AA:214:C:C2	1:AA:215:C:C5	3.07	0.43
1:AA:704:A:C4	1:AA:705:G:C8	3.07	0.43
2:AB:60:ILE:H	2:AB:60:ILE:HG12	1.68	0.43
3:AC:61:ALA:O	3:AC:62:LYS:HG3	2.19	0.43
3:AC:62:LYS:HD2	3:AC:62:LYS:O	2.19	0.43
6:AF:98:GLU:O	6:AF:99:ALA:C	2.61	0.43
11:AK:52:PHE:CE2	11:AK:62:ALA:HB1	2.53	0.43
13:AM:28:THR:HG23	13:AM:29:ARG:N	2.34	0.43
20:AT:44:LYS:HB2	20:AT:87:ALA:C	2.43	0.43
21:AU:25:LYS:HG3	21:AU:26:ALA:N	2.34	0.43
23:AW:34:C:H2'	23:AW:35:A:C8	2.54	0.43
31:BA:528:A:C2	31:BA:2043:C:H4'	2.54	0.43
31:BA:1746:A:H2'	31:BA:1747:U:C6	2.53	0.43
33:BC:245:VAL:HG12	33:BC:246:THR:O	2.18	0.43
42:BM:26:VAL:CG1	42:BM:133:LYS:HA	2.49	0.43
42:BM:64:TRP:HB2	42:BM:104:GLU:HB2	2.00	0.43
42:BM:66:ARG:NH1	42:BM:104:GLU:OE2	2.51	0.43
47:BR:94:THR:HG23	47:BR:94:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:722:G:H3'	1:AA:722:G:N3	2.34	0.43
24:AX:22:A:O2'	24:AX:23:G:OP2	2.25	0.43
31:BA:580:U:H2'	31:BA:581:C:C6	2.54	0.43
31:BA:2831:G:OP2	34:BD:59:ARG:NH1	2.52	0.43
1:AA:1071:C:H2'	1:AA:1072:G:H8	1.84	0.43
2:AB:28:LYS:N	2:AB:29:PRO:HD2	2.33	0.43
2:AB:66:LYS:HG2	2:AB:90:PHE:HE1	1.84	0.43
11:AK:122:ARG:HG3	21:AU:35:ARG:HG3	2.01	0.43
24:AX:9:G:H5'	24:AX:47:G:N2	2.34	0.43
29:B4:16:ILE:CD1	29:B4:25:VAL:HG22	2.45	0.43
34:BD:105:LYS:O	34:BD:106:LYS:HG3	2.19	0.43
45:BP:33:VAL:HG22	45:BP:38:LYS:HB3	2.00	0.43
50:BU:74:ASN:O	50:BU:75:ALA:HB3	2.18	0.43
1:AA:687:A:C8	1:AA:701:U:C4	3.07	0.42
2:AB:66:LYS:HG2	2:AB:90:PHE:CE1	2.54	0.42
2:AB:148:LEU:O	2:AB:148:LEU:HG	2.19	0.42
5:AE:35:ALA:O	5:AE:50:TYR:O	2.37	0.42
10:AJ:78:GLU:O	10:AJ:79:PRO:C	2.62	0.42
24:AX:19:G:H1'	24:AX:59:A:C2	2.53	0.42
26:B1:9:ILE:HG22	26:B1:53:LYS:HB2	2.01	0.42
31:BA:139:U:C6	49:BT:1:MET:HE1	2.54	0.42
31:BA:493:G:H2'	31:BA:494:G:O4'	2.19	0.42
31:BA:837:C:N3	31:BA:941:A:N6	2.66	0.42
31:BA:1062:G:C2'	31:BA:1063:G:O4'	2.67	0.42
31:BA:1321:A:C4	31:BA:1322:A:C8	3.06	0.42
31:BA:1322:A:C5	31:BA:1323:C:C5	3.06	0.42
31:BA:2143:C:H2'	31:BA:2144:G:C8	2.54	0.42
31:BA:2514:U:H2'	31:BA:2515:C:C6	2.54	0.42
38:BH:43:ASN:O	38:BH:47:PHE:N	2.38	0.42
39:BJ:78:THR:O	39:BJ:78:THR:HG22	2.19	0.42
49:BT:92:ASN:O	49:BT:93:LEU:HD12	2.18	0.42
1:AA:1316:G:N1	1:AA:1319:A:OP2	2.52	0.42
2:AB:78:GLU:HA	2:AB:81:LYS:CE	2.48	0.42
4:AD:13:ARG:HD2	4:AD:32:CYS:SG	2.59	0.42
23:AY:49:G:O6	23:AY:66:A:N6	2.51	0.42
31:BA:1790:C:H2'	31:BA:1791:A:C5	2.53	0.42
31:BA:2109:U:H3'	31:BA:2110:G:C8	2.54	0.42
37:BG:156:PRO:O	37:BG:171:THR:HG23	2.19	0.42
49:BT:4:GLU:O	49:BT:5:GLU:C	2.62	0.42
1:AA:523:A:H61	12:AL:89:ASP:CB	2.32	0.42
2:AB:64:LYS:HA	2:AB:64:LYS:HD3	1.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:95:PHE:O	5:AE:125:ALA:O	2.37	0.42
31:BA:2191:A:H2'	31:BA:2192:U:C6	2.54	0.42
31:BA:2297:A:N1	31:BA:2321:U:H5	2.18	0.42
33:BC:146:MET:HE1	33:BC:182:ARG:CZ	2.49	0.42
50:BU:32:GLY:O	50:BU:67:VAL:HG23	2.20	0.42
1:AA:373:A:O2'	1:AA:451:A:N7	2.52	0.42
1:AA:384:G:H2'	1:AA:385:C:C6	2.55	0.42
1:AA:512:U:P	4:AD:44:ARG:HH22	2.42	0.42
5:AE:107:ALA:O	5:AE:112:ARG:NH1	2.52	0.42
12:AL:34:CYS:CA	12:AL:55:VAL:HG22	2.50	0.42
31:BA:2228:G:H2'	31:BA:2229:U:C6	2.54	0.42
32:BB:13:G:O2'	32:BB:15:A:OP2	2.37	0.42
50:BU:50:PRO:HA	50:BU:54:GLN:CG	2.50	0.42
1:AA:206:C:C6	1:AA:206:C:C3'	3.02	0.42
1:AA:920:U:H2'	1:AA:921:U:C6	2.55	0.42
1:AA:996:A:H2'	1:AA:997:U:C6	2.54	0.42
1:AA:1313:U:OP2	19:AS:3:ARG:NH2	2.52	0.42
3:AC:148:GLY:HA3	3:AC:203:PHE:HB3	2.01	0.42
4:AD:29:ASP:OD1	4:AD:29:ASP:N	2.53	0.42
5:AE:15:LEU:HD23	5:AE:15:LEU:H	1.83	0.42
17:AQ:17:MET:O	17:AQ:18:GLU:HB2	2.20	0.42
26:B1:47:VAL:HG12	26:B1:48:ILE:N	2.34	0.42
27:B2:12:ARG:NE	27:B2:44:VAL:HG21	2.32	0.42
30:B5:41:HIS:O	30:B5:42:PRO:C	2.62	0.42
31:BA:1179:G:H2'	31:BA:1180:U:H4'	2.02	0.42
31:BA:2025:C:H2'	31:BA:2026:U:C6	2.54	0.42
31:BA:2119:A:N6	31:BA:2169:A:C5	2.87	0.42
31:BA:2150:C:H2'	31:BA:2151:U:O4'	2.19	0.42
40:BK:109:SER:C	40:BK:110:GLU:HG3	2.44	0.42
53:BX:39:TRP:CH2	53:BX:44:LYS:HD3	2.55	0.42
1:AA:983:A:N3	1:AA:983:A:C2'	2.83	0.42
3:AC:142:MET:SD	3:AC:146:ALA:O	2.78	0.42
21:AU:37:PHE:O	21:AU:38:TYR:C	2.60	0.42
21:AU:40:LYS:O	21:AU:43:THR:HG22	2.20	0.42
23:AY:15:G:N1	23:AY:59:U:C2	2.88	0.42
31:BA:1447:C:O2'	31:BA:1544:A:N3	2.48	0.42
1:AA:635:A:H2'	1:AA:636:U:C6	2.55	0.42
1:AA:1060:U:H5''	10:AJ:53:ILE:HD12	2.02	0.42
2:AB:60:ILE:HD13	2:AB:63:ARG:NH2	2.34	0.42
7:AG:24:ALA:O	7:AG:27:VAL:HG22	2.20	0.42
11:AK:126:LYS:HA	21:AU:34:ARG:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AS:19:VAL:HG21	19:AS:44:MET:HG2	2.01	0.42
23:AY:58:A:H4'	23:AY:59:U:OP1	2.19	0.42
31:BA:1169:A:H2'	31:BA:1170:C:O4'	2.20	0.42
41:BL:81:ASP:C	41:BL:83:ALA:H	2.27	0.42
41:BL:85:VAL:HG11	41:BL:90:VAL:HG12	2.02	0.42
45:BP:37:LYS:NZ	45:BP:39:ARG:HD3	2.35	0.42
4:AD:148:LYS:H	4:AD:148:LYS:HG3	1.57	0.42
4:AD:153:SER:O	4:AD:154:ARG:C	2.62	0.42
18:AR:47:THR:O	18:AR:48:ARG:C	2.62	0.42
31:BA:2138:G:H2'	31:BA:2139:U:O4'	2.19	0.42
47:BR:53:PHE:O	47:BR:54:VAL:C	2.63	0.42
1:AA:207:C:H2'	1:AA:208:U:O4'	2.18	0.42
1:AA:297:G:N2	1:AA:300:A:OP2	2.44	0.42
1:AA:413:G:H1'	1:AA:428:G:H21	1.85	0.42
1:AA:976:G:N2	1:AA:1362:A:O2'	2.53	0.42
1:AA:1498:U:O4	57:AA:1694:84G:N	2.53	0.42
2:AB:23:TRP:CZ3	2:AB:25:PRO:HA	2.55	0.42
5:AE:102:GLY:C	5:AE:103:THR:HG1	2.21	0.42
23:AY:36:C:H2'	23:AY:37:A:O4'	2.19	0.42
30:B5:62:LYS:O	30:B5:63:ARG:C	2.63	0.42
31:BA:833:A:H2'	31:BA:834:G:C8	2.55	0.42
31:BA:2098:U:H2'	31:BA:2099:U:O4'	2.20	0.42
1:AA:1273:C:H2'	1:AA:1274:A:O4'	2.20	0.42
3:AC:10:ILE:HG23	3:AC:11:ARG:HG3	2.00	0.42
13:AM:7:ILE:HG12	36:BF:112:ARG:HE	1.84	0.42
26:B1:33:LYS:HD2	26:B1:33:LYS:HA	1.81	0.42
31:BA:5:A:H2'	31:BA:6:A:C8	2.55	0.42
31:BA:1066:U:H5''	31:BA:1066:U:C6	2.54	0.42
31:BA:1085:A:H3'	31:BA:1085:A:C8	2.55	0.42
31:BA:1526:C:H2'	31:BA:1527:G:O4'	2.20	0.42
31:BA:1730:C:O2'	31:BA:1731:G:C4	2.73	0.42
31:BA:2799:A:O2'	31:BA:2800:A:H5''	2.19	0.42
36:BF:47:LYS:HE2	36:BF:47:LYS:HA	2.02	0.42
38:BH:30:LEU:O	38:BH:34:GLY:O	2.37	0.42
1:AA:524:G:H2'	1:AA:525:C:C6	2.55	0.41
1:AA:978:A:C4	1:AA:1319:A:C2	3.08	0.41
1:AA:1404:C:H2'	1:AA:1405:G:C8	2.54	0.41
4:AD:192:SER:O	4:AD:193:ALA:HB3	2.20	0.41
9:AI:13:LYS:O	9:AI:14:SER:HB3	2.20	0.41
31:BA:1847:A:O2'	31:BA:1848:A:P	2.76	0.41
34:BD:1:MET:HE3	34:BD:100:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BG:166:ASP:OD2	37:BG:166:ASP:C	2.63	0.41
40:BK:99:ILE:HG23	40:BK:118:LEU:HB2	2.01	0.41
1:AA:594:U:H2'	1:AA:595:A:O4'	2.19	0.41
3:AC:7:PRO:HG2	3:AC:184:TYR:HB3	2.02	0.41
17:AQ:61:ILE:HG22	17:AQ:73:TRP:CE3	2.46	0.41
20:AT:69:LYS:HB3	20:AT:69:LYS:HE3	1.70	0.41
31:BA:151:C:H2'	31:BA:152:A:H8	1.85	0.41
31:BA:885:C:H4'	31:BA:892:A:N3	2.35	0.41
31:BA:1558:C:O4'	31:BA:1560:G:C8	2.73	0.41
31:BA:2038:G:H2'	31:BA:2039:U:O4'	2.20	0.41
31:BA:2074:U:H2'	31:BA:2075:U:C6	2.55	0.41
31:BA:2168:G:C5	31:BA:2169:A:C5	3.08	0.41
31:BA:2680:U:O2'	31:BA:2681:C:H5'	2.19	0.41
33:BC:110:LEU:HD12	33:BC:110:LEU:N	2.35	0.41
45:BP:34:GLU:O	45:BP:34:GLU:OE1	2.38	0.41
1:AA:728:A:H2'	1:AA:729:A:C8	2.55	0.41
2:AB:203:ASN:OD1	2:AB:204:ASP:N	2.53	0.41
5:AE:23:LYS:C	5:AE:24:THR:HG22	2.45	0.41
7:AG:87:VAL:HG23	7:AG:87:VAL:O	2.19	0.41
10:AJ:10:LEU:HB2	10:AJ:18:ILE:HD11	2.01	0.41
10:AJ:31:ARG:NH2	10:AJ:32:THR:HB	2.35	0.41
12:AL:14:ARG:NE	12:AL:15:LYS:H	2.19	0.41
21:AU:15:ALA:HB1	21:AU:17:ARG:HG2	2.01	0.41
25:B0:28:LEU:CD1	25:B0:37:LYS:HD2	2.50	0.41
31:BA:2682:A:C8	34:BD:11:MET:HE2	2.55	0.41
32:BB:5:U:OP1	32:BB:61:G:O2'	2.35	0.41
45:BP:5:ILE:O	45:BP:9:GLU:HG3	2.20	0.41
1:AA:1042:A:H2'	1:AA:1043:G:O4'	2.20	0.41
7:AG:50:LEU:HD22	7:AG:124:LEU:HD11	1.99	0.41
12:AL:42:PRO:HB3	12:AL:89:ASP:OD2	2.21	0.41
23:AY:19:G:H4'	23:AY:20:G:OP2	2.19	0.41
31:BA:1794:A:H2'	31:BA:1795:C:C6	2.55	0.41
31:BA:2747:G:O6	31:BA:2755:C:H5''	2.21	0.41
41:BL:110:VAL:O	41:BL:111:ILE:O	2.38	0.41
49:BT:37:ASP:OD1	49:BT:38:ALA:N	2.43	0.41
1:AA:58:C:O2	1:AA:58:C:H2'	2.19	0.41
1:AA:1127:G:C2	1:AA:1128:C:C6	3.09	0.41
5:AE:105:ILE:HD12	5:AE:123:VAL:HG22	2.03	0.41
9:AI:90:TYR:O	9:AI:91:ASP:OD1	2.38	0.41
23:AY:26:A:C6	23:AY:44:G:O6	2.74	0.41
31:BA:607:U:C5	31:BA:620:G:C4	3.07	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BA:1245:G:OP1	41:BL:13:LYS:NZ	2.53	0.41
32:BB:29:A:H2'	32:BB:30:C:O4'	2.20	0.41
33:BC:196:GLY:O	33:BC:198:ALA:N	2.52	0.41
40:BK:93:GLN:O	40:BK:94:PRO:C	2.63	0.41
1:AA:96:U:O2'	1:AA:97:G:OP1	2.31	0.41
1:AA:1238:A:H2	1:AA:1241:G:N3	2.18	0.41
7:AG:84:THR:O	7:AG:84:THR:HG23	2.20	0.41
26:B1:23:THR:OG1	31:BA:2286:G:O6	2.33	0.41
