



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 03:53 AM UTC

PDB ID : 6ZQG / pdb_00006zqg
EMDB ID : EMD-11363
Title : Cryo-EM structure of the 90S pre-ribosome from *Saccharomyces cerevisiae*, state Dis-C
Authors : Cheng, J.; Lau, B.; Venuta, G.L.; Berninghausen, O.; Hurt, E.; Beckmann, R.
Deposited on : 2020-07-09
Resolution : 3.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

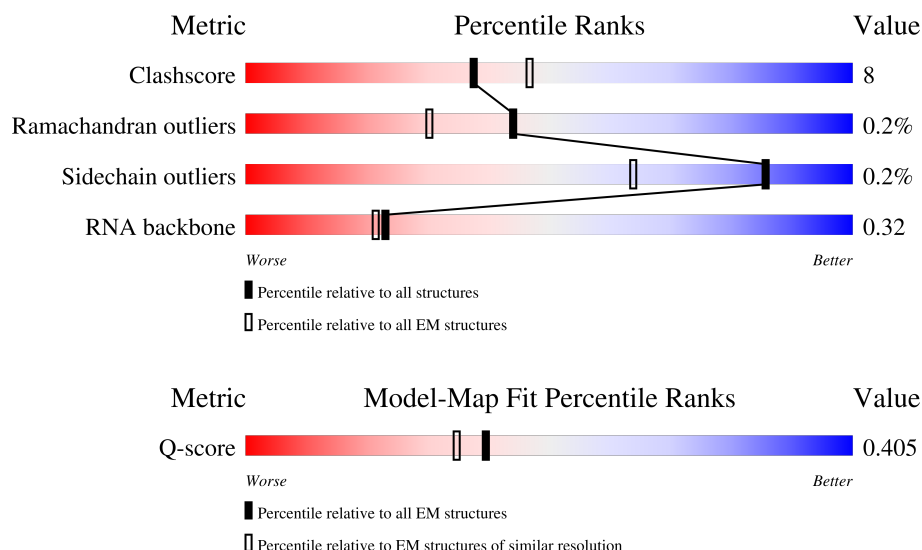
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



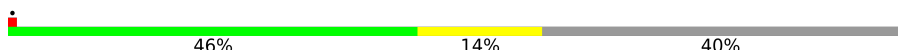
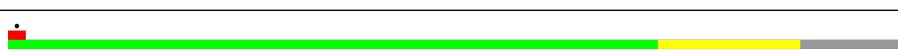
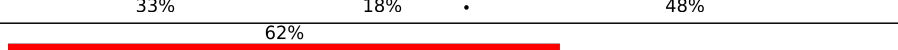
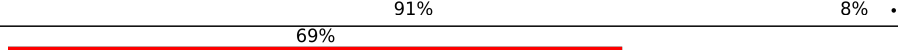
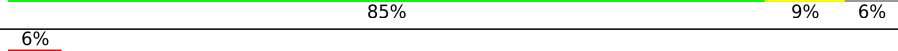
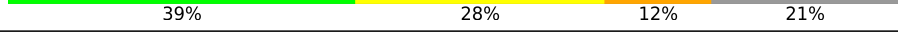
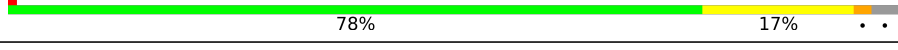
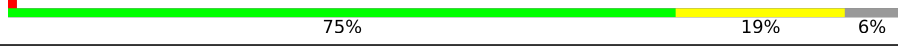
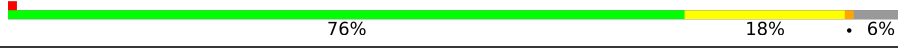
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	UB	810	
2	UC	610	
3	US	552	

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Mol	Chain	Length	Quality of chain
4	UX	189	
5	CJ	290	
6	CK	593	
7	CL	1183	
8	CM	367	
9	JF	252	
9	JG	252	
10	JH	483	
11	JL	318	
12	JJ	274	
13	DF	225	
14	DQ	143	
15	DS	147	
16	DT	144	
17	Dc	67	
18	D3	1758	
19	DA	255	
20	DE	261	
21	DG	236	
22	DH	190	
23	DI	200	
24	DJ	197	
25	DL	156	
26	DN	151	
27	DO	137	

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Mol	Chain	Length	Quality of chain
28	DZ	108	
29	DW	130	
30	DX	145	
31	DY	135	
32	Db	82	
33	UN	899	
34	JD	1267	
35	D4	23	
36	D5	9	

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 80072 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 protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	UB	403	Total	C	N	O	S	0	0
			2207	1328	441	435	3		

- Molecule 2 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	UC	47	Total	C	N	O	0	0
			393	243	86	64		

- Molecule 3 is a protein called Noc4,Nucleolar complex protein 4,Noc4.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	US	484	Total	C	N	O	0	0
			2411	1443	484	484		

- Molecule 4 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	UX	143	Total	C	N	O	S	0	0
			1132	729	199	194	10		

- Molecule 5 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	CJ	219	Total	C	N	O	0	0
			1083	645	219	219		

- Molecule 6 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	CK	92	Total	C	N	O	0	0
			645	398	116	131		

- Molecule 7 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CL	710	Total	C	N	O	S	0	0
			5758	3696	1019	1016	27		

- Molecule 8 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CM	360	Total	C	N	O	S	0	0
			2781	1781	473	516	11		

- Molecule 9 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	JF	216	Total	C	N	O	0	0
			1071	639	216	216		
9	JG	221	Total	C	N	O	0	0
			1096	654	221	221		

- Molecule 10 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	JH	261	Total	C	N	O	0	0
			1295	773	261	261		

- Molecule 11 is a protein called Dimethyladenosine transferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	JL	283	Total	C	N	O	S	0	0
			2262	1439	401	408	14		

- Molecule 12 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	JJ	181	Total	C	N	O	S	0	0
			1436	917	261	254	4		

- Molecule 13 is a protein called Rps5p.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	DF	196	Total	C	N	O	0	0
			970	578	196	196		

- Molecule 14 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	DQ	125	Total	C	N	O	0	0
			616	366	125	125		

- Molecule 15 is a protein called 40S ribosomal protein S18-A,40S ribosomal protein S18-A,Rps18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	DS	77	Total	C	N	O	S	0	0
			630	403	115	110	2		

- Molecule 16 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	DT	143	Total	C	N	O	0	0
			700	414	143	143		

- Molecule 17 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Dc	63	Total	C	N	O	0	0
			310	184	63	63		

- Molecule 18 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	D3	1387	Total	C	N	O	P	0	0
			29536	13208	5223	9718	1387		

- Molecule 19 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	DA	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 20 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	DE	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 21 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	DG	226	Total	C	N	O	S	0	0
			1799	1129	346	321	3		

- Molecule 22 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	DH	184	Total	C	N	O	S	0	0
			1481	951	265	265			

- Molecule 23 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	DI	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 24 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	DJ	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 25 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	DL	143	Total	C	N	O	S	0	0
			1154	739	218	194	3		

- Molecule 26 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	DN	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 27 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	DO	127	Total	C	N	O	S	0	0
			941	578	186	174	3		

- Molecule 28 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	DZ	67	Total	C	N	O	0	0
			332	198	67	67		

- Molecule 29 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	DW	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 30 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	DX	143	Total	C	N	O	S	0	0
			1115	705	219	189	2		

- Molecule 31 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	DY	133	Total	C	N	O	0	0
			1067	673	207	187		

- Molecule 32 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Db	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 33 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	UN	108	Total	C	N	O	S	0	0
			920	561	184	165	10		

- Molecule 34 is a protein called Probable ATP-dependent RNA helicase DHR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	JD	829	Total	C	N	O	S	0	0
			4600	2795	916	887	2		

- Molecule 35 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	D4	23	Total	C	N	O	P	0	0
			496	220	87	165	24		

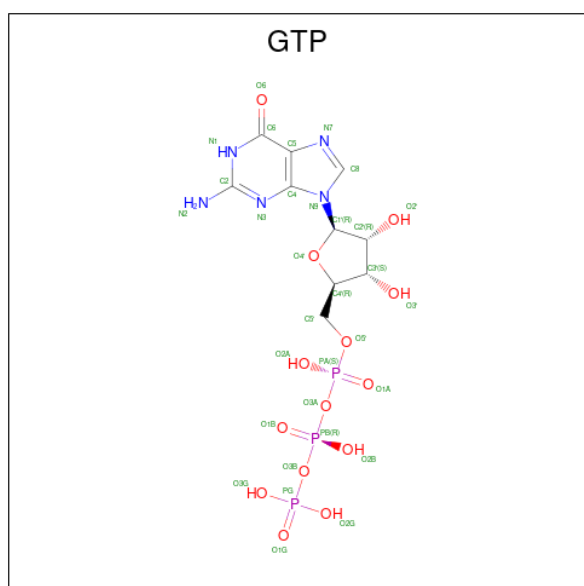
- Molecule 36 is a RNA chain called Poly-U RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	D5	9	Total	C	N	O	P	0	0
			180	81	18	72	9		

- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
37	UX	1	Total	Zn	0
			1	1	

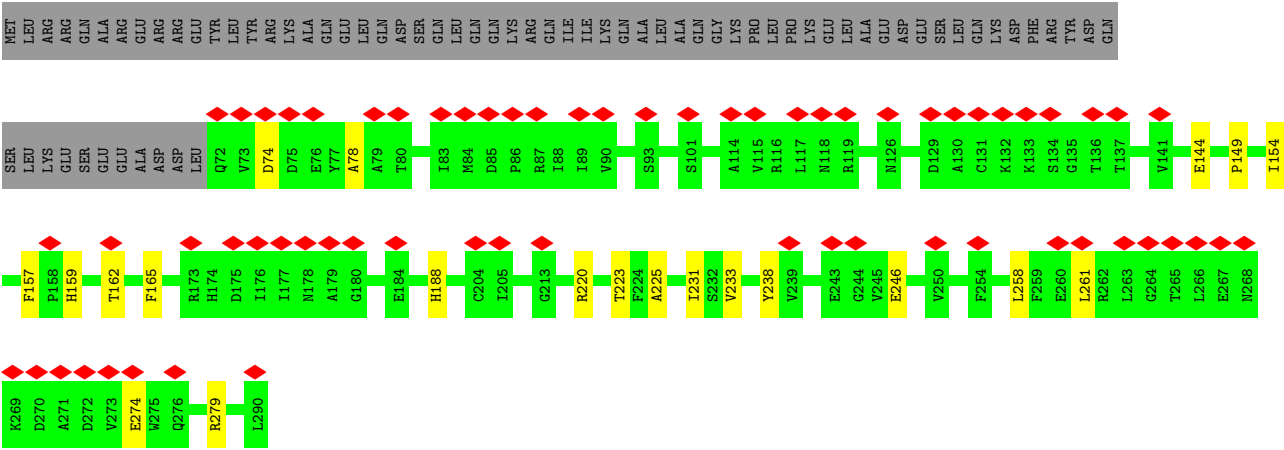
- Molecule 38 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



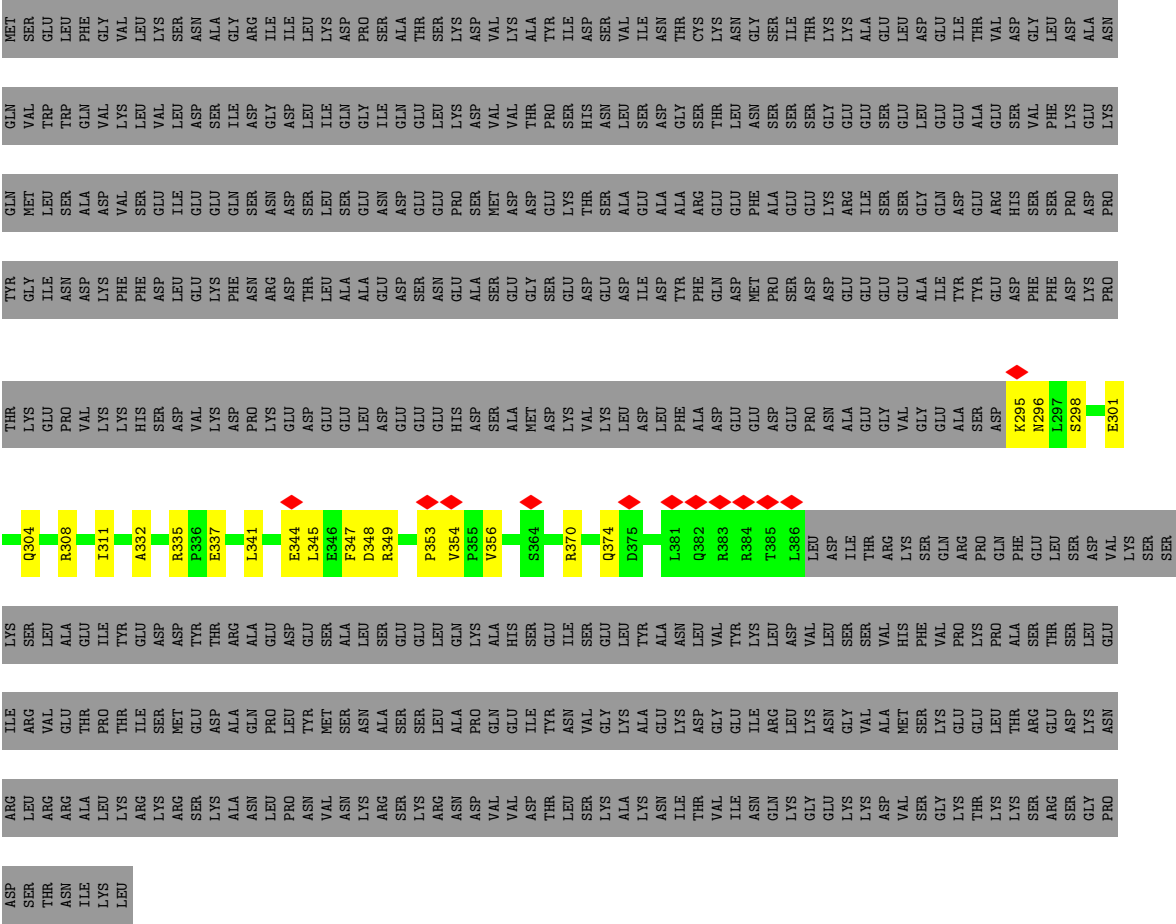
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Mol	Chain	Residues	Atoms		AltConf
39	D3	37	Total	Mg	0
			37	37	
39	DG	1	Total	Mg	0
			1	1	





● Molecule 6: U3 small nucleolar RNA-associated protein MPP10



● Molecule 7: Ribosome biogenesis protein BMS1

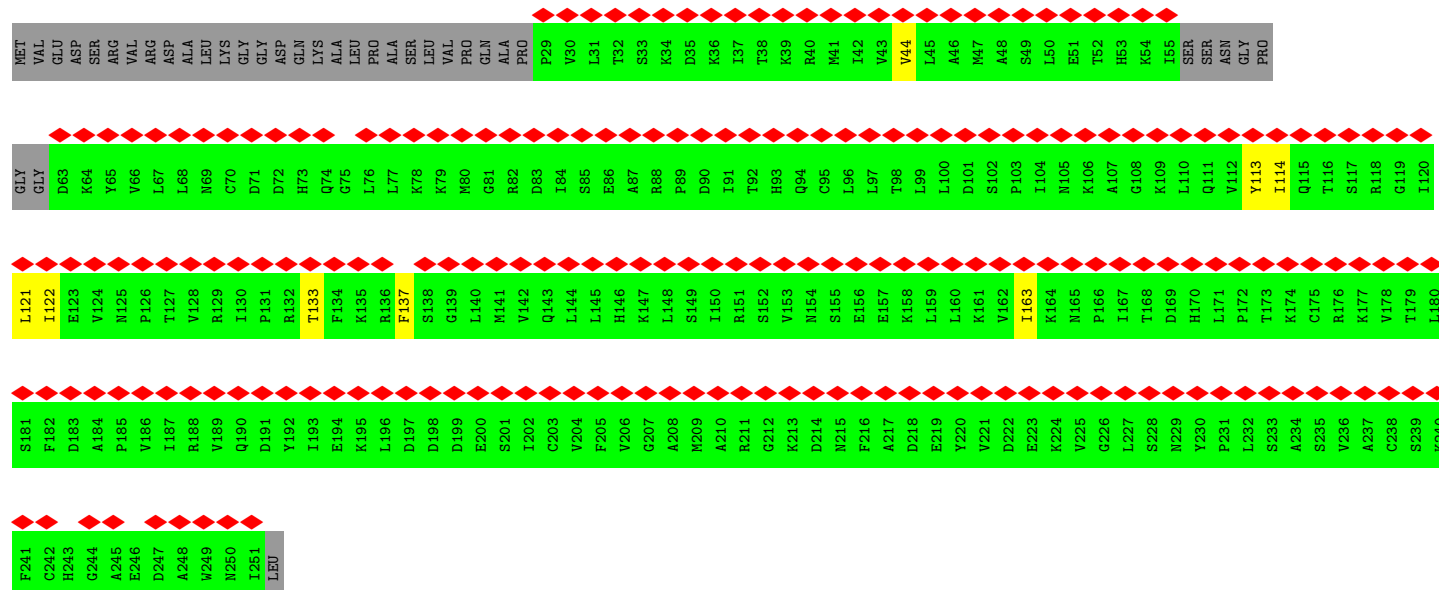






• Molecule 9: Ribosomal RNA small subunit methyltransferase NEP1

Chain JF: 84% 83% 14%



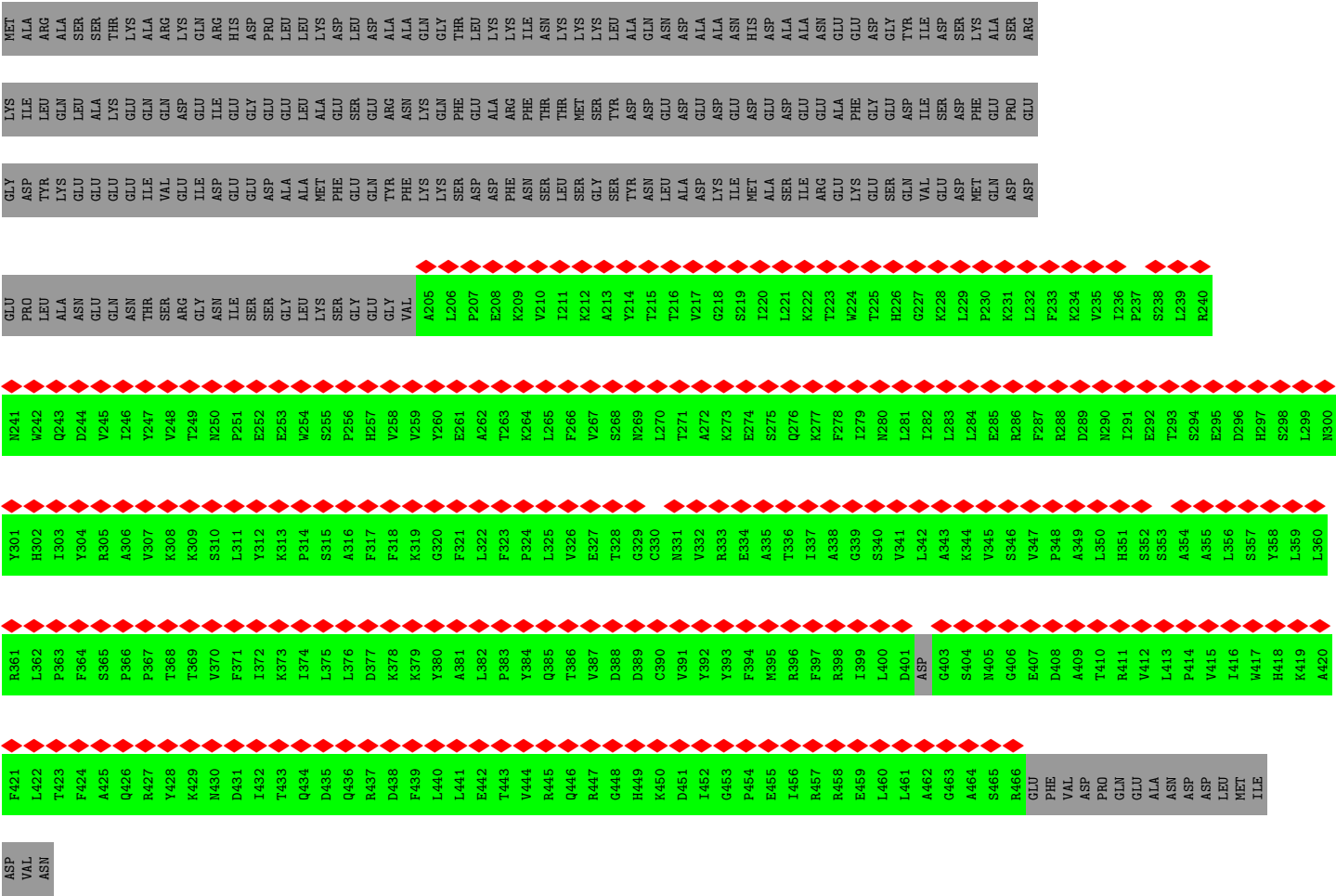
• Molecule 9: Ribosomal RNA small subunit methyltransferase NEP1

Chain JG: 82% 85% 12%



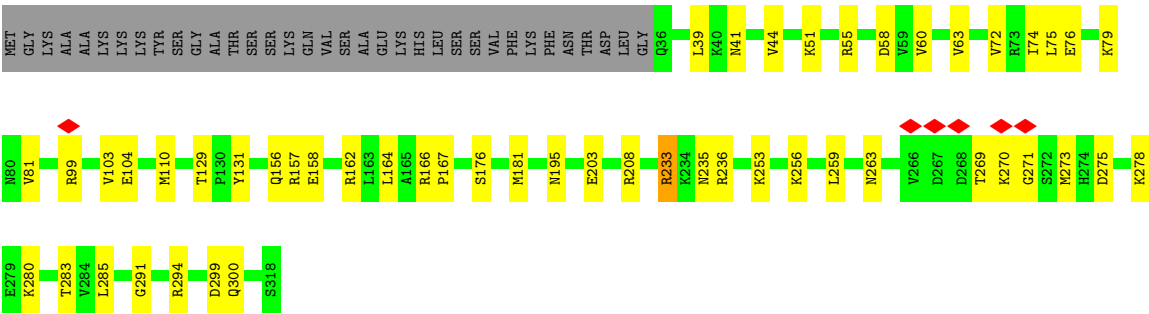
• Molecule 10: Essential nuclear protein 1

Chain JH: 53% 54% 46%



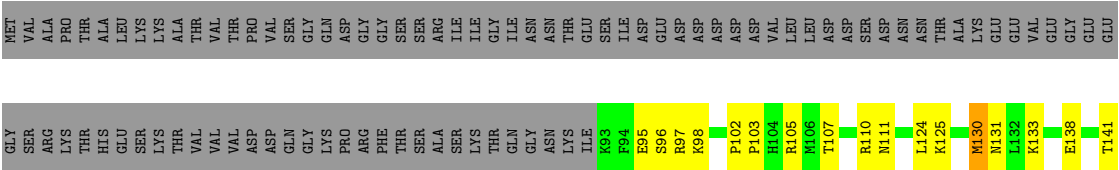
• Molecule 11: Dimethyladenosine transferase

