



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:18 AM UTC

PDB ID : 6RBE / pdb_00006rbe
EMDB ID : EMD-4793
Title : State 2 of yeast Tsr1-TAP Rps20-Deltaloop pre-40S particles
Authors : Shayan, R.; Mitterer, V.; Ferreira-Cerca, S.; Murat, G.; Enne, T.; Rinaldi, D.; Weigl, S.; Omanic, H.; Gleizes, P.E.; Kressler, D.; Pertschy, B.; Plisson-Chastang, C.
Deposited on : 2019-04-10
Resolution : 3.80 Å (reported)
Based on initial models : ?, 4V88

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:

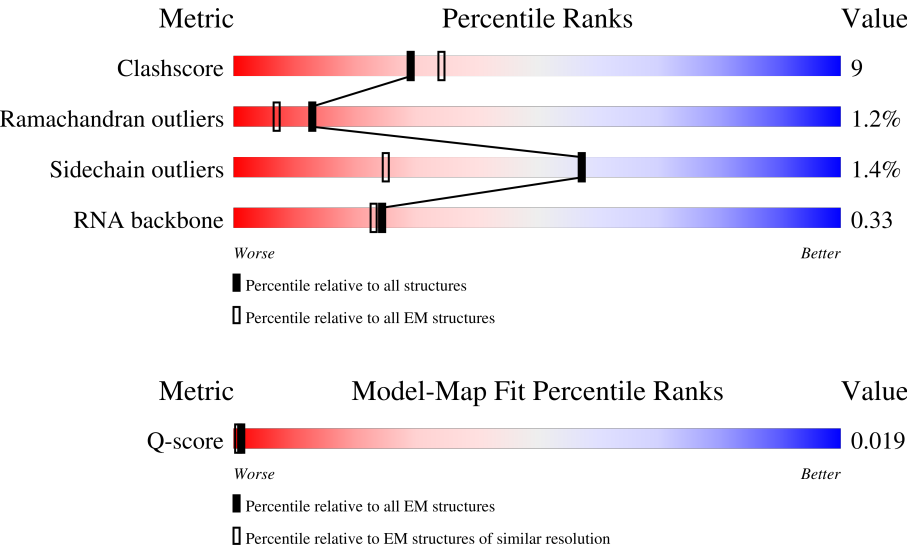
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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	13733 (2.97 - 3.97)

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	2	1800	
2	A	252	
3	B	255	

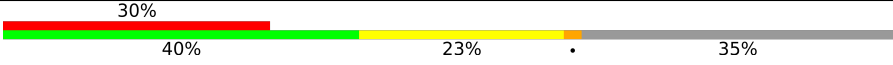
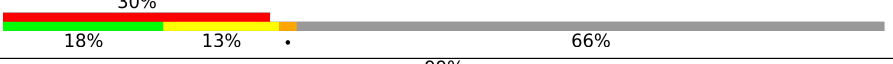
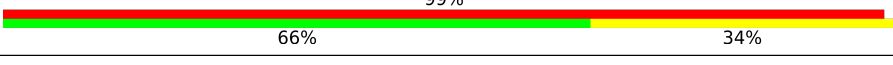
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Mol	Chain	Length	Quality of chain
4	C	254	
5	E	261	
6	G	236	
7	H	190	
8	I	200	
9	J	197	
10	L	156	
11	N	151	
12	O	137	
13	R	136	
14	V	87	
15	W	130	
16	X	145	
17	Y	135	
18	b	82	
19	d	56	
20	e	63	
21	D	240	
22	F	225	
23	K	105	
24	M	143	
25	P	142	
26	Q	143	
27	S	146	
28	T	144	

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Mol	Chain	Length	Quality of chain
29	U	121	
30	Z	108	
31	c	67	
32	f	152	
33	g	319	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 72721 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1750	Total	C	N	O	P	0	0
			37285	16669	6597	12269	1750		

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	206	Total	C	N	O	S	0	0
			1577	1014	278	283	2		

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	113	Total	C	N	O	S	0	0
			918	584	169	164	1		

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 5 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 6 is a protein called 40S ribosomal protein S6-A.

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

- Molecule 7 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 8 is a protein called 40S ribosomal protein S8-A.

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

- Molecule 9 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 10 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	155	Total	C	N	O	S	0	0
			1213	774	230	206	3		

- Molecule 11 is a protein called 40S ribosomal protein S13.

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

- Molecule 12 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	O	18	Total	C	N	O	0	0
			141	83	35	23		

- Molecule 13 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	120	Total	C	N	O	S	0	0
			926	577	177	170	2		

- Molecule 14 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 15 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 16 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 17 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	134	Total	C	N	O	S	0	0
			1073	676	208	189			

- Molecule 18 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 19 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	d	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 20 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	e	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 21 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	D	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 22 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	F	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 23 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	K	96	Total	C	N	O	S	0	0
			772	499	126	145	2		

- Molecule 24 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	124	Total	C	N	O	S	0	0
			890	560	156	172	2		

- Molecule 25 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	124	Total	C	N	O	S	0	0
			977	622	182	166	7		

- Molecule 26 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	141	Total	C	N	O		0	0
			1105	708	203	194			

- Molecule 27 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 28 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 29 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	98	Total	C	N	O	S	0	0
			792	502	144	145	1		

- Molecule 30 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	70	Total	C	N	O	S	0	0
			563	360	104	99			

- Molecule 31 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	51	Total	C	N	O	S	0	0
			397	249	73	71	4		

- Molecule 33 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	318	Total	C	N	O	S	0	0
			2437	1541	418	470	8		