29:B4:37:GLN:HE21	31:BA:1125:G:H5''	1.85	0.41
31:BA:281:C:N4	31:BA:282:A:H62	2.19	0.41
31:BA:353:C:C2	31:BA:354:A:C8	3.08	0.41
31:BA:607:U:C5	31:BA:620:G:C5	3.09	0.41
31:BA:962:G:H21	31:BA:2250:G:H1	1.68	0.41
31:BA:1083:U:C2	31:BA:1086:A:N6	2.89	0.41
31:BA:1607:C:N4	31:BA:1622:G:OP2	2.35	0.41
31:BA:2590:A:H2'	31:BA:2591:C:H6	1.85	0.41
35:BE:7:ASP:OD1	35:BE:8:ALA:N	2.54	0.41
1:AA:309:A:O2'	1:AA:607:A:N1	2.50	0.41
2:AB:58:ASN:O	2:AB:59:LYS:C	2.63	0.41
4:AD:29:ASP:O	4:AD:30:THR:OG1	2.16	0.41
5:AE:111:MET:SD	5:AE:127:ALA:HB2	2.60	0.41
8:AH:106:THR:HG23	8:AH:108:LYS:N	2.24	0.41
17:AQ:49:GLU:O	17:AQ:50:ASN:CG	2.64	0.41
29:B4:36:ARG:HG2	29:B4:37:GLN:N	2.36	0.41
31:BA:70:G:H4'	31:BA:71:A:OP1	2.21	0.41
31:BA:274:C:N3	31:BA:275:C:H1'	2.36	0.41
31:BA:1069:A:H2'	31:BA:1074:G:O6	2.20	0.41
31:BA:1432:G:H2'	31:BA:1433:A:C8	2.54	0.41
32:BB:45:A:C4	32:BB:46:A:C8	3.08	0.41
42:BM:69:PRO:O	42:BM:93:VAL:O	2.39	0.41
2:AB:94:HIS:O	2:AB:95:ARG:C	2.64	0.41
19:AS:79:THR:HG23	19:AS:79:THR:O	2.21	0.41
25:B0:25:VAL:HG23	25:B0:26:THR:N	2.35	0.41
31:BA:636:G:N1	41:BL:76:GLU:OE1	2.46	0.41
31:BA:947:A:H2'	31:BA:948:C:C6	2.55	0.41
31:BA:1936:A:H2	31:BA:1943:U:N3	2.19	0.41
50:BU:7:ARG:NH2	50:BU:26:LYS:O	2.53	0.41
1:AA:160:A:H3'	1:AA:161:A:C8	2.56	0.41
1:AA:590:U:OP2	8:AH:31:LYS:NZ	2.53	0.41
1:AA:1133:G:H2'	1:AA:1134:G:C8	2.56	0.41
6:AF:3:HIS:ND1	6:AF:65:GLU:HG3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:23:GLU:HA	6:AF:26:THR:OG1	2.21	0.41
9:AI:55:VAL:O	9:AI:55:VAL:HG23	2.20	0.41
14:AN:83:LYS:HA	14:AN:83:LYS:HD3	1.62	0.41
17:AQ:75:LEU:HD12	17:AQ:75:LEU:C	2.46	0.41
20:AT:39:ILE:HG22	20:AT:47:ALA:HB1	2.03	0.41
26:B1:40:ASP:O	26:B1:44:ARG:N	2.51	0.41
31:BA:139:U:H6	31:BA:139:U:O5'	2.03	0.41
31:BA:273:G:H2'	31:BA:274:C:O4'	2.21	0.41
31:BA:760:G:H2'	31:BA:761:A:O4'	2.21	0.41
31:BA:866:A:C6	31:BA:867:C:C5	3.09	0.41
31:BA:1360:G:N7	31:BA:1361:G:C8	2.89	0.41
31:BA:1433:A:H2'	31:BA:1434:A:O4'	2.20	0.41
31:BA:1577:C:H2'	31:BA:1578:U:O4'	2.20	0.41
31:BA:1847:A:O2'	31:BA:1848:A:H8	2.03	0.41
31:BA:1858:A:H2'	31:BA:1859:U:O4'	2.20	0.41
31:BA:2063:C:O2	31:BA:2063:C:H2'	2.20	0.41
31:BA:2099:U:H2'	31:BA:2100:G:C8	2.56	0.41
31:BA:2113:U:H2'	31:BA:2114:A:C8	2.56	0.41
31:BA:2116:G:O6	31:BA:2165:C:N4	2.54	0.41
31:BA:2140:G:H2'	31:BA:2141:G:C8	2.55	0.41
32:BB:8:C:O3'	44:BO:25:ARG:NH2	2.52	0.41
33:BC:9:THR:O	33:BC:10:SER:CB	2.69	0.41
34:BD:25:THR:HG21	34:BD:193:VAL:HG13	2.03	0.41
37:BG:45:HIS:O	37:BG:49:THR:O	2.39	0.41
38:BH:44:ILE:HG13	38:BH:45:GLU:N	2.34	0.41
48:BS:59:GLU:HA	48:BS:64:ALA:CB	2.51	0.41
1:AA:1346:A:OP1	9:AI:122:ARG:NH1	2.42	0.41
1:AA:1410:A:H2'	1:AA:1411:C:C6	2.55	0.41
23:AW:33:U:H2'	23:AW:35:A:OP2	2.20	0.41
31:BA:1149:G:H2'	31:BA:1150:C:C6	2.56	0.41
31:BA:1386:C:H2'	31:BA:1387:A:C8	2.55	0.41
31:BA:2119:A:N6	31:BA:2167:U:O2'	2.54	0.41
32:BB:42:C:C6	36:BF:66:LEU:HB2	2.56	0.41
1:AA:976:G:N1	1:AA:1362:A:O2'	2.52	0.40
3:AC:113:ALA:CB	3:AC:183:ASP:O	2.69	0.40
4:AD:29:ASP:C	4:AD:31:LYS:H	2.29	0.40
4:AD:99:ASP:OD1	4:AD:100:ASN:N	2.53	0.40
8:AH:18:GLN:NE2	8:AH:72:VAL:HG22	2.36	0.40
11:AK:21:ALA:HB2	11:AK:82:LEU:HD12	2.03	0.40
23:AY:9:A:O2'	23:AY:10:G:N7	2.54	0.40
31:BA:139:U:P	31:BA:139:U:H3'	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BA:356:G:H2'	31:BA:357:C:C6	2.56	0.40
31:BA:1353:A:H2'	31:BA:1354:A:C8	2.56	0.40
31:BA:1590:A:H2'	31:BA:1591:A:H8	1.86	0.40
43:BN:45:ARG:O	43:BN:49:GLU:HG3	2.21	0.40
44:BO:31:THR:O	44:BO:32:PRO:C	2.63	0.40
1:AA:695:A:H2'	1:AA:696:A:C8	2.56	0.40
1:AA:1126:U:P	10:AJ:7:ARG:HH22	2.44	0.40
5:AE:111:MET:HA	5:AE:114:VAL:HG12	2.03	0.40
7:AG:13:LEU:HD12	7:AG:14:PRO:O	2.22	0.40
15:AO:20:ASN:OD1	15:AO:20:ASN:C	2.64	0.40
17:AQ:76:VAL:O	17:AQ:77:ARG:C	2.63	0.40
21:AU:6:VAL:O	21:AU:6:VAL:HG23	2.20	0.40
31:BA:2168:G:C6	31:BA:2169:A:C6	3.09	0.40
31:BA:2312:U:O2	36:BF:37:ASN:ND2	2.55	0.40
31:BA:2723:C:H2'	31:BA:2724:U:O4'	2.22	0.40
32:BB:66:A:H61	32:BB:107:G:H2'	1.85	0.40
1:AA:203:G:N1	1:AA:215:C:C4	2.90	0.40
8:AH:108:LYS:HA	8:AH:108:LYS:HD2	1.85	0.40
17:AQ:15:ASP:O	17:AQ:17:MET:N	2.52	0.40
23:AW:19:G:H3'	23:AW:20:G:H5'	2.03	0.40
23:AW:74:C:H3'	23:AW:75:C:H6	1.83	0.40
25:B0:16:ARG:HD2	31:BA:1266:G:OP1	2.21	0.40
31:BA:645:C:H2'	31:BA:647:G:N7	2.35	0.40
31:BA:685:A:O2'	31:BA:773:U:O4	2.26	0.40
31:BA:839:U:H2'	31:BA:840:C:C6	2.56	0.40
31:BA:884:U:H1'	31:BA:893:C:O2	2.21	0.40
31:BA:2740:A:H2'	31:BA:2741:A:C8	2.57	0.40
38:BH:11:ASN:OD1	38:BH:11:ASN:O	2.39	0.40
40:BK:89:ASN:C	40:BK:89:ASN:ND2	2.73	0.40
41:BL:86:GLU:O	41:BL:86:GLU:CD	2.64	0.40
43:BN:22:ARG:HG3	43:BN:70:THR:HA	2.04	0.40
53:BX:3:ARG:O	53:BX:12:PRO:HD3	2.21	0.40
1:AA:206:C:N4	1:AA:213:G:O6	2.54	0.40
1:AA:972:C:OP2	10:AJ:59:LYS:NZ	2.49	0.40
11:AK:13:ARG:O	11:AK:14:LYS:HB2	2.20	0.40
21:AU:37:PHE:CE2	21:AU:40:LYS:HB2	2.56	0.40
31:BA:181:A:H2'	31:BA:182:A:C8	2.55	0.40
31:BA:1682:G:H2'	31:BA:1683:U:C6	2.56	0.40
31:BA:1928:A:H2'	31:BA:1929:G:O4'	2.22	0.40
31:BA:2642:G:OP1	39:BJ:78:THR:HG21	2.22	0.40
1:AA:948:C:P	13:AM:105:ASN:O	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1236:A:H2'	1:AA:1237:C:C6	2.56	0.40
3:AC:7:PRO:HG2	3:AC:184:TYR:CB	2.51	0.40
6:AF:1:MET:SD	6:AF:65:GLU:OE2	2.80	0.40
10:AJ:15:HIS:HA	10:AJ:18:ILE:HG22	2.02	0.40
14:AN:51:LEU:O	14:AN:53:ARG:N	2.54	0.40
24:AX:54:G:C2'	24:AX:55:U:O5'	2.70	0.40
31:BA:1087:G:H22	31:BA:1102:C:H42	1.68	0.40
31:BA:1570:A:H2'	31:BA:1571:A:C8	2.56	0.40
31:BA:2627:G:O2'	31:BA:2781:A:N1	2.53	0.40
31:BA:2822:G:O2'	31:BA:2824:C:OP2	2.34	0.40
40:BK:105:ARG:HH12	40:BK:122:VAL:HA	1.87	0.40
41:BL:123:ARG:HA	41:BL:143:GLU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	189 (88%)	24 (11%)	3 (1%)	9	7
3	AC	204/233 (88%)	181 (89%)	22 (11%)	1 (0%)	25	28
4	AD	203/206 (98%)	186 (92%)	15 (7%)	2 (1%)	13	12
5	AE	148/167 (89%)	125 (84%)	23 (16%)	0	100	100
6	AF	98/135 (73%)	86 (88%)	12 (12%)	0	100	100
7	AG	149/179 (83%)	140 (94%)	9 (6%)	0	100	100
8	AH	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
9	AI	125/130 (96%)	110 (88%)	12 (10%)	3 (2%)	5	3
10	AJ	96/103 (93%)	81 (84%)	12 (12%)	3 (3%)	3	1
11	AK	115/129 (89%)	102 (89%)	12 (10%)	1 (1%)	14	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AL	121/124 (98%)	101 (84%)	18 (15%)	2 (2%)	7	5
13	AM	112/118 (95%)	101 (90%)	10 (9%)	1 (1%)	14	14
14	AN	92/101 (91%)	79 (86%)	12 (13%)	1 (1%)	12	10
15	AO	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	11	9
16	AP	80/82 (98%)	68 (85%)	12 (15%)	0	100	100
17	AQ	78/84 (93%)	70 (90%)	7 (9%)	1 (1%)	10	8
18	AR	53/75 (71%)	51 (96%)	2 (4%)	0	100	100
19	AS	77/92 (84%)	71 (92%)	6 (8%)	0	100	100
20	AT	83/87 (95%)	79 (95%)	3 (4%)	1 (1%)	11	9
21	AU	49/71 (69%)	44 (90%)	4 (8%)	1 (2%)	6	4
25	B0	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
26	B1	48/55 (87%)	44 (92%)	3 (6%)	1 (2%)	5	3
27	B2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
28	B3	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
29	B4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
30	B5	56/70 (80%)	51 (91%)	5 (9%)	0	100	100
33	BC	269/273 (98%)	252 (94%)	15 (6%)	2 (1%)	19	19
34	BD	207/209 (99%)	197 (95%)	9 (4%)	1 (0%)	25	28
35	BE	199/201 (99%)	193 (97%)	5 (2%)	1 (0%)	25	28
36	BF	175/179 (98%)	164 (94%)	11 (6%)	0	100	100
37	BG	174/177 (98%)	167 (96%)	6 (3%)	1 (1%)	22	23
38	BH	45/149 (30%)	33 (73%)	10 (22%)	2 (4%)	2	1
39	BJ	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
40	BK	120/123 (98%)	109 (91%)	10 (8%)	1 (1%)	16	16
41	BL	141/144 (98%)	120 (85%)	19 (14%)	2 (1%)	9	7
42	BM	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
43	BN	118/127 (93%)	102 (86%)	15 (13%)	1 (1%)	16	16
44	BO	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
45	BP	112/115 (97%)	101 (90%)	11 (10%)	0	100	100
46	BQ	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
47	BR	101/103 (98%)	95 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	BS	108/110 (98%)	98 (91%)	9 (8%)	1 (1%)	14	14
49	BT	91/100 (91%)	86 (94%)	4 (4%)	1 (1%)	12	10
50	BU	100/104 (96%)	89 (89%)	10 (10%)	1 (1%)	13	12
51	BV	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
52	BW	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
53	BX	75/78 (96%)	75 (100%)	0	0	100	100
54	BY	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
55	BZ	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	7	5
All	All	5432/5912 (92%)	4991 (92%)	404 (7%)	37 (1%)	21	19