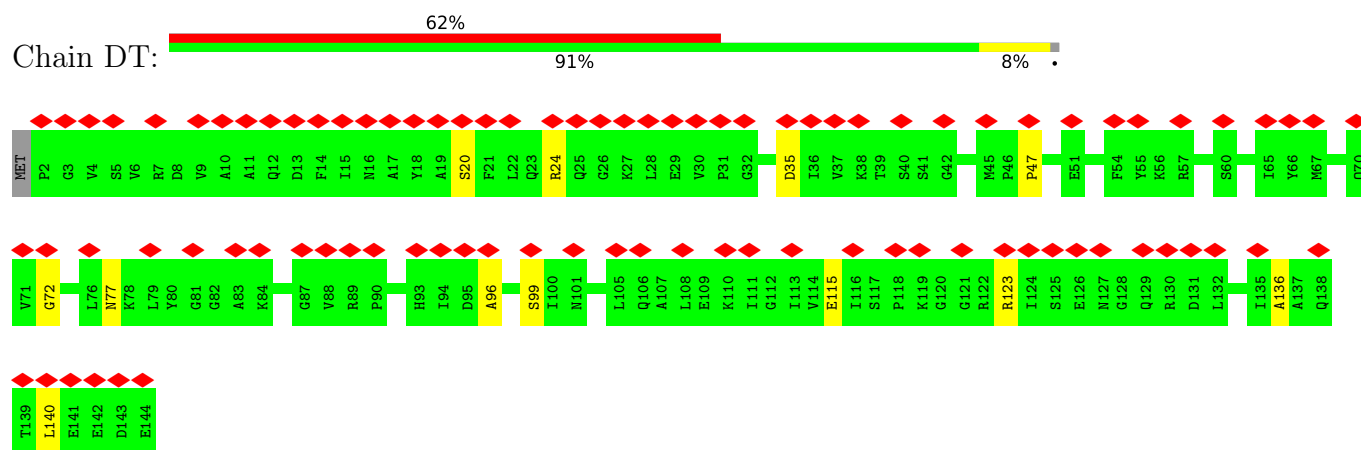
Chain JL: 73% 16% 11%



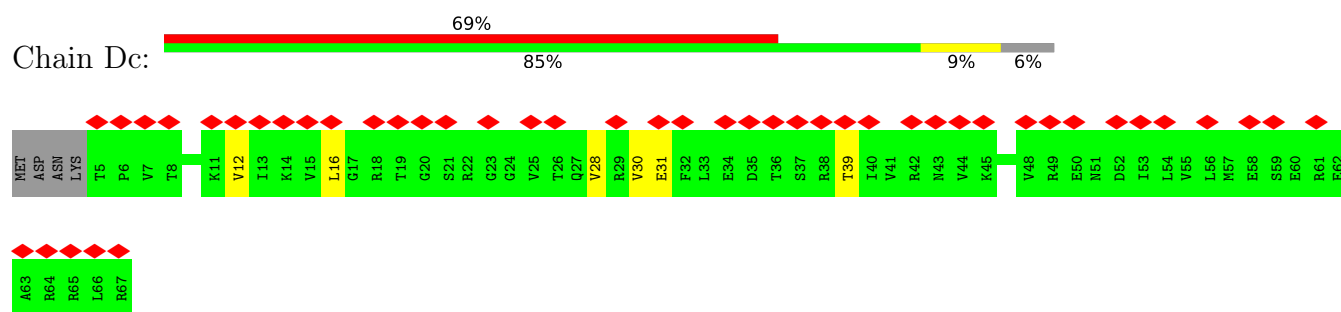
• Molecule 12: Pre-rRNA-processing protein PNO1

Chain JJ: 53% 13% 34%

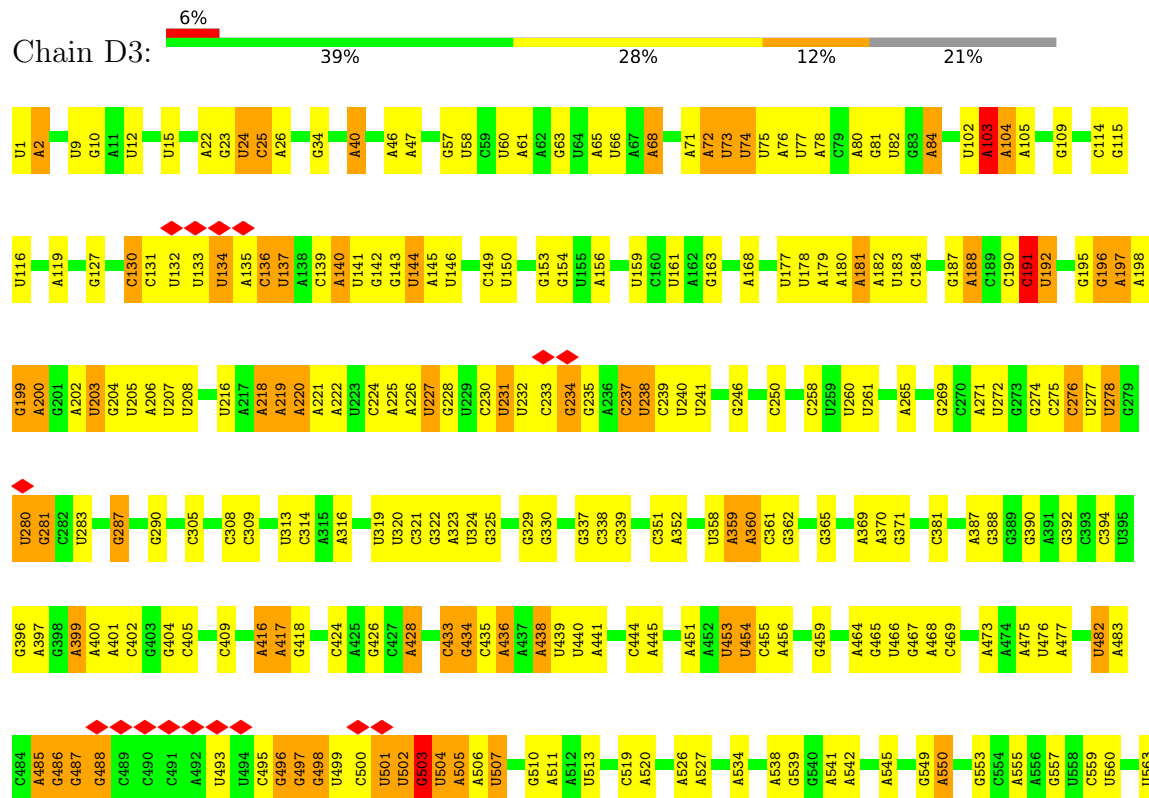


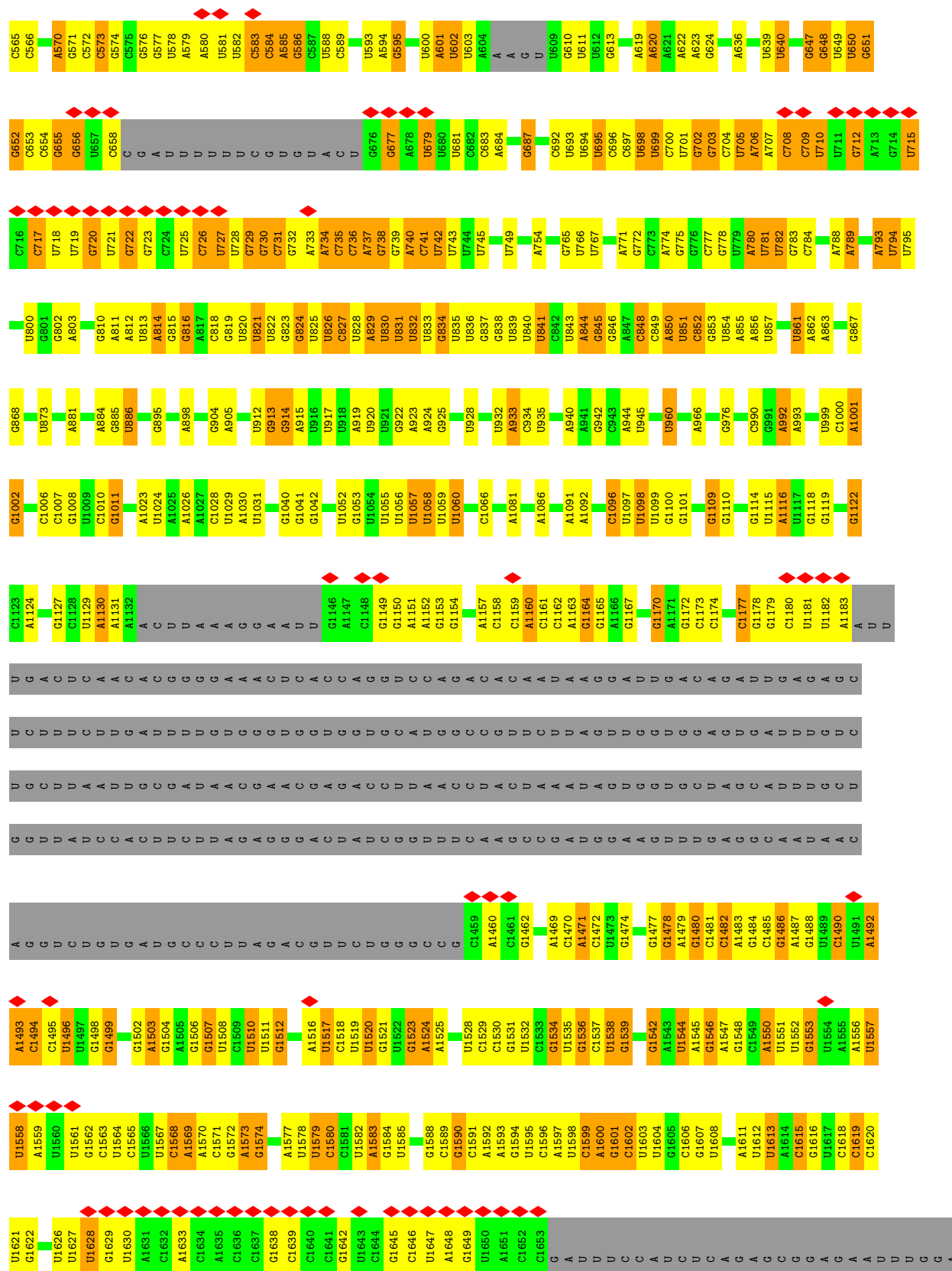


• Molecule 17: 40S ribosomal protein S28-A

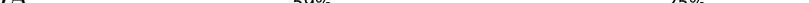


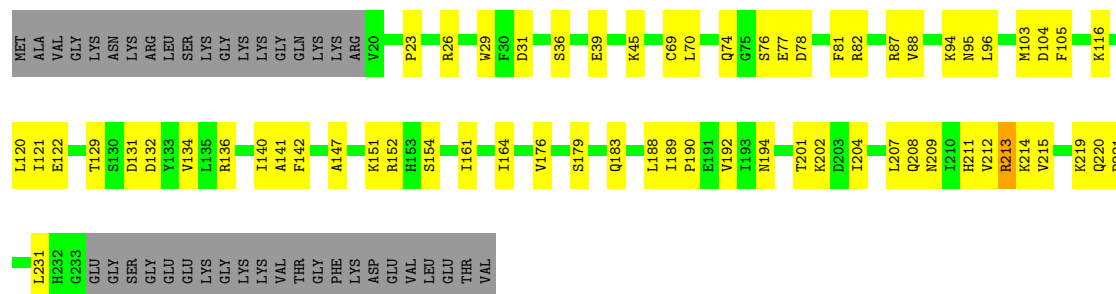
• Molecule 18: 18S rRNA



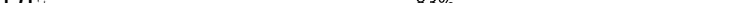


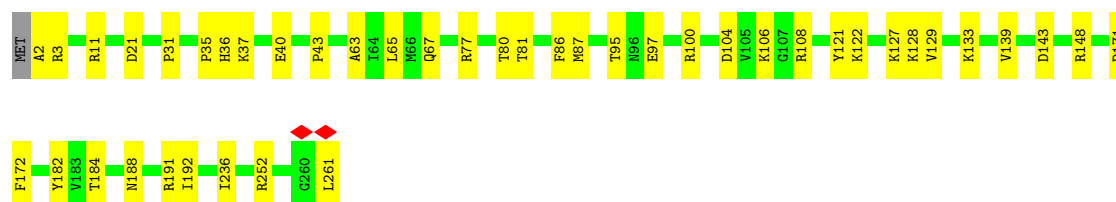
- Molecule 19: 40S ribosomal protein S1-A

Chain DA: 



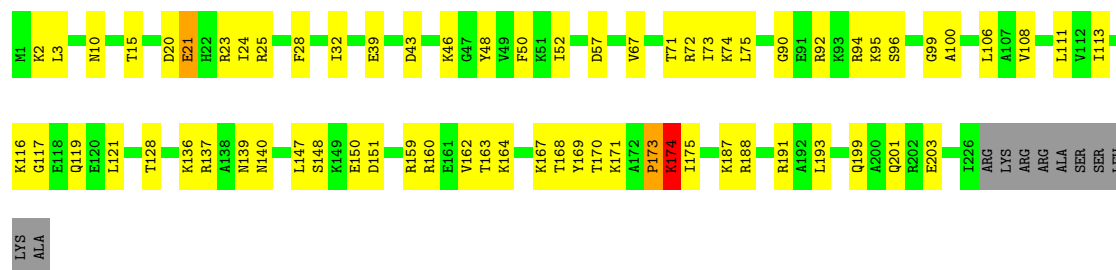
- Molecule 20: 40S ribosomal protein S4-A

Chain DE:  83% 16%

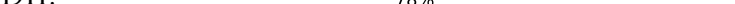


- Molecule 21: 40S ribosomal protein S6-A

Chain DG: 67% 28% . .



- Molecule 22: 40S ribosomal protein S7-A

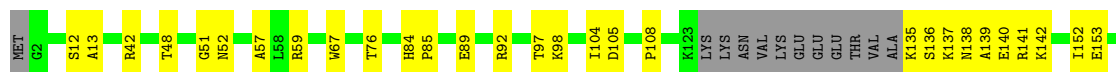
Chain DH:  78% 17% . .





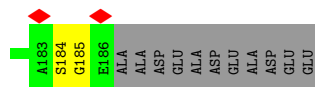
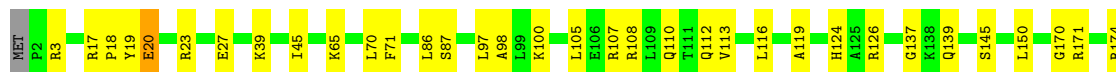
- Molecule 23: 40S ribosomal protein S8-A

Chain DI: 75% 19% 6%



- Molecule 24: 40S ribosomal protein S9-A

Chain DJ: 76% 18% 6%



- Molecule 25: 40S ribosomal protein S11-A

Chain DL: 78% 14% 8%



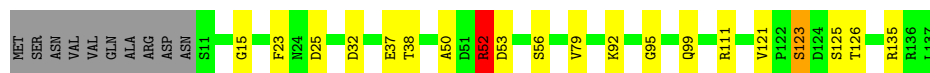
- Molecule 26: 40S ribosomal protein S13

Chain DN: 86% 13% 1%



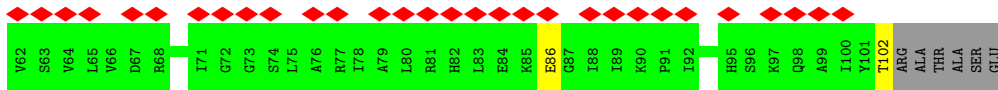
- Molecule 27: 40S ribosomal protein S14-A

Chain DO: 78% 13% 7%



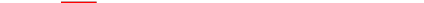
- Molecule 28: 40S ribosomal protein S25-A

Chain DZ: 49% 59% 38%

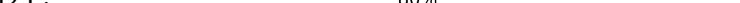


- Chain DW:  78% 21%



- Chain DX:  82% 16% ..

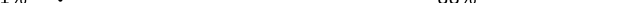


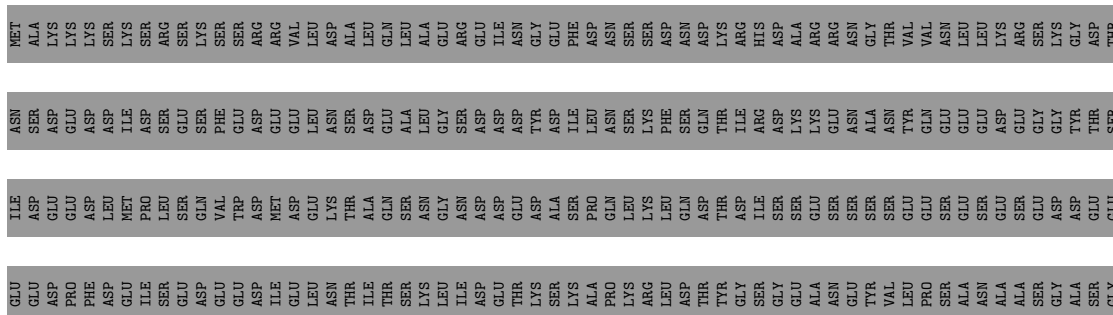
- Chain DY:  80% 18% ..

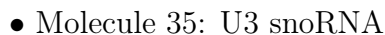


- Chain Db: 76% 23% .



- Chain UN:  11% . 88%





9%



- Molecule 36: Poly-U RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102097	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.099	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	508.32, 508.32, 508.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, M7G, ZN

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	UB	0.21	0/2206	0.58	2/3035 (0.1%)
2	UC	0.89	0/395	0.99	0/517
3	US	0.17	0/2406	0.53	4/3355 (0.1%)
4	UX	0.85	0/1154	0.88	0/1557
5	CJ	0.28	0/1082	0.75	0/1506
6	CK	0.45	0/649	0.80	0/877
7	CL	0.94	0/5887	0.91	5/7931 (0.1%)
8	CM	0.89	0/2832	0.84	2/3825 (0.1%)
9	JF	0.14	0/1069	0.40	0/1488
9	JG	0.15	0/1094	0.44	0/1523
10	JH	0.10	0/1293	0.32	0/1801
11	JL	0.91	0/2305	0.88	0/3116
12	JJ	0.91	1/1462 (0.1%)	0.95	2/1969 (0.1%)
13	DF	0.16	0/969	0.53	0/1349
14	DQ	0.18	0/615	0.58	0/854
15	DS	0.19	0/641	0.63	0/866
16	DT	0.16	0/699	0.53	0/968
17	Dc	0.17	0/309	0.47	0/428
18	D3	0.99	0/33028	0.67	5/51447 (0.0%)
19	DA	0.89	0/1735	0.97	0/2335
20	DE	1.18	1/2109 (0.0%)	0.97	2/2839 (0.1%)
21	DG	0.76	0/1823	0.83	1/2439 (0.0%)
22	DH	0.71	0/1506	0.84	1/2028 (0.0%)
23	DI	0.99	0/1514	0.95	0/2021
24	DJ	1.06	1/1519 (0.1%)	0.96	3/2035 (0.1%)
25	DL	1.21	0/1180	0.94	0/1591
26	DN	0.97	0/1215	0.98	0/1638
27	DO	0.95	0/952	1.09	5/1279 (0.4%)
28	DZ	0.25	0/331	0.74	2/460 (0.4%)
29	DW	1.22	0/1038	1.10	3/1395 (0.2%)
30	DX	1.14	0/1133	1.03	2/1510 (0.1%)
31	DY	1.12	1/1081 (0.1%)	0.94	0/1441

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Db	0.91	0/620	0.89	0/838
33	UN	0.81	0/926	0.85	0/1213
34	JD	0.44	0/4616	0.78	2/6348 (0.0%)
35	D4	0.84	0/521	0.54	0/809
36	D5	0.18	0/197	0.48	0/302
All	All	0.88	4/84111 (0.0%)	0.76	41/120933 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	UB	0	1
7	CL	0	1
11	JL	0	1
19	DA	0	3
22	DH	0	4
23	DI	0	1
24	DJ	0	2
25	DL	0	1
26	DN	0	1
27	DO	0	2
31	DY	0	2
32	Db	0	2
33	UN	0	1
34	JD	0	3
All	All	0	25

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	JJ	105	ARG	CA-C	-9.38	1.41	1.53
31	DY	59	GLY	C-O	-5.94	1.16	1.23
24	DJ	108	ARG	CB-CG	-5.12	1.37	1.52
20	DE	3	ARG	C-O	-5.08	1.17	1.24

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	CL	897	CYS	CA-C-N	-8.01	115.44	121.61
7	CL	897	CYS	C-N-CA	-8.01	115.44	121.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	JD	1174	ALA	CA-C-N	-7.63	112.29	121.90
34	JD	1174	ALA	C-N-CA	-7.63	112.29	121.90
29	DW	28	ARG	CA-C-N	7.57	145.17	127.00
29	DW	28	ARG	C-N-CA	7.57	145.17	127.00
1	UB	412	PRO	N-CA-CB	7.39	110.22	103.20
18	D3	503	G	C2'-C3'-O3'	7.11	124.36	113.70
3	US	75	PRO	N-CA-CB	6.95	110.65	103.00
1	UB	400	PRO	N-CA-CB	6.77	110.70	103.52
24	DJ	108	ARG	CB-CG-CD	6.61	126.50	111.30
30	DX	44	GLY	N-CA-C	-6.45	104.50	111.21
3	US	37	PRO	N-CA-CB	6.35	110.55	103.44
18	D3	702	G	C3'-C2'-O2'	6.23	123.95	114.60
22	DH	8	ILE	N-CA-C	-6.02	106.89	112.43
29	DW	28	ARG	C-N-CD	-6.00	107.41	120.60
21	DG	174	LYS	N-CA-C	-5.84	98.36	110.80
30	DX	9	LEU	CA-CB-CG	5.83	136.72	116.30
18	D3	1800	A	C2'-C3'-O3'	5.82	118.22	109.50
12	JJ	187	VAL	N-CA-C	-5.78	106.65	113.42
7	CL	943	LYS	N-CA-C	-5.72	100.38	109.76
7	CL	223	LEU	CB-CG-CD2	-5.70	93.60	110.70
18	D3	191	C	O4'-C1'-N1	5.60	116.60	108.20
20	DE	2	ALA	CA-C-N	5.52	132.09	121.54
20	DE	2	ALA	C-N-CA	5.52	132.09	121.54
24	DJ	3	ARG	N-CA-C	-5.45	100.19	107.88
3	US	285	ILE	CA-C-N	5.22	123.53	120.24
3	US	285	ILE	C-N-CA	5.22	123.53	120.24
7	CL	141	LEU	CA-CB-CG	5.21	134.54	116.30
12	JJ	130	MET	CG-SD-CE	-5.21	89.44	100.90
27	DO	52	ARG	CA-C-N	5.17	129.48	121.83
27	DO	52	ARG	C-N-CA	5.17	129.48	121.83
28	DZ	57	TYR	CA-C-N	5.17	131.00	121.70
28	DZ	57	TYR	C-N-CA	5.17	131.00	121.70
27	DO	25	ASP	CB-CA-C	-5.12	101.65	111.78
24	DJ	108	ARG	NE-CZ-NH1	-5.09	116.41	121.50
8	CM	304	GLY	CA-C-N	-5.04	113.96	122.67
8	CM	304	GLY	C-N-CA	-5.04	113.96	122.67
27	DO	23	PHE	CA-C-N	5.03	131.15	121.54
27	DO	23	PHE	C-N-CA	5.03	131.15	121.54
18	D3	103	A	C4'-C3'-O3'	5.03	116.94	109.40

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	CL	51	GLU	Peptide
19	DA	147	ALA	Peptide
19	DA	151	LYS	Peptide
19	DA	69	CYS	Peptide
22	DH	133	THR	Peptide
22	DH	154	LEU	Peptide
22	DH	30	SER	Peptide
22	DH	31	SER	Peptide
23	DI	51	GLY	Peptide
24	DJ	137	GLY	Peptide
24	DJ	20	GLU	Peptide
25	DL	5	LEU	Peptide
26	DN	58	HIS	Peptide
27	DO	123	SER	Peptide
27	DO	52	ARG	Peptide
31	DY	122	GLY	Peptide
31	DY	17	LEU	Peptide
32	Db	3	LEU	Peptide
32	Db	4	VAL	Peptide
34	JD	1148	PRO	Peptide
34	JD	501	MET	Peptide
34	JD	588	PHE	Peptide
11	JL	233	ARG	Peptide
1	UB	784	ILE	Peptide
33	UN	402	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	UB	2207	0	1231	24	0
2	UC	393	0	444	10	0
3	US	2411	0	1035	7	0
4	UX	1132	0	1186	17	0
5	CJ	1083	0	478	11	0
6	CK	645	0	541	19	0
7	CL	5758	0	5885	122	0
8	CM	2781	0	2878	51	0
9	JF	1071	0	467	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	JG	1096	0	478	4	0
10	JH	1295	0	570	0	0
11	JL	2262	0	2330	32	0
12	JJ	1436	0	1515	23	0
13	DF	970	0	462	2	0
14	DQ	616	0	285	3	0
15	DS	630	0	652	18	0
16	DT	700	0	334	8	0
17	Dc	310	0	134	3	0
18	D3	29536	0	14872	424	0
19	DA	1709	0	1784	42	0
20	DE	2068	0	2154	27	0
21	DG	1799	0	1879	51	0
22	DH	1481	0	1572	24	0
23	DI	1489	0	1525	27	0
24	DJ	1494	0	1573	21	0
25	DL	1154	0	1220	14	0
26	DN	1192	0	1255	12	0
27	DO	941	0	979	13	0
28	DZ	332	0	149	1	0
29	DW	1021	0	1060	26	0
30	DX	1115	0	1191	16	0
31	DY	1067	0	1127	19	0
32	Db	610	0	633	11	0
33	UN	920	0	972	8	0
34	JD	4600	0	2789	37	0
35	D4	496	0	253	2	0
36	D5	180	0	91	0	0
37	UX	1	0	0	0	0
38	CL	32	0	12	1	0
39	CL	1	0	0	0	0
39	D3	37	0	0	0	0
39	DG	1	0	0	0	0
All	All	80072	0	57995	1004	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 8.