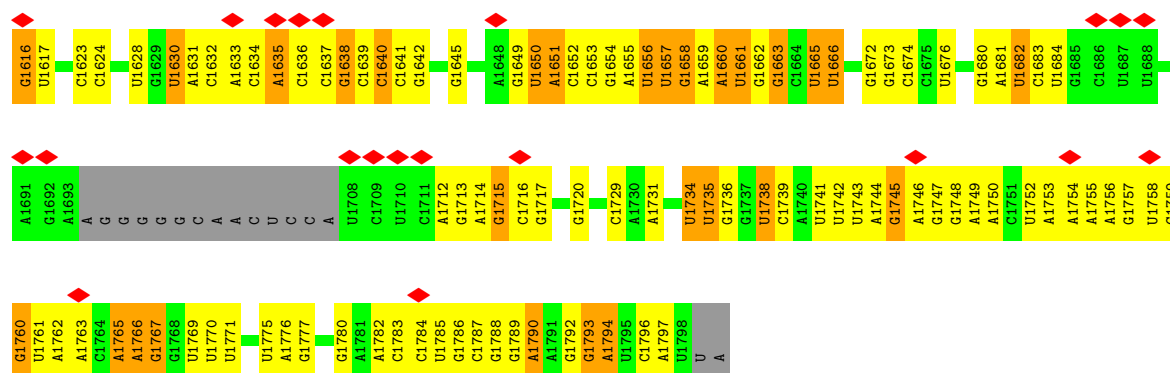
3 Residue-property plots

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

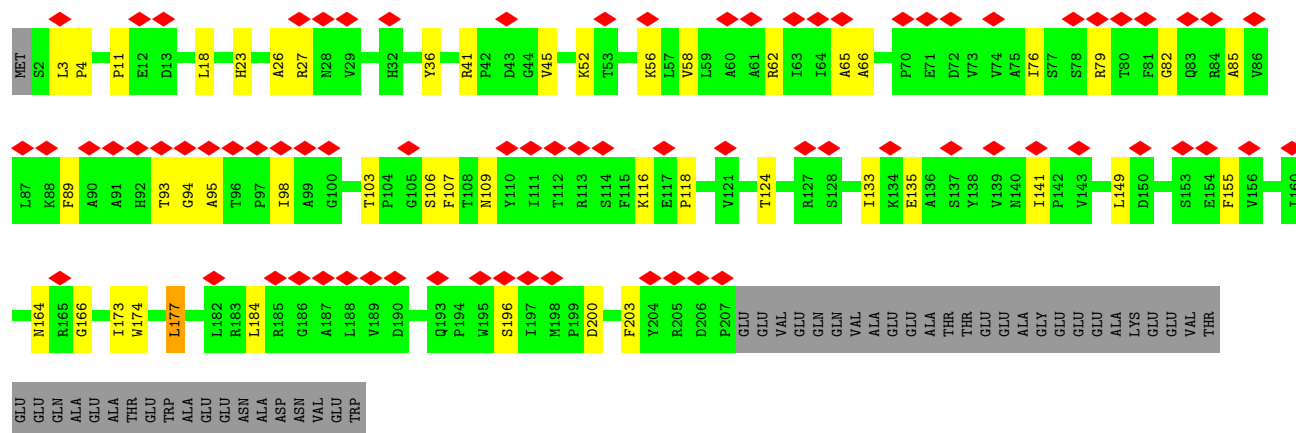
• Molecule 1: 18S ribosomal RNA



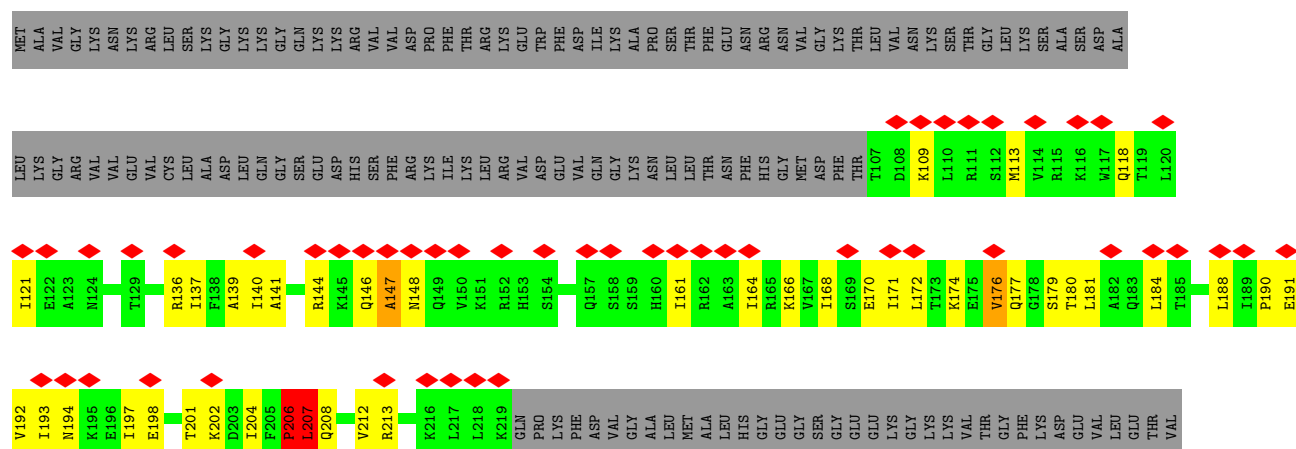




• Molecule 2: 40S ribosomal protein S0-A