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	34	ALA
2	AB	74	ARG
4	AD	192	SER
12	AL	76	GLU
38	BH	3	VAL
38	BH	9	VAL
41	BL	111	ILE
43	BN	88	ALA
49	BT	38	ALA
50	BU	52	LEU
9	AI	55	VAL
9	AI	58	VAL
9	AI	121	ALA
10	AJ	57	VAL
14	AN	92	GLU
37	BG	56	ASP
41	BL	82	LEU
10	AJ	81	GLU
11	AK	36	ASP
15	AO	46	HIS
17	AQ	18	GLU
33	BC	238	ARG
33	BC	240	PHE
3	AC	66	VAL
13	AM	4	ILE
4	AD	28	ILE

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Mol	Chain	Res	Type
10	AJ	36	VAL
21	AU	38	TYR
34	BD	152	PRO
2	AB	75	ALA
12	AL	24	LEU
35	BE	83	VAL
55	BZ	4	THR
40	BK	35	VAL
48	BS	29	VAL
26	B1	5	ILE
20	AT	42	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/198 (91%)	171 (95%)	9 (5%)	20	26
3	AC	170/190 (90%)	170 (100%)	0	100	100
4	AD	172/173 (99%)	158 (92%)	14 (8%)	9	10
5	AE	113/126 (90%)	111 (98%)	2 (2%)	54	69
6	AF	87/116 (75%)	84 (97%)	3 (3%)	32	42
7	AG	124/147 (84%)	122 (98%)	2 (2%)	58	73
8	AH	104/105 (99%)	102 (98%)	2 (2%)	52	67
9	AI	105/107 (98%)	105 (100%)	0	100	100
10	AJ	86/90 (96%)	79 (92%)	7 (8%)	9	10
11	AK	90/99 (91%)	89 (99%)	1 (1%)	70	82
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%)	78 (99%)	1 (1%)	65	78
15	AO	75/77 (97%)	75 (100%)	0	100	100
16	AP	65/65 (100%)	62 (95%)	3 (5%)	23	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AQ	74/78 (95%)	71 (96%)	3 (4%)	26	34
18	AR	48/65 (74%)	48 (100%)	0	100	100
19	AS	70/79 (89%)	68 (97%)	2 (3%)	37	50
20	AT	65/66 (98%)	62 (95%)	3 (5%)	23	30
21	AU	44/61 (72%)	39 (89%)	5 (11%)	4	4
25	B0	47/48 (98%)	47 (100%)	0	100	100
26	B1	45/49 (92%)	44 (98%)	1 (2%)	47	61
27	B2	38/38 (100%)	38 (100%)	0	100	100
28	B3	51/52 (98%)	51 (100%)	0	100	100
29	B4	34/34 (100%)	34 (100%)	0	100	100
30	B5	55/62 (89%)	53 (96%)	2 (4%)	30	40
33	BC	216/218 (99%)	216 (100%)	0	100	100
34	BD	164/164 (100%)	163 (99%)	1 (1%)	84	91
35	BE	165/165 (100%)	165 (100%)	0	100	100
36	BF	148/150 (99%)	146 (99%)	2 (1%)	62	77
37	BG	137/138 (99%)	134 (98%)	3 (2%)	47	61
38	BH	38/114 (33%)	38 (100%)	0	100	100
39	BJ	116/116 (100%)	116 (100%)	0	100	100
40	BK	103/104 (99%)	102 (99%)	1 (1%)	73	84
41	BL	102/103 (99%)	102 (100%)	0	100	100
42	BM	109/109 (100%)	109 (100%)	0	100	100
43	BN	100/103 (97%)	100 (100%)	0	100	100
44	BO	86/87 (99%)	85 (99%)	1 (1%)	67	80
45	BP	99/100 (99%)	96 (97%)	3 (3%)	36	48
46	BQ	89/90 (99%)	89 (100%)	0	100	100
47	BR	84/84 (100%)	84 (100%)	0	100	100
48	BS	93/93 (100%)	93 (100%)	0	100	100
49	BT	80/84 (95%)	78 (98%)	2 (2%)	42	56
50	BU	83/85 (98%)	82 (99%)	1 (1%)	67	80
51	BV	78/78 (100%)	78 (100%)	0	100	100
52	BW	56/63 (89%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	BX	67/68 (98%)	67 (100%)	0	100	100
54	BY	55/55 (100%)	54 (98%)	1 (2%)	54	69
55	BZ	48/49 (98%)	48 (100%)	0	100	100
All	All	4532/4829 (94%)	4457 (98%)	75 (2%)	56	71

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	59	LYS
2	AB	64	LYS
2	AB	66	LYS
2	AB	73	LYS
2	AB	74	ARG
2	AB	81	LYS
2	AB	82	ASP
2	AB	85	LEU
2	AB	87	CYS
4	AD	12	SER
4	AD	68	LEU
4	AD	69	GLU
4	AD	73	ARG
4	AD	147	GLU
4	AD	148	LYS
4	AD	151	LYS
4	AD	153	SER
4	AD	154	ARG
4	AD	155	VAL
4	AD	156	LYS
4	AD	159	LEU
4	AD	192	SER
4	AD	194	ASP
5	AE	149	SER
5	AE	152	MET
6	AF	2	ARG
6	AF	90	MET
6	AF	93	LYS
7	AG	13	LEU
7	AG	17	LYS
8	AH	106	THR
8	AH	107	SER
10	AJ	35	GLN

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Mol	Chain	Res	Type
10	AJ	37	ARG
10	AJ	76	ILE
10	AJ	78	GLU
10	AJ	80	THR
10	AJ	81	GLU
10	AJ	82	LYS
11	AK	37	ARG
14	AN	83	LYS
16	AP	8	ARG
16	AP	18	GLN
16	AP	20	VAL
17	AQ	17	MET
17	AQ	21	ILE
17	AQ	69	LYS
19	AS	11	ILE
19	AS	13	LEU
20	AT	44	LYS
20	AT	67	ILE
20	AT	69	LYS
21	AU	35	ARG
21	AU	36	GLU
21	AU	38	TYR
21	AU	40	LYS
21	AU	43	THR
26	B1	25	LYS
30	B5	62	LYS
30	B5	63	ARG
34	BD	157	LYS
36	BF	14	LYS
36	BF	94	GLU
37	BG	42	GLU
37	BG	43	VAL
37	BG	56	ASP
40	BK	99	ILE
44	BO	35	ILE
45	BP	65	SER
45	BP	66	ASN
45	BP	89	ARG
49	BT	3	ARG
49	BT	4	GLU
50	BU	49	VAL
54	BY	36	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	58	ASN
2	AB	177	ASN
3	AC	25	ASN
4	AD	71	GLN
4	AD	152	GLN
6	AF	68	GLN
8	AH	18	GLN
9	AI	32	GLN
11	AK	40	ASN
11	AK	119	ASN
13	AM	14	HIS
16	AP	29	ASN
20	AT	21	ASN
26	B1	19	HIS
26	B1	26	ASN
27	B2	26	ASN
30	B5	65	ASN
33	BC	53	HIS
33	BC	134	ASN
33	BC	260	ASN
34	BD	42	ASN
34	BD	140	HIS
34	BD	164	GLN
34	BD	173	GLN
35	BE	165	HIS
38	BH	2	GLN
41	BL	104	GLN
43	BN	107	ASN
44	BO	98	GLN
45	BP	41	GLN
45	BP	52	ASN
46	BQ	20	GLN
46	BQ	71	GLN
46	BQ	72	ASN
52	BW	76	ASN
53	BX	36	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1538/1539 (99%)	208 (13%)	13 (0%)
22	AV	9/89 (10%)	0	0
23	AW	72/76 (94%)	15 (20%)	3 (4%)
23	AY	72/76 (94%)	23 (31%)	3 (4%)
24	AX	76/77 (98%)	18 (23%)	1 (1%)
31	BA	2895/2903 (99%)	407 (14%)	18 (0%)
32	BB	117/120 (97%)	9 (7%)	0
All	All	4779/4880 (97%)	680 (14%)	38 (0%)

All (680) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	22	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	51	A
1	AA	52	C
1	AA	69	G
1	AA	74	A
1	AA	83	C
1	AA	84	U
1	AA	87	C
1	AA	95	C
1	AA	97	G
1	AA	108	G
1	AA	116	A
1	AA	117	G
1	AA	120	A
1	AA	121	U
1	AA	130	A
1	AA	131	A
1	AA	143	A
1	AA	144	G
1	AA	160	A
1	AA	161	A
1	AA	162	A
1	AA	163	C
1	AA	164	G
1	AA	182	A
1	AA	183	C

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Mol	Chain	Res	Type
1	AA	189	A
1	AA	197	A
1	AA	205	A
1	AA	206	C
1	AA	207	C
1	AA	210	C
1	AA	211	G
1	AA	212	G
1	AA	226	G
1	AA	240	G
1	AA	245	U
1	AA	247	G
1	AA	251	G
1	AA	266	G
1	AA	267	C
1	AA	289	G
1	AA	321	A
1	AA	328	C
1	AA	329	A
1	AA	332	G
1	AA	347	G
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	397	A
1	AA	406	G
1	AA	412	A
1	AA	413	G
1	AA	421	U
1	AA	422	C
1	AA	423	G
1	AA	424	G
1	AA	429	U
1	AA	448	A
1	AA	458	U
1	AA	467	U
1	AA	468	A
1	AA	481	G
1	AA	484	G
1	AA	485	U

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Mol	Chain	Res	Type
1	AA	486	U
1	AA	495	A
1	AA	496	A
1	AA	497	G
1	AA	511	C
1	AA	512	U
1	AA	518	C
1	AA	527	G
1	AA	531	U
1	AA	532	A
1	AA	547	A
1	AA	559	A
1	AA	564	C
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	581	G
1	AA	596	A
1	AA	653	U
1	AA	665	A
1	AA	687	A
1	AA	695	A
1	AA	721	G
1	AA	723	U
1	AA	724	G
1	AA	731	G
1	AA	755	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	815	A
1	AA	817	C
1	AA	828	U
1	AA	829	G
1	AA	841	C
1	AA	843	U
1	AA	844	G
1	AA	845	A
1	AA	846	G
1	AA	858	G
1	AA	914	A

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Mol	Chain	Res	Type
1	AA	922	G
1	AA	926	G
1	AA	934	C
1	AA	935	A
1	AA	960	U
1	AA	966	G
1	AA	969	A
1	AA	971	G
1	AA	972	C
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	983	A
1	AA	992	U
1	AA	993	G
1	AA	1004	A
1	AA	1020	G
1	AA	1026	G
1	AA	1027	C
1	AA	1030	U
1	AA	1032	G
1	AA	1034	G
1	AA	1037	C
1	AA	1044	A
1	AA	1054	C
1	AA	1065	U
1	AA	1079	G
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1124	G
1	AA	1125	U
1	AA	1135	U
1	AA	1136	C
1	AA	1137	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1145	A
1	AA	1146	A
1	AA	1159	U
1	AA	1160	G

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Mol	Chain	Res	Type
1	AA	1161	C
1	AA	1167	A
1	AA	1181	G
1	AA	1184	G
1	AA	1196	A
1	AA	1197	A
1	AA	1202	U
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C
1	AA	1227	A
1	AA	1238	A
1	AA	1240	U
1	AA	1241	G
1	AA	1260	G
1	AA	1280	A
1	AA	1286	U
1	AA	1287	A
1	AA	1293	C
1	AA	1299	A
1	AA	1300	G
1	AA	1302	C
1	AA	1305	G
1	AA	1317	C
1	AA	1318	A
1	AA	1320	C
1	AA	1337	G
1	AA	1338	G
1	AA	1346	A
1	AA	1353	G
1	AA	1363	A
1	AA	1364	U
1	AA	1370	G
1	AA	1378	C
1	AA	1397	C
1	AA	1398	A
1	AA	1440	U
1	AA	1441	A
1	AA	1446	A
1	AA	1487	G
1	AA	1492	A
1	AA	1494	G

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Mol	Chain	Res	Type
1	AA	1497	G
1	AA	1503	A
1	AA	1506	U
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1535	C
1	AA	1536	C
1	AA	1539	C
23	AW	5	G
23	AW	19	G
23	AW	20	G
23	AW	21	A
23	AW	29	U
23	AW	36	C
23	AW	44	G
23	AW	45	G
23	AW	47	U
23	AW	48	C
23	AW	54	5MU
23	AW	59	U
23	AW	60	C
23	AW	73	A
23	AW	76	A
24	AX	2	G
24	AX	16	C
24	AX	18	U
24	AX	19	G
24	AX	21	U
24	AX	22	A
24	AX	24	C
24	AX	25	U
24	AX	47	G
24	AX	48	U
24	AX	49	C
24	AX	55	U
24	AX	56	U
24	AX	60	A
24	AX	61	U
24	AX	62	C
24	AX	63	C
24	AX	77	A

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Mol	Chain	Res	Type
23	AY	5	G
23	AY	9	A
23	AY	15	G
23	AY	20	G
23	AY	21	A
23	AY	31	C
23	AY	33	U
23	AY	34	C
23	AY	35	A
23	AY	38	A
23	AY	44	G
23	AY	45	G
23	AY	46	7MG
23	AY	47	U
23	AY	48	C
23	AY	54	5MU
23	AY	58	A
23	AY	59	U
23	AY	60	C
23	AY	61	C
23	AY	66	A
23	AY	73	A
23	AY	76	A
31	BA	10	A
31	BA	15	G
31	BA	26	G
31	BA	34	U
31	BA	46	G
31	BA	55	G
31	BA	58	G
31	BA	71	A
31	BA	74	A
31	BA	75	G
31	BA	83	A
31	BA	84	A
31	BA	96	C
31	BA	101	A
31	BA	103	A
31	BA	118	A
31	BA	119	A
31	BA	120	U
31	BA	138	U