All (1004) 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)
1:UB:701:ALA:HB2	3:US:417:HIS:HA	1.27	1.14
18:D3:187:G:N2	18:D3:198:A:N7	2.04	1.06
18:D3:736:C:H6	18:D3:736:C:H5'	1.24	1.02
1:UB:701:ALA:CB	3:US:417:HIS:HA	1.91	1.00
18:D3:895:G:H1	18:D3:917:U:H3	1.02	0.99
18:D3:1588:G:H1	18:D3:1608:U:H3	0.99	0.93
1:UB:701:ALA:CB	3:US:417:HIS:CB	2.47	0.92
1:UB:701:ALA:HB1	3:US:417:HIS:CB	2.00	0.92
7:CL:943:LYS:HG2	18:D3:1594:G:H5'	1.49	0.91
13:DF:149:VAL:O	13:DF:155:ALA:HA	1.71	0.90
18:D3:736:C:H5'	18:D3:736:C:C6	2.06	0.89
18:D3:1471:A:N6	18:D3:1538:U:H3	1.70	0.89
34:JD:1153:LEU:O	34:JD:1170:LEU:HA	1.74	0.88
18:D3:1504:G:N2	18:D3:1563:C:O2	2.09	0.86
18:D3:1471:A:H62	18:D3:1538:U:H3	0.87	0.85
18:D3:737:A:OP2	18:D3:737:A:H2'	1.75	0.85
18:D3:488:G:C6	18:D3:498:G:N2	2.45	0.85
34:JD:445:VAL:HA	34:JD:512:SER:O	1.77	0.84
18:D3:1646:C:N4	18:D3:1754:A:N6	2.25	0.83
1:UB:701:ALA:CB	3:US:417:HIS:CA	2.56	0.83
18:D3:488:G:O6	18:D3:498:G:N2	2.13	0.82
18:D3:505:A:N1	18:D3:507:U:C4	2.48	0.81
1:UB:701:ALA:HB2	3:US:417:HIS:CA	2.11	0.79
18:D3:496:G:H3'	18:D3:497:G:H4'	1.65	0.79
34:JD:1218:GLY:HA3	34:JD:1228:GLY:HA3	1.65	0.79
8:CM:301:MET:HE1	8:CM:311:LEU:HB2	1.66	0.78
5:CJ:225:ALA:O	5:CJ:231:ILE:HA	1.84	0.77
18:D3:187:G:H21	18:D3:198:A:H62	1.32	0.77
18:D3:976:G:H1	18:D3:1023:A:HO2'	1.32	0.77
18:D3:824:G:N2	18:D3:849:C:O2	2.18	0.76
18:D3:1583:A:H61	18:D3:1611:A:H3'	1.51	0.76
18:D3:1550:A:C6	18:D3:1562:G:C6	2.74	0.75
12:JJ:110:ARG:HD3	12:JJ:130:MET:HE1	1.67	0.74
34:JD:733:PRO:HA	34:JD:759:VAL:O	1.87	0.74
7:CL:174:LEU:HD23	7:CL:206:TYR:HB3	1.67	0.74
7:CL:267:ARG:HH12	7:CL:798:MET:HG2	1.52	0.74
18:D3:868:G:H1	18:D3:960:U:H3	1.35	0.74
21:DG:74:LYS:HA	21:DG:95:LYS:O	1.86	0.74
20:DE:87:MET:HE1	20:DE:236:ILE:HD13	1.68	0.74
23:DI:57:ALA:HB2	23:DI:177:GLY:HA2	1.69	0.74
18:D3:693:U:C2	18:D3:695:U:O4	2.40	0.73
18:D3:933:A:OP1	19:DA:116:LYS:NZ	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CJ:223:THR:O	5:CJ:233:VAL:HA	1.88	0.73
18:D3:826:U:H4'	18:D3:826:U:OP1	1.87	0.72
18:D3:1646:C:N4	18:D3:1754:A:H61	1.86	0.72
20:DE:122:LYS:NZ	20:DE:143:ASP:OD2	2.19	0.72
18:D3:708:C:N3	18:D3:710:U:C5	2.57	0.72
18:D3:1556:A:H4'	18:D3:1557:U:H2'	1.72	0.72
18:D3:736:C:H6	18:D3:736:C:C5'	2.01	0.71
18:D3:1096:C:N4	29:DW:18:GLU:OE1	2.23	0.71
11:JL:235:ASN:O	11:JL:294:ARG:NH2	2.23	0.71
21:DG:162:VAL:O	21:DG:168:THR:HA	1.90	0.71
19:DA:208:GLN:HG3	19:DA:209:ASN:HB2	1.71	0.71
18:D3:195:G:O6	23:DI:137:LYS:NZ	2.23	0.71
18:D3:227:U:C2	18:D3:834:G:C6	2.77	0.71
18:D3:1498:G:N2	18:D3:1510:U:O2	2.24	0.71
27:DO:15:GLY:O	27:DO:79:VAL:HA	1.91	0.70
18:D3:486:G:H5''	18:D3:497:G:H1	1.56	0.70
18:D3:23:G:C6	18:D3:603:U:O2	2.45	0.70
18:D3:104:A:OP2	18:D3:308:C:N4	2.23	0.70
18:D3:177:U:O2	21:DG:191:ARG:NH1	2.26	0.69
21:DG:162:VAL:HB	21:DG:169:TYR:HB2	1.74	0.69
18:D3:188:A:OP2	23:DI:138:ASN:ND2	2.25	0.69
22:DH:143:LEU:O	29:DW:42:GLN:NE2	2.26	0.69
18:D3:1484:G:H1	18:D3:1591:C:H1'	1.56	0.69
18:D3:1484:G:N2	18:D3:1591:C:O2	2.26	0.69
19:DA:82:ARG:HA	19:DA:104:ASP:O	1.92	0.69
34:JD:621:ALA:HB3	34:JD:773:VAL:HA	1.75	0.69
18:D3:220:A:C8	18:D3:832:U:C2	2.81	0.69
17:Dc:16:LEU:H	17:Dc:28:VAL:HA	1.57	0.69
18:D3:68:A:OP1	21:DG:160:ARG:NH2	2.25	0.69
18:D3:905:A:O3'	27:DO:52:ARG:NH2	2.27	0.68
18:D3:1471:A:N7	18:D3:1538:U:O4	2.26	0.68
27:DO:125:SER:OG	27:DO:126:THR:N	2.26	0.68
18:D3:1646:C:H42	18:D3:1754:A:N6	1.90	0.68
22:DH:31:SER:HB3	22:DH:35:LYS:HD2	1.73	0.68
21:DG:164:LYS:HB3	21:DG:167:LYS:HB2	1.76	0.68
31:DY:27:VAL:HG11	31:DY:35:VAL:HG11	1.74	0.68
18:D3:821:U:N3	18:D3:852:C:O2	2.26	0.68
18:D3:23:G:O6	18:D3:603:U:O2	2.12	0.68
34:JD:1157:LEU:HA	34:JD:1166:ARG:O	1.94	0.68
18:D3:867:G:H5'	26:DN:4:MET:HE3	1.76	0.67
18:D3:496:G:H5'	18:D3:497:G:H5''	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:195:G:N7	23:DI:141:ARG:NH2	2.43	0.67
11:JL:299:ASP:OD2	34:JD:106:LYS:NZ	2.28	0.67
11:JL:181:MET:SD	11:JL:300:GLN:NE2	2.68	0.67
18:D3:821:U:O4	18:D3:852:C:N3	2.28	0.67
24:DJ:17:ARG:HD2	24:DJ:18:PRO:HD2	1.76	0.67
18:D3:1480:G:C2	18:D3:1528:U:O2	2.48	0.66
18:D3:1573:A:H4'	18:D3:1574:G:H5'	1.77	0.66
2:UC:538:ARG:NH1	7:CL:151:GLU:OE2	2.28	0.66
18:D3:187:G:H21	18:D3:198:A:N6	1.94	0.66
18:D3:207:U:O2	23:DI:178:ARG:NH1	2.25	0.66
18:D3:230:C:N4	18:D3:231:U:C4	2.64	0.66
26:DN:130:ARG:NH2	26:DN:139:TRP:O	2.29	0.66
18:D3:715:U:H3	18:D3:723:G:H1	1.43	0.66
26:DN:20:ARG:HH21	29:DW:56:HIS:CG	2.14	0.66
24:DJ:139:GLN:NE2	31:DY:64:PHE:O	2.28	0.65
32:Db:40:CYS:SG	32:Db:41:LEU:N	2.70	0.65
18:D3:76:A:N6	18:D3:80:A:O2'	2.27	0.65
18:D3:789:A:O2'	20:DE:106:LYS:NZ	2.27	0.65
7:CL:166:ARG:NH2	18:D3:435:C:OP1	2.29	0.65
7:CL:248:ARG:HG2	7:CL:272:TYR:HB2	1.77	0.65
7:CL:889:LEU:HD22	7:CL:922:ILE:HG23	1.78	0.65
11:JL:162:ARG:O	11:JL:176:SER:OG	2.14	0.65
18:D3:218:A:C6	18:D3:830:U:N3	2.64	0.65
18:D3:1550:A:N1	18:D3:1562:G:C6	2.65	0.65
26:DN:4:MET:SD	26:DN:124:ARG:NH1	2.70	0.65
4:UX:56:ASN:ND2	4:UX:169:GLY:O	2.29	0.65
7:CL:830:ARG:NH1	30:DX:138:GLU:OE2	2.29	0.65
23:DI:84:HIS:NE2	23:DI:97:THR:OG1	2.29	0.65
18:D3:1498:G:H1	18:D3:1510:U:H3	1.45	0.65
18:D3:396:G:N2	18:D3:399:A:OP2	2.30	0.64
18:D3:1170:G:N2	18:D3:1571:C:O2'	2.30	0.64
7:CL:309:PRO:HB3	7:CL:313:TYR:HD2	1.61	0.64
12:JJ:193:LEU:HD22	12:JJ:197:HIS:HB3	1.78	0.64
23:DI:48:THR:OG1	23:DI:52:ASN:O	2.15	0.64
23:DI:67:TRP:NE1	23:DI:185:GLU:OE2	2.29	0.64
2:UC:553:LYS:HB3	18:D3:586:G:H21	1.62	0.64
34:JD:1151:TYR:CB	34:JD:1173:ILE:O	2.46	0.64
7:CL:736:GLU:OE2	7:CL:739:LYS:NZ	2.30	0.64
18:D3:710:U:C4	18:D3:730:G:C6	2.86	0.64
11:JL:208:ARG:NH2	35:D4:2:U:OP1	2.21	0.64
12:JJ:95:GLU:OE1	27:DO:111:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:140:A:OP2	21:DG:187:LYS:NZ	2.26	0.64
19:DA:82:ARG:NH2	19:DA:188:LEU:O	2.31	0.64
18:D3:698:U:OP1	18:D3:733:A:N6	2.31	0.64
18:D3:227:U:C2	18:D3:834:G:O6	2.51	0.63
18:D3:729:G:N2	18:D3:730:G:O2'	2.31	0.63
4:UX:149:LYS:NZ	4:UX:168:PRO:O	2.32	0.63
18:D3:187:G:N2	18:D3:198:A:H62	1.96	0.63
7:CL:64:GLU:OE2	7:CL:766:ASN:ND2	2.32	0.63
18:D3:1498:G:C2	18:D3:1510:U:O2	2.52	0.63
18:D3:66:U:OP1	21:DG:136:LYS:NZ	2.32	0.63
7:CL:193:ARG:NH2	7:CL:197:GLU:OE2	2.30	0.63
19:DA:154:SER:OG	19:DA:154:SER:O	2.15	0.63
18:D3:485:A:C8	18:D3:485:A:H5''	2.34	0.62
18:D3:324:U:OP1	25:DL:133:LYS:NZ	2.27	0.62
18:D3:224:C:H2'	18:D3:225:A:H8	1.63	0.62
18:D3:647:G:H2'	18:D3:648:G:H8	1.63	0.62
18:D3:1477:G:O6	18:D3:1531:G:C6	2.53	0.62
7:CL:996:LEU:HD23	7:CL:998:SER:H	1.65	0.62
8:CM:158:SER:H	8:CM:162:GLY:HA2	1.65	0.62
25:DL:133:LYS:O	25:DL:136:ARG:NH1	2.32	0.62
12:JJ:259:VAL:O	12:JJ:263:LEU:HB2	1.99	0.62
19:DA:76:SER:OG	19:DA:78:ASP:OD1	2.17	0.62
24:DJ:170:GLY:O	24:DJ:174:ARG:NE	2.32	0.62
18:D3:227:U:O2	18:D3:834:G:C6	2.53	0.62
18:D3:846:G:H5''	18:D3:846:G:N3	2.14	0.62
22:DH:9:LEU:HD21	22:DH:21:ALA:HB2	1.80	0.62
18:D3:803:A:N3	22:DH:104:ARG:NH2	2.46	0.62
18:D3:1057:U:H3	18:D3:1060:U:H3'	1.65	0.62
30:DX:46:SER:OG	30:DX:48:HIS:O	2.16	0.62
34:JD:1092:VAL:H	34:JD:1122:ALA:HB2	1.65	0.62
5:CJ:154:ILE:O	5:CJ:162:THR:HA	2.00	0.62
18:D3:488:G:O6	18:D3:498:G:C2	2.52	0.62
6:CK:298:SER:OG	6:CK:301:GLU:OE1	2.16	0.62
18:D3:258:C:O2	23:DI:178:ARG:NH2	2.33	0.62
8:CM:286:SER:HA	8:CM:317:GLN:HE21	1.65	0.61
15:DS:40:ARG:HH11	18:D3:1539:G:H4'	1.65	0.61
7:CL:819:GLU:O	7:CL:852:ARG:NH2	2.34	0.61
6:CK:344:GLU:OE2	7:CL:960:ARG:NH2	2.33	0.61
18:D3:504:U:H2'	18:D3:505:A:H4'	1.82	0.61
18:D3:1530:C:H2'	18:D3:1531:G:H8	1.64	0.61
20:DE:63:ALA:O	20:DE:67:GLN:NE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DW:87:GLU:HA	29:DW:90:THR:HG22	1.81	0.61
32:Db:48:SER:OG	32:Db:49:HIS:ND1	2.32	0.61
1:UB:785:VAL:HG11	30:DX:119:GLY:HA2	1.82	0.61
18:D3:500:C:O5'	18:D3:500:C:H6	1.83	0.61
7:CL:71:ILE:HD12	7:CL:245:LEU:HD22	1.82	0.61
7:CL:943:LYS:CG	18:D3:1594:G:H5'	2.27	0.61
18:D3:709:C:H5	18:D3:730:G:H21	1.49	0.61
18:D3:40:A:N6	18:D3:466:U:O4	2.33	0.61
25:DL:57:LYS:HD2	25:DL:131:ILE:HG23	1.83	0.61
18:D3:1470:C:H3'	18:D3:1573:A:H62	1.66	0.61
9:JF:44:VAL:HA	9:JF:113:TYR:O	2.01	0.60
34:JD:1235:ALA:HB3	34:JD:1251:ILE:O	2.00	0.60
2:UC:580:ARG:NH2	4:UX:49:SER:O	2.35	0.60
18:D3:283:U:H5''	21:DG:188:ARG:HD2	1.82	0.60
18:D3:647:G:H22	18:D3:687:G:H1	1.49	0.60
18:D3:405:C:O2'	21:DG:92:ARG:O	2.18	0.60
23:DI:152:ILE:HG13	23:DI:153:GLU:H	1.66	0.60
29:DW:112:ASP:OD1	29:DW:112:ASP:N	2.28	0.60
30:DX:9:LEU:O	30:DX:10:ASN:ND2	2.31	0.60
1:UB:787:THR:HG23	18:D3:1116:A:H4'	1.82	0.60
7:CL:134:ILE:HG21	7:CL:811:VAL:HG21	1.83	0.60
18:D3:780:A:H62	31:DY:10:ARG:HH21	1.48	0.60
30:DX:27:ASN:O	30:DX:31:LYS:HB2	2.01	0.60
11:JL:156:GLN:NE2	11:JL:158:GLU:OE2	2.31	0.60
18:D3:738:G:H2'	18:D3:739:G:C8	2.37	0.60
18:D3:1160:A:O2'	18:D3:1620:C:N3	2.30	0.60
7:CL:831:ARG:NH2	7:CL:835:HIS:O	2.34	0.60
33:UN:466:ARG:NH1	35:D4:15:U:OP1	2.33	0.60
34:JD:514:ILE:HA	34:JD:556:ILE:O	2.02	0.60
20:DE:129:VAL:HG12	20:DE:139:VAL:HG12	1.83	0.59
8:CM:193:GLY:O	8:CM:225:ILE:HA	2.02	0.59
18:D3:1472:C:N3	18:D3:1534:G:C2	2.71	0.59
24:DJ:145:SER:O	24:DJ:145:SER:OG	2.16	0.59
18:D3:504:U:H6	18:D3:504:U:O5'	1.86	0.59
18:D3:717:C:N3	18:D3:720:G:N1	2.51	0.59
18:D3:781:U:OP2	31:DY:9:THR:OG1	2.19	0.59
11:JL:285:LEU:HB3	11:JL:291:GLY:HA3	1.84	0.59
34:JD:1092:VAL:O	34:JD:1121:LEU:N	2.34	0.59
7:CL:14:LYS:HG2	7:CL:19:LYS:HD3	1.84	0.59
19:DA:121:ILE:HG12	19:DA:161:ILE:HG23	1.84	0.59
21:DG:67:VAL:HG23	21:DG:99:GLY:HA2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:CL:210:VAL:O	7:CL:210:VAL:HG13	2.01	0.59
7:CL:130:ASP:OD1	7:CL:853:ARG:NH2	2.35	0.59
18:D3:485:A:C8	18:D3:485:A:C5'	2.86	0.59
18:D3:1477:G:C6	18:D3:1531:G:C6	2.90	0.59
18:D3:1550:A:C6	18:D3:1562:G:N1	2.71	0.59
18:D3:640:U:O2	22:DH:179:LYS:NZ	2.29	0.59
18:D3:1583:A:H62	18:D3:1612:U:H5	1.50	0.59
18:D3:549:G:HO2'	18:D3:550:A:H8	1.51	0.59
18:D3:1588:G:N2	18:D3:1608:U:O2	2.30	0.59
25:DL:57:LYS:HD2	25:DL:131:ILE:HD12	1.85	0.59
7:CL:135:ALA:O	7:CL:238:ARG:NH2	2.29	0.58
18:D3:149:C:OP1	31:DY:121:THR:OG1	2.20	0.58
18:D3:912:U:OP1	18:D3:913:G:O2'	2.21	0.58
7:CL:105:ILE:HD11	7:CL:354:ILE:HD11	1.86	0.58
18:D3:1627:U:H5''	18:D3:1628:U:H5'	1.85	0.58
7:CL:562:GLU:OE2	7:CL:566:ARG:NH1	2.36	0.58
7:CL:826:LYS:HE3	7:CL:926:ILE:HD13	1.85	0.58
20:DE:148:ARG:NH1	21:DG:201:GLN:OE1	2.36	0.58
21:DG:57:ASP:HA	21:DG:106:LEU:HA	1.85	0.58
18:D3:23:G:O6	18:D3:603:U:C2	2.57	0.58
18:D3:1127:G:OP2	34:JD:107:ARG:NH1	2.36	0.58
18:D3:1478:G:H2'	18:D3:1479:A:H8	1.68	0.58
18:D3:1480:G:N1	18:D3:1528:U:C2	2.72	0.58
6:CK:345:LEU:HD13	7:CL:1005:SER:HB2	1.85	0.58
23:DI:137:LYS:HZ3	23:DI:141:ARG:HH22	1.52	0.58
32:Db:36:LYS:HB3	32:Db:43:ILE:HG22	1.86	0.58
11:JL:271:GLY:N	11:JL:275:ASP:OD2	2.36	0.58
18:D3:717:C:C4	18:D3:720:G:N2	2.72	0.58
18:D3:130:C:N4	18:D3:177:U:OP1	2.37	0.57
7:CL:1018:VAL:O	7:CL:1029:TRP:NE1	2.37	0.57
18:D3:428:A:N3	18:D3:440:U:O2'	2.33	0.57
18:D3:720:G:O2'	18:D3:722:G:N7	2.34	0.57
18:D3:1122:G:OP2	34:JD:95:LYS:NZ	2.35	0.57
26:DN:132:VAL:HG13	26:DN:134:VAL:HG23	1.87	0.57
18:D3:505:A:N1	18:D3:507:U:O4	2.36	0.57
18:D3:1542:G:H1	18:D3:1568:C:HO2'	1.49	0.57
5:CJ:144:GLU:HA	5:CJ:149:PRO:HA	1.85	0.57
18:D3:1163:A:N3	18:D3:1613:U:O2'	2.31	0.57
18:D3:1164:G:H2'	18:D3:1165:G:H8	1.69	0.57
29:DW:41:MET:HG2	29:DW:129:VAL:HG11	1.86	0.57
18:D3:163:G:OP2	18:D3:163:G:N2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:656:G:H1	18:D3:679:U:H1'	1.69	0.57
7:CL:228:SER:O	7:CL:228:SER:OG	2.15	0.57
18:D3:683:C:H2'	18:D3:684:A:H8	1.68	0.57
19:DA:29:TRP:O	19:DA:94:LYS:NZ	2.36	0.57
15:DS:14:ILE:HA	15:DS:22:VAL:O	2.05	0.57
18:D3:65:A:H2	18:D3:84:A:H62	1.51	0.57
18:D3:1542:G:O2'	18:D3:1544:U:O4	2.22	0.57
19:DA:104:ASP:OD1	19:DA:105:PHE:N	2.37	0.57
31:DY:29:HIS:O	31:DY:29:HIS:ND1	2.38	0.57
24:DJ:27:GLU:OE1	24:DJ:39:LYS:NZ	2.37	0.57
8:CM:285:LYS:NZ	8:CM:316:GLU:OE1	2.38	0.56
8:CM:289:VAL:HG21	8:CM:294:LEU:HD13	1.87	0.56
34:JD:536:VAL:O	34:JD:540:ALA:N	2.38	0.56
18:D3:195:G:H2'	18:D3:196:G:C8	2.40	0.56
18:D3:651:G:H2'	18:D3:652:G:C8	2.39	0.56
2:UC:562:ARG:NH2	18:D3:476:U:OP2	2.38	0.56
7:CL:282:SER:O	7:CL:282:SER:OG	2.22	0.56
18:D3:144:U:O4	21:DG:137:ARG:NH1	2.39	0.56
18:D3:1472:C:C2	18:D3:1534:G:C2	2.93	0.56
21:DG:116:LYS:NZ	21:DG:117:GLY:O	2.34	0.56
7:CL:170:VAL:HG12	7:CL:205:PHE:HB2	1.87	0.56
7:CL:954:SER:N	7:CL:957:GLU:OE1	2.34	0.56
18:D3:482:U:N3	18:D3:507:U:O4	2.38	0.56
18:D3:706:A:N6	18:D3:731:C:O3'	2.38	0.56
4:UX:89:CYS:SG	4:UX:90:LEU:N	2.78	0.56
18:D3:1550:A:N6	18:D3:1562:G:O6	2.39	0.56
26:DN:12:SER:O	26:DN:12:SER:OG	2.19	0.56
7:CL:984:GLU:OE1	18:D3:1558:U:O2'	2.24	0.56
18:D3:438:A:O2'	18:D3:465:G:N2	2.39	0.56
18:D3:1498:G:N1	18:D3:1510:U:N3	2.52	0.56
6:CK:304:GLN:HB3	6:CK:308:ARG:HH22	1.71	0.55
9:JG:175:CYS:HA	9:JG:201:SER:H	1.72	0.55
19:DA:76:SER:OG	19:DA:77:GLU:N	2.40	0.55
1:UB:749:LYS:NZ	18:D3:1177:C:O3'	2.40	0.55
15:DS:12:GLN:HG2	15:DS:59:GLY:HA2	1.88	0.55
11:JL:256:LYS:HG3	11:JL:273:MET:HE1	1.86	0.55
15:DS:82:PRO:HG2	15:DS:85:PHE:HB2	1.89	0.55
18:D3:208:U:O2'	23:DI:180:ASP:OD2	2.23	0.55
18:D3:1127:G:N7	34:JD:107:ARG:NH2	2.53	0.55
15:DS:87:ASN:O	18:D3:1546:G:N2	2.40	0.55
18:D3:1588:G:O6	18:D3:1608:U:O4	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DW:6:VAL:HG12	29:DW:34:ILE:HD11	1.89	0.55
6:CK:311:ILE:HG23	7:CL:1032:LEU:HD23	1.88	0.55
7:CL:9:ARG:NH1	18:D3:619:A:O4'	2.40	0.55
18:D3:712:G:O6	18:D3:727:U:O4	2.24	0.55
30:DX:90:ASP:OD1	30:DX:90:ASP:N	2.39	0.55
8:CM:260:ASP:OD1	8:CM:261:ILE:N	2.39	0.55
18:D3:715:U:O2	18:D3:723:G:N2	2.38	0.55
18:D3:1484:G:N2	18:D3:1591:C:C2	2.73	0.55
21:DG:147:LEU:HD13	21:DG:151:ASP:HB2	1.89	0.55
7:CL:952:PHE:HD2	7:CL:958:VAL:HG22	1.72	0.55
8:CM:110:SER:OG	8:CM:112:LYS:O	2.25	0.55
12:JJ:96:SER:OG	12:JJ:97:ARG:N	2.37	0.55
12:JJ:107:THR:O	12:JJ:111:ASN:HB2	2.07	0.55
18:D3:830:U:O2'	18:D3:831:U:O4'	2.25	0.54
18:D3:218:A:H2'	18:D3:219:A:H5''	1.89	0.54
21:DG:148:SER:N	21:DG:151:ASP:OD2	2.40	0.54
12:JJ:98:LYS:HB2	12:JJ:138:GLU:HG2	1.89	0.54
18:D3:269:G:C6	18:D3:287:G:C2	2.96	0.54
18:D3:777:C:H4'	20:DE:261:LEU:HD11	1.88	0.54
18:D3:802:G:N2	29:DW:107:SER:HG	2.05	0.54
7:CL:166:ARG:NH1	7:CL:231:LYS:O	2.40	0.54
7:CL:281:PRO:HG2	7:CL:286:THR:HG21	1.89	0.54
8:CM:68:SER:HB2	8:CM:73:THR:HB	1.89	0.54
8:CM:180:MET:HE1	8:CM:311:LEU:HD13	1.89	0.54
18:D3:220:A:N7	18:D3:832:U:N3	2.55	0.54
18:D3:237:C:H4'	18:D3:238:U:H5'	1.89	0.54
18:D3:1647:U:H2'	18:D3:1648:A:H8	1.72	0.54
27:DO:92:LYS:HD3	27:DO:121:VAL:HG22	1.88	0.54
5:CJ:188:HIS:N	5:CJ:220:ARG:O	2.36	0.54
8:CM:361:ASN:O	8:CM:364:LYS:NZ	2.29	0.54
18:D3:620:A:N7	18:D3:1109:G:C2	2.76	0.54
19:DA:88:VAL:HG11	19:DA:96:LEU:HD12	1.89	0.54
22:DH:144:VAL:HA	29:DW:42:GLN:HE21	1.72	0.54
24:DJ:65:LYS:HA	24:DJ:70:LEU:HD11	1.89	0.54
7:CL:607:ASP:OD1	7:CL:607:ASP:N	2.39	0.54
22:DH:63:PRO:O	22:DH:66:SER:OG	2.19	0.54
34:JD:1061:VAL:O	34:JD:1065:GLU:N	2.36	0.54
2:UC:580:ARG:NH1	4:UX:51:LEU:O	2.41	0.54
5:CJ:238:TYR:HA	5:CJ:246:GLU:O	2.07	0.54
18:D3:220:A:H3'	18:D3:832:U:H1'	1.88	0.54
18:D3:734:A:C8	18:D3:734:A:H3'	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:1164:G:H2'	18:D3:1165:G:C8	2.43	0.54
18:D3:319:U:H4'	18:D3:323:A:C8	2.43	0.54
19:DA:78:ASP:OD1	19:DA:78:ASP:N	2.40	0.54
22:DH:67:LEU:HD11	22:DH:94:ALA:HB2	1.90	0.54
12:JJ:216:ILE:HA	12:JJ:263:LEU:HD21	1.90	0.54
16:DT:72:GLY:HA3	18:D3:1498:G:H5''	1.89	0.54
27:DO:53:ASP:HB2	27:DO:56:SER:HB2	1.90	0.54
7:CL:977:LYS:NZ	18:D3:1597:A:OP1	2.30	0.53
18:D3:852:C:H2'	18:D3:853:G:C8	2.43	0.53
18:D3:895:G:H21	27:DO:38:THR:HG21	1.73	0.53
7:CL:960:ARG:HD3	7:CL:961:PHE:HE1	1.73	0.53
18:D3:704:C:H3'	18:D3:705:U:H4'	1.90	0.53
8:CM:306:GLU:OE2	8:CM:355:LYS:NZ	2.41	0.53
9:JF:113:TYR:HA	9:JF:122:ILE:O	2.09	0.53
23:DI:89:GLU:OE2	23:DI:92:ARG:NH2	2.38	0.53
30:DX:109:ARG:NE	30:DX:111:GLY:O	2.40	0.53
18:D3:717:C:N4	18:D3:720:G:N2	2.56	0.53
19:DA:132:ASP:OD1	19:DA:132:ASP:N	2.36	0.53
24:DJ:17:ARG:NH2	24:DJ:19:TYR:H	2.06	0.53
34:JD:731:VAL:HA	34:JD:757:CYS:O	2.09	0.53
4:UX:77:GLN:O	18:D3:1098:U:O2'	2.25	0.53
18:D3:134:U:H4'	18:D3:136:C:H41	1.73	0.53
18:D3:585:A:H3'	18:D3:586:G:H2'	1.89	0.53
28:DZ:86:GLU:HA	28:DZ:102:THR:HA	1.91	0.53
18:D3:1056:U:O3'	19:DA:202:LYS:NZ	2.41	0.53
18:D3:704:C:H2'	18:D3:734:A:H2	1.74	0.53
8:CM:124:SER:OG	8:CM:125:HIS:N	2.39	0.53
18:D3:358:U:O2'	18:D3:360:A:OP1	2.26	0.53
25:DL:27:THR:HG22	25:DL:28:SER:H	1.73	0.53
16:DT:136:ALA:O	16:DT:140:LEU:N	2.42	0.53
29:DW:55:ASP:HB3	32:Db:25:VAL:HG13	1.91	0.53
7:CL:843:ASP:OD1	7:CL:1035:THR:OG1	2.26	0.52
18:D3:1506:G:H2'	18:D3:1507:G:C8	2.44	0.52
18:D3:1518:C:H2'	18:D3:1519:U:C6	2.44	0.52
19:DA:81:PHE:HD2	19:DA:82:ARG:HG3	1.75	0.52
20:DE:104:ASP:N	20:DE:104:ASP:OD1	2.41	0.52
7:CL:923:ASP:OD1	7:CL:923:ASP:N	2.42	0.52
8:CM:312:ARG:NH2	8:CM:344:GLU:OE1	2.34	0.52
15:DS:17:LEU:O	15:DS:20:THR:OG1	2.25	0.52
18:D3:513:U:O4	24:DJ:171:ARG:NH2	2.43	0.52
18:D3:741:C:O2'	18:D3:742:U:O4'	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:DJ:119:ALA:O	24:DJ:124:HIS:ND1	2.42	0.52
1:UB:784:ILE:HD11	30:DX:73:ARG:HH12	1.74	0.52
18:D3:218:A:C6	18:D3:830:U:C4	2.97	0.52
18:D3:1477:G:H2'	18:D3:1478:G:C8	2.45	0.52
23:DI:85:PRO:O	25:DL:11:ARG:NH2	2.34	0.52
1:UB:734:ARG:NH1	18:D3:1173:C:OP1	2.43	0.52
18:D3:895:G:O6	18:D3:917:U:O4	2.28	0.52
7:CL:729:GLN:NE2	7:CL:733:GLU:OE2	2.39	0.52
8:CM:204:LEU:HD23	8:CM:268:PRO:HG3	1.92	0.52
18:D3:1157:A:N6	18:D3:1618:C:O2	2.43	0.52
19:DA:87:ARG:NH1	19:DA:220:GLN:OE1	2.43	0.52
18:D3:434:G:O2'	18:D3:435:C:O2	2.27	0.52
18:D3:846:G:N3	18:D3:846:G:C5'	2.73	0.52
18:D3:992:A:OP2	18:D3:1011:G:N1	2.30	0.52
1:UB:657:PHE:O	1:UB:661:ILE:N	2.42	0.51
18:D3:1511:U:H2'	18:D3:1512:G:H8	1.75	0.51
29:DW:30:SER:O	29:DW:30:SER:OG	2.26	0.51
7:CL:14:LYS:HE2	7:CL:19:LYS:HB3	1.92	0.51
9:JF:114:ILE:O	9:JF:121:LEU:HA	2.09	0.51
11:JL:55:ARG:N	11:JL:58:ASP:OD2	2.36	0.51
18:D3:1594:G:N1	18:D3:1603:U:N3	2.58	0.51
18:D3:487:G:H1	18:D3:500:C:H42	1.59	0.51
18:D3:1486:G:O6	18:D3:1520:U:C4	2.64	0.51
19:DA:103:MET:HB3	19:DA:215:VAL:HG12	1.93	0.51
19:DA:134:VAL:HB	19:DA:219:LYS:HB2	1.91	0.51
8:CM:286:SER:OG	8:CM:289:VAL:O	2.24	0.51
18:D3:168:A:OP1	21:DG:140:ASN:ND2	2.44	0.51
18:D3:1583:A:N1	18:D3:1611:A:H5''	2.26	0.51
24:DJ:113:VAL:HG12	24:DJ:119:ALA:HB2	1.92	0.51
18:D3:23:G:C2	18:D3:24:U:H1'	2.46	0.51
18:D3:1483:A:H2'	18:D3:1484:G:C8	2.45	0.51
21:DG:50:PHE:HE1	21:DG:113:ILE:HG12	1.76	0.51
21:DG:52:ILE:HA	21:DG:111:LEU:HD23	1.91	0.51
7:CL:174:LEU:CD2	7:CL:206:TYR:HB3	2.39	0.51
11:JL:75:LEU:HD22	11:JL:81:VAL:HG21	1.93	0.51
18:D3:503:G:H3'	18:D3:504:U:H5	1.75	0.51
18:D3:1504:G:H21	18:D3:1563:C:H1'	1.74	0.51
20:DE:31:PRO:HG3	20:DE:43:PRO:HG3	1.93	0.51
22:DH:8:ILE:HA	22:DH:42:GLN:HG3	1.92	0.51
7:CL:773:THR:O	7:CL:776:GLN:N	2.40	0.51
11:JL:233:ARG:HG2	11:JL:236:ARG:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:DS:27:LYS:HA	15:DS:57:ARG:HA	1.92	0.51
18:D3:1484:G:O2'	18:D3:1606:C:O3'	2.28	0.51
21:DG:160:ARG:O	21:DG:170:THR:HA	2.10	0.51
18:D3:738:G:H2'	18:D3:739:G:H8	1.73	0.51
7:CL:844:PRO:HG3	7:CL:1032:LEU:HB2	1.93	0.51
19:DA:141:ALA:HB1	19:DA:207:LEU:HD11	1.93	0.51
19:DA:194:ASN:HD21	19:DA:211:HIS:HA	1.76	0.51
6:CK:337:GLU:OE2	7:CL:954:SER:OG	2.27	0.50
18:D3:734:A:H2'	18:D3:735:C:C2	2.46	0.50
20:DE:182:TYR:HD1	20:DE:192:ILE:HG12	1.76	0.50
9:JF:121:LEU:CB	9:JF:163:ILE:O	2.59	0.50
18:D3:824:G:H2'	18:D3:825:U:H6	1.77	0.50
23:DI:104:ILE:HG13	23:DI:105:ASP:H	1.76	0.50
7:CL:244:MET:HB3	7:CL:812:MET:HB3	1.93	0.50
7:CL:934:LEU:O	7:CL:1002:ILE:HA	2.11	0.50
11:JL:299:ASP:OD1	11:JL:299:ASP:N	2.44	0.50
18:D3:1585:U:O2	18:D3:1611:A:N7	2.44	0.50
7:CL:905:SER:OG	7:CL:906:ASP:N	2.45	0.50
9:JF:133:THR:O	9:JF:137:PHE:N	2.42	0.50
18:D3:1486:G:H2'	18:D3:1487:A:C8	2.46	0.50
2:UC:535:ASP:HB3	2:UC:537:LYS:H	1.77	0.50
2:UC:557:ASP:OD2	2:UC:567:LYS:NZ	2.27	0.50
7:CL:719:ASN:N	7:CL:719:ASN:OD1	2.44	0.50
18:D3:824:G:H2'	18:D3:825:U:C6	2.46	0.50
30:DX:109:ARG:HH12	30:DX:116:ASP:HB2	1.77	0.50
1:UB:756:ARG:NH1	6:CK:353:PRO:O	2.45	0.50
18:D3:394:C:O2'	21:DG:90:GLY:O	2.26	0.50
18:D3:636:A:H5''	29:DW:31:SER:HB3	1.93	0.50
18:D3:1008:G:OP1	27:DO:135:ARG:NH1	2.45	0.50
34:JD:1244:GLN:OE1	34:JD:1245:TRP:N	2.44	0.50
7:CL:125:LEU:HD22	7:CL:912:ARG:HH21	1.77	0.50
7:CL:198:VAL:HG12	7:CL:199:TYR:H	1.77	0.50
11:JL:60:VAL:HG11	11:JL:74:ILE:HG21	1.93	0.50
18:D3:1480:G:C2	18:D3:1528:U:C2	2.99	0.50
21:DG:43:ASP:OD1	21:DG:43:ASP:N	2.43	0.50
25:DL:124:THR:HB	25:DL:141:LYS:HG2	1.92	0.50
29:DW:24:GLN:HE22	32:Db:6:ASP:HA	1.76	0.50
18:D3:1800:A:O2'	18:D3:1801:A:O5'	2.25	0.50
11:JL:280:LYS:O	11:JL:283:THR:OG1	2.29	0.50
4:UX:106:LEU:HA	4:UX:109:LEU:HD23	1.94	0.49
7:CL:267:ARG:NH1	7:CL:798:MET:HG2	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:225:A:N6	18:D3:837:G:O6	2.45	0.49
23:DI:135:LYS:N	23:DI:140:GLU:OE1	2.45	0.49
34:JD:1195:THR:OG1	34:JD:1196:GLY:N	2.35	0.49
8:CM:85:ALA:HA	8:CM:115:SER:O	2.12	0.49
15:DS:53:ASP:HB3	15:DS:56:LYS:HG3	1.93	0.49
18:D3:834:G:H2'	18:D3:835:U:C2	2.47	0.49
19:DA:94:LYS:C	19:DA:95:ASN:HD22	2.19	0.49
7:CL:803:ASN:O	7:CL:1026:LYS:NZ	2.39	0.49
22:DH:49:ILE:HD11	22:DH:172:VAL:HG22	1.94	0.49
24:DJ:20:GLU:O	24:DJ:23:ARG:N	2.35	0.49
7:CL:921:GLU:HB3	8:CM:365:LYS:HG3	1.95	0.49
34:JD:788:ASN:N	34:JD:793:VAL:O	2.38	0.49
18:D3:150:U:O4	31:DY:124:ARG:NH2	2.45	0.49
18:D3:827:C:H2'	18:D3:828:U:C6	2.47	0.49
7:CL:719:ASN:HA	7:CL:722:LYS:HE2	1.93	0.49
7:CL:831:ARG:HD3	7:CL:838:ILE:HG22	1.92	0.49
18:D3:1564:U:H2'	18:D3:1565:C:C6	2.48	0.49
7:CL:87:ARG:NH2	7:CL:99:ASN:OD1	2.46	0.49
7:CL:105:ILE:HG13	7:CL:356:ALA:HB2	1.95	0.49
7:CL:870:ARG:NH1	18:D3:574:G:OP1	2.45	0.49
4:UX:72:ILE:O	4:UX:76:ILE:HG12	2.13	0.49
7:CL:140:LEU:HD11	7:CL:152:THR:HG23	1.95	0.49
18:D3:142:G:H5''	21:DG:139:ASN:HD21	1.78	0.49
18:D3:647:G:N2	18:D3:687:G:H22	2.11	0.49
18:D3:649:U:O2'	18:D3:650:U:O5'	2.26	0.49
18:D3:734:A:H3'	18:D3:734:A:H8	1.77	0.49
21:DG:10:ASN:OD1	21:DG:128:THR:OG1	2.23	0.49
7:CL:983:PRO:HB2	7:CL:986:HIS:HB2	1.94	0.48
8:CM:148:GLU:HB2	8:CM:171:ASP:HB2	1.95	0.48
19:DA:176:VAL:O	19:DA:179:SER:OG	2.27	0.48
22:DH:48:GLU:OE2	22:DH:88:ARG:NH2	2.46	0.48
8:CM:233:GLU:OE2	8:CM:233:GLU:N	2.46	0.48
14:DQ:11:GLY:N	14:DQ:18:ALA:O	2.43	0.48
18:D3:734:A:C8	18:D3:734:A:C3'	2.96	0.48
20:DE:100:ARG:NH2	20:DE:121:TYR:O	2.45	0.48
15:DS:71:GLN:HA	15:DS:74:GLN:HG2	1.95	0.48
18:D3:828:U:O4	18:D3:829:A:N6	2.36	0.48
18:D3:992:A:O2'	18:D3:1785:U:O2	2.30	0.48
18:D3:1498:G:H2'	18:D3:1499:G:C8	2.48	0.48
5:CJ:157:PHE:O	5:CJ:159:HIS:N	2.47	0.48
8:CM:47:ASP:OD1	8:CM:47:ASP:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:269:G:C5	18:D3:287:G:C2	3.01	0.48
18:D3:693:U:N3	18:D3:695:U:O4	2.46	0.48
18:D3:1041:G:H2'	18:D3:1042:G:C8	2.48	0.48
21:DG:24:ILE:HG22	21:DG:28:PHE:HE1	1.78	0.48
23:DI:12:SER:OG	23:DI:13:ALA:N	2.47	0.48
16:DT:20:SER:O	16:DT:24:ARG:N	2.42	0.48
18:D3:1001:A:H3'	18:D3:1002:G:C8	2.48	0.48
18:D3:1490:C:N3	18:D3:1492:A:N6	2.60	0.48
7:CL:549:ILE:HB	7:CL:567:TRP:CD1	2.49	0.48
7:CL:968:THR:OG1	7:CL:972:ILE:N	2.45	0.48
18:D3:220:A:OP2	18:D3:831:U:O2'	2.18	0.48
18:D3:851:U:H2'	18:D3:852:C:C2	2.48	0.48
20:DE:35:PRO:HB2	20:DE:36:HIS:CD2	2.49	0.48
5:CJ:165:PHE:HA	5:CJ:258:LEU:HA	1.94	0.48
21:DG:173:PRO:HB2	21:DG:174:LYS:H	1.47	0.48
22:DH:136:VAL:HG23	22:DH:155:ASP:HA	1.95	0.48
6:CK:347:PHE:HE2	6:CK:349:ARG:HH11	1.61	0.48
12:JJ:224:ILE:HG12	12:JJ:233:ILE:HG12	1.95	0.48
18:D3:220:A:N7	18:D3:832:U:C4	2.81	0.48
18:D3:1472:C:C2	18:D3:1534:G:N1	2.82	0.48
31:DY:57:VAL:HG13	31:DY:60:PHE:HE2	1.79	0.48
18:D3:237:C:H2'	18:D3:834:G:H4'	1.95	0.48
20:DE:252:ARG:HD3	24:DJ:71:PHE:HE1	1.77	0.48
34:JD:1216:ARG:HH12	34:JD:1219:SER:C	2.22	0.48
6:CK:337:GLU:HG3	7:CL:953:SER:HB3	1.95	0.48
18:D3:320:U:H3'	18:D3:321:C:H2'	1.96	0.48
18:D3:577:G:N2	18:D3:581:U:O2'	2.46	0.48
18:D3:849:C:H2'	18:D3:850:A:C8	2.49	0.48
29:DW:30:SER:HA	29:DW:34:ILE:HD12	1.96	0.48
1:UB:753:LYS:NZ	6:CK:356:VAL:H	2.12	0.47
6:CK:341:LEU:HD23	7:CL:960:ARG:HD2	1.96	0.47