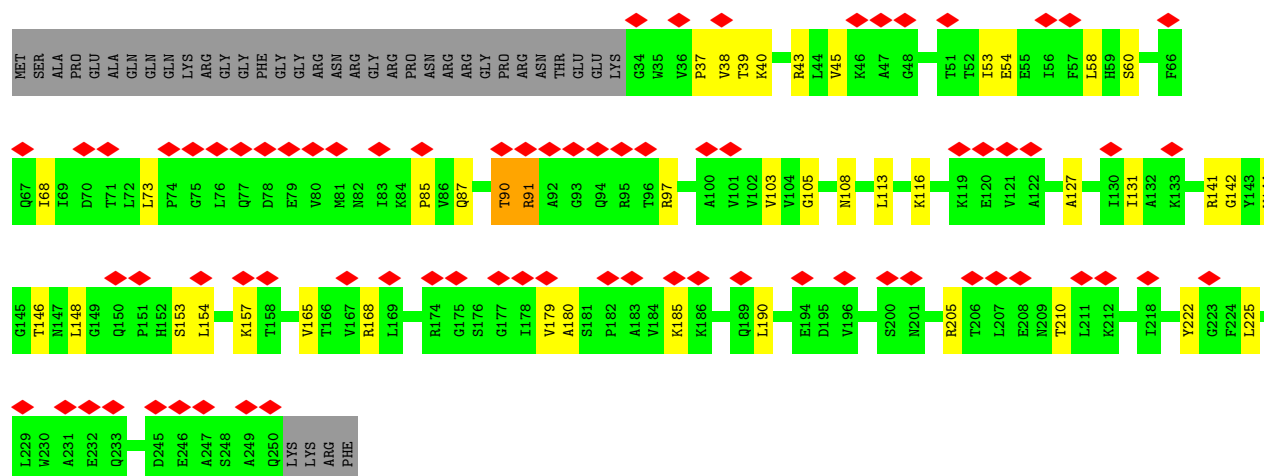


• Molecule 3: 40S ribosomal protein S1-A

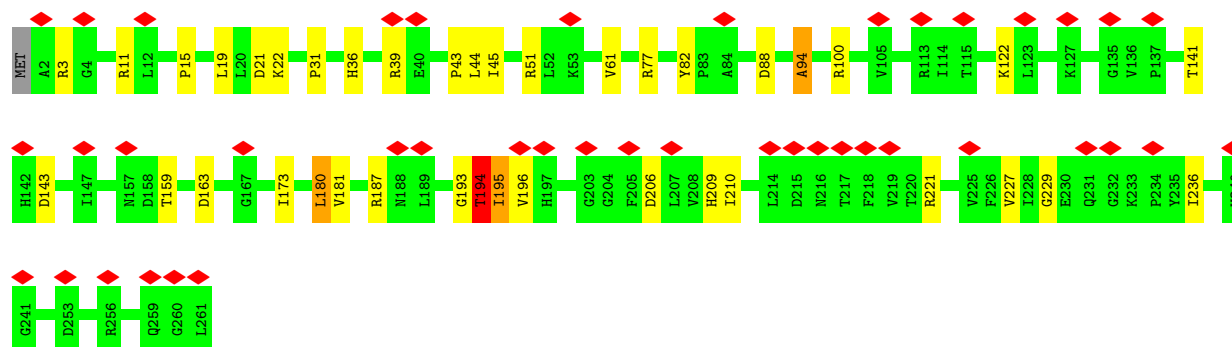
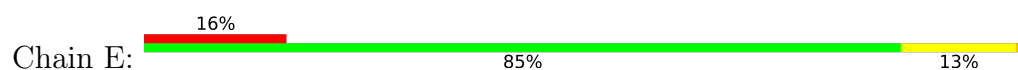


• Molecule 4: 40S ribosomal protein S2

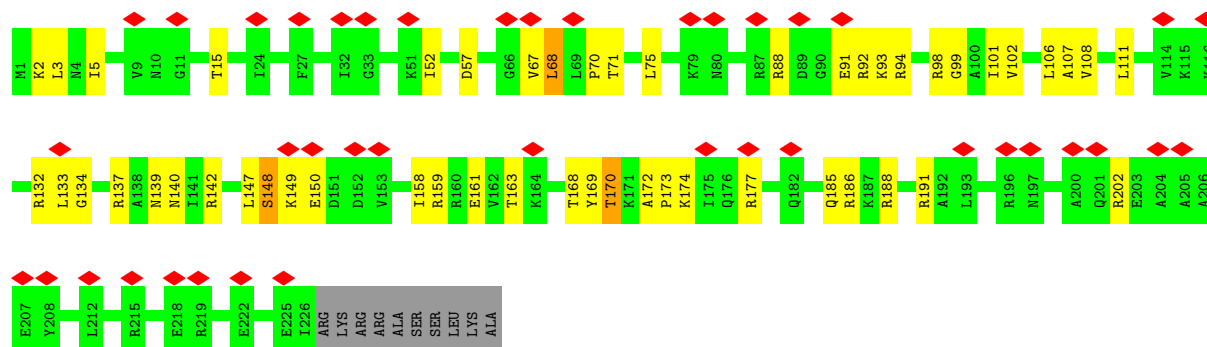
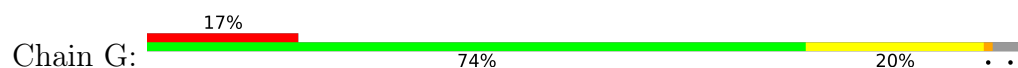