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Mol	Chain	Res	Type
31	BA	139	U
31	BA	140	C
31	BA	141	G
31	BA	149	A
31	BA	162	U
31	BA	163	C
31	BA	166	U
31	BA	181	A
31	BA	196	A
31	BA	199	A
31	BA	215	G
31	BA	216	A
31	BA	221	A
31	BA	222	A
31	BA	228	C
31	BA	233	A
31	BA	248	G
31	BA	255	A
31	BA	266	G
31	BA	272	A
31	BA	275	C
31	BA	276	U
31	BA	277	G
31	BA	278	A
31	BA	279	A
31	BA	281	C
31	BA	285	G
31	BA	286	U
31	BA	309	A
31	BA	311	A
31	BA	329	G
31	BA	330	A
31	BA	359	G
31	BA	361	G
31	BA	362	A
31	BA	371	A
31	BA	372	G
31	BA	386	G
31	BA	396	G
31	BA	405	U
31	BA	411	G
31	BA	412	A

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Mol	Chain	Res	Type
31	BA	424	G
31	BA	480	A
31	BA	481	G
31	BA	490	C
31	BA	491	G
31	BA	502	A
31	BA	505	A
31	BA	509	C
31	BA	530	G
31	BA	531	C
31	BA	532	A
31	BA	546	U
31	BA	548	G
31	BA	549	G
31	BA	563	A
31	BA	573	U
31	BA	575	A
31	BA	586	A
31	BA	603	A
31	BA	614	A
31	BA	622	G
31	BA	627	A
31	BA	637	A
31	BA	645	C
31	BA	647	G
31	BA	654	A
31	BA	677	A
31	BA	686	U
31	BA	694	U
31	BA	695	G
31	BA	730	A
31	BA	738	G
31	BA	747	U
31	BA	764	A
31	BA	771	G
31	BA	775	G
31	BA	776	G
31	BA	782	A
31	BA	784	G
31	BA	785	G
31	BA	805	G
31	BA	812	C

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Mol	Chain	Res	Type
31	BA	819	A
31	BA	827	U
31	BA	828	U
31	BA	830	G
31	BA	845	A
31	BA	846	U
31	BA	847	U
31	BA	858	G
31	BA	859	G
31	BA	878	A
31	BA	883	G
31	BA	884	U
31	BA	885	C
31	BA	896	A
31	BA	897	C
31	BA	910	A
31	BA	914	G
31	BA	915	C
31	BA	927	A
31	BA	931	U
31	BA	941	A
31	BA	946	C
31	BA	961	C
31	BA	974	G
31	BA	983	A
31	BA	985	C
31	BA	995	C
31	BA	996	A
31	BA	1005	C
31	BA	1012	U
31	BA	1013	C
31	BA	1026	G
31	BA	1033	U
31	BA	1046	A
31	BA	1047	G
31	BA	1056	G
31	BA	1057	A
31	BA	1058	U
31	BA	1060	U
31	BA	1061	U
31	BA	1062	G
31	BA	1063	G

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Mol	Chain	Res	Type
31	BA	1064	C
31	BA	1065	U
31	BA	1066	U
31	BA	1067	A
31	BA	1068	G
31	BA	1070	A
31	BA	1071	G
31	BA	1072	C
31	BA	1073	A
31	BA	1083	U
31	BA	1084	A
31	BA	1085	A
31	BA	1088	A
31	BA	1089	A
31	BA	1092	C
31	BA	1096	A
31	BA	1098	A
31	BA	1101	U
31	BA	1104	C
31	BA	1106	G
31	BA	1108	U
31	BA	1111	A
31	BA	1112	G
31	BA	1116	G
31	BA	1132	U
31	BA	1133	A
31	BA	1135	C
31	BA	1136	G
31	BA	1139	G
31	BA	1142	A
31	BA	1172	C
31	BA	1173	U
31	BA	1174	U
31	BA	1175	A
31	BA	1176	U
31	BA	1179	G
31	BA	1180	U
31	BA	1206	G
31	BA	1238	G
31	BA	1250	G
31	BA	1253	A
31	BA	1255	U

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Mol	Chain	Res	Type
31	BA	1256	G
31	BA	1266	G
31	BA	1271	G
31	BA	1272	A
31	BA	1300	G
31	BA	1301	A
31	BA	1345	C
31	BA	1352	U
31	BA	1365	A
31	BA	1368	G
31	BA	1379	U
31	BA	1383	A
31	BA	1384	A
31	BA	1395	A
31	BA	1416	G
31	BA	1417	C
31	BA	1428	C
31	BA	1434	A
31	BA	1452	G
31	BA	1453	A
31	BA	1482	G
31	BA	1493	C
31	BA	1504	A
31	BA	1508	A
31	BA	1509	A
31	BA	1510	G
31	BA	1515	A
31	BA	1524	G
31	BA	1533	C
31	BA	1534	U
31	BA	1535	A
31	BA	1536	C
31	BA	1537	G
31	BA	1540	G
31	BA	1566	A
31	BA	1569	A
31	BA	1578	U
31	BA	1584	U
31	BA	1585	C
31	BA	1608	A
31	BA	1610	A
31	BA	1647	U

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Mol	Chain	Res	Type
31	BA	1648	U
31	BA	1649	G
31	BA	1652	A
31	BA	1674	G
31	BA	1677	A
31	BA	1715	G
31	BA	1716	U
31	BA	1728	C
31	BA	1729	U
31	BA	1730	C
31	BA	1733	G
31	BA	1738	G
31	BA	1758	U
31	BA	1764	C
31	BA	1773	A
31	BA	1791	A
31	BA	1800	C
31	BA	1801	A
31	BA	1802	A
31	BA	1808	A
31	BA	1816	C
31	BA	1829	A
31	BA	1848	A
31	BA	1858	A
31	BA	1870	C
31	BA	1872	A
31	BA	1873	G
31	BA	1903	G
31	BA	1906	G
31	BA	1913	A
31	BA	1914	C
31	BA	1919	A
31	BA	1927	A
31	BA	1929	G
31	BA	1930	G
31	BA	1937	A
31	BA	1955	U
31	BA	1965	C
31	BA	1967	C
31	BA	1970	A
31	BA	1971	U
31	BA	1972	G

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Mol	Chain	Res	Type
31	BA	1991	U
31	BA	1993	U
31	BA	1997	C
31	BA	2022	U
31	BA	2023	C
31	BA	2031	A
31	BA	2033	A
31	BA	2043	C
31	BA	2055	C
31	BA	2056	G
31	BA	2060	A
31	BA	2061	G
31	BA	2062	A
31	BA	2069	G
31	BA	2100	G
31	BA	2102	G
31	BA	2110	G
31	BA	2111	U
31	BA	2112	G
31	BA	2113	U
31	BA	2114	A
31	BA	2115	G
31	BA	2116	G
31	BA	2117	A
31	BA	2118	U
31	BA	2119	A
31	BA	2123	G
31	BA	2125	G
31	BA	2126	A
31	BA	2127	G
31	BA	2128	G
31	BA	2129	C
31	BA	2131	U
31	BA	2132	U
31	BA	2133	G
31	BA	2135	A
31	BA	2137	U
31	BA	2140	G
31	BA	2145	C
31	BA	2148	G
31	BA	2150	C
31	BA	2157	G

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Mol	Chain	Res	Type
31	BA	2158	A
31	BA	2159	G
31	BA	2162	G
31	BA	2164	C
31	BA	2168	G
31	BA	2169	A
31	BA	2170	A
31	BA	2171	A
31	BA	2172	U
31	BA	2177	C
31	BA	2181	U
31	BA	2183	A
31	BA	2187	U
31	BA	2190	G
31	BA	2193	G
31	BA	2194	U
31	BA	2198	A
31	BA	2204	G
31	BA	2211	A
31	BA	2212	A
31	BA	2225	A
31	BA	2226	C
31	BA	2238	G
31	BA	2239	G
31	BA	2250	G
31	BA	2279	G
31	BA	2283	C
31	BA	2287	A
31	BA	2297	A
31	BA	2305	U
31	BA	2309	A
31	BA	2310	C
31	BA	2311	A
31	BA	2322	A
31	BA	2325	G
31	BA	2327	A
31	BA	2333	A
31	BA	2347	C
31	BA	2361	G
31	BA	2383	G
31	BA	2385	C
31	BA	2396	G

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Mol	Chain	Res	Type
31	BA	2402	U
31	BA	2406	A
31	BA	2407	A
31	BA	2423	U
31	BA	2425	A
31	BA	2429	G
31	BA	2430	A
31	BA	2435	A
31	BA	2441	U
31	BA	2448	A
31	BA	2474	U
31	BA	2476	A
31	BA	2491	U
31	BA	2502	G
31	BA	2505	G
31	BA	2506	U
31	BA	2518	A
31	BA	2520	C
31	BA	2529	G
31	BA	2547	A
31	BA	2554	U
31	BA	2566	A
31	BA	2567	G
31	BA	2573	C
31	BA	2602	A
31	BA	2609	U
31	BA	2613	U
31	BA	2615	U
31	BA	2629	U
31	BA	2689	U
31	BA	2690	U
31	BA	2714	G
31	BA	2726	A
31	BA	2733	A
31	BA	2744	G
31	BA	2748	A
31	BA	2778	A
31	BA	2794	C
31	BA	2807	U
31	BA	2820	A
31	BA	2821	A
31	BA	2835	A

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Mol	Chain	Res	Type
31	BA	2849	U
31	BA	2867	G
31	BA	2872	A
31	BA	2873	A
31	BA	2880	C
31	BA	2883	A
31	BA	2884	U
31	BA	2887	A
31	BA	2891	U
31	BA	2903	U
32	BB	15	A
32	BB	44	G
32	BB	56	G
32	BB	88	C
32	BB	89	U
32	BB	90	C
32	BB	91	C
32	BB	99	A
32	BB	109	A

All (38) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	96	U
1	AA	115	G
1	AA	160	A
1	AA	428	G
1	AA	575	G
1	AA	1036	A
1	AA	1078	U
1	AA	1124	G
1	AA	1145	A
1	AA	1160	G
1	AA	1201	A
1	AA	1317	C
1	AA	1408	1MA
23	AW	44	G
23	AW	46	7MG
23	AW	59	U
24	AX	47	G
23	AY	44	G
23	AY	46	7MG

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Mol	Chain	Res	Type
23	AY	58	A
31	BA	25	U
31	BA	138	U
31	BA	271	G
31	BA	404	A
31	BA	479	A
31	BA	784	G
31	BA	846	U
31	BA	1095	A
31	BA	1383	A
31	BA	1583	A
31	BA	1847	A
31	BA	1913	A
31	BA	2109	U
31	BA	2112	G
31	BA	2124	G
31	BA	2169	A
31	BA	2286	G
31	BA	2308	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	1MA	AA	1408	1	17,25,26	0.96	2 (11%)	17,37,40	1.70	4 (23%)
23	PSU	AW	55	23	18,21,22	1.10	1 (5%)	21,30,33	1.96	5 (23%)
23	7MG	AW	46	23	23,26,27	1.43	4 (17%)	27,39,42	2.57	7 (25%)
23	4SU	AY	8	23	18,21,22	3.94	8 (44%)	25,30,33	2.33	5 (20%)
23	5MU	AY	54	23	19,22,23	0.35	0	27,32,35	1.19	3 (11%)
23	4SU	AW	8	23	18,21,22	3.89	8 (44%)	25,30,33	2.29	5 (20%)
23	PSU	AY	55	23	18,21,22	1.07	1 (5%)	21,30,33	1.88	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	7MG	AY	46	23	23,26,27	1.34	3 (13%)	27,39,42	2.81	9 (33%)
23	5MU	AW	54	23	19,22,23	0.38	0	27,32,35	1.16	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
1	1MA	AA	1408	1	-	0/3/25/26	0/3/3/3
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
23	7MG	AW	46	23	-	2/7/37/38	0/3/3/3
23	4SU	AY	8	23	-	0/7/25/26	0/2/2/2
23	5MU	AY	54	23	-	3/7/25/26	0/2/2/2
23	4SU	AW	8	23	-	0/7/25/26	0/2/2/2
23	PSU	AY	55	23	-	0/7/25/26	0/2/2/2
23	7MG	AY	46	23	-	1/7/37/38	0/3/3/3
23	5MU	AW	54	23	-	2/7/25/26	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AY	8	4SU	C4-N3	8.53	1.46	1.37
23	AW	8	4SU	C4-N3	8.35	1.46	1.37
23	AY	8	4SU	C2-N3	7.30	1.50	1.38
23	AW	8	4SU	C2-N3	7.12	1.50	1.38
23	AY	8	4SU	C2-N1	7.04	1.49	1.38
23	AW	8	4SU	C2-N1	6.84	1.49	1.38
23	AY	8	4SU	C6-C5	5.90	1.48	1.35
23	AW	8	4SU	C6-C5	5.88	1.48	1.35
23	AW	8	4SU	C5-C4	5.49	1.49	1.42
23	AY	8	4SU	C5-C4	5.44	1.49	1.42
23	AW	8	4SU	C4-S4	-5.03	1.59	1.68
23	AY	8	4SU	C4-S4	-5.01	1.59	1.68
23	AW	46	7MG	C4-N9	-4.05	1.32	1.37
23	AW	55	PSU	C6-C5	3.58	1.39	1.35
23	AY	55	PSU	C6-C5	3.55	1.39	1.35
23	AY	46	7MG	C5-C4	3.16	1.47	1.37
23	AY	8	4SU	C6-N1	3.10	1.45	1.38
23	AW	8	4SU	C6-N1	3.06	1.45	1.38
23	AY	46	7MG	C4-N9	-2.99	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	46	7MG	C5-C4	2.99	1.46	1.37
23	AW	46	7MG	C6-N1	-2.73	1.33	1.38
1	AA	1408	1MA	C8-N7	-2.62	1.30	1.34
23	AY	46	7MG	C6-N1	-2.56	1.34	1.38
1	AA	1408	1MA	C5-C4	-2.31	1.37	1.43
23	AW	8	4SU	O2-C2	-2.24	1.19	1.23
23	AY	8	4SU	O2-C2	-2.13	1.19	1.23
23	AW	46	7MG	C5-N7	-2.02	1.33	1.35