11:JL:157:ARG:NH2	11:JL:203:GLU:OE1	2.46	0.47
21:DG:39:GLU:HG3	21:DG:46:LYS:HG2	1.95	0.47
7:CL:280:LEU:HD12	7:CL:281:PRO:HD2	1.96	0.47
7:CL:321:GLU:C	7:CL:322:ARG:HD2	2.39	0.47
8:CM:113:LYS:HD2	8:CM:171:ASP:HA	1.97	0.47
18:D3:433:C:N4	18:D3:436:A:OP1	2.46	0.47
18:D3:844:A:H2'	18:D3:845:G:C8	2.49	0.47
19:DA:31:ASP:OD1	19:DA:31:ASP:N	2.41	0.47
7:CL:933:LYS:HA	7:CL:1003:LEU:O	2.14	0.47
18:D3:78:A:H1'	21:DG:175:ILE:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:219:A:C5	18:D3:843:U:H1'	2.49	0.47
18:D3:351:C:O4'	30:DX:13:ARG:NH1	2.47	0.47
18:D3:739:G:H2'	18:D3:740:A:C8	2.50	0.47
21:DG:2:LYS:HB3	21:DG:108:VAL:HG22	1.96	0.47
31:DY:122:GLY:O	31:DY:124:ARG:N	2.47	0.47
8:CM:83:GLY:HA2	8:CM:114:PHE:CE1	2.50	0.47
12:JJ:102:PRO:HD2	12:JJ:163:THR:HG23	1.97	0.47
18:D3:1542:G:N2	18:D3:1569:A:C8	2.76	0.47
18:D3:1603:U:H2'	18:D3:1604:U:C6	2.49	0.47
19:DA:39:GLU:N	19:DA:74:GLN:OE1	2.40	0.47
20:DE:171:ASP:OD1	20:DE:172:PHE:N	2.47	0.47
33:UN:383:MET:HE2	34:JD:1206:PRO:HD3	1.96	0.47
11:JL:41:ASN:HB2	11:JL:195:ASN:HB3	1.96	0.47
18:D3:710:U:N3	18:D3:730:G:C6	2.83	0.47
18:D3:1548:G:N1	18:D3:1564:U:N3	2.63	0.47
18:D3:1753:A:H2'	18:D3:1754:A:C8	2.49	0.47
22:DH:50:ASP:OD1	22:DH:50:ASP:N	2.47	0.47
18:D3:22:A:H2'	18:D3:23:G:C8	2.49	0.47
18:D3:1486:G:N2	18:D3:1592:A:H4'	2.30	0.47
20:DE:81:THR:O	20:DE:81:THR:OG1	2.28	0.47
21:DG:159:ARG:HA	21:DG:171:LYS:O	2.14	0.47
30:DX:86:PHE:HB2	30:DX:120:VAL:HG11	1.95	0.47
8:CM:123:ALA:HB1	8:CM:261:ILE:HG21	1.96	0.47
18:D3:150:U:OP1	31:DY:123:LYS:NZ	2.48	0.47
18:D3:840:U:O2'	18:D3:841:U:O4'	2.33	0.47
15:DS:48:LYS:HE2	16:DT:35:ASP:HA	1.96	0.47
21:DG:191:ARG:HA	21:DG:191:ARG:HD3	1.68	0.47
25:DL:74:THR:HG22	25:DL:122:ILE:HG12	1.97	0.47
9:JG:208:ALA:HB2	9:JG:234:ALA:H	1.80	0.47
15:DS:16:ARG:HA	15:DS:20:THR:O	2.15	0.47
18:D3:1471:A:C6	18:D3:1536:G:O6	2.68	0.47
34:JD:1021:LYS:O	34:JD:1025:MET:N	2.48	0.47
6:CK:348:ASP:OD1	6:CK:349:ARG:N	2.41	0.46
25:DL:33:ARG:HH11	25:DL:61:THR:HG21	1.80	0.46
1:UB:764:ARG:O	1:UB:767:ILE:N	2.46	0.46
7:CL:748:ASP:OD1	7:CL:748:ASP:N	2.46	0.46
18:D3:1494:C:H2'	18:D3:1495:C:C6	2.50	0.46
18:D3:1594:G:HO2'	18:D3:1600:A:H61	1.58	0.46
20:DE:37:LYS:HB2	20:DE:40:GLU:HG2	1.96	0.46
20:DE:188:ASN:HB3	20:DE:191:ARG:HD3	1.97	0.46
21:DG:71:THR:OG1	21:DG:72:ARG:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:JD:1205:SER:HB2	34:JD:1208:GLU:HB3	1.97	0.46
8:CM:190:SER:OG	8:CM:191:ILE:N	2.46	0.46
18:D3:196:G:H2'	18:D3:197:A:H8	1.80	0.46
18:D3:1592:A:H2'	18:D3:1593:A:C8	2.50	0.46
7:CL:56:VAL:HG22	30:DX:52:ILE:HG12	1.96	0.46
18:D3:487:G:O5'	18:D3:487:G:H8	1.98	0.46
18:D3:1152:A:H2'	18:D3:1153:G:H8	1.79	0.46
23:DI:42:ARG:NH1	23:DI:59:ARG:HE	2.13	0.46
24:DJ:112:GLN:O	24:DJ:116:LEU:HD23	2.16	0.46
1:UB:753:LYS:HD2	1:UB:753:LYS:HA	1.62	0.46
18:D3:453:U:H2'	18:D3:454:U:H5''	1.96	0.46
18:D3:726:C:N4	18:D3:727:U:O4	2.48	0.46
18:D3:814:A:N6	18:D3:816:G:C6	2.84	0.46
18:D3:1472:C:C2	18:D3:1534:G:N2	2.84	0.46
7:CL:548:ASN:HB3	7:CL:551:LYS:HG2	1.96	0.46
18:D3:1545:A:N1	18:D3:1567:U:N3	2.63	0.46
19:DA:74:GLN:HE21	19:DA:189:ILE:HG21	1.80	0.46
24:DJ:45:ILE:HG13	24:DJ:105:LEU:HD11	1.97	0.46
1:UB:701:ALA:HB2	3:US:416:LEU:O	2.16	0.46
4:UX:81:ASP:OD1	4:UX:82:ILE:N	2.49	0.46
20:DE:95:THR:O	20:DE:97:GLU:HG3	2.16	0.46
32:Db:34:ASP:O	32:Db:79:PHE:HA	2.16	0.46
16:DT:115:GLU:O	16:DT:123:ARG:N	2.46	0.46
18:D3:202:A:H2'	18:D3:203:U:O4'	2.15	0.46
19:DA:212:VAL:O	19:DA:214:LYS:N	2.46	0.46
18:D3:734:A:C8	18:D3:734:A:O5'	2.69	0.46
11:JL:99:ARG:NH1	11:JL:104:GLU:OE2	2.41	0.46
21:DG:3:LEU:O	21:DG:15:THR:HA	2.16	0.46
7:CL:636:LEU:HA	7:CL:636:LEU:HD23	1.80	0.45
18:D3:231:U:O2	18:D3:234:G:N1	2.31	0.45
26:DN:29:SER:O	26:DN:32:SER:OG	2.33	0.45
18:D3:504:U:C6	18:D3:504:U:H3'	2.52	0.45
18:D3:1495:C:O5'	18:D3:1495:C:H6	1.99	0.45
18:D3:1496:U:H1'	18:D3:1512:G:N2	2.31	0.45
7:CL:88:SER:HB3	7:CL:214:ARG:HB2	1.98	0.45
7:CL:629:ASP:O	7:CL:632:LYS:HB2	2.15	0.45
8:CM:225:ILE:N	18:D3:1130:A:H61	2.14	0.45
12:JJ:221:ARG:HE	12:JJ:271:LYS:NZ	2.13	0.45
18:D3:154:G:OP1	21:DG:2:LYS:NZ	2.36	0.45
18:D3:1512:G:C8	18:D3:1512:G:OP2	2.70	0.45
23:DI:76:THR:HG22	23:DI:108:PRO:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:JD:1256:PHE:HA	34:JD:1259:ILE:HG22	1.97	0.45
7:CL:81:GLY:HA2	38:CL:2001:GTP:O3A	2.16	0.45
7:CL:611:PHE:HZ	8:CM:137:LEU:HD11	1.81	0.45
7:CL:970:SER:OG	7:CL:999:ASP:OD1	2.22	0.45
16:DT:77:ASN:HA	16:DT:96:ALA:HB3	1.98	0.45
18:D3:73:U:O2	18:D3:74:U:N3	2.50	0.45
18:D3:191:C:O2'	18:D3:192:U:O5'	2.32	0.45
18:D3:485:A:C5'	18:D3:485:A:H8	2.28	0.45
4:UX:51:LEU:HG	4:UX:52:PHE:O	2.17	0.45
5:CJ:74:ASP:O	5:CJ:78:ALA:N	2.50	0.45
7:CL:606:VAL:HG22	7:CL:607:ASP:H	1.81	0.45
15:DS:32:LEU:O	15:DS:43:SER:OG	2.32	0.45
18:D3:221:A:H2'	18:D3:222:A:C8	2.51	0.45
19:DA:31:ASP:HB3	19:DA:45:LYS:HD3	1.99	0.45
21:DG:73:ILE:O	21:DG:96:SER:HA	2.16	0.45
11:JL:51:LYS:HA	11:JL:51:LYS:HD2	1.76	0.45
18:D3:24:U:H2'	18:D3:25:C:C4	2.51	0.45
18:D3:754:A:N6	18:D3:793:A:N7	2.64	0.45
18:D3:802:G:H21	29:DW:107:SER:HG	1.61	0.45
18:D3:855:A:O2'	18:D3:856:A:H3'	2.16	0.45
18:D3:1511:U:H2'	18:D3:1512:G:C8	2.51	0.45
1:UB:774:SER:O	1:UB:778:HIS:ND1	2.50	0.45
8:CM:201:SER:HA	8:CM:202:PRO:HD3	1.81	0.45
11:JL:259:LEU:O	11:JL:263:ASN:N	2.50	0.45
13:DF:78:ALA:O	18:D3:1615:C:N4	2.35	0.45
18:D3:329:G:H5''	23:DI:98:LYS:HB3	1.97	0.45
18:D3:814:A:C6	18:D3:816:G:C6	3.05	0.45
18:D3:1594:G:HO2'	18:D3:1600:A:N6	2.15	0.45
21:DG:21:GLU:O	21:DG:25:ARG:N	2.48	0.45
6:CK:295:LYS:HD2	6:CK:296:ASN:HB2	1.99	0.45
18:D3:218:A:C6	18:D3:830:U:C2	3.05	0.45
18:D3:712:G:C6	18:D3:727:U:C4	3.05	0.45
18:D3:1174:C:O2'	18:D3:1601:G:O2'	2.33	0.45
18:D3:1545:A:C2	18:D3:1567:U:C2	3.05	0.45
19:DA:122:GLU:OE2	19:DA:213:ARG:NH2	2.50	0.45
20:DE:133:LYS:HB2	20:DE:133:LYS:HE3	1.74	0.45
34:JD:804:ALA:N	34:JD:836:GLN:O	2.50	0.45
6:CK:304:GLN:HB3	6:CK:308:ARG:NH2	2.30	0.45
8:CM:23:LEU:HD23	8:CM:23:LEU:HA	1.83	0.45
18:D3:782:U:H4'	31:DY:12:VAL:HG11	1.99	0.45
18:D3:1492:A:O2'	18:D3:1493:A:O4'	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:1528:U:O4	18:D3:1529:C:N4	2.50	0.45
26:DN:39:LYS:HE3	26:DN:39:LYS:HB2	1.78	0.45
7:CL:9:ARG:NH1	18:D3:619:A:N3	2.66	0.44
18:D3:1479:A:H2'	18:D3:1480:G:C8	2.52	0.44
19:DA:70:LEU:O	19:DA:74:GLN:N	2.51	0.44
32:Db:31:TYR:HE1	32:Db:33:LEU:HD23	1.81	0.44
11:JL:63:VAL:HG12	11:JL:129:THR:HG21	1.99	0.44
11:JL:72:VAL:O	11:JL:76:GLU:HG2	2.16	0.44
16:DT:47:PRO:HA	18:D3:1477:G:H4'	2.00	0.44
18:D3:601:A:H2'	18:D3:602:U:O4'	2.17	0.44
18:D3:736:C:C6	18:D3:736:C:C4'	3.00	0.44
18:D3:884:A:OP1	19:DA:136:ARG:NH2	2.50	0.44
18:D3:1506:G:H4'	18:D3:1551:U:H5'	1.99	0.44
19:DA:129:THR:OG1	19:DA:131:ASP:O	2.31	0.44
30:DX:46:SER:OG	30:DX:47:SER:N	2.50	0.44
1:UB:746:LYS:NZ	18:D3:1179:G:N7	2.61	0.44
12:JJ:159:ILE:HD12	12:JJ:159:ILE:HG23	1.80	0.44
18:D3:1:U:O2'	18:D3:2:A:H5''	2.17	0.44
18:D3:600:U:H2'	18:D3:601:A:O4'	2.18	0.44
20:DE:21:ASP:OD1	20:DE:21:ASP:N	2.49	0.44
4:UX:105:GLU:OE1	33:UN:439:ARG:NH1	2.49	0.44
18:D3:1552:U:H3'	18:D3:1553:G:C8	2.53	0.44
32:Db:67:THR:HG22	32:Db:68:GLY:H	1.83	0.44
4:UX:76:ILE:HD11	4:UX:119:LEU:HG	2.00	0.44
8:CM:54:ARG:HD3	8:CM:54:ARG:HA	1.80	0.44
18:D3:25:C:H42	18:D3:601:A:H61	1.65	0.44
18:D3:119:A:H1'	18:D3:397:A:C5	2.53	0.44
18:D3:496:G:H8	18:D3:498:G:O5'	2.00	0.44
18:D3:701:U:C6	18:D3:701:U:O5'	2.70	0.44
18:D3:835:U:H2'	18:D3:836:U:C6	2.52	0.44
18:D3:1162:C:H2'	18:D3:1163:A:C8	2.52	0.44
18:D3:1477:G:C6	18:D3:1531:G:N1	2.86	0.44
18:D3:1503:A:H3'	18:D3:1504:G:H8	1.82	0.44
18:D3:1517:U:H2'	18:D3:1518:C:H5	1.83	0.44
19:DA:120:LEU:HD12	19:DA:142:PHE:CE2	2.53	0.44
21:DG:150:GLU:OE1	21:DG:150:GLU:N	2.51	0.44
32:Db:31:TYR:CG	32:Db:81:ARG:HD2	2.52	0.44
8:CM:95:PRO:HG3	8:CM:124:SER:HB3	1.99	0.44
15:DS:49:LYS:HD2	15:DS:49:LYS:HA	1.83	0.44
18:D3:504:U:C6	18:D3:504:U:C3'	3.00	0.44
18:D3:699:U:H3	18:D3:739:G:H1	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:CL:137:LEU:HD12	7:CL:166:ARG:O	2.18	0.44
7:CL:350:LYS:HB3	7:CL:350:LYS:HE2	1.82	0.44
7:CL:772:MET:HE1	7:CL:780:ILE:HD11	1.99	0.44
18:D3:218:A:N6	18:D3:830:U:C2	2.85	0.44
30:DX:130:VAL:HG21	30:DX:135:LEU:HD21	1.99	0.44
8:CM:198:THR:O	8:CM:239:PRO:HA	2.18	0.44
11:JL:167:PRO:HG2	11:JL:299:ASP:HB3	2.00	0.44
12:JJ:130:MET:HB3	12:JJ:130:MET:HE2	1.78	0.44
18:D3:58:U:O2'	18:D3:451:A:N3	2.49	0.44
18:D3:224:C:H2'	18:D3:225:A:C8	2.50	0.44
18:D3:740:A:N6	18:D3:741:C:N4	2.66	0.44
1:UB:667:LEU:O	1:UB:670:ALA:HB3	2.18	0.44
7:CL:156:LEU:HD23	7:CL:156:LEU:HA	1.78	0.44
8:CM:291:ARG:HH11	8:CM:291:ARG:HD3	1.68	0.44
18:D3:416:A:H5'	18:D3:417:A:N7	2.33	0.44
18:D3:1546:G:H2'	18:D3:1547:A:C8	2.53	0.44
18:D3:1548:G:C2	18:D3:1564:U:C2	3.06	0.44
24:DJ:184:SER:OG	24:DJ:185:GLY:N	2.50	0.44
7:CL:943:LYS:HB3	7:CL:943:LYS:HE2	1.60	0.43
18:D3:736:C:C6	18:D3:736:C:C5'	2.85	0.43
18:D3:885:G:N2	27:DO:123:SER:O	2.51	0.43
18:D3:1589:C:H2'	18:D3:1590:G:C8	2.53	0.43
19:DA:219:LYS:HB3	19:DA:219:LYS:HE3	1.70	0.43
21:DG:20:ASP:HB3	21:DG:23:ARG:HD3	2.00	0.43
22:DH:87:ASP:O	22:DH:88:ARG:NH1	2.43	0.43
1:UB:753:LYS:HZ3	6:CK:356:VAL:H	1.65	0.43
7:CL:977:LYS:NZ	18:D3:1598:U:OP2	2.34	0.43
14:DQ:11:GLY:O	14:DQ:18:ALA:N	2.51	0.43
18:D3:1173:C:H2'	18:D3:1174:C:H6	1.83	0.43
18:D3:1482:C:OP2	18:D3:1521:G:N2	2.51	0.43
24:DJ:110:GLN:NE2	24:DJ:126:ARG:HB2	2.33	0.43
7:CL:301:ILE:HD12	7:CL:783:PHE:CE2	2.53	0.43
7:CL:830:ARG:NH2	7:CL:831:ARG:O	2.51	0.43
18:D3:218:A:N6	18:D3:830:U:N3	2.65	0.43
18:D3:593:U:HO2'	18:D3:595:G:HO2'	1.53	0.43
18:D3:834:G:H3'	18:D3:835:U:C5	2.53	0.43
18:D3:1525:A:N3	18:D3:1589:C:O2'	2.48	0.43
26:DN:84:ILE:HD13	26:DN:149:LEU:HD21	1.99	0.43
29:DW:61:ILE:HG21	29:DW:61:ILE:HD13	1.73	0.43
34:JD:5:ARG:HH21	34:JD:7:ARG:NE	2.15	0.43
7:CL:126:ASN:OD1	7:CL:853:ARG:NE	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:CL:748:ASP:OD1	7:CL:749:THR:N	2.50	0.43
7:CL:859:ILE:HG21	7:CL:1011:VAL:HG12	2.01	0.43
8:CM:83:GLY:HA2	8:CM:114:PHE:HE1	1.84	0.43
11:JL:275:ASP:O	11:JL:278:LYS:HB3	2.19	0.43
17:Dc:31:GLU:HA	17:Dc:39:THR:HA	2.00	0.43
18:D3:136:C:H4'	18:D3:137:U:H5'	2.00	0.43
18:D3:486:G:H4'	18:D3:486:G:OP1	2.18	0.43
18:D3:1523:G:OP2	18:D3:1523:G:N2	2.39	0.43
21:DG:75:LEU:HA	21:DG:75:LEU:HD23	1.80	0.43
22:DH:44:LYS:HG3	22:DH:63:PRO:HD3	2.00	0.43
24:DJ:97:LEU:HD23	24:DJ:97:LEU:HA	1.86	0.43
8:CM:106:LEU:HA	8:CM:106:LEU:HD23	1.84	0.43
8:CM:337:VAL:HG13	8:CM:354:ILE:HG13	2.01	0.43
8:CM:338:PHE:CE2	8:CM:340:LYS:HB3	2.53	0.43
11:JL:58:ASP:O	11:JL:79:LYS:HG2	2.19	0.43
14:DQ:13:LYS:N	14:DQ:16:ALA:O	2.52	0.43
18:D3:692:C:H2'	18:D3:693:U:H6	1.84	0.43
18:D3:1477:G:C5	18:D3:1531:G:C2	3.07	0.43
18:D3:1478:G:H2'	18:D3:1479:A:C8	2.50	0.43
18:D3:1524:A:H2'	18:D3:1525:A:C8	2.52	0.43
18:D3:1551:U:H2'	18:D3:1552:U:C6	2.54	0.43
18:D3:1552:U:N3	18:D3:1556:A:C8	2.73	0.43
7:CL:143:ASP:OD1	7:CL:146:PHE:N	2.36	0.43
7:CL:157:ASN:HD22	7:CL:911:PHE:HZ	1.65	0.43
7:CL:855:GLN:HE22	7:CL:1031:GLY:HA3	1.83	0.43
8:CM:176:GLN:HE21	8:CM:305:LYS:HB3	1.83	0.43
9:JG:114:ILE:O	9:JG:121:LEU:HA	2.18	0.43
18:D3:199:G:O2'	18:D3:200:A:O4'	2.32	0.43
18:D3:1579:U:H2'	18:D3:1580:C:C6	2.54	0.43
20:DE:128:LYS:HB3	20:DE:128:LYS:HE2	1.81	0.43
22:DH:50:ASP:HA	22:DH:56:LYS:HD3	2.00	0.43
22:DH:83:LYS:HE3	22:DH:83:LYS:HB3	1.77	0.43
34:JD:827:SER:O	34:JD:831:GLU:N	2.44	0.43
7:CL:626:LYS:HB2	7:CL:626:LYS:HE2	1.70	0.43
7:CL:940:LYS:HB3	7:CL:947:PHE:HB2	2.01	0.43
18:D3:1519:U:H3'	18:D3:1520:U:H2'	1.99	0.43
34:JD:447:ILE:HA	34:JD:514:ILE:O	2.19	0.43
7:CL:869:THR:O	7:CL:869:THR:OG1	2.30	0.43
7:CL:870:ARG:NH2	18:D3:573:C:O2'	2.39	0.43
7:CL:871:MET:HB2	7:CL:928:ILE:HG22	2.00	0.43
18:D3:485:A:H8	18:D3:485:A:O5'	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:1173:C:H2'	18:D3:1174:C:C6	2.54	0.43
18:D3:1511:U:C2'	18:D3:1512:G:H5'	2.49	0.43
18:D3:1529:C:C4	18:D3:1530:C:N4	2.87	0.43
33:UN:382:LEU:HD23	33:UN:382:LEU:HA	1.89	0.43
11:JL:110:MET:HE2	11:JL:110:MET:HB3	1.76	0.43
29:DW:29:PRO:HB3	29:DW:58:SER:HB3	2.00	0.43
1:UB:756:ARG:HH12	6:CK:354:VAL:C	2.25	0.43
18:D3:218:A:N1	18:D3:830:U:C4	2.87	0.43
18:D3:1542:G:N2	18:D3:1569:A:OP1	2.48	0.43
19:DA:190:PRO:HG2	19:DA:192:VAL:HG23	2.01	0.43
12:JJ:204:ARG:HH12	12:JJ:253:GLY:HA2	1.84	0.42
18:D3:1161:C:H1'	18:D3:1619:C:H42	1.84	0.42
18:D3:1599:C:O2'	18:D3:1602:C:O2	2.34	0.42
19:DA:201:THR:HG23	19:DA:204:ILE:HD12	2.01	0.42
21:DG:32:ILE:HG12	21:DG:100:ALA:HB1	2.00	0.42
31:DY:29:HIS:NE2	31:DY:69:SER:OG	2.43	0.42
31:DY:81:GLU:HA	31:DY:84:LYS:HG2	2.00	0.42
8:CM:312:ARG:NE	8:CM:349:ASP:OD2	2.31	0.42
12:JJ:131:ASN:OD1	12:JJ:133:LYS:N	2.53	0.42
18:D3:276:C:O2'	18:D3:278:U:O4	2.33	0.42
18:D3:570:A:H2'	18:D3:571:G:C8	2.55	0.42
18:D3:780:A:H62	31:DY:10:ARG:NH2	2.13	0.42
18:D3:1484:G:H2'	18:D3:1485:C:C6	2.54	0.42
29:DW:55:ASP:OD1	29:DW:55:ASP:N	2.28	0.42
34:JD:826:SER:O	34:JD:830:PHE:N	2.46	0.42
8:CM:274:LYS:O	8:CM:278:GLN:HG3	2.18	0.42
11:JL:75:LEU:HD12	11:JL:103:VAL:HB	2.01	0.42
11:JL:269:THR:OG1	11:JL:275:ASP:OD2	2.35	0.42
12:JJ:225:VAL:HG12	12:JJ:232:HIS:HB2	2.00	0.42
18:D3:500:C:C6	18:D3:500:C:H3'	2.53	0.42
23:DI:196:LEU:O	23:DI:200:LYS:NZ	2.52	0.42
2:UC:542:TYR:OH	2:UC:548:LYS:NZ	2.52	0.42
12:JJ:263:LEU:HD12	12:JJ:263:LEU:HA	1.75	0.42
18:D3:501:U:H1'	18:D3:502:U:C5	2.54	0.42
18:D3:1545:A:H2'	18:D3:1546:G:C8	2.54	0.42
19:DA:36:SER:HB2	19:DA:231:LEU:O	2.18	0.42
19:DA:94:LYS:O	19:DA:95:ASN:ND2	2.45	0.42
22:DH:9:LEU:HD13	22:DH:17:GLU:HB3	2.01	0.42
7:CL:838:ILE:HD11	18:D3:578:U:N3	2.35	0.42
11:JL:253:LYS:HB2	11:JL:253:LYS:HE3	1.75	0.42
12:JJ:102:PRO:HA	12:JJ:103:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:199:G:H2'	18:D3:200:A:C8	2.55	0.42
18:D3:712:G:N1	18:D3:727:U:C4	2.87	0.42
18:D3:734:A:H8	18:D3:734:A:O5'	2.03	0.42
18:D3:1150:G:H2'	18:D3:1151:A:C8	2.54	0.42
21:DG:121:LEU:HD23	21:DG:121:LEU:HA	1.88	0.42
22:DH:147:ASN:OD1	22:DH:147:ASN:N	2.52	0.42
25:DL:29:LYS:NZ	25:DL:32:LYS:HA	2.35	0.42
32:Db:14:SER:O	32:Db:18:LYS:HG3	2.20	0.42
34:JD:117:LEU:HA	34:JD:117:LEU:HD23	1.81	0.42
4:UX:102:VAL:HG22	4:UX:137:ALA:HB1	2.00	0.42
7:CL:43:MET:HE2	18:D3:359:A:N6	2.34	0.42
18:D3:72:A:N7	21:DG:169:TYR:OH	2.45	0.42
18:D3:205:U:H2'	18:D3:206:A:H8	1.85	0.42
18:D3:504:U:C2'	18:D3:505:A:H4'	2.48	0.42
18:D3:886:U:O2	27:DO:123:SER:N	2.49	0.42
18:D3:1479:A:H2'	18:D3:1480:G:H8	1.84	0.42
18:D3:1538:U:H2'	18:D3:1539:G:H2'	2.01	0.42
20:DE:86:PHE:CE2	20:DE:184:THR:HG21	2.55	0.42
21:DG:199:GLN:O	21:DG:203:GLU:HG2	2.19	0.42
34:JD:26:ILE:O	34:JD:29:LYS:HG2	2.19	0.42
8:CM:191:ILE:HB	8:CM:223:VAL:HG22	2.02	0.42
18:D3:182:A:H2'	18:D3:183:U:C6	2.55	0.42
18:D3:559:C:H2'	18:D3:560:U:C6	2.54	0.42
18:D3:922:G:H2'	18:D3:923:A:H8	1.85	0.42
18:D3:1152:A:H2'	18:D3:1153:G:C8	2.54	0.42
18:D3:1545:A:N1	18:D3:1567:U:C4	2.88	0.42
18:D3:1619:C:H2'	18:D3:1620:C:C6	2.54	0.42
24:DJ:86:LEU:HD12	24:DJ:87:SER:H	1.84	0.42
26:DN:61:THR:OG1	26:DN:62:GLN:N	2.51	0.42
29:DW:78:ARG:HE	29:DW:126:LEU:HD23	1.85	0.42
2:UC:576:LEU:HG	2:UC:580:ARG:HD3	2.02	0.42
12:JJ:124:LEU:HD12	12:JJ:124:LEU:HA	1.87	0.42
12:JJ:125:LYS:O	12:JJ:146:THR:HG22	2.19	0.42
18:D3:710:U:N3	18:D3:730:G:C5	2.87	0.42
22:DH:126:LEU:HA	22:DH:126:LEU:HD23	1.78	0.42
33:UN:435:ARG:NH1	33:UN:480:LYS:O	2.53	0.42
7:CL:78:PRO:HD3	7:CL:122:ALA:HB1	2.01	0.42
7:CL:879:THR:HB	7:CL:880:TYR:H	1.66	0.42
16:DT:99:SER:N	18:D3:1502:G:O6	2.53	0.42
17:Dc:12:VAL:HA	17:Dc:30:VAL:HA	2.01	0.42
18:D3:1486:G:H2'	18:D3:1487:A:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:1517:U:O2	18:D3:1517:U:O2'	2.32	0.42
18:D3:1583:A:N6	18:D3:1612:U:OP2	2.53	0.42
23:DI:138:ASN:HB3	23:DI:142:LYS:NZ	2.34	0.42
25:DL:2:SER:N	25:DL:82:ARG:HG2	2.34	0.42
25:DL:53:TYR:CD1	25:DL:113:PRO:HG2	2.55	0.42
29:DW:103:ILE:HG22	29:DW:126:LEU:HD12	2.00	0.42
30:DX:107:PHE:CE2	30:DX:109:ARG:HD2	2.55	0.42
34:JD:1093:ALA:HA	34:JD:1121:LEU:H	1.85	0.42
5:CJ:261:LEU:O	5:CJ:274:GLU:N	2.53	0.42
6:CK:332:ALA:HA	6:CK:335:ARG:HG2	2.02	0.42
8:CM:202:PRO:HG3	8:CM:229:VAL:HG11	2.01	0.42
12:JJ:141:THR:OG1	12:JJ:146:THR:HG21	2.20	0.42
18:D3:924:A:H2'	18:D3:925:G:C8	2.55	0.42
21:DG:92:ARG:HE	21:DG:92:ARG:HB2	1.63	0.42
22:DH:34:LEU:HD12	22:DH:34:LEU:HA	1.93	0.42
34:JD:33:ARG:HD3	34:JD:33:ARG:HA	1.77	0.42
2:UC:544:ILE:HD13	2:UC:544:ILE:HG21	1.72	0.41
7:CL:613:PRO:HD3	8:CM:292:ASN:HD22	1.84	0.41
18:D3:739:G:O2'	18:D3:740:A:H5'	2.21	0.41
19:DA:164:ILE:HG23	19:DA:201:THR:HG21	2.02	0.41
8:CM:351:ILE:HD13	8:CM:351:ILE:HA	1.91	0.41
15:DS:46:VAL:HG11	15:DS:73:MET:HE1	2.01	0.41
26:DN:121:ARG:HH11	26:DN:121:ARG:HD2	1.70	0.41
7:CL:142:ILE:HG21	7:CL:142:ILE:HD13	1.84	0.41
11:JL:270:LYS:N	11:JL:275:ASP:OD2	2.53	0.41
18:D3:500:C:C6	18:D3:500:C:C3'	3.03	0.41
18:D3:583:C:H2'	18:D3:584:C:H5''	2.02	0.41
18:D3:861:U:O2'	29:DW:56:HIS:O	2.30	0.41
18:D3:1602:C:H2'	18:D3:1603:U:C6	2.55	0.41
19:DA:152:ARG:H	19:DA:152:ARG:HG2	1.64	0.41
23:DI:137:LYS:NZ	23:DI:141:ARG:HH22	2.19	0.41
31:DY:108:ARG:HH11	31:DY:108:ARG:HD2	1.72	0.41
34:JD:411:ILE:O	34:JD:580:VAL:HA	2.20	0.41
18:D3:280:U:O2'	18:D3:281:G:OP2	2.34	0.41
18:D3:330:G:OP2	23:DI:172:ARG:NH1	2.53	0.41
18:D3:584:C:OP1	18:D3:584:C:H4'	2.20	0.41
18:D3:703:G:H2'	18:D3:704:C:H5'	2.02	0.41
23:DI:165:LEU:HD22	23:DI:183:ILE:HD13	2.02	0.41
24:DJ:107:ARG:HA	24:DJ:107:ARG:HD2	1.69	0.41
24:DJ:150:LEU:HA	24:DJ:150:LEU:HD12	1.85	0.41
11:JL:39:LEU:HD11	11:JL:44:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:325:G:OP1	25:DL:134:THR:OG1	2.36	0.41
20:DE:77:ARG:HD3	20:DE:77:ARG:HA	1.78	0.41
21:DG:193:LEU:HA	21:DG:193:LEU:HD23	1.82	0.41
25:DL:3:THR:OG1	25:DL:113:PRO:HG3	2.20	0.41
7:CL:830:ARG:HG3	7:CL:831:ARG:O	2.20	0.41
12:JJ:169:ASP:N	12:JJ:169:ASP:OD1	2.49	0.41
15:DS:60:GLU:HG3	15:DS:61:LEU:HD12	2.02	0.41
18:D3:483:A:N1	18:D3:505:A:H1'	2.35	0.41
18:D3:793:A:H4'	18:D3:794:U:C5	2.56	0.41
20:DE:127:LYS:HA	20:DE:127:LYS:HD2	1.89	0.41
21:DG:48:TYR:OH	21:DG:119:GLN:O	2.26	0.41
22:DH:75:THR:O	22:DH:78:THR:OG1	2.34	0.41
23:DI:152:ILE:HG13	23:DI:153:GLU:N	2.32	0.41
29:DW:38:LEU:HD23	29:DW:38:LEU:HA	1.80	0.41
34:JD:1252:THR:OG1	34:JD:1253:ARG:N	2.53	0.41
5:CJ:279:ARG:N	18:D3:1596:C:O2	2.44	0.41
7:CL:552:LEU:HB3	7:CL:563:CYS:SG	2.60	0.41
8:CM:18:ARG:HD3	8:CM:98:TYR:CZ	2.55	0.41
15:DS:17:LEU:HD12	15:DS:22:VAL:HB	2.03	0.41
18:D3:788:A:OP2	20:DE:108:ARG:NH1	2.54	0.41
26:DN:99:ARG:O	26:DN:103:GLU:HG2	2.20	0.41
29:DW:14:ILE:HD13	29:DW:14:ILE:HG21	1.86	0.41
4:UX:158:ALA:O	4:UX:162:GLN:HG2	2.20	0.41
7:CL:561:GLU:O	7:CL:565:ARG:HG3	2.20	0.41
7:CL:720:ALA:O	7:CL:724:GLU:HG2	2.19	0.41
8:CM:60:THR:O	8:CM:60:THR:OG1	2.38	0.41
18:D3:143:G:P	21:DG:139:ASN:HD22	2.44	0.41
18:D3:584:C:H5'	18:D3:586:G:H3'	2.03	0.41
18:D3:1057:U:O2	18:D3:1058:U:O2'	2.36	0.41
27:DO:50:ALA:C	27:DO:52:ARG:H	2.28	0.41
4:UX:65:VAL:HG12	4:UX:152:ILE:CG1	2.51	0.41
4:UX:103:MET:HE2	4:UX:103:MET:HB2	1.91	0.41
7:CL:227:ILE:HD13	7:CL:227:ILE:HG21	1.82	0.41
7:CL:237:TRP:CZ2	7:CL:850:GLY:HA2	2.56	0.41
7:CL:631:ILE:HD12	7:CL:631:ILE:HA	1.92	0.41
8:CM:104:LEU:HD22	8:CM:141:MET:SD	2.60	0.41
8:CM:217:LYS:HE3	8:CM:217:LYS:HB3	1.92	0.41
8:CM:298:ILE:HD13	8:CM:298:ILE:HA	1.94	0.41
18:D3:103:A:H8	18:D3:103:A:H2'	1.63	0.41
18:D3:650:U:H2'	18:D3:651:G:C8	2.56	0.41
18:D3:736:C:C6	18:D3:736:C:C3'	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:848:C:H2'	18:D3:849:C:C6	2.55	0.41
18:D3:914:G:H5''	18:D3:914:G:H8	1.86	0.41
18:D3:919:A:H2'	18:D3:920:U:C6	2.56	0.41
20:DE:65:LEU:HD22	20:DE:80:THR:HA	2.02	0.41
21:DG:75:LEU:O	21:DG:94:ARG:HA	2.21	0.41
21:DG:159:ARG:HH21	21:DG:170:THR:HG23	1.86	0.41
21:DG:163:THR:O	21:DG:163:THR:OG1	2.39	0.41
22:DH:98:ILE:HD13	22:DH:118:LEU:HD12	2.02	0.41
29:DW:27:ILE:HD13	29:DW:27:ILE:HG21	1.84	0.41
33:UN:375:LYS:O	33:UN:379:GLU:HG2	2.20	0.41
1:UB:767:ILE:HD13	1:UB:767:ILE:HA	1.90	0.41
7:CL:137:LEU:HD13	7:CL:230:MET:HE1	2.02	0.41
12:JJ:231:ILE:HD13	12:JJ:247:VAL:HG11	2.02	0.41
15:DS:41:ARG:HG3	15:DS:85:PHE:CZ	2.56	0.41
18:D3:829:A:H2	18:D3:830:U:H3	1.67	0.41
27:DO:32:ASP:OD2	27:DO:37:GLU:HB2	2.21	0.41
31:DY:5:VAL:HA	31:DY:28:LEU:O	2.21	0.41
6:CK:335:ARG:NH2	7:CL:957:GLU:OE2	2.48	0.40
6:CK:370:ARG:O	6:CK:374:GLN:CB	2.69	0.40
7:CL:177:PHE:CD2	7:CL:183:LEU:HD12	2.56	0.40
7:CL:632:LYS:HB2	7:CL:632:LYS:HE2	1.84	0.40
8:CM:26:LEU:HD23	8:CM:26:LEU:HA	1.83	0.40
11:JL:131:TYR:CD2	11:JL:156:GLN:HB2	2.56	0.40
18:D3:1570:A:H2'	18:D3:1571:C:O4'	2.21	0.40
18:D3:1615:C:H4'	18:D3:1616:G:H8	1.85	0.40
22:DH:31:SER:O	22:DH:34:LEU:N	2.52	0.40
24:DJ:100:LYS:H	24:DJ:100:LYS:HG2	1.70	0.40
7:CL:89:LEU:HD23	7:CL:89:LEU:HA	1.87	0.40
7:CL:906:ASP:N	7:CL:906:ASP:OD1	2.40	0.40
18:D3:701:U:O5'	18:D3:701:U:H6	2.04	0.40
18:D3:855:A:N1	18:D3:857:U:O2	2.55	0.40
18:D3:1506:G:N1	18:D3:1507:G:C6	2.89	0.40
18:D3:1571:C:H3'	18:D3:1572:G:H21	1.86	0.40
23:DI:136:SER:O	23:DI:139:ALA:N	2.41	0.40
8:CM:103:MET:O	8:CM:107:ALA:HB2	2.21	0.40
18:D3:81:G:C6	18:D3:82:U:C4	3.10	0.40
18:D3:655:G:C6	18:D3:677:G:C6	3.09	0.40
18:D3:1547:A:H2'	18:D3:1548:G:C8	2.56	0.40
19:DA:23:PRO:HA	19:DA:26:ARG:NH1	2.36	0.40
27:DO:95:GLY:O	27:DO:99:GLN:NE2	2.54	0.40
29:DW:24:GLN:NE2	32:Db:6:ASP:HA	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:DX:69:ARG:O	30:DX:93:LEU:HD11	2.21	0.40
31:DY:40:LEU:HA	31:DY:40:LEU:HD23	1.89	0.40
4:UX:90:LEU:HD12	4:UX:94:CYS:SG	2.61	0.40
7:CL:948:ILE:O	7:CL:986:HIS:HA	2.21	0.40
9:JG:176:ARG:O	9:JG:203:CYS:N	2.52	0.40
18:D3:180:A:H2'	18:D3:181:A:O4'	2.21	0.40
18:D3:526:A:OP2	31:DY:93:ARG:NH2	2.54	0.40
18:D3:1799:U:C4	33:UN:389:ARG:HD3	2.56	0.40
19:DA:179:SER:HB2	19:DA:183:GLN:HB2	2.03	0.40
29:DW:25:VAL:O	29:DW:62:VAL:HA	2.21	0.40
1:UB:734:ARG:HH12	18:D3:1173:C:P	2.44	0.40
15:DS:24:GLY:O	15:DS:58:ALA:N	2.55	0.40
18:D3:182:A:H2'	18:D3:183:U:H6	1.86	0.40
18:D3:369:A:H2'	18:D3:371:G:OP2	2.21	0.40
18:D3:683:C:H2'	18:D3:684:A:C8	2.51	0.40
19:DA:140:ILE:HB	19:DA:213:ARG:HD2	2.04	0.40
20:DE:11:ARG:HE	20:DE:11:ARG:HB2	1.75	0.40
31:DY:55:VAL:HG22	31:DY:75:VAL:HG23	2.02	0.40
33:UN:460:THR:O	33:UN:460:THR:OG1	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	UB	391/810 (48%)	372 (95%)	14 (4%)	5 (1%)	9	39
2	UC	45/610 (7%)	40 (89%)	5 (11%)	0	100	100
3	US	474/552 (86%)	463 (98%)	11 (2%)	0	100	100
4	UX	141/189 (75%)	124 (88%)	17 (12%)	0	100	100
5	CJ	217/290 (75%)	195 (90%)	22 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	CK	90/593 (15%)	83 (92%)	7 (8%)	0	100	100
7	CL	698/1183 (59%)	633 (91%)	64 (9%)	1 (0%)	48	79
8	CM	358/367 (98%)	326 (91%)	32 (9%)	0	100	100
9	JF	212/252 (84%)	211 (100%)	1 (0%)	0	100	100
9	JG	217/252 (86%)	209 (96%)	8 (4%)	0	100	100
10	JH	257/483 (53%)	252 (98%)	5 (2%)	0	100	100
11	JL	281/318 (88%)	260 (92%)	21 (8%)	0	100	100
12	JJ	179/274 (65%)	167 (93%)	12 (7%)	0	100	100
13	DF	194/225 (86%)	185 (95%)	9 (5%)	0	100	100
14	DQ	123/143 (86%)	114 (93%)	9 (7%)	0	100	100
15	DS	75/147 (51%)	67 (89%)	8 (11%)	0	100	100
16	DT	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
17	Dc	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
19	DA	212/255 (83%)	170 (80%)	40 (19%)	2 (1%)	14	47
20	DE	258/261 (99%)	229 (89%)	29 (11%)	0	100	100
21	DG	224/236 (95%)	202 (90%)	19 (8%)	3 (1%)	9	39
22	DH	182/190 (96%)	158 (87%)	23 (13%)	1 (0%)	24	57
23	DI	184/200 (92%)	154 (84%)	30 (16%)	0	100	100
24	DJ	183/197 (93%)	163 (89%)	19 (10%)	1 (0%)	24	57
25	DL	141/156 (90%)	125 (89%)	16 (11%)	0	100	100
26	DN	148/151 (98%)	129 (87%)	18 (12%)	1 (1%)	18	51
27	DO	125/137 (91%)	102 (82%)	23 (18%)	0	100	100
28	DZ	65/108 (60%)	51 (78%)	14 (22%)	0	100	100
29	DW	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
30	DX	141/145 (97%)	123 (87%)	18 (13%)	0	100	100
31	DY	131/135 (97%)	120 (92%)	11 (8%)	0	100	100
32	Db	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
33	UN	104/899 (12%)	100 (96%)	4 (4%)	0	100	100
34	JD	815/1267 (64%)	743 (91%)	72 (9%)	0	100	100
All	All	7273/11448 (64%)	6654 (92%)	605 (8%)	14 (0%)	44	74