• Molecule 5: 40S ribosomal protein S4-A

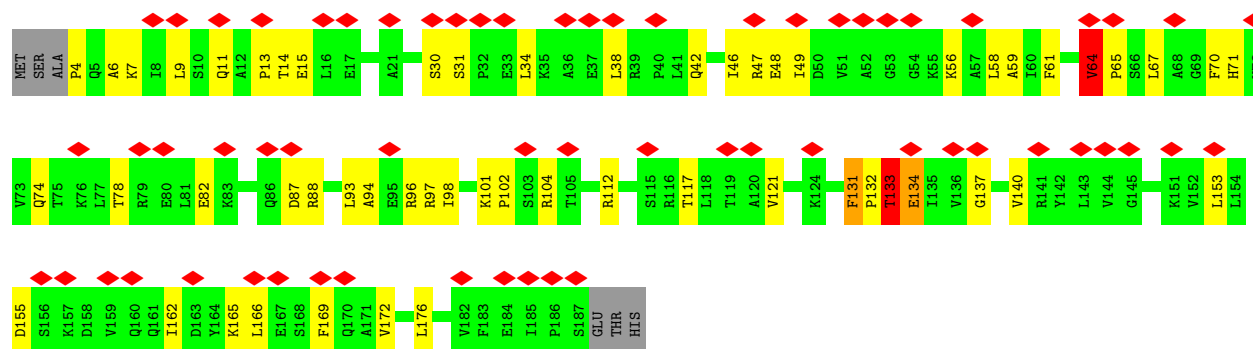


• Molecule 6: 40S ribosomal protein S6-A

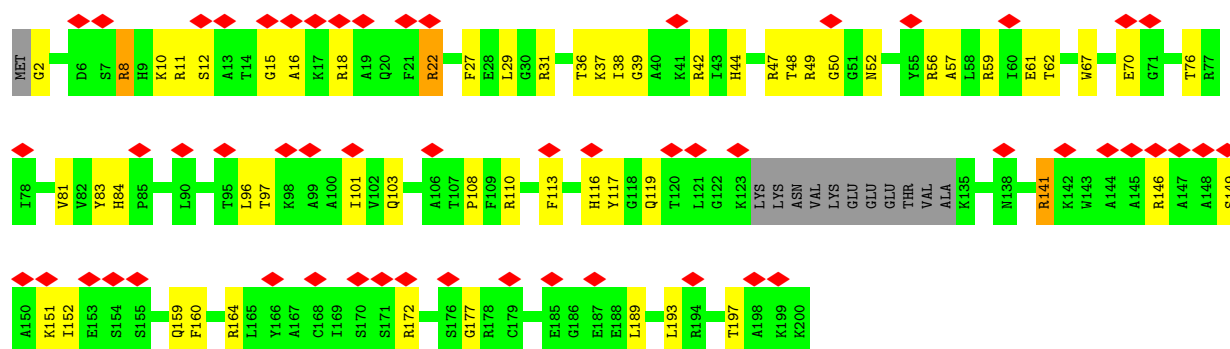


• Molecule 7: 40S ribosomal protein S7-A

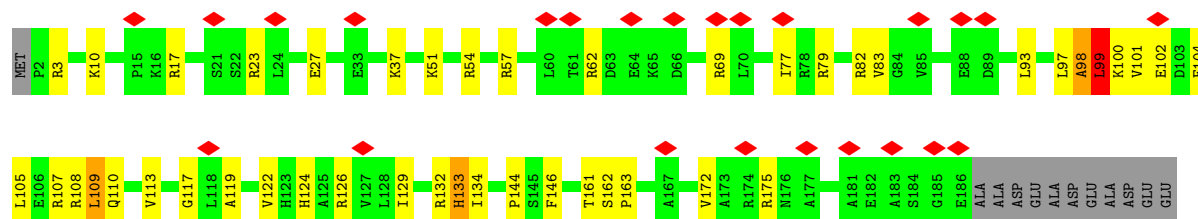




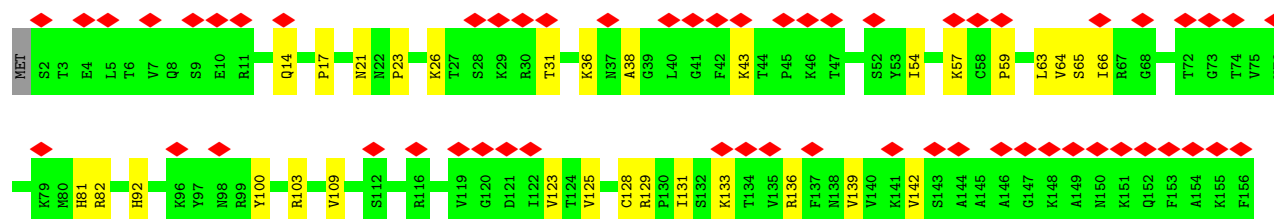
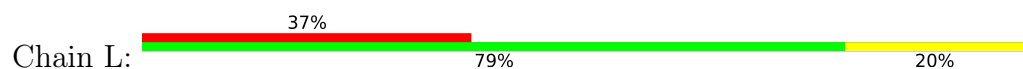
• Molecule 8: 40S ribosomal protein S8-A



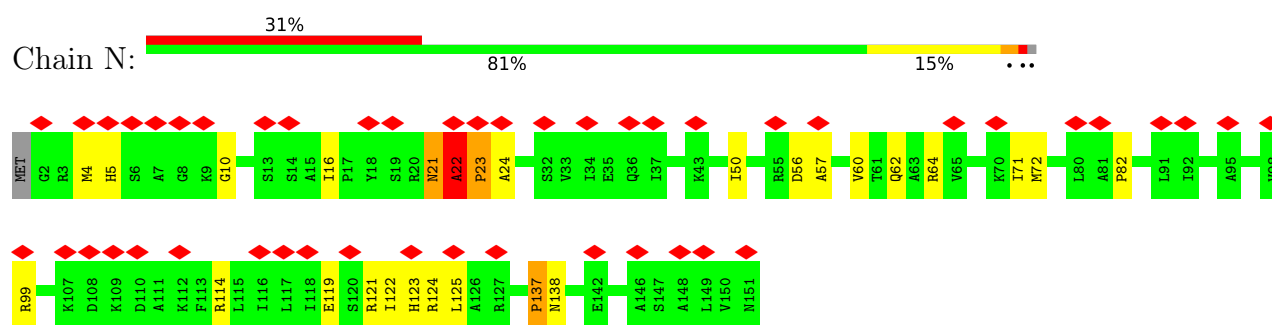
• Molecule 9: 40S ribosomal protein S9-A