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AY	46	7MG	N9-C4-N3	9.35	139.16	125.46
23	AW	46	7MG	N9-C4-N3	8.47	137.87	125.46
23	AY	8	4SU	C4-N3-C2	-7.99	119.66	127.31
23	AW	8	4SU	C4-N3-C2	-7.93	119.71	127.31
23	AW	46	7MG	N9-C8-N7	-5.99	94.90	103.37
23	AY	46	7MG	C5-C4-N3	-5.71	117.42	128.13
23	AW	8	4SU	C5-C4-N3	5.49	119.86	114.75
23	AY	46	7MG	N9-C8-N7	-5.43	95.69	103.37
23	AY	8	4SU	C5-C4-N3	5.42	119.79	114.75
23	AW	55	PSU	C4-N3-C2	-4.90	119.62	126.37
23	AW	55	PSU	N1-C2-N3	4.88	120.31	115.17
23	AW	46	7MG	C5-C4-N3	-4.76	119.20	128.13
23	AY	55	PSU	C4-N3-C2	-4.72	119.87	126.37
23	AY	55	PSU	N1-C2-N3	4.64	120.06	115.17
23	AY	46	7MG	C2-N3-C4	4.41	119.89	112.30
23	AY	8	4SU	C5-C4-S4	-3.97	119.78	124.31
23	AY	8	4SU	N3-C2-N1	3.92	120.00	114.89
23	AW	46	7MG	C2-N3-C4	3.89	119.00	112.30
23	AW	8	4SU	N3-C2-N1	3.85	119.90	114.89
23	AY	54	5MU	O3'-C3'-C4'	3.77	121.92	111.08
1	AA	1408	1MA	O3'-C3'-C4'	3.69	121.68	111.08
23	AW	54	5MU	O3'-C3'-C4'	3.64	121.55	111.08
23	AW	8	4SU	C5-C4-S4	-3.61	120.19	124.31
23	AW	54	5MU	O3'-C3'-C2'	3.34	122.51	111.82
1	AA	1408	1MA	O3'-C3'-C2'	3.33	122.48	111.82
23	AY	54	5MU	O3'-C3'-C2'	3.25	122.23	111.82
23	AW	55	PSU	O2-C2-N1	-2.92	119.78	122.79
23	AY	55	PSU	O2-C2-N1	-2.83	119.87	122.79
23	AW	46	7MG	C5-C4-N9	-2.66	102.93	106.33
23	AY	46	7MG	C5-C6-N1	2.63	115.57	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AY	54	5MU	C2'-C3'-C4'	2.49	107.42	102.61
23	AY	55	PSU	C6-N1-C2	-2.44	120.42	122.69
23	AY	46	7MG	C3'-C2'-C1'	2.44	106.08	101.46
1	AA	1408	1MA	C5-C6-N1	-2.38	110.53	113.95
23	AW	55	PSU	C6-N1-C2	-2.37	120.49	122.69
23	AW	55	PSU	C6-C5-C4	2.37	119.77	118.17
1	AA	1408	1MA	N1-C6-N6	2.30	125.50	119.71
23	AY	46	7MG	C5-C4-N9	-2.27	103.42	106.33
23	AW	46	7MG	C5-C6-N1	2.22	114.84	110.94
23	AY	46	7MG	O4'-C1'-N9	2.16	112.23	109.30
23	AY	46	7MG	O6-C6-C5	-2.15	122.34	127.62
23	AY	8	4SU	O2-C2-N1	-2.04	120.14	122.80
23	AW	46	7MG	O6-C6-C5	-2.03	122.64	127.62
23	AW	8	4SU	O2-C2-N1	-2.01	120.17	122.80

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	AW	54	5MU	O4'-C4'-C5'-O5'
23	AY	46	7MG	C4'-C5'-O5'-P
23	AY	54	5MU	O4'-C4'-C5'-O5'
23	AW	54	5MU	C3'-C4'-C5'-O5'
23	AY	54	5MU	C3'-C4'-C5'-O5'
23	AW	46	7MG	C2'-C1'-N9-C8
23	AY	54	5MU	C4'-C5'-O5'-P
23	AW	46	7MG	O4'-C1'-N9-C8

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AY	55	PSU	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 313 ligands modelled in this entry, 311 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	84G	AA	1694	-	39,40,40	1.81	8 (20%)	48,57,57	1.19	8 (16%)
57	84G	AA	1695	-	39,40,40	0.55	1 (2%)	48,57,57	1.04	3 (6%)

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
57	84G	AA	1694	-	-	2/23/76/76	0/3/3/3
57	84G	AA	1695	-	-	3/23/76/76	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	AA	1694	84G	C3-N1	6.64	1.48	1.34
57	AA	1694	84G	O6-C16	3.62	1.51	1.41
57	AA	1694	84G	C21-C20	-3.60	1.49	1.53
57	AA	1694	84G	O1-C3	-3.01	1.17	1.23
57	AA	1694	84G	C11-C12	-2.97	1.45	1.52
57	AA	1694	84G	C20-N5	2.64	1.51	1.47
57	AA	1694	84G	C19-C20	-2.37	1.50	1.53
57	AA	1694	84G	O3-C9	2.22	1.47	1.44
57	AA	1695	84G	C2-C3	-2.06	1.50	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	AA	1694	84G	O3-C9-C11	3.03	113.10	109.91
57	AA	1694	84G	C-C1-C2	-2.63	108.92	112.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	AA	1695	84G	C17-C19-C20	-2.44	107.97	110.67
57	AA	1694	84G	C16-O5-C15	-2.38	112.33	117.98
57	AA	1694	84G	C11-C9-C10	-2.34	108.35	112.83
57	AA	1694	84G	C5-C4-N1	-2.25	107.34	110.78
57	AA	1695	84G	C5-C4-N1	-2.19	107.43	110.78
57	AA	1695	84G	C4-N1-C3	-2.17	119.48	123.25
57	AA	1694	84G	C8-O2-C7	-2.13	112.92	117.98
57	AA	1694	84G	C4-N1-C3	-2.07	119.64	123.25
57	AA	1694	84G	C7-C14-C15	2.06	113.29	109.11

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	AA	1694	84G	O6-C17-C18-O7
57	AA	1694	84G	C19-C17-C18-O7
57	AA	1695	84G	C14-C7-O2-C8
57	AA	1695	84G	C6-C7-O2-C8
57	AA	1695	84G	O-C2-C3-O1

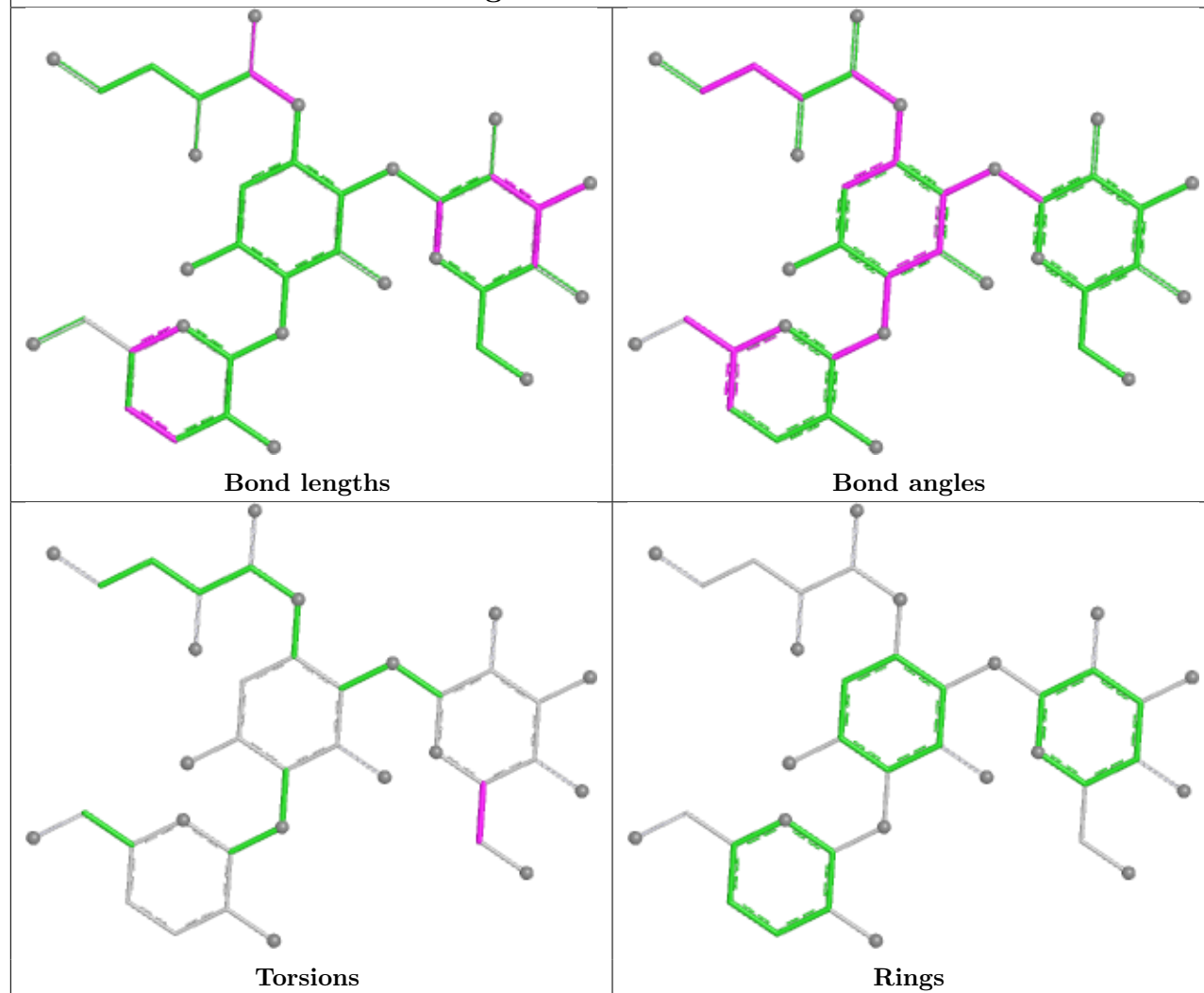
There are no ring outliers.

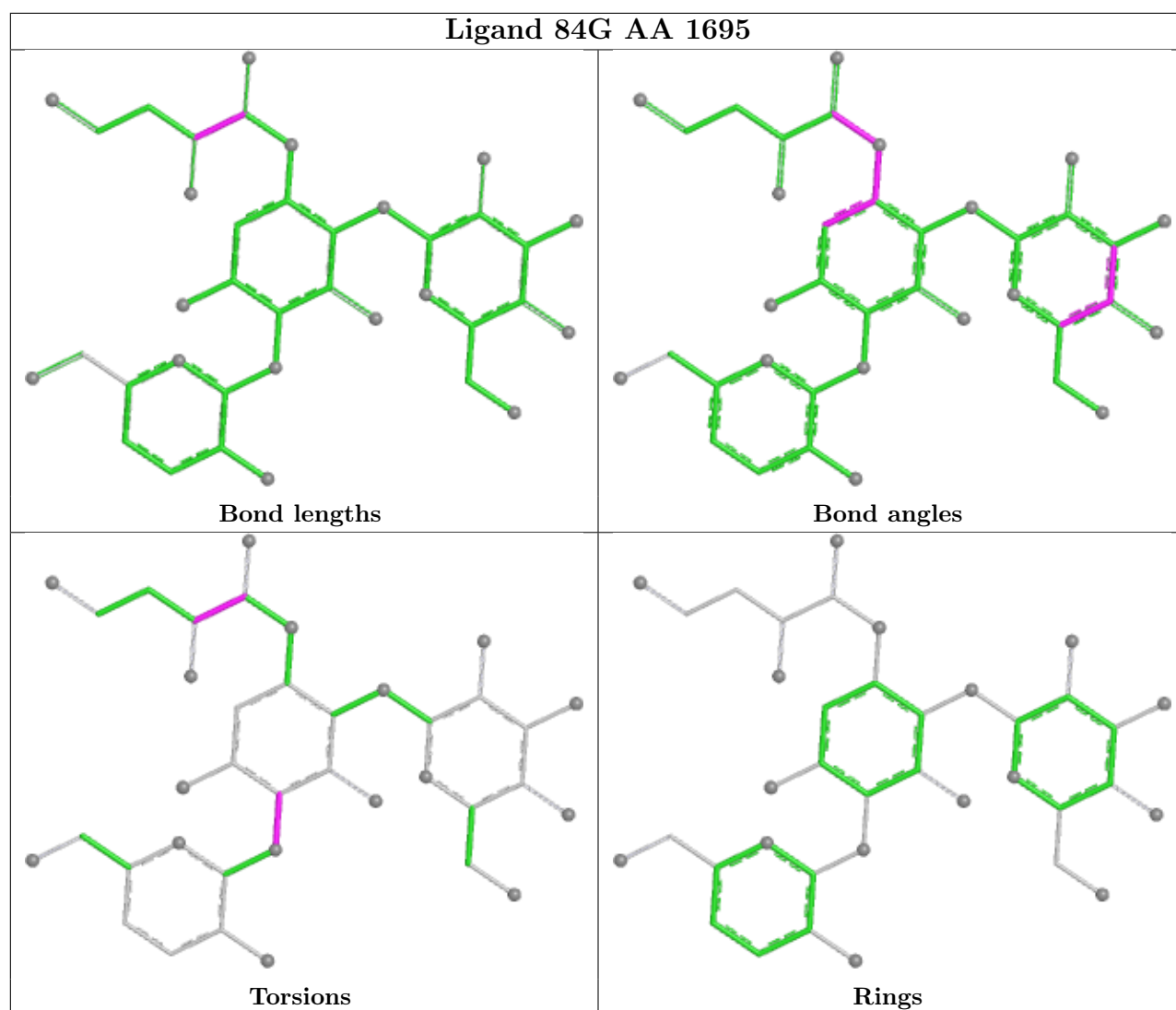
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AA	1694	84G	1	0

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

Ligand 84G AA 1694





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

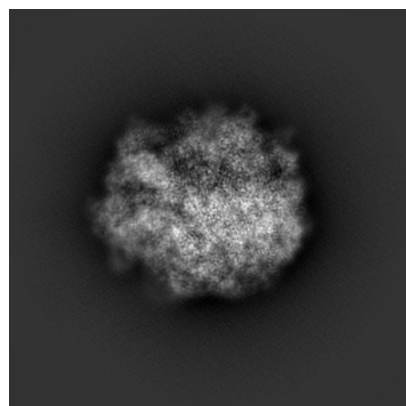
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44192. These allow visual inspection of the internal detail of the map and identification of artifacts.