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	UB	698	ILE
1	UB	699	PRO
1	UB	706	LYS
19	DA	213	ARG
21	DG	173	PRO
7	CL	208	SER
22	DH	155	ASP
26	DN	28	LEU
1	UB	702	LEU
1	UB	707	PRO
21	DG	174	LYS
24	DJ	98	ALA
21	DG	21	GLU
19	DA	221	PRO

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	
1	UB	52/732 (7%)	52 (100%)	0	100	100
2	UC	42/538 (8%)	42 (100%)	0	100	100
4	UX	126/169 (75%)	126 (100%)	0	100	100
6	CK	51/535 (10%)	51 (100%)	0	100	100
7	CL	624/1039 (60%)	620 (99%)	4 (1%)	78	79
8	CM	307/312 (98%)	307 (100%)	0	100	100
11	JL	255/283 (90%)	253 (99%)	2 (1%)	73	77
12	JJ	158/238 (66%)	158 (100%)	0	100	100
15	DS	69/110 (63%)	68 (99%)	1 (1%)	59	71
19	DA	191/224 (85%)	191 (100%)	0	100	100
20	DE	221/222 (100%)	221 (100%)	0	100	100
21	DG	188/201 (94%)	188 (100%)	0	100	100
22	DH	165/170 (97%)	165 (100%)	0	100	100
23	DI	150/161 (93%)	150 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	DJ	158/166 (95%)	158 (100%)	0	100	100
25	DL	129/137 (94%)	129 (100%)	0	100	100
26	DN	127/128 (99%)	127 (100%)	0	100	100
27	DO	96/105 (91%)	96 (100%)	0	100	100
29	DW	110/111 (99%)	110 (100%)	0	100	100
30	DX	118/120 (98%)	118 (100%)	0	100	100
31	DY	111/113 (98%)	111 (100%)	0	100	100
32	Db	70/71 (99%)	70 (100%)	0	100	100
33	UN	98/808 (12%)	98 (100%)	0	100	100
34	JD	133/1140 (12%)	133 (100%)	0	100	100
All	All	3749/7833 (48%)	3742 (100%)	7 (0%)	85	85