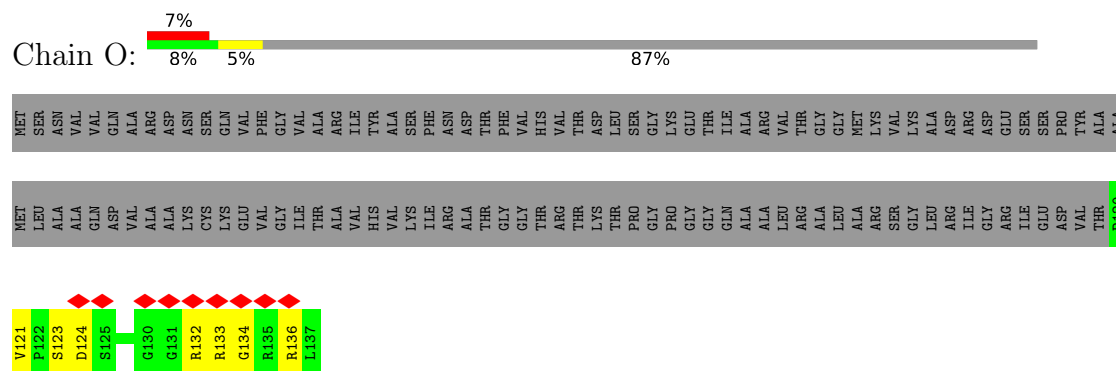
• Molecule 10: 40S ribosomal protein S11-A



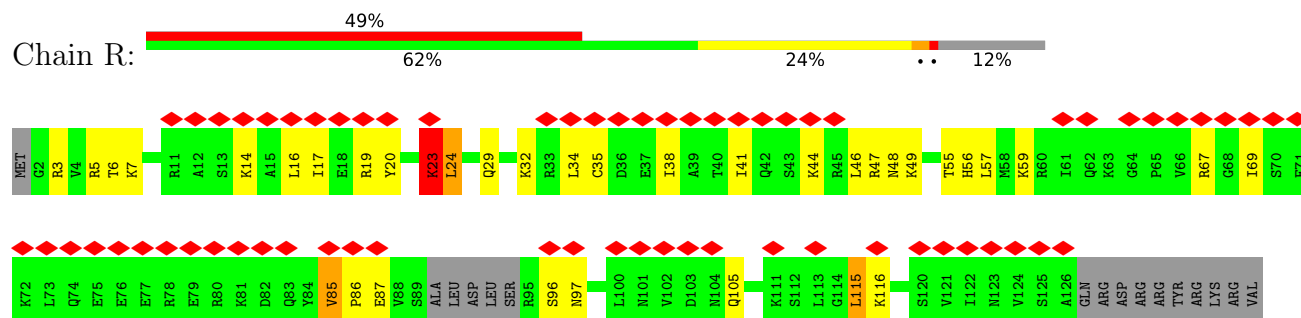
• Molecule 11: 40S ribosomal protein S13



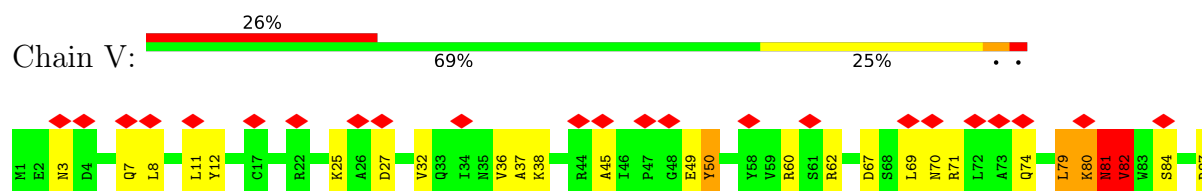
• Molecule 12: 40S ribosomal protein S14-A



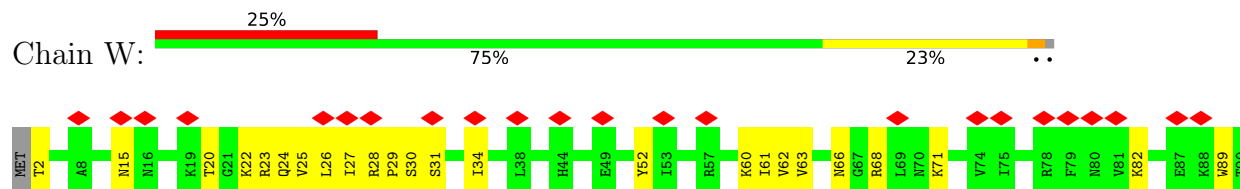
• Molecule 13: 40S ribosomal protein S17-A

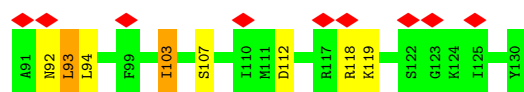


• Molecule 14: 40S ribosomal protein S21-A

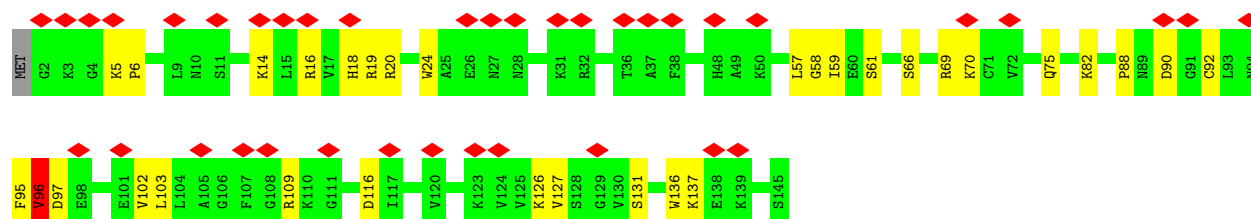
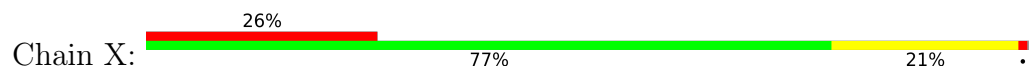