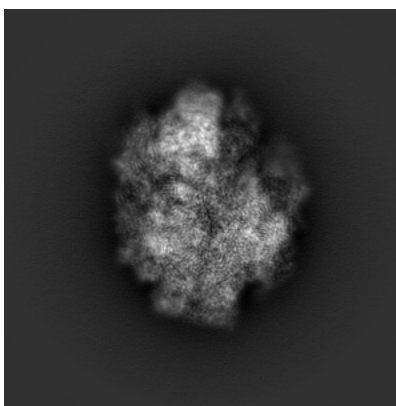
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

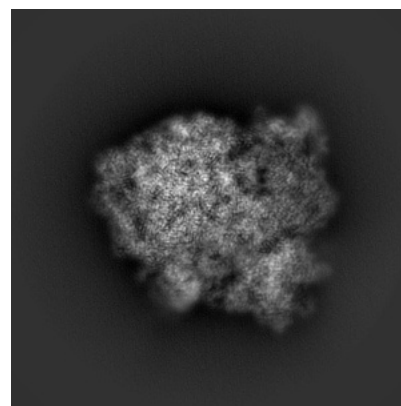
6.1.1 Primary map



X

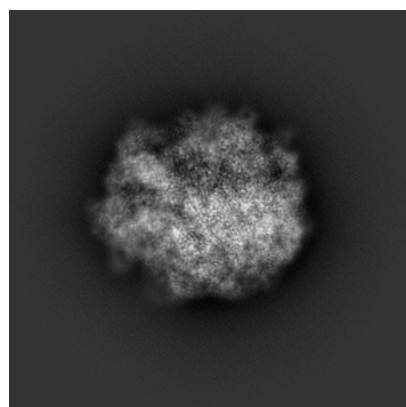


Y

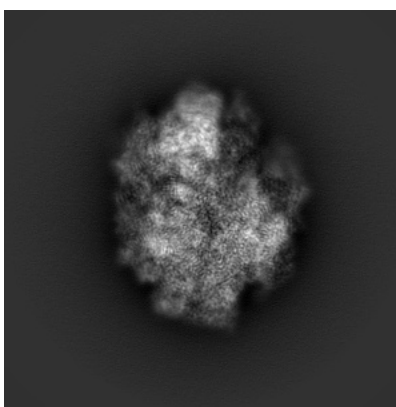


Z

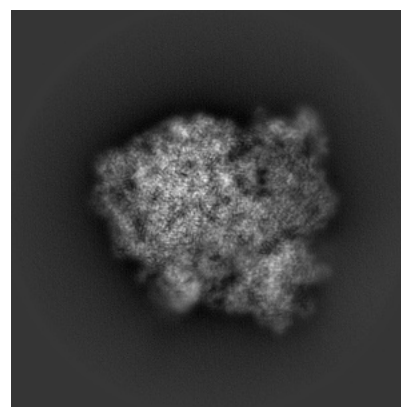
6.1.2 Raw map



X



Y

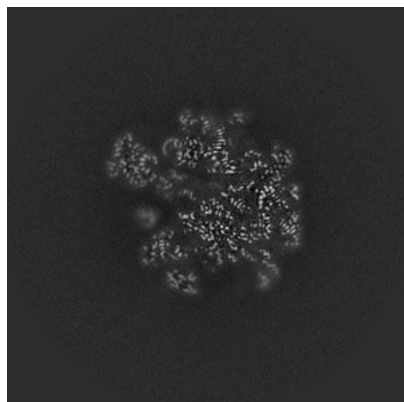


Z

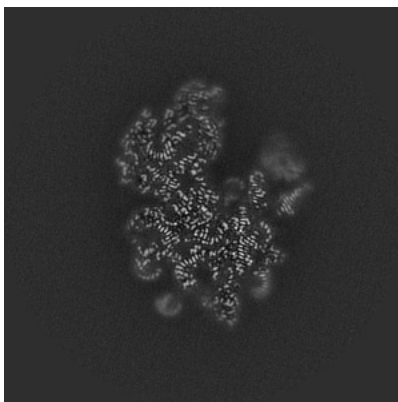
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

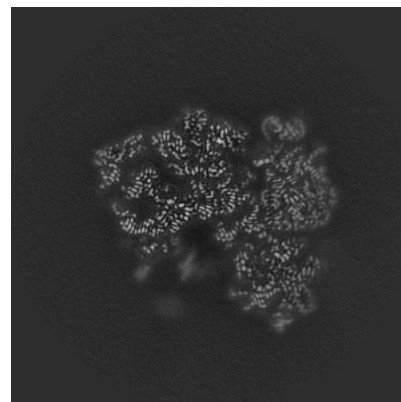
6.2.1 Primary map



X Index: 256

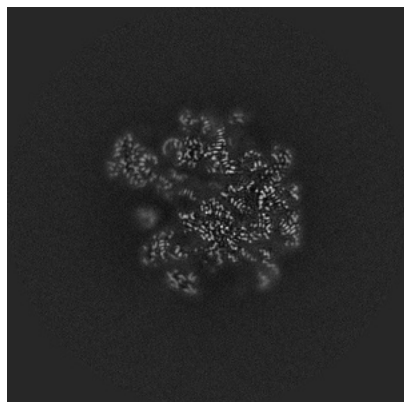


Y Index: 256

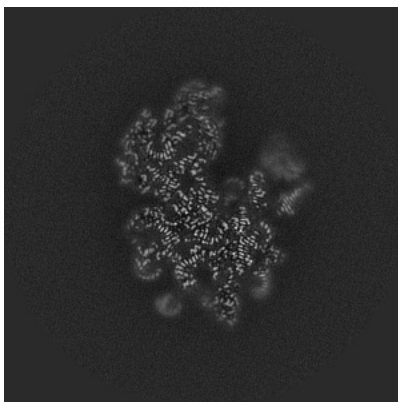


Z Index: 256

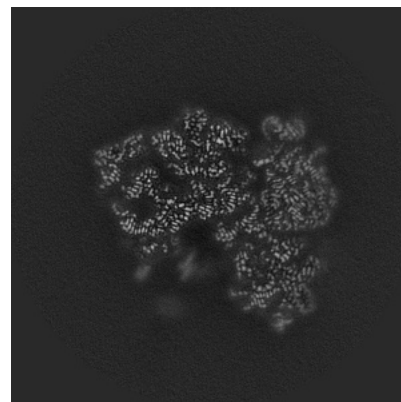
6.2.2 Raw map



X Index: 256



Y Index: 256

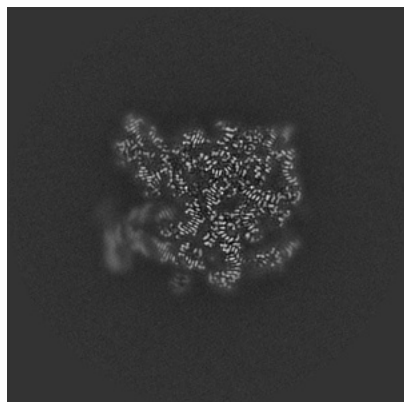


Z Index: 256

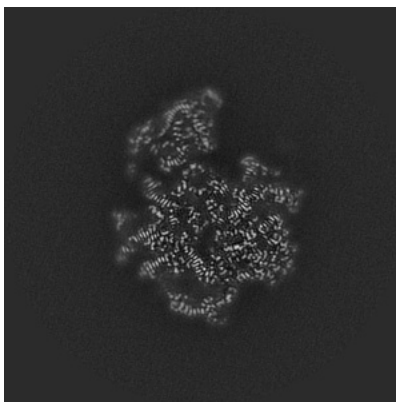
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

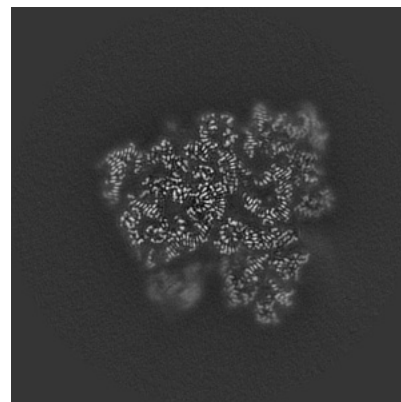
6.3.1 Primary map



X Index: 216

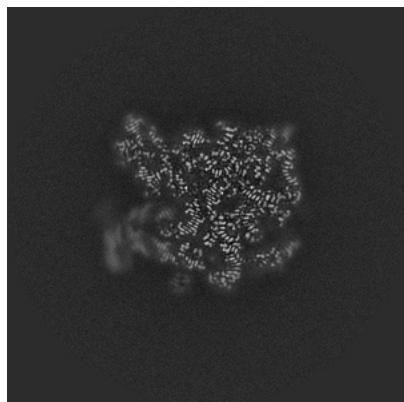


Y Index: 289

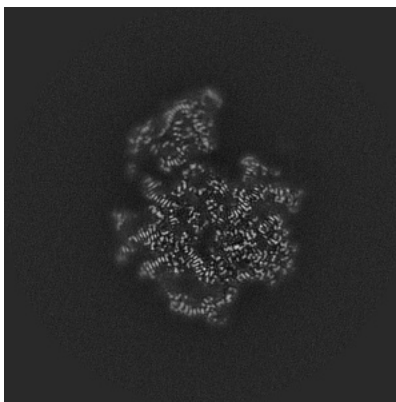


Z Index: 228

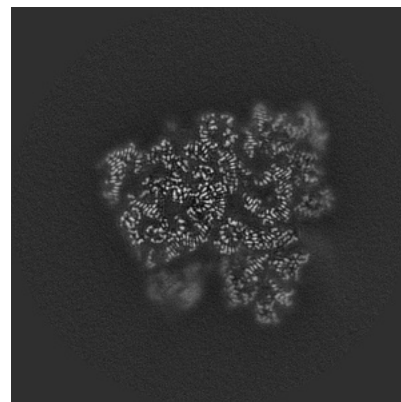
6.3.2 Raw map



X Index: 216



Y Index: 289

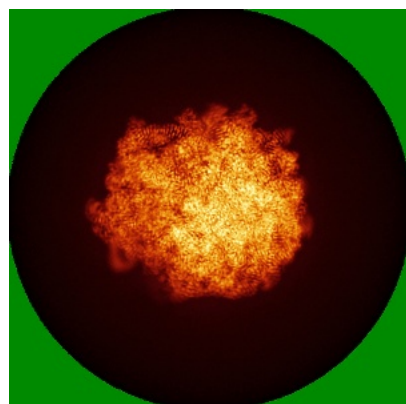


Z Index: 228

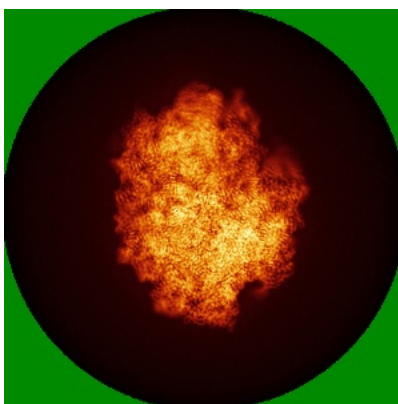
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

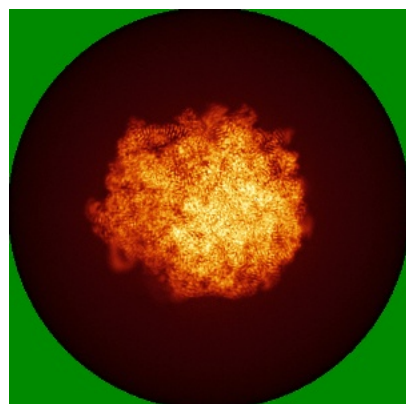


Y

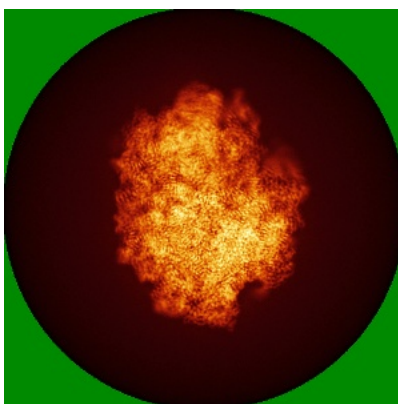


Z

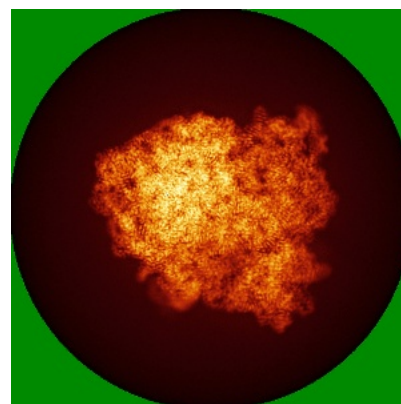
6.4.2 Raw map



X



Y

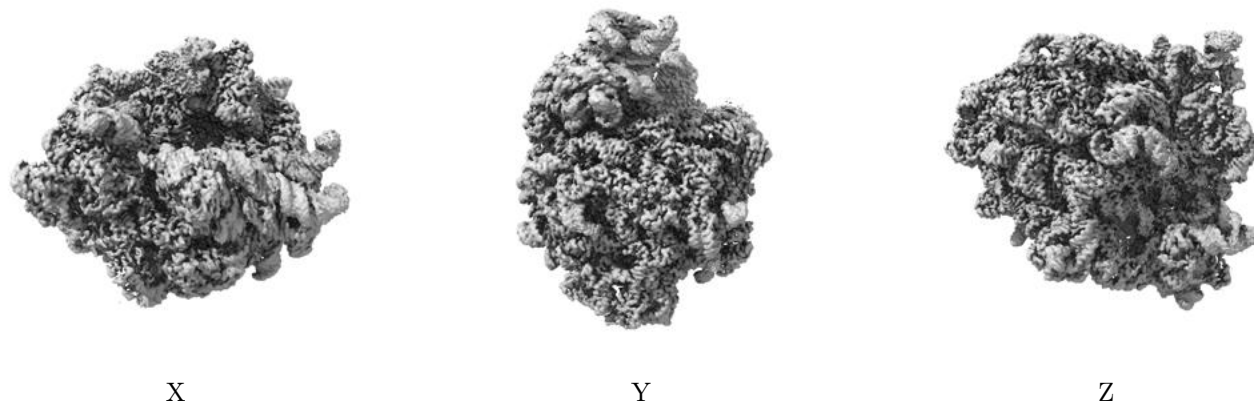


Z

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

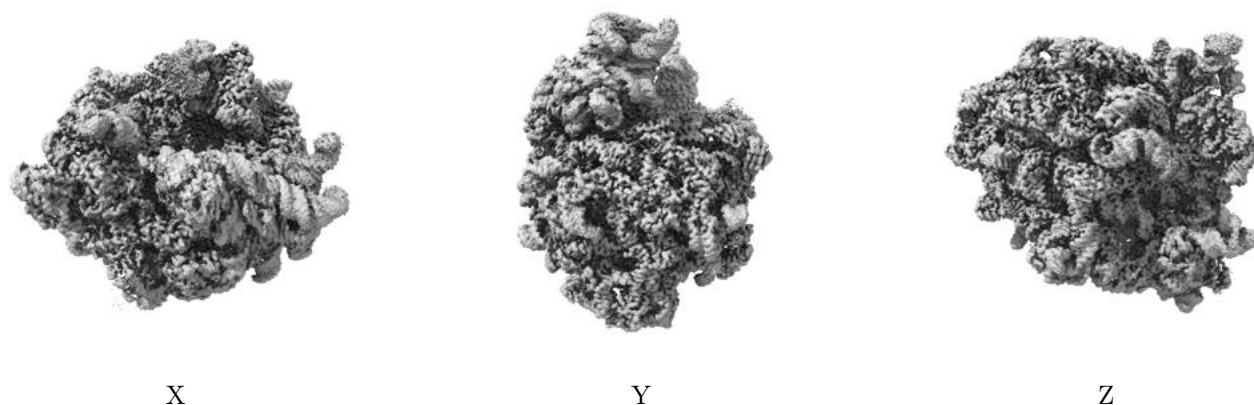
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