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	CL	174	LEU
7	CL	176	LEU
7	CL	548	ASN
7	CL	943	LYS
11	JL	164	LEU
11	JL	166	ARG
15	DS	71	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
2	UC	573	GLN
7	CL	761	GLN
7	CL	855	GLN
8	CM	15	GLN
11	JL	194	ASN
11	JL	300	GLN
19	DA	95	ASN
19	DA	194	ASN
19	DA	199	ASN
19	DA	209	ASN
19	DA	232	HIS

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Mol	Chain	Res	Type
20	DE	36	HIS
20	DE	50	ASN
20	DE	188	ASN
20	DE	258	GLN
21	DG	139	ASN
23	DI	32	GLN
23	DI	94	ASN
29	DW	24	GLN
33	UN	444	HIS
33	UN	475	GLN
34	JD	28	ASN
34	JD	1241	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	D3	1380/1758 (78%)	492 (35%)	34 (2%)
35	D4	21/23 (91%)	7 (33%)	0
36	D5	8/9 (88%)	6 (75%)	1 (12%)
All	All	1409/1790 (78%)	505 (35%)	35 (2%)

All (505) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	D3	2	A
18	D3	9	U
18	D3	10	G
18	D3	12	U
18	D3	15	U
18	D3	24	U
18	D3	25	C
18	D3	26	A
18	D3	34	G
18	D3	40	A
18	D3	46	A
18	D3	47	A
18	D3	57	G
18	D3	60	U
18	D3	61	A
18	D3	63	G
18	D3	68	A

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Mol	Chain	Res	Type
18	D3	71	A
18	D3	72	A
18	D3	73	U
18	D3	74	U
18	D3	75	U
18	D3	77	U
18	D3	84	A
18	D3	102	U
18	D3	103	A
18	D3	104	A
18	D3	105	A
18	D3	109	G
18	D3	114	C
18	D3	115	G
18	D3	116	U
18	D3	127	G
18	D3	130	C
18	D3	131	C
18	D3	132	U
18	D3	133	U
18	D3	134	U
18	D3	135	A
18	D3	136	C
18	D3	137	U
18	D3	140	A
18	D3	141	U
18	D3	144	U
18	D3	145	A
18	D3	146	U
18	D3	153	G
18	D3	156	A
18	D3	159	U
18	D3	161	U
18	D3	178	U
18	D3	179	A
18	D3	181	A
18	D3	184	C
18	D3	188	A
18	D3	190	C
18	D3	191	C
18	D3	192	U
18	D3	196	G

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Mol	Chain	Res	Type
18	D3	197	A
18	D3	199	G
18	D3	200	A
18	D3	203	U
18	D3	204	G
18	D3	216	U
18	D3	219	A
18	D3	220	A
18	D3	226	A
18	D3	227	U
18	D3	228	G
18	D3	231	U
18	D3	232	U
18	D3	233	C
18	D3	234	G
18	D3	235	G
18	D3	237	C
18	D3	238	U
18	D3	239	C
18	D3	240	U
18	D3	241	U
18	D3	246	G
18	D3	250	C
18	D3	260	U
18	D3	261	U
18	D3	265	A
18	D3	271	A
18	D3	272	U
18	D3	274	G
18	D3	275	C
18	D3	276	C
18	D3	277	U
18	D3	278	U
18	D3	280	U
18	D3	281	G
18	D3	287	G
18	D3	290	G
18	D3	305	C
18	D3	309	C
18	D3	313	U
18	D3	314	C
18	D3	316	A