• Molecule 15: 40S ribosomal protein S22-A

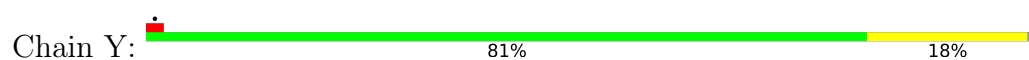




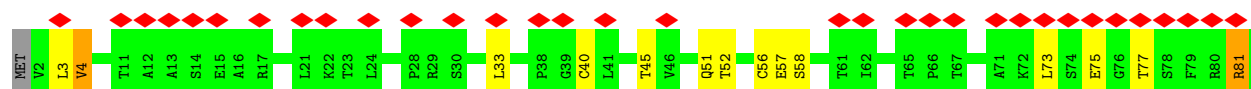
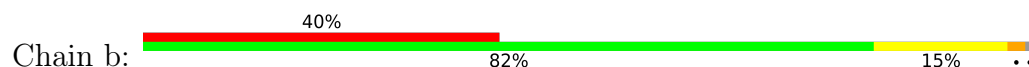
- Molecule 16: 40S ribosomal protein S23-A



- Molecule 17: 40S ribosomal protein S24-A



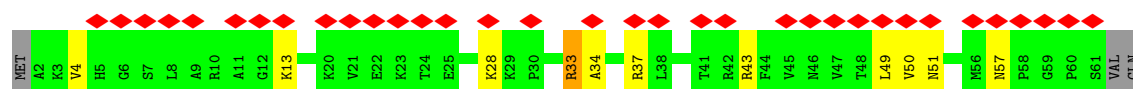
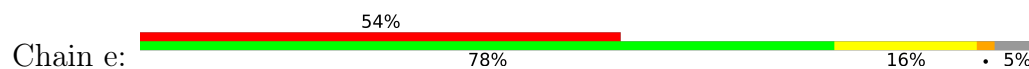
- Molecule 18: 40S ribosomal protein S27-A



- Molecule 19: 40S ribosomal protein S29-A

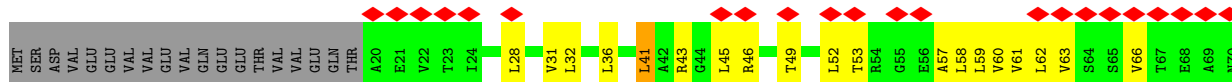


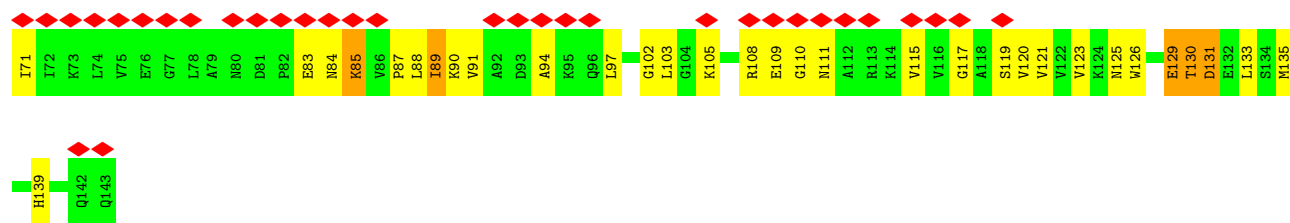
- Molecule 20: 40S ribosomal protein S30-A



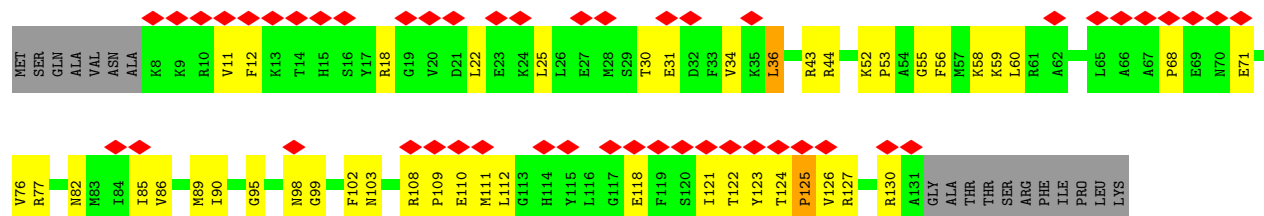
- Molecule 21: 40S ribosomal protein S3



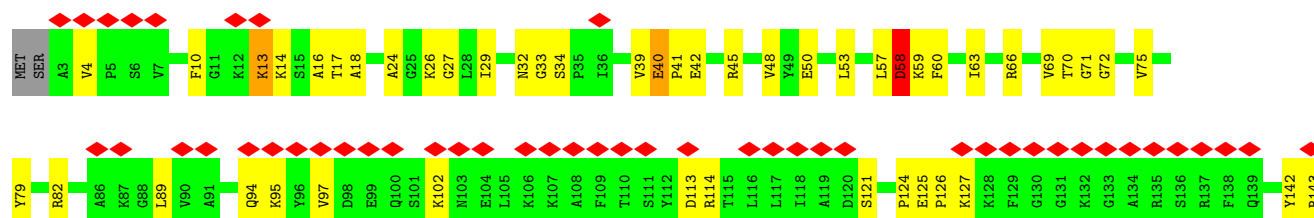




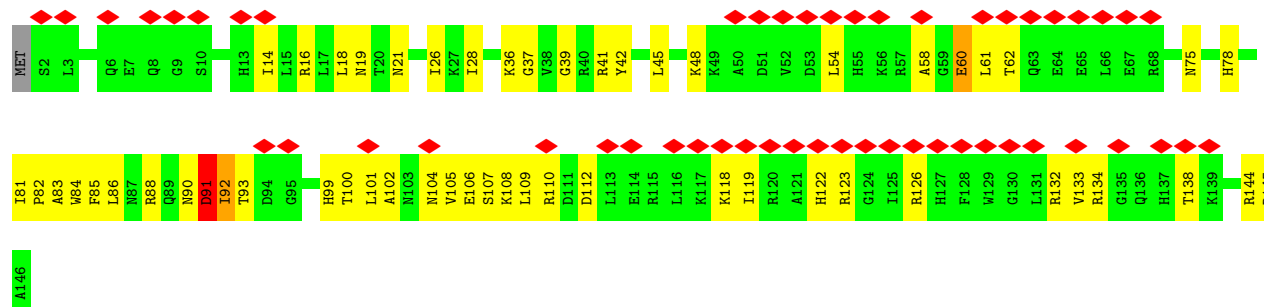
• Molecule 25: 40S ribosomal protein S15