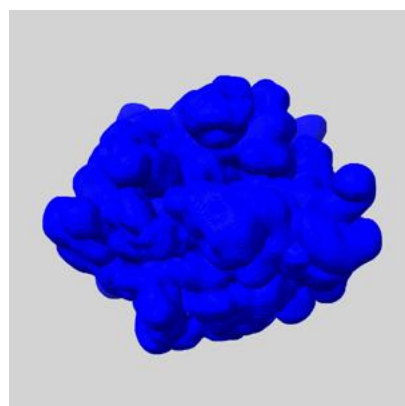
6.6 Mask visualisation [i](#)

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

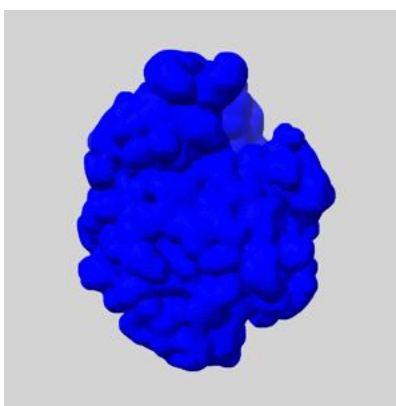
A mask typically either:

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

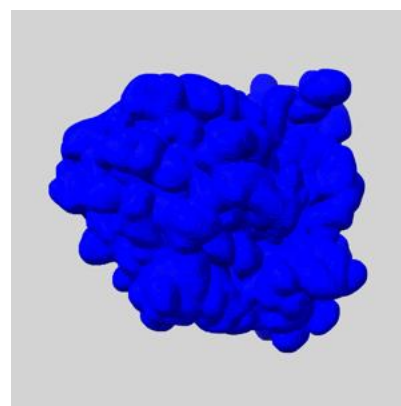
6.6.1 emd_44192_msk_1.map [i](#)



X



Y

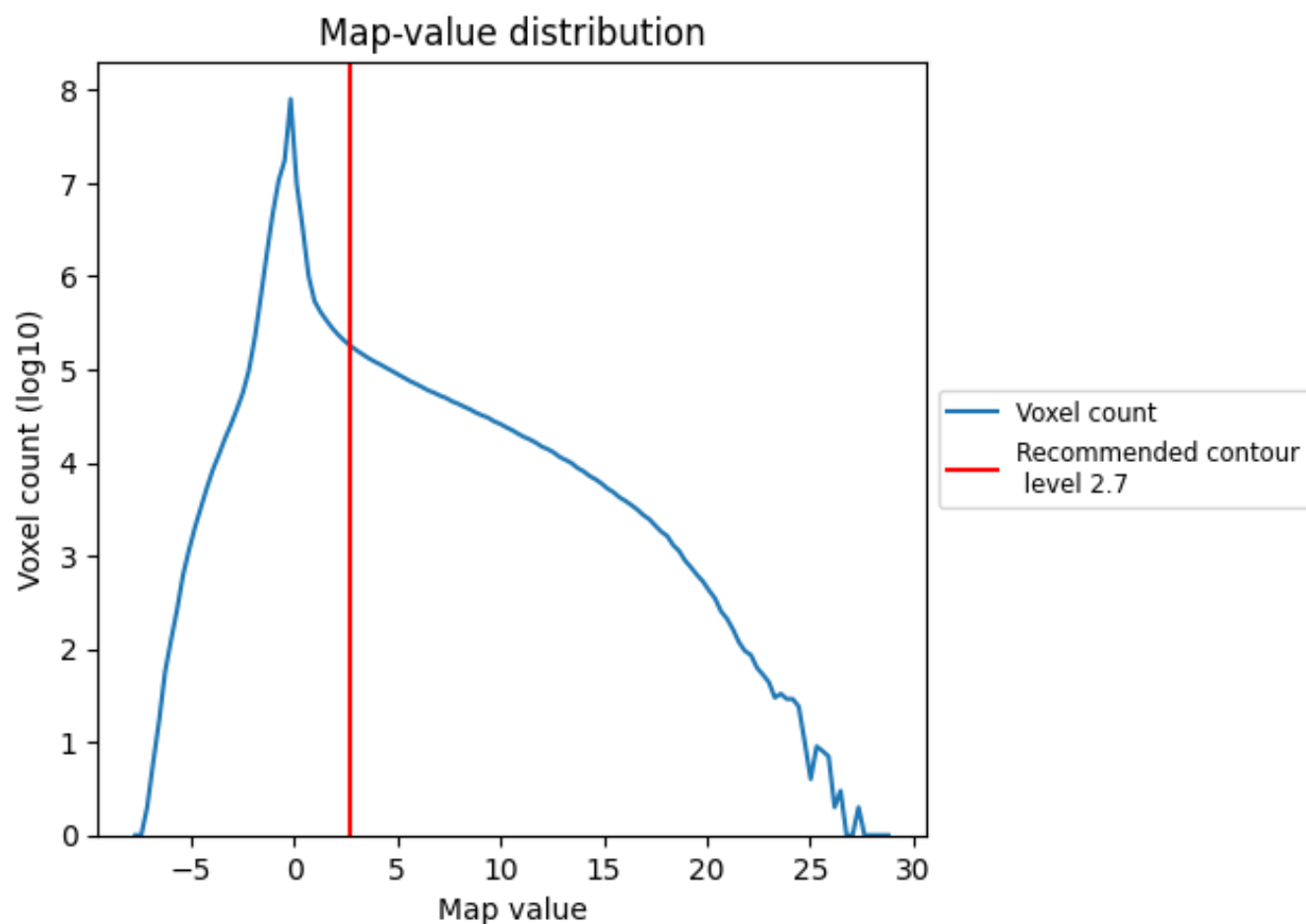


Z

7 Map analysis [i](#)

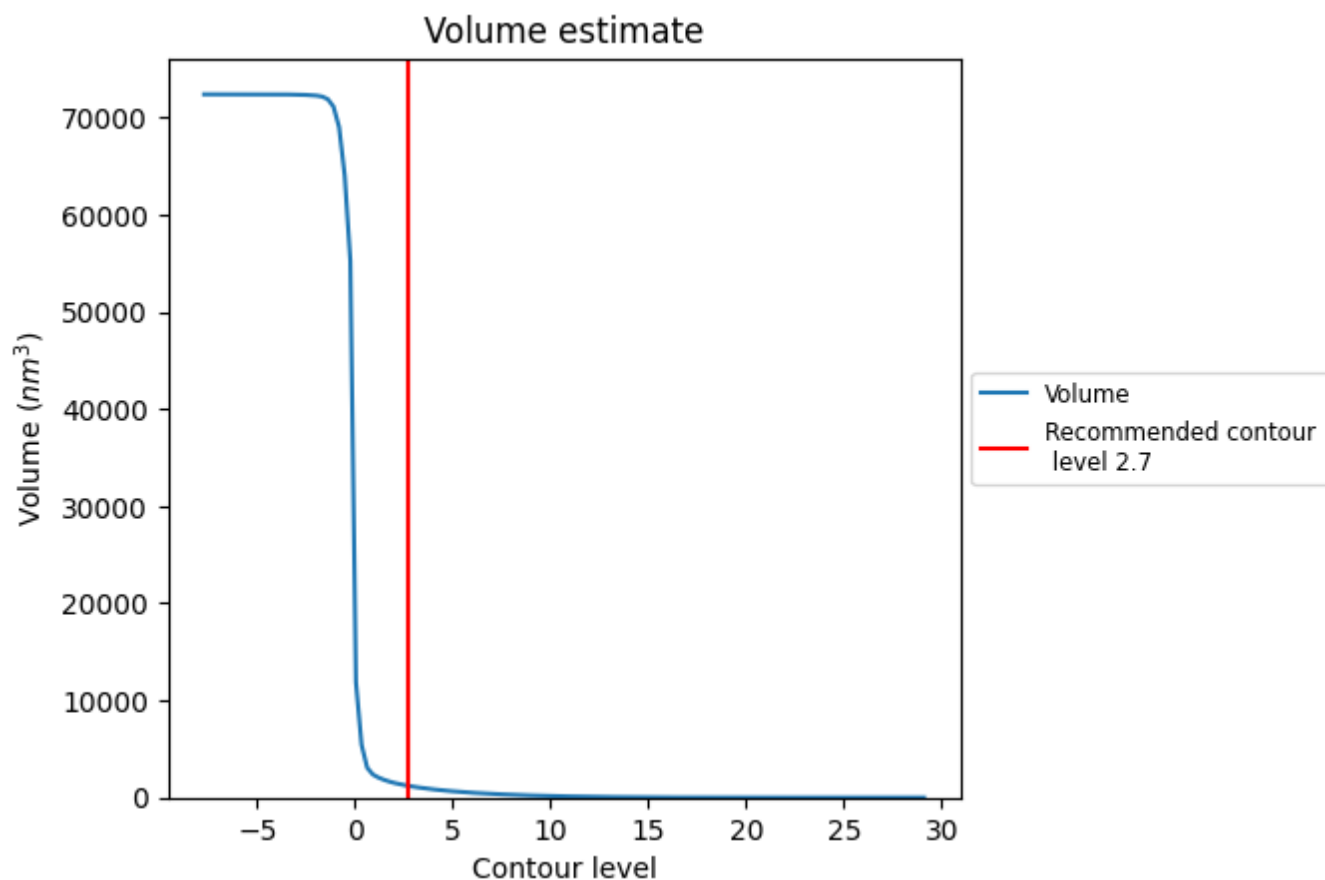
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

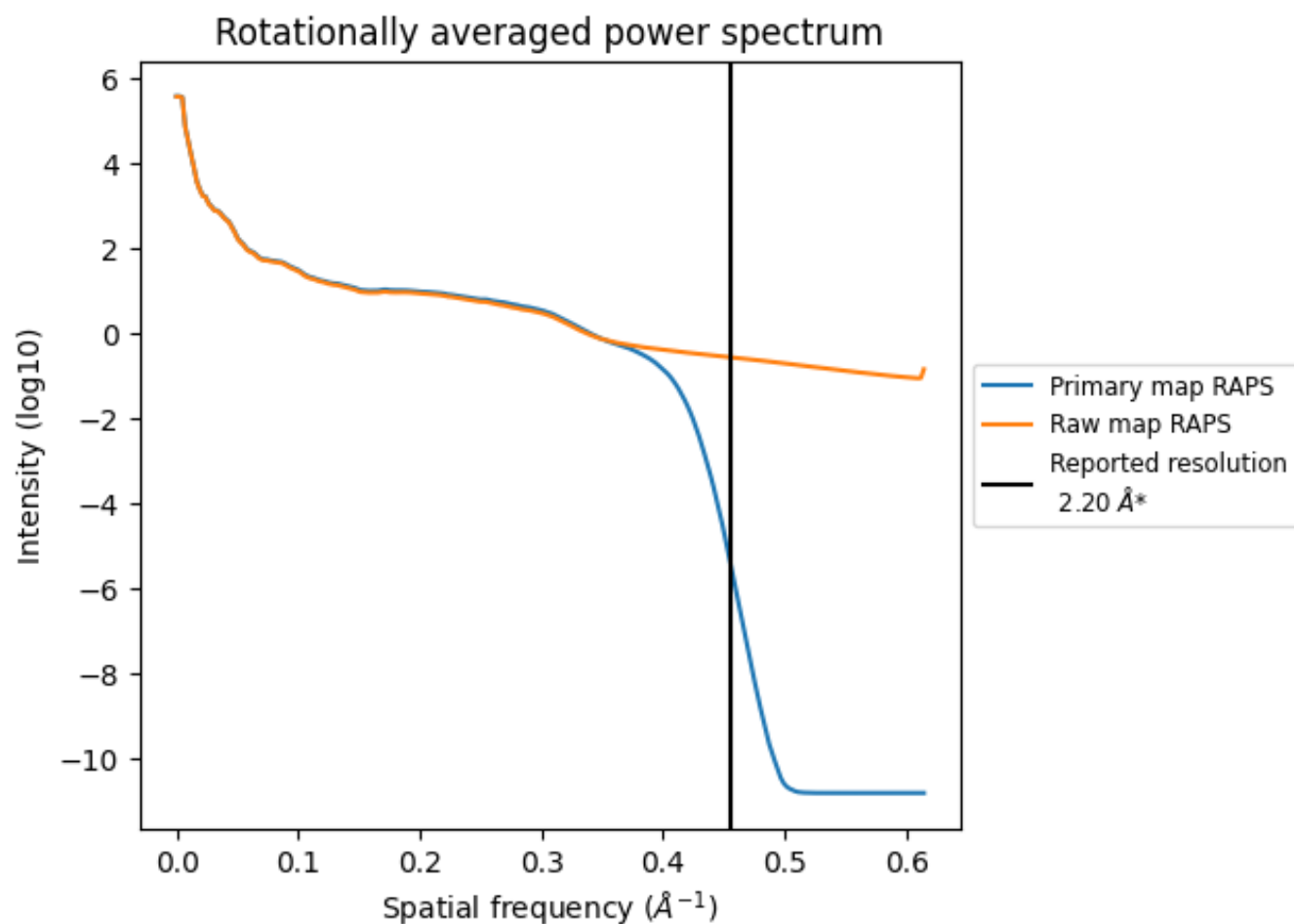
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1217 nm³; this corresponds to an approximate mass of 1099 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 ⓘ