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Mol	Chain	Res	Type
18	D3	322	G
18	D3	337	G
18	D3	338	C
18	D3	339	C
18	D3	352	A
18	D3	359	A
18	D3	360	A
18	D3	361	C
18	D3	362	G
18	D3	365	G
18	D3	370	A
18	D3	381	C
18	D3	387	A
18	D3	388	G
18	D3	390	G
18	D3	392	G
18	D3	399	A
18	D3	400	A
18	D3	401	A
18	D3	402	C
18	D3	404	G
18	D3	409	C
18	D3	416	A
18	D3	417	A
18	D3	418	G
18	D3	424	C
18	D3	426	G
18	D3	428	A
18	D3	433	C
18	D3	434	G
18	D3	436	A
18	D3	438	A
18	D3	439	U
18	D3	441	A
18	D3	444	C
18	D3	445	A
18	D3	453	U
18	D3	454	U
18	D3	455	C
18	D3	456	A
18	D3	459	G
18	D3	464	A

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Mol	Chain	Res	Type
18	D3	467	G
18	D3	468	A
18	D3	469	C
18	D3	473	A
18	D3	475	A
18	D3	477	A
18	D3	482	U
18	D3	485	A
18	D3	486	G
18	D3	487	G
18	D3	488	G
18	D3	493	U
18	D3	495	C
18	D3	496	G
18	D3	497	G
18	D3	498	G
18	D3	499	U
18	D3	501	U
18	D3	502	U
18	D3	503	G
18	D3	504	U
18	D3	505	A
18	D3	506	A
18	D3	507	U
18	D3	510	G
18	D3	511	A
18	D3	519	C
18	D3	520	A
18	D3	527	A
18	D3	534	A
18	D3	538	A
18	D3	539	G
18	D3	541	A
18	D3	542	A
18	D3	545	A
18	D3	550	A
18	D3	553	G
18	D3	555	A
18	D3	557	G
18	D3	563	U
18	D3	564	G
18	D3	565	C

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Mol	Chain	Res	Type
18	D3	566	C
18	D3	570	A
18	D3	572	C
18	D3	573	C
18	D3	576	G
18	D3	579	A
18	D3	580	A
18	D3	582	U
18	D3	583	C
18	D3	584	C
18	D3	585	A
18	D3	586	G
18	D3	588	U
18	D3	589	C
18	D3	594	A
18	D3	595	G
18	D3	601	A
18	D3	602	U
18	D3	610	G
18	D3	611	U
18	D3	613	G
18	D3	620	A
18	D3	622	A
18	D3	623	A
18	D3	624	G
18	D3	639	U
18	D3	640	U
18	D3	647	G
18	D3	648	G
18	D3	650	U
18	D3	651	G
18	D3	652	G
18	D3	653	C
18	D3	654	C
18	D3	655	G
18	D3	656	G
18	D3	658	C
18	D3	677	G
18	D3	679	U
18	D3	681	U
18	D3	687	G
18	D3	694	U

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Mol	Chain	Res	Type
18	D3	696	C
18	D3	697	C
18	D3	698	U
18	D3	699	U
18	D3	700	C
18	D3	702	G
18	D3	703	G
18	D3	705	U
18	D3	706	A
18	D3	707	A
18	D3	708	C
18	D3	709	C
18	D3	710	U
18	D3	712	G
18	D3	715	U
18	D3	717	C
18	D3	718	U
18	D3	719	U
18	D3	720	G
18	D3	721	U
18	D3	722	G
18	D3	725	U
18	D3	726	C
18	D3	727	U
18	D3	728	U
18	D3	729	G
18	D3	730	G
18	D3	731	C
18	D3	732	G
18	D3	734	A
18	D3	735	C
18	D3	736	C
18	D3	737	A
18	D3	738	G
18	D3	740	A
18	D3	741	C
18	D3	742	U
18	D3	743	U
18	D3	745	U
18	D3	749	U
18	D3	765	G
18	D3	766	U

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Mol	Chain	Res	Type
18	D3	767	U
18	D3	771	A
18	D3	772	G
18	D3	774	A
18	D3	775	G
18	D3	778	G
18	D3	780	A
18	D3	781	U
18	D3	782	U
18	D3	783	G
18	D3	784	C
18	D3	789	A
18	D3	793	A
18	D3	794	U
18	D3	795	U
18	D3	800	U
18	D3	810	G
18	D3	811	A
18	D3	812	A
18	D3	813	U
18	D3	814	A
18	D3	815	G
18	D3	816	G
18	D3	818	C
18	D3	819	G
18	D3	820	U
18	D3	821	U
18	D3	822	U
18	D3	823	G
18	D3	824	G
18	D3	826	U
18	D3	827	C
18	D3	829	A
18	D3	830	U
18	D3	831	U
18	D3	832	U
18	D3	833	U
18	D3	834	G
18	D3	838	G
18	D3	839	U
18	D3	841	U
18	D3	844	A

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Mol	Chain	Res	Type
18	D3	845	G
18	D3	848	C
18	D3	850	A
18	D3	851	U
18	D3	852	C
18	D3	854	U
18	D3	861	U
18	D3	862	A
18	D3	863	A
18	D3	873	U
18	D3	881	A
18	D3	886	U
18	D3	898	A
18	D3	904	G
18	D3	913	G
18	D3	914	G
18	D3	915	A
18	D3	928	U
18	D3	932	U
18	D3	933	A
18	D3	934	C
18	D3	935	U
18	D3	940	A
18	D3	942	G
18	D3	944	A
18	D3	945	U
18	D3	960	U
18	D3	966	A
18	D3	990	C
18	D3	992	A
18	D3	993	A
18	D3	999	U
18	D3	1000	C
18	D3	1001	A
18	D3	1002	G
18	D3	1006	C
18	D3	1007	C
18	D3	1010	C
18	D3	1011	G
18	D3	1024	U
18	D3	1026	A
18	D3	1028	C

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Mol	Chain	Res	Type
18	D3	1029	U
18	D3	1030	A
18	D3	1031	U
18	D3	1040	G
18	D3	1052	U
18	D3	1053	G
18	D3	1055	U
18	D3	1057	U
18	D3	1058	U
18	D3	1059	U
18	D3	1060	U
18	D3	1066	C
18	D3	1081	A
18	D3	1086	A
18	D3	1091	A
18	D3	1092	A
18	D3	1096	C
18	D3	1097	U
18	D3	1098	U
18	D3	1099	U
18	D3	1100	G
18	D3	1101	G
18	D3	1109	G
18	D3	1110	G
18	D3	1114	G
18	D3	1115	U
18	D3	1116	A
18	D3	1118	G
18	D3	1119	G
18	D3	1122	G
18	D3	1124	A
18	D3	1129	U
18	D3	1130	A
18	D3	1131	A
18	D3	1149	G
18	D3	1154	G
18	D3	1158	C
18	D3	1159	C
18	D3	1160	A
18	D3	1164	G
18	D3	1167	G
18	D3	1170	G

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Mol	Chain	Res	Type
18	D3	1172	G
18	D3	1177	C
18	D3	1178	G
18	D3	1180	C
18	D3	1181	U
18	D3	1182	U
18	D3	1183	A
18	D3	1460	A
18	D3	1462	G
18	D3	1469	A
18	D3	1471	A
18	D3	1474	G
18	D3	1478	G
18	D3	1480	G
18	D3	1481	C
18	D3	1482	C
18	D3	1486	G
18	D3	1488	G
18	D3	1490	C
18	D3	1492	A
18	D3	1493	A
18	D3	1494	C
18	D3	1496	U
18	D3	1499	G
18	D3	1503	A
18	D3	1507	G
18	D3	1508	U
18	D3	1510	U
18	D3	1512	G
18	D3	1516	A
18	D3	1517	U
18	D3	1520	U
18	D3	1523	G
18	D3	1524	A
18	D3	1532	U
18	D3	1534	G
18	D3	1535	U
18	D3	1536	G
18	D3	1537	C
18	D3	1538	U
18	D3	1539	G
18	D3	1542	G

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Mol	Chain	Res	Type
18	D3	1544	U
18	D3	1546	G
18	D3	1550	A
18	D3	1553	G
18	D3	1557	U
18	D3	1558	U
18	D3	1559	A
18	D3	1561	U
18	D3	1568	C
18	D3	1569	A
18	D3	1573	A
18	D3	1574	G
18	D3	1577	A
18	D3	1578	U
18	D3	1579	U
18	D3	1580	C
18	D3	1582	U
18	D3	1583	A
18	D3	1584	G
18	D3	1590	G
18	D3	1595	U
18	D3	1599	C
18	D3	1600	A
18	D3	1601	G
18	D3	1602	C
18	D3	1607	G
18	D3	1613	U
18	D3	1615	C
18	D3	1619	C
18	D3	1621	U
18	D3	1622	G
18	D3	1626	U
18	D3	1628	U
18	D3	1629	G
18	D3	1630	U
18	D3	1633	A
18	D3	1638	G
18	D3	1639	C
18	D3	1642	G
18	D3	1645	G
18	D3	1649	G
18	D3	1750	A

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Mol	Chain	Res	Type
18	D3	1751	C
18	D3	1777	G
18	D3	1780	G
18	D3	1781	A
18	D3	1782	A
18	D3	1783	C
18	D3	1792	G
18	D3	1794	A
18	D3	1796	C
18	D3	1801	A
18	D3	1802	A
18	D3	1803	G
18	D3	1804	A
35	D4	2	U
35	D4	6	C
35	D4	8	U
35	D4	14	A
35	D4	15	U
35	D4	16	A
35	D4	18	G
36	D5	4	U
36	D5	5	U
36	D5	6	U
36	D5	8	U
36	D5	9	U
36	D5	10	U

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	D3	24	U
18	D3	73	U
18	D3	103	A
18	D3	114	C
18	D3	130	C
18	D3	132	U
18	D3	135	A
18	D3	139	C
18	D3	196	G
18	D3	199	G
18	D3	218	A
18	D3	280	U

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Mol	Chain	Res	Type
18	D3	417	A
18	D3	433	C
18	D3	485	A
18	D3	498	G
18	D3	503	G
18	D3	510	G
18	D3	579	A
18	D3	695	U
18	D3	721	U
18	D3	736	C
18	D3	829	A
18	D3	834	G
18	D3	913	G
18	D3	1109	G
18	D3	1115	U
18	D3	1481	C
18	D3	1535	U
18	D3	1568	C
18	D3	1573	A
18	D3	1600	A
18	D3	1800	A
18	D3	1802	A
36	D5	5	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 40 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
38	GTP	CL	2001	39	33,34,34	1.16	3 (9%)	50,54,54	1.74	7 (14%)

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
38	GTP	CL	2001	39	-	3/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	CL	2001	GTP	C5-C4	3.10	1.47	1.38
38	CL	2001	GTP	C6-N1	-2.56	1.34	1.38
38	CL	2001	GTP	C5-N7	-2.14	1.34	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	CL	2001	GTP	C5-C4-N3	-6.22	118.49	128.39
38	CL	2001	GTP	C2-N3-C4	5.05	121.00	112.30
38	CL	2001	GTP	N9-C4-N3	4.63	135.20	125.95
38	CL	2001	GTP	C6-C5-N7	3.17	136.06	130.29
38	CL	2001	GTP	C4-C5-N7	-2.52	106.67	110.67
38	CL	2001	GTP	C3'-C2'-C1'	2.18	105.58	101.46
38	CL	2001	GTP	O6-C6-C5	-2.13	120.92	126.53

There are no chirality outliers.

All (3) torsion outliers are listed below:

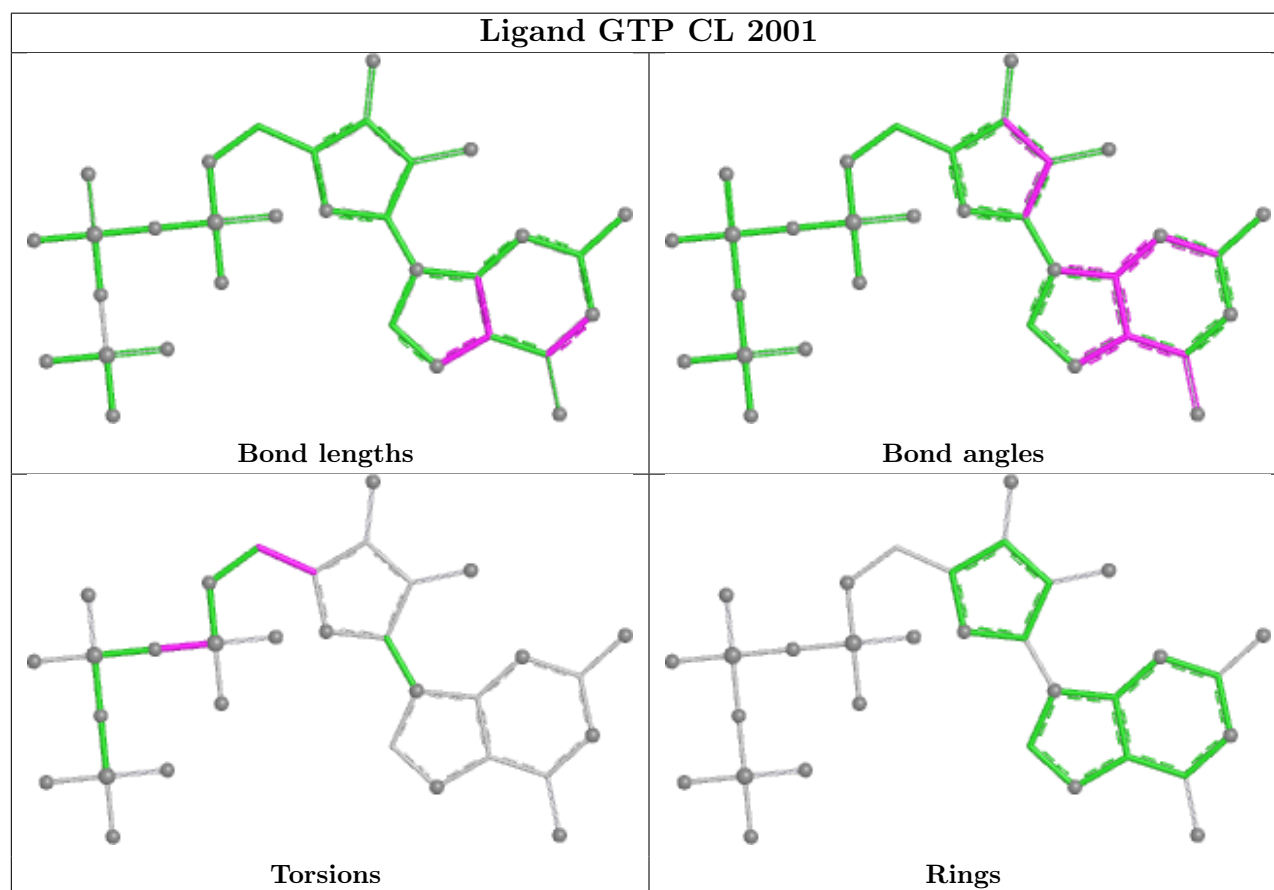
Mol	Chain	Res	Type	Atoms
38	CL	2001	GTP	O4'-C4'-C5'-O5'
38	CL	2001	GTP	C3'-C4'-C5'-O5'
38	CL	2001	GTP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	CL	2001	GTP	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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

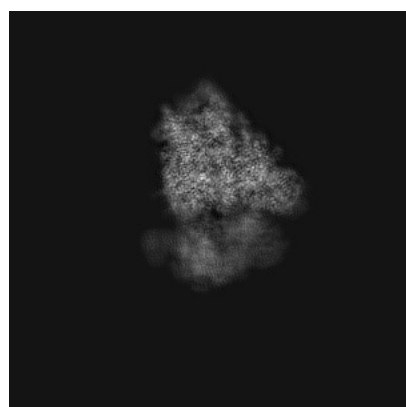
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11363. These allow visual inspection of the internal detail of the map and identification of artifacts.

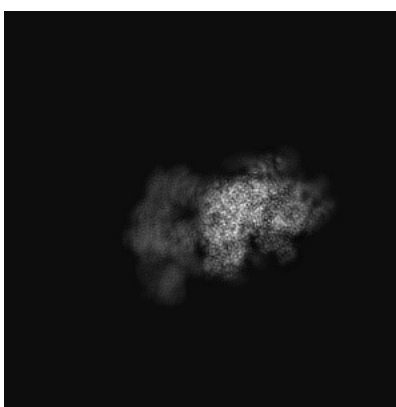
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

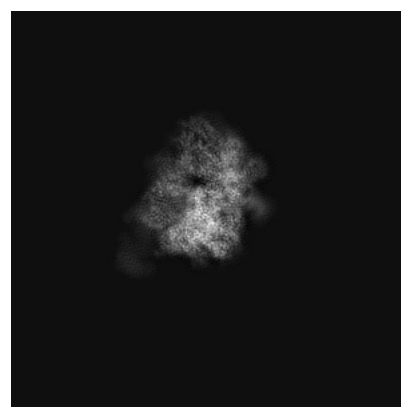
6.1.1 Primary map



X



Y

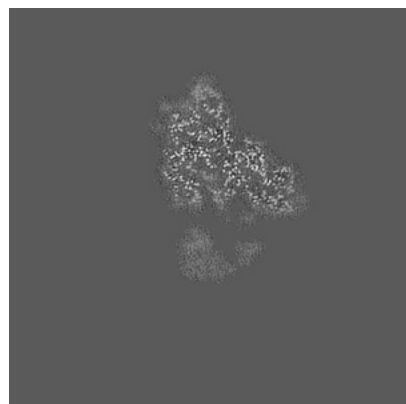


Z

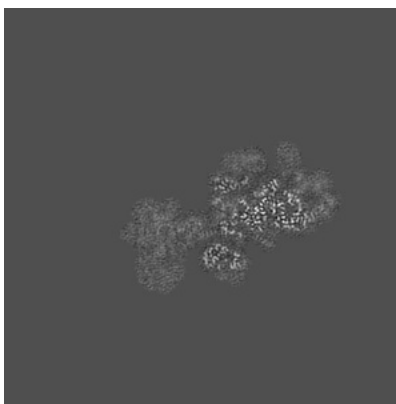
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

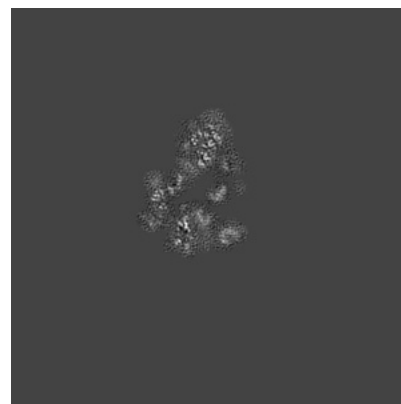
6.2.1 Primary map



X Index: 240



Y Index: 240

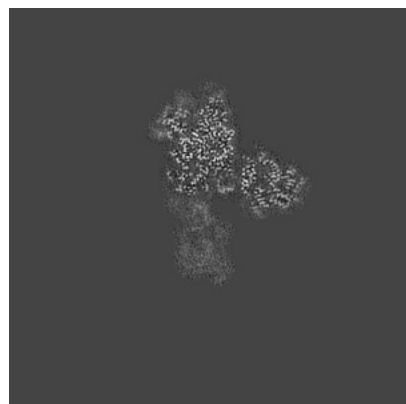


Z Index: 240

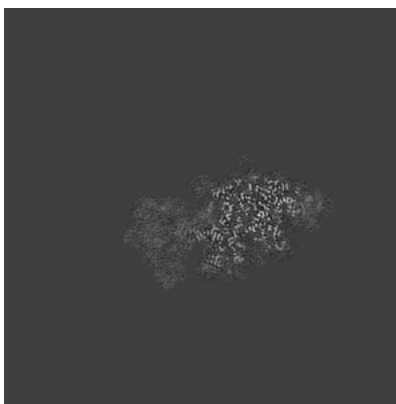
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

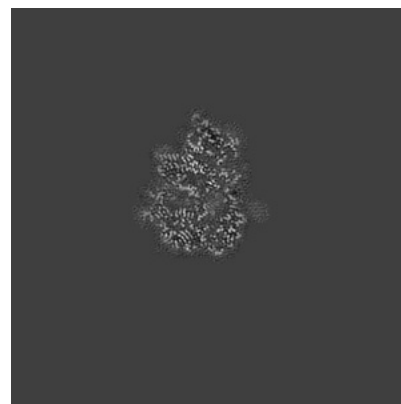
6.3.1 Primary map



X Index: 226



Y Index: 219

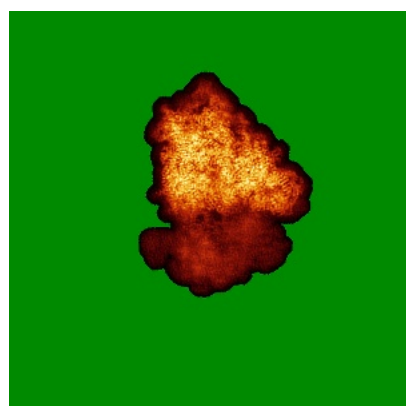


Z Index: 278

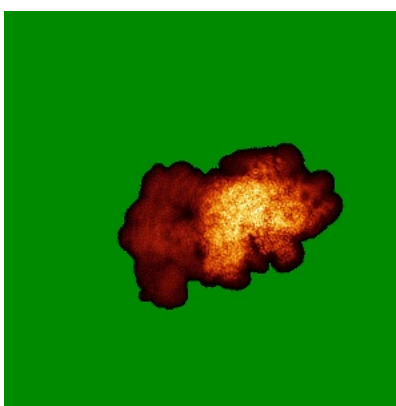
The images above show the largest variance slices of the map in three orthogonal directions.