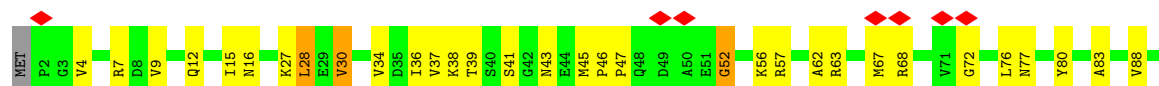
• Molecule 26: 40S ribosomal protein S16-A



• Molecule 27: 40S ribosomal protein S18-A



• Molecule 28: 40S ribosomal protein S19-A





L301	F241	W181	M121	F61	MET
F302	S242	N182	I122	K62	A2
A303	L243	L183	I123	G63	S3
G304	A244	N184	S124	H64	N4
Y305	F245	Q185	G125	S65	E5
T306	S246	F186	S126	H66	V6
D307	P247	Q187	R127	I67	L7
N308	N248	I188	D128	V68	V8
V309	R249	E189	K129	Q69	L9
I310	Y250	A190	T130	D70	R10
R311	W251	D191	I131	C71	G11
V312	L252	F192	K132	T72	T12
W313	A253	L193	V133	L73	L13
Q314	A254	G194	W134	T74	E14
V315	A255	H195	T135	A75	G15
M316	T256	N196	I136	D76	H16
T317	A257	S197	K137	G77	M17
A318	T258	N198	G138	A78	G18
N319	G259	I199	Q139	Y79	W19
	L260	N200	C140	A80	V20
	K261	T201	L141	L81	T21
	V262	L202	A142	S82	S22
	F263	T203	T143	A83	L23
	S264	A204	L144	S84	A24
	L265	S205	L145	W85	T25
	D266	P206	G146	D86	S26
	P267	D207	H147	K87	A27
	Q268	G208	N148	T88	G28
	Y269	T209	D149	L89	Q29
	L270	L210	W150	R90	P30
	V271	T211	V151	L91	N31
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	D273	S213	Q153	D93	L33
	L274	A214	V154	V94	L34
	R275	G215	R155	A95	S35
	P276	T216	V156	T96	A36
	E277	D217	V157	G97	S37
	F278	G218	P158	E98	R38
	A279	E219	N159	T99	D39
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	A285	N224	D164	S44	S44
	E286	L225	D165	G105	W45
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	H288	A227	V167	K107	L47
	A289	K228	T168	S108	T48
	V290	K229	I169	D109	G49
	S291	A230	I170	V110	D50
	L292	M231	S171	M111	D51
	A293	T232	A172	S112	Q52
	W294	T233	G173	V113	A53
	S295	L234	N174	D114	F54
	A296	S235	D175	I115	G55
	D297	A236	K176	D116	V56
	G298	Q237	M177	K117	P57
	Q299	D238	V178	K118	V58
	T300	E239	A179	L119	A59
		W240	K180	S120	S60

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	42901	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 ($e^-/\text{\AA}^2$)	32.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.528	Depositor
Minimum map value	-0.170	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	409.72803, 409.72803, 409.72803	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	2	0.32	0/41697	0.53	9/64961 (0.0%)
2	A	0.38	0/1617	0.95	7/2215 (0.3%)
3	B	0.31	0/929	0.99	8/1250 (0.6%)
4	C	0.45	1/1665 (0.1%)	0.81	2/2263 (0.1%)
5	E	0.43	0/2109	0.91	6/2839 (0.2%)
6	G	0.36	0/1823	0.80	0/2439
7	H	0.36	0/1506	1.00	3/2028 (0.1%)
8	I	0.40	0/1514	0.87	1/2021 (0.0%)
9	J	0.40	0/1519	0.88	3/2035 (0.1%)
10	L	0.42	0/1239	0.77	0/1673
11	N	0.31	0/1215	0.96	7/1638 (0.4%)
12	O	0.36	0/142	1.08	1/185 (0.5%)
13	R	0.35	0/935	0.99	4/1254 (0.3%)
14	V	0.41	0/693	0.93	4/935 (0.4%)
15	W	0.51	0/1038	0.83	1/1395 (0.1%)
16	X	0.42	0/1139	0.94	2/1518 (0.1%)
17	Y	0.40	0/1087	0.86	2/1449 (0.1%)
18	b	0.33	0/620	0.99	2/838 (0.2%)
19	d	0.27	0/452	0.82	0/600
20	e	0.34	0/483	0.83	1/643 (0.2%)
21	D	0.30	0/1759	0.81	0/2368
22	F	0.33	0/1629	0.88	2/2202 (0.1%)
23	K	0.35	0/789	0.97	1/1067 (0.1%)
24	M	0.38	0/898	1.25	10/1220 (0.8%)
25	P	0.32	0/998	0.87	0/1341
26	Q	0.33	0/1125	1.22	7/1510 (0.5%)
27	S	0.32	0/1211	0.86	0/1628
28	T	0.38	0/1130	0.92	5/1517 (0.3%)
29	U	0.29	0/798	0.78	0/1075
30	Z	0.32	0/571	1.03	3/768 (0.4%)
31	c	0.28	0/499	0.82	0/670
32	f	0.34	0/404	0.96	0/542
33	g	0.33	0/2490	0.77	2/3389 (0.1%)
All	All	0.34	1/77723 (0.0%)	0.72	93/113476 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	3
3	B	0	2
4	C	0	4
5	E	0	2
6	G	0	1
7	H	0	4
8	I	0	2
9	J	0	6
11	N	0	4
12	O	0	1
13	R	0	2
14	V	0	4
15	W	0	2
16	X	0	3
17	Y	0	2
21	D	0	2
22	F	0	8
23	K	0	3
24	M	0	8
25	P	0	2
26	Q	0	3
27	S	0	3
28	T	0	2
29	U	0	2
30	Z	0	3
32	f	0	4
33	g	0	1
All	All	0	83