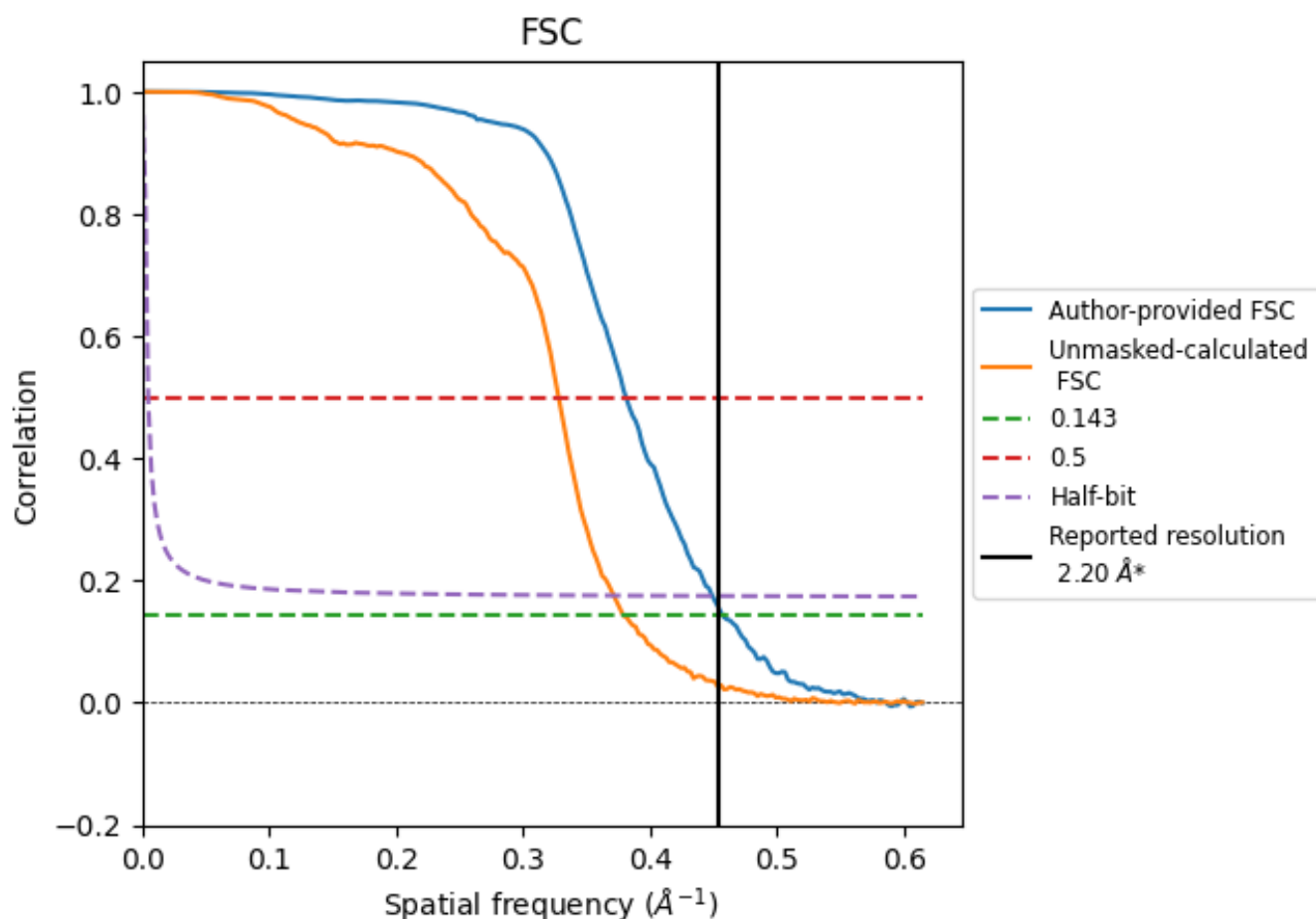


*Reported resolution corresponds to spatial frequency of 0.455 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.455 \AA^{-1}

8.2 Resolution estimates [i](#)

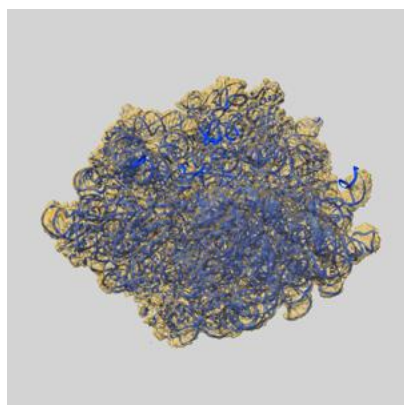
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.19	2.62	2.23
Unmasked-calculated*	2.64	3.05	2.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.64 differs from the reported value 2.2 by more than 10 %

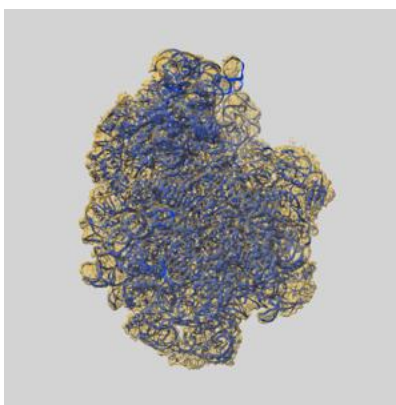
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44192 and PDB model 9B4Z. Per-residue inclusion information can be found in section [3](#) on page [14](#).

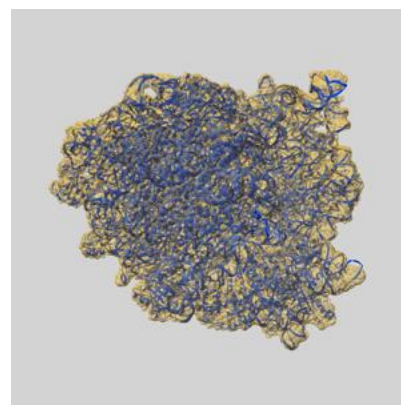
9.1 Map-model overlay [i](#)



X



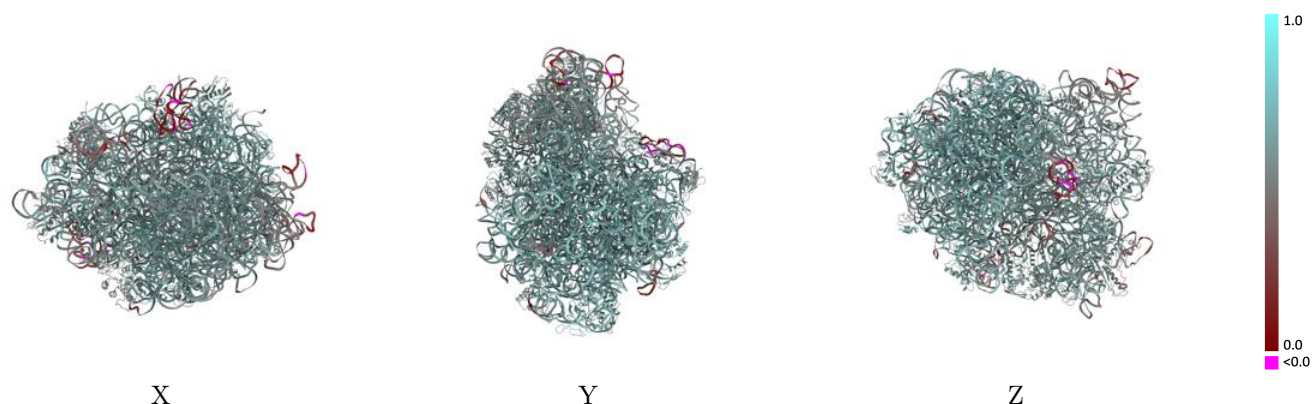
Y



Z

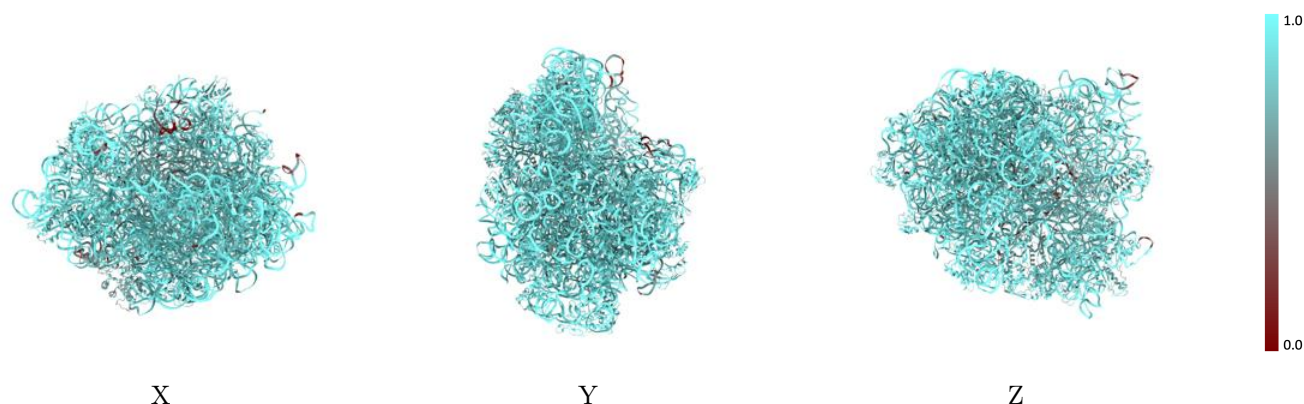
The images above show the 3D surface view of the map at the recommended contour level 2.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



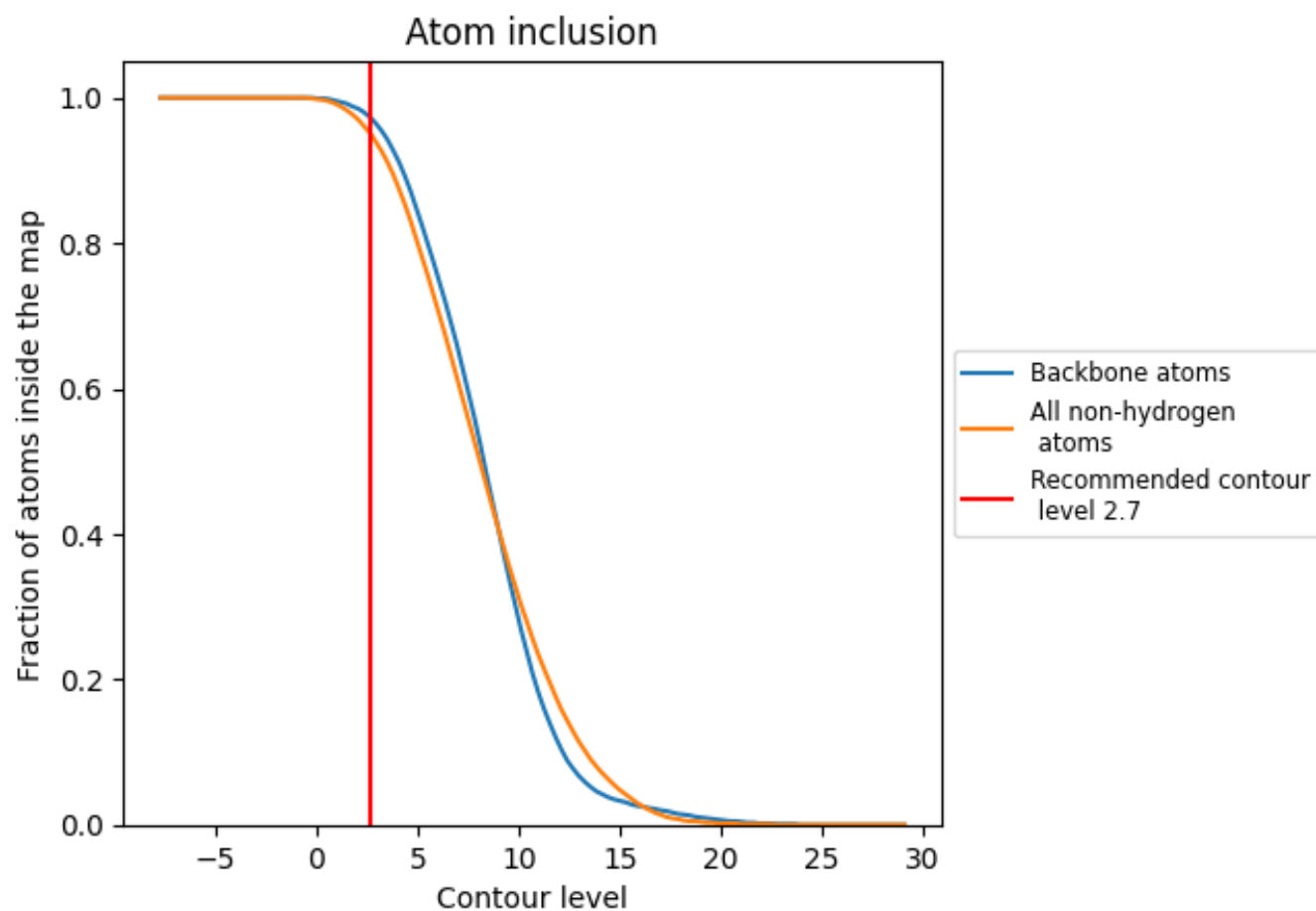
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.7).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (2.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9500	 0.5950
AA	 0.9780	 0.5840
AB	 0.6370	 0.4990
AC	 0.8980	 0.5740
AD	 0.8570	 0.5260
AE	 0.9080	 0.5830
AF	 0.8960	 0.5540
AG	 0.8650	 0.5380
AH	 0.9190	 0.5930
AI	 0.9090	 0.5530
AJ	 0.8530	 0.5210
AK	 0.9130	 0.5810
AL	 0.8750	 0.5790
AM	 0.9070	 0.5510
AN	 0.9110	 0.5490
AO	 0.9120	 0.5730
AP	 0.8580	 0.5240
AQ	 0.8620	 0.5410
AR	 0.9290	 0.5900
AS	 0.9080	 0.5520
AT	 0.8940	 0.5210
AU	 0.6670	 0.4040
AV	 0.9540	 0.6100
AW	 0.7640	 0.5390
AX	 0.8780	 0.5670
AY	 0.7750	 0.3350
B0	 0.9250	 0.6280
B1	 0.8900	 0.6000
B2	 0.9490	 0.6560
B3	 0.9670	 0.6650
B4	 0.9420	 0.6130
B5	 0.8750	 0.5330
BA	 0.9770	 0.6150
BB	 0.9940	 0.6190
BC	 0.9490	 0.6510



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Chain	Atom inclusion	Q-score
BD	 0.9530	 0.6380
BE	 0.9320	 0.6190
BF	 0.9000	 0.5630
BG	 0.9070	 0.5700
BH	 0.7020	 0.4800
BJ	 0.9460	 0.6390
BK	 0.9300	 0.6320
BL	 0.9480	 0.6190
BM	 0.9450	 0.6380
BN	 0.9620	 0.6400
BO	 0.9480	 0.6050
BP	 0.9200	 0.6190
BQ	 0.9740	 0.6620
BR	 0.9270	 0.6040
BS	 0.9270	 0.6300
BT	 0.8960	 0.5900
BU	 0.9350	 0.5910
BV	 0.9160	 0.6060
BW	 0.9410	 0.6410
BX	 0.9380	 0.6300
BY	 0.8830	 0.5610
BZ	 0.9270	 0.6200