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

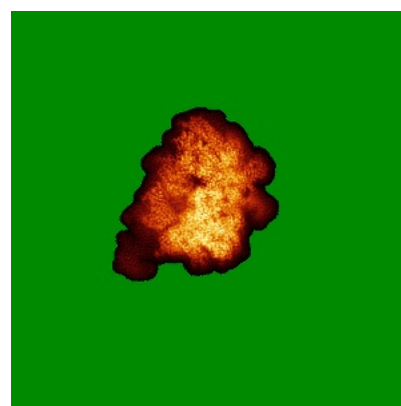
6.4.1 Primary map



X



Y



Z

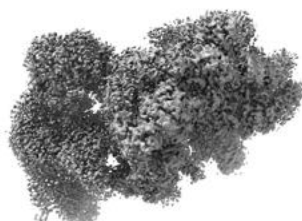
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

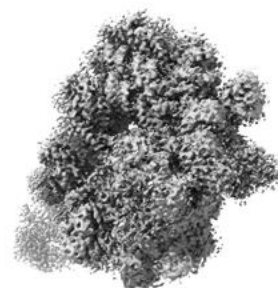
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

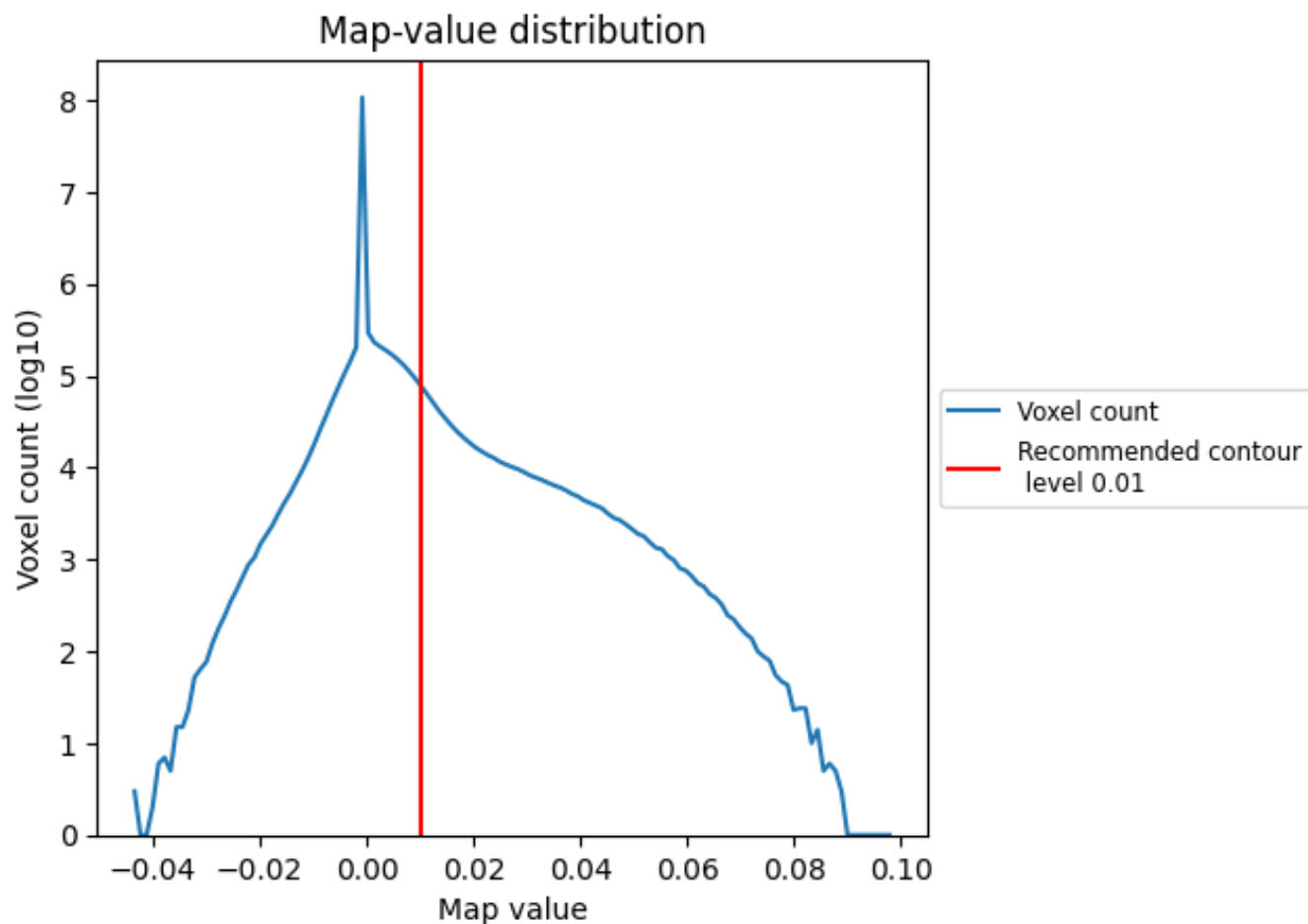
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

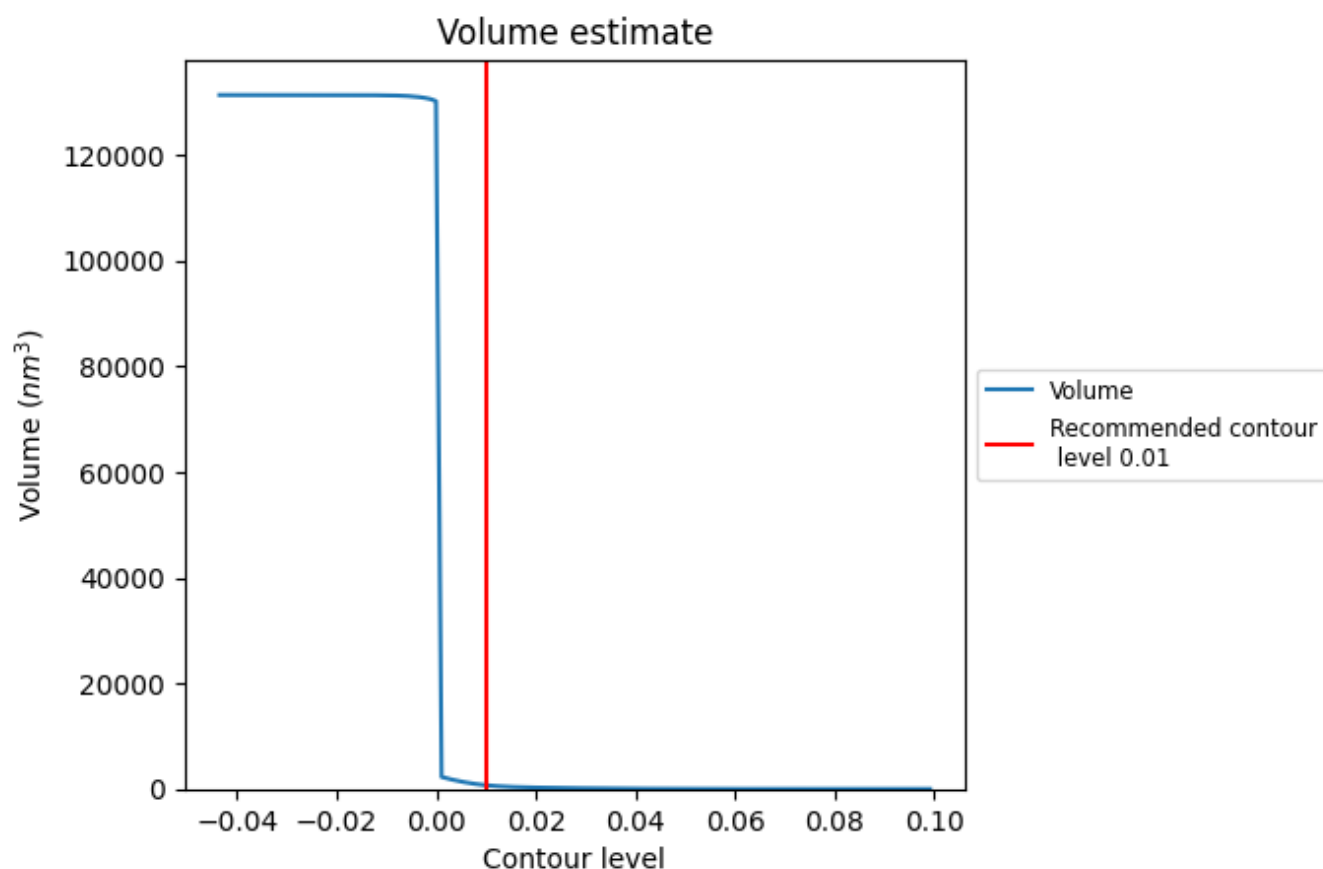
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

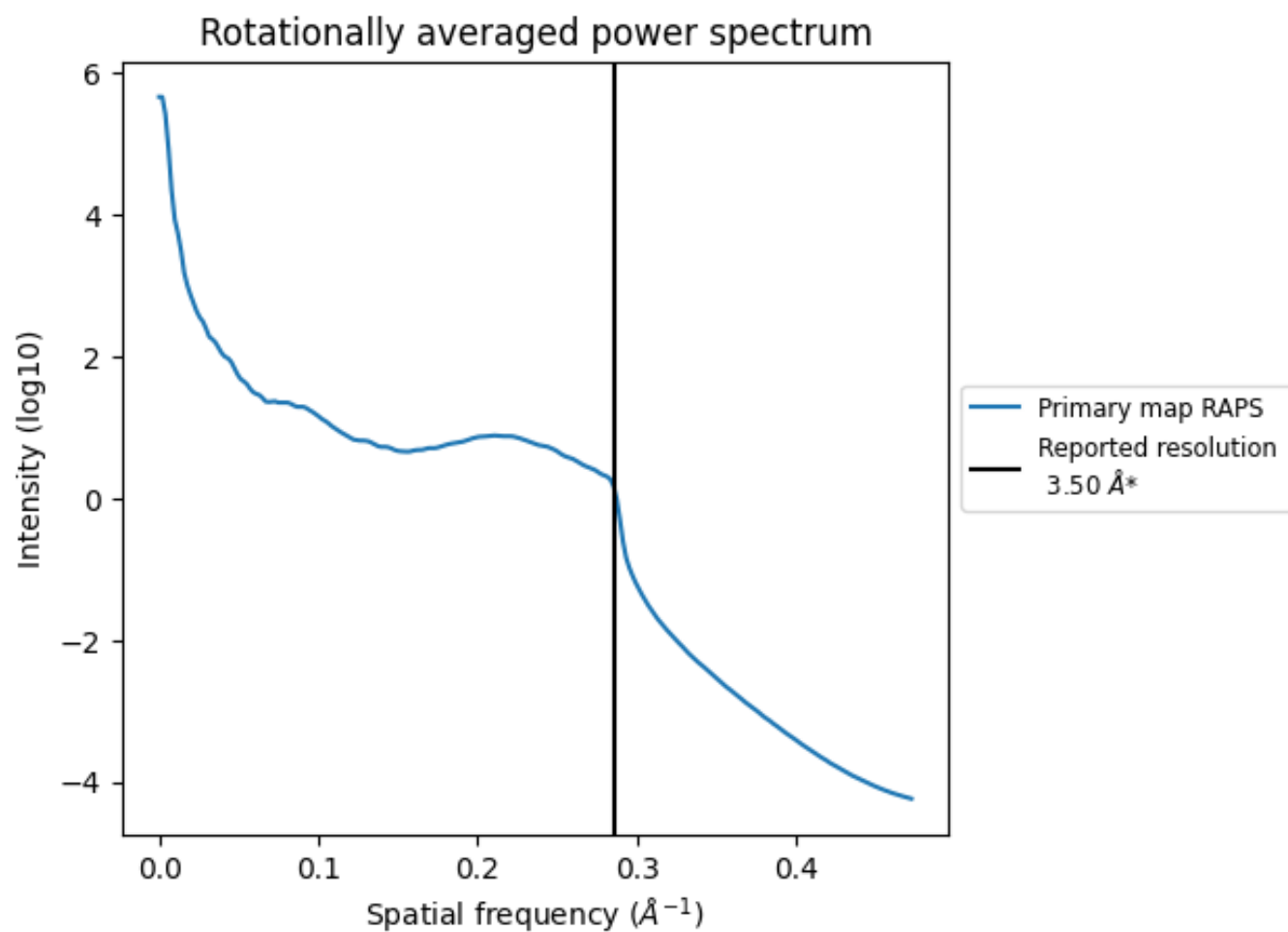
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 707 nm^3 ; this corresponds to an approximate mass of 638 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 ⓘ

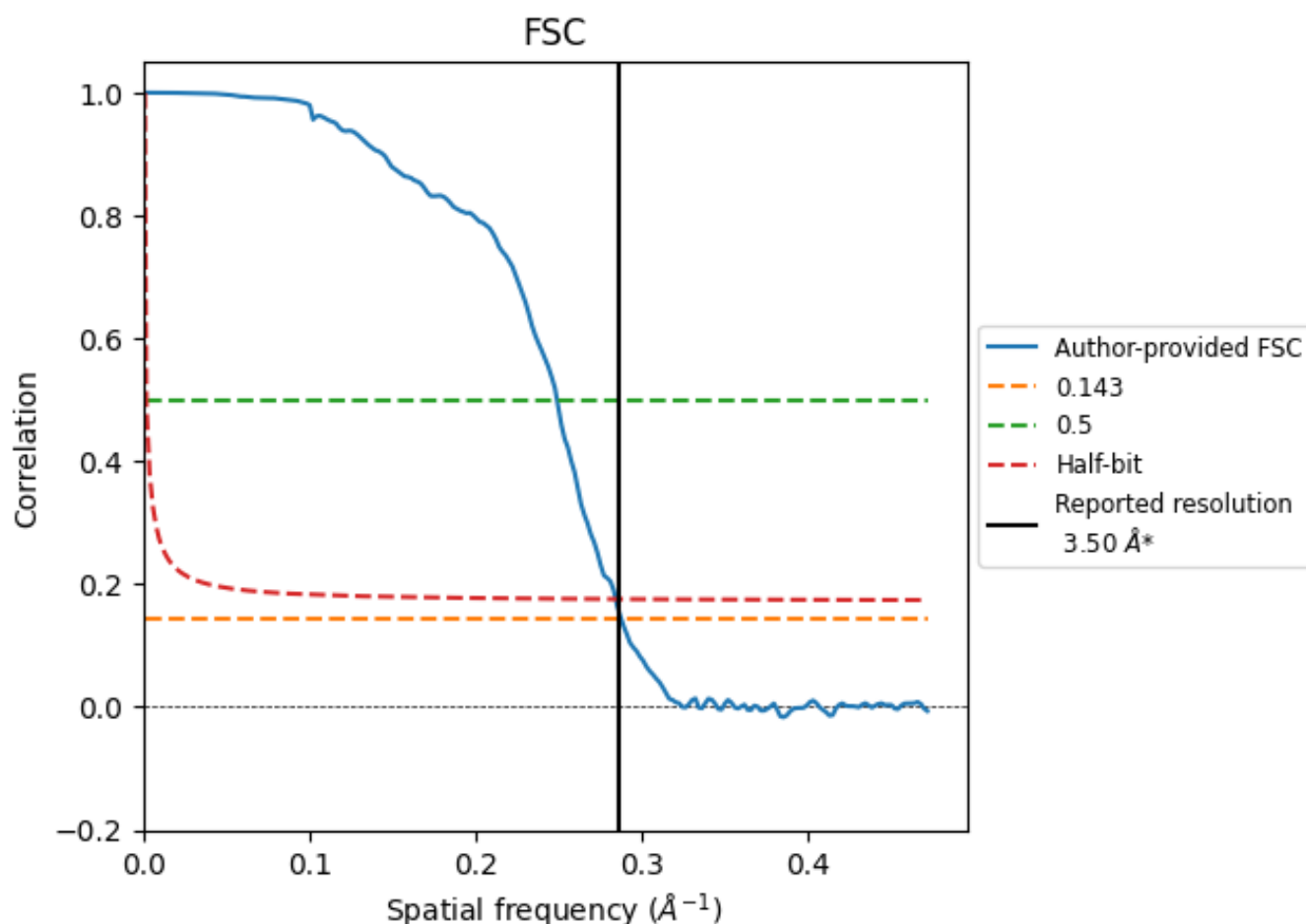


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

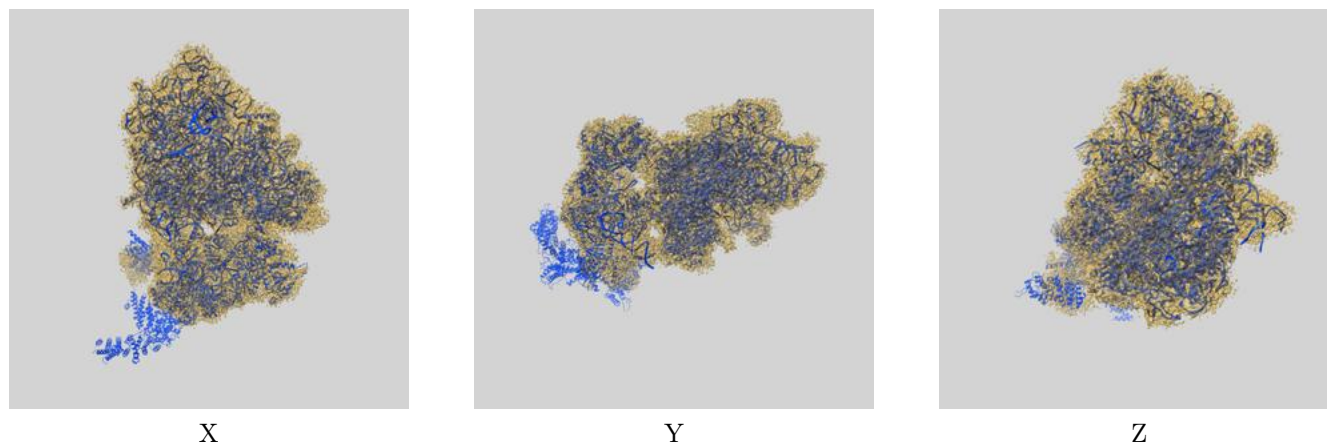
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.47	4.01	3.52
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

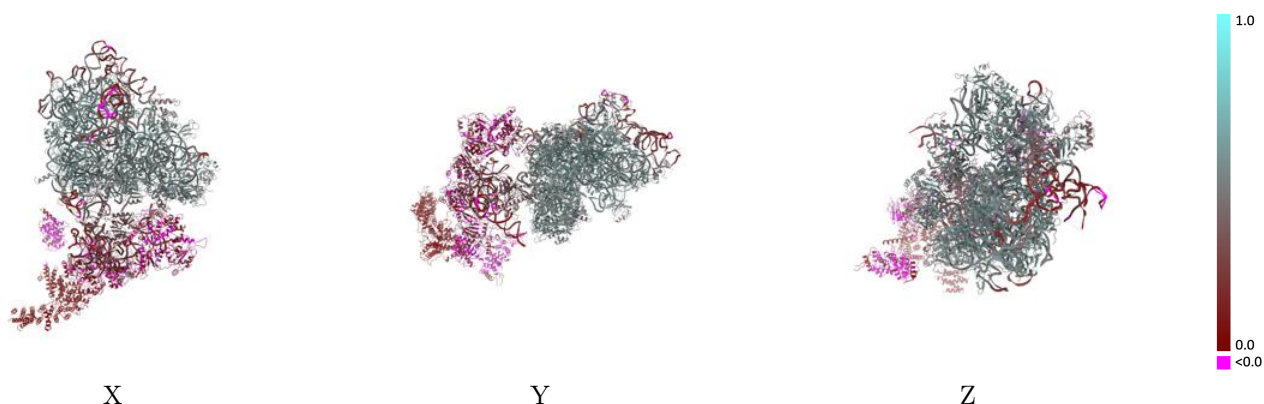
This section contains information regarding the fit between EMDB map EMD-11363 and PDB model 6ZQG. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



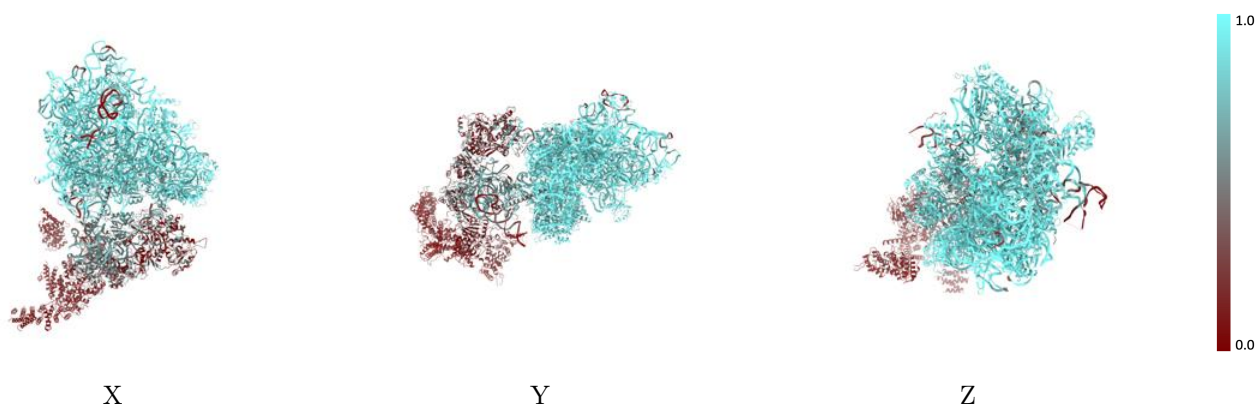
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



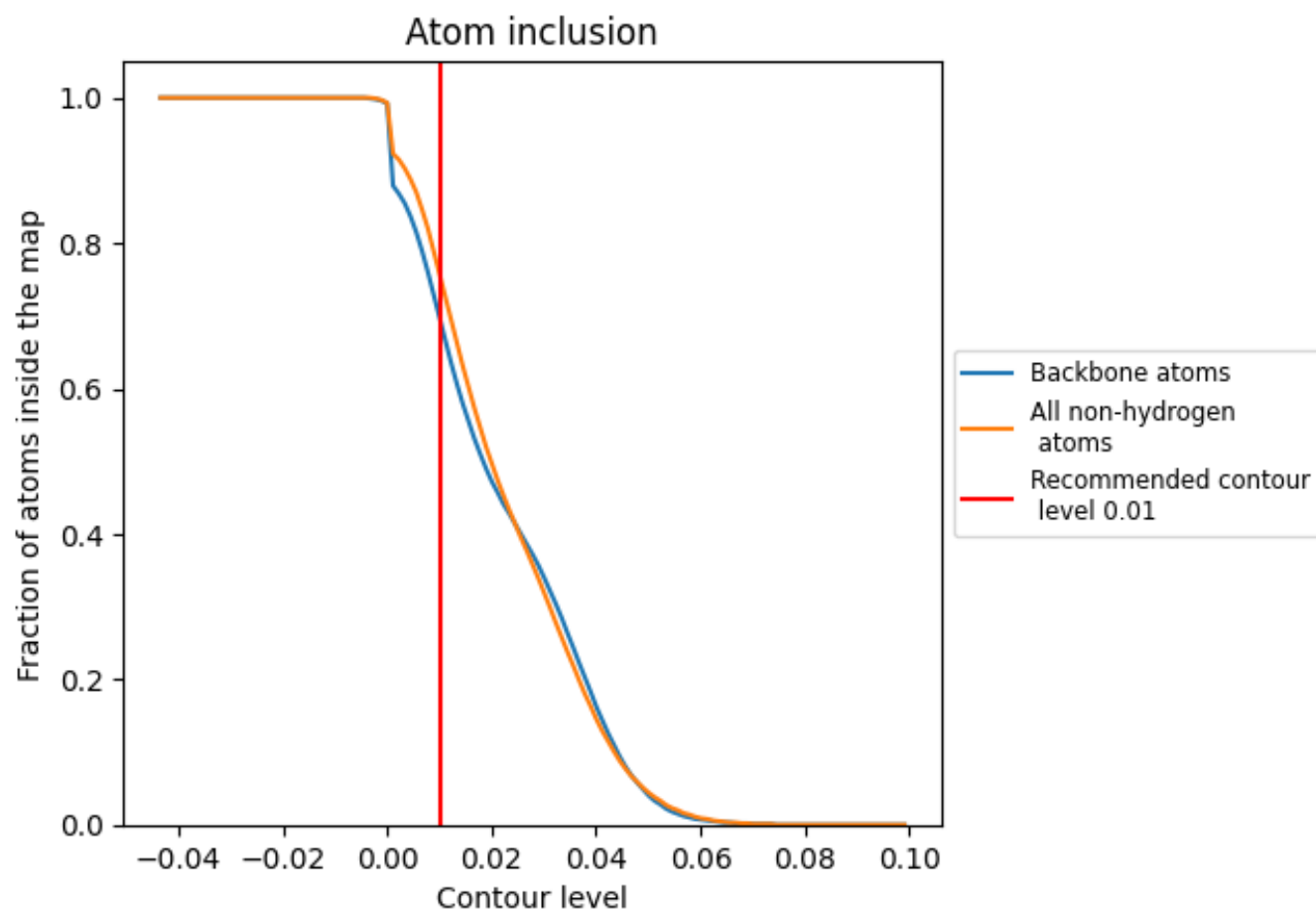
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7580	 0.4050
CJ	 0.6030	 0.3060
CK	 0.7460	 0.4080
CL	 0.9180	 0.5250
CM	 0.9410	 0.5440
D3	 0.8660	 0.4250
D4	 0.9800	 0.4900
D5	 0.3830	 0.2000
DA	 0.9430	 0.5380
DE	 0.9620	 0.5680
DF	 0.4190	 0.1550
DG	 0.9430	 0.5120
DH	 0.9130	 0.4860
DI	 0.9580	 0.5480
DJ	 0.9440	 0.5550
DL	 0.9310	 0.5520
DN	 0.9570	 0.5520
DO	 0.9590	 0.5380
DQ	 0.3510	 0.1660
DS	 0.3250	 0.1450
DT	 0.4190	 0.1510
DW	 0.9680	 0.5730
DX	 0.9030	 0.5490
DY	 0.9440	 0.5520
DZ	 0.2620	 0.1620
Db	 0.9300	 0.5260
Dc	 0.3160	 0.1410
JD	 0.4490	 0.2300
JF	 0.0740	 0.0360
JG	 0.1510	 0.1140
JH	 0.0460	 -0.0270
JJ	 0.9160	 0.5250
JL	 0.9140	 0.5300
UB	 0.0760	 0.0720
UC	 0.9130	 0.5480



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Chain	Atom inclusion	Q-score
UN	 0.8740	 0.5350
US	 0.0000	 -0.0000
UX	 0.9100	 0.5380