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	225	LEU	C-N	-6.55	1.20	1.33

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Q	124	PRO	CA-C-N	15.63	150.63	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Q	124	PRO	C-N-CA	15.63	150.63	120.94
26	Q	40	GLU	CA-C-N	13.23	136.38	119.84
26	Q	40	GLU	C-N-CA	13.23	136.38	119.84
11	N	22	ALA	CA-C-N	10.80	133.34	119.84
11	N	22	ALA	C-N-CA	10.80	133.34	119.84
23	K	3	MET	N-CA-C	-9.12	97.67	108.25
17	Y	47	VAL	N-CA-C	-8.34	105.36	113.53
13	R	85	VAL	CA-C-N	-7.13	110.93	119.84
13	R	85	VAL	C-N-CA	-7.13	110.93	119.84
16	X	96	VAL	CA-C-N	6.98	134.87	121.54
16	X	96	VAL	C-N-CA	6.98	134.87	121.54
4	C	90	THR	CA-C-N	-6.81	111.34	122.65
4	C	90	THR	C-N-CA	-6.81	111.34	122.65
11	N	21	ASN	CA-C-N	6.61	137.94	121.80
11	N	21	ASN	C-N-CA	6.61	137.94	121.80
11	N	137	PRO	CA-C-N	6.56	134.07	121.54
11	N	137	PRO	C-N-CA	6.56	134.07	121.54
28	T	113	ILE	N-CA-C	-6.48	105.84	113.42
1	2	1051	G	P-O3'-C3'	6.44	129.85	120.20
20	e	50	VAL	N-CA-C	-6.34	106.15	112.17
3	B	179	SER	CA-C-N	6.32	133.60	121.54
3	B	179	SER	C-N-CA	6.32	133.60	121.54
24	M	89	ILE	CA-C-N	6.24	133.46	121.54
24	M	89	ILE	C-N-CA	6.24	133.46	121.54
22	F	49	GLU	CA-C-N	6.15	133.29	121.54
22	F	49	GLU	C-N-CA	6.15	133.29	121.54
33	g	164	ASP	CA-C-N	6.14	133.26	121.54
33	g	164	ASP	C-N-CA	6.14	133.26	121.54
3	B	147	ALA	CA-C-N	6.10	133.19	121.54
3	B	147	ALA	C-N-CA	6.10	133.19	121.54
18	b	81	ARG	CA-C-N	6.09	132.67	121.70
18	b	81	ARG	C-N-CA	6.09	132.67	121.70
5	E	194	THR	CA-C-N	6.09	132.93	121.97
5	E	194	THR	C-N-CA	6.09	132.93	121.97
3	B	206	PRO	CA-C-N	6.07	133.14	121.54
3	B	206	PRO	C-N-CA	6.07	133.14	121.54
15	W	30	SER	N-CA-C	6.05	117.98	110.91
9	J	133	HIS	CB-CA-C	-6.01	103.83	111.22
24	M	83	GLU	N-CA-C	-5.99	99.41	108.52
13	R	23	LYS	CA-C-N	5.98	132.96	121.54
13	R	23	LYS	C-N-CA	5.98	132.96	121.54
3	B	176	VAL	CA-C-N	5.97	132.94	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	176	VAL	C-N-CA	5.97	132.94	121.54
8	I	141	ARG	CB-CG-CD	-5.92	97.67	111.30
1	2	131	C	C2'-C3'-O3'	5.86	118.29	109.50
17	Y	60	PHE	N-CA-C	5.79	117.68	110.91
14	V	81	ASN	CA-C-N	5.76	132.34	121.97
14	V	81	ASN	C-N-CA	5.76	132.34	121.97
24	M	129	GLU	CA-C-N	5.74	132.50	121.54
24	M	129	GLU	C-N-CA	5.74	132.50	121.54
24	M	117	GLY	N-CA-C	5.68	118.58	112.33
2	A	95	ALA	N-CA-C	5.55	117.95	111.02
2	A	27	ARG	CA-C-N	5.54	129.13	120.82
2	A	27	ARG	C-N-CA	5.54	129.13	120.82
2	A	65	ALA	CA-C-N	5.52	132.08	121.54
2	A	65	ALA	C-N-CA	5.52	132.08	121.54
11	N	23	PRO	N-CA-C	5.47	123.74	112.47
1	2	497	G	P-O3'-C3'	5.42	128.32	120.20
24	M	53	THR	CA-C-N	5.41	131.53	121.62
24	M	53	THR	C-N-CA	5.41	131.53	121.62
26	Q	113	ASP	N-CA-C	5.39	118.29	110.42
30	Z	87	GLY	CA-C-N	5.38	127.54	120.60
30	Z	87	GLY	C-N-CA	5.38	127.54	120.60
1	2	827	C	N1-C1'-C2'	5.35	120.03	112.00
5	E	94	ALA	CA-C-N	5.35	131.75	121.54
5	E	94	ALA	C-N-CA	5.35	131.75	121.54
26	Q	48	VAL	N-CA-C	-5.34	106.65	112.80
1	2	1370	U	P-O3'-C3'	5.32	128.17	120.20
14	V	80	LYS	N-CA-C	-5.31	100.77	109.80
7	H	133	THR	CA-C-N	5.29	131.65	121.54
7	H	133	THR	C-N-CA	5.29	131.65	121.54
1	2	1051	G	C2'-C3'-O3'	5.29	117.43	109.50
2	A	116	LYS	CA-C-N	-5.27	116.77	123.15
2	A	116	LYS	C-N-CA	-5.27	116.77	123.15
28	T	34	VAL	CA-C-N	5.25	131.57	121.54
28	T	34	VAL	C-N-CA	5.25	131.57	121.54
9	J	3	ARG	CA-C-N	-5.25	113.64	120.67
9	J	3	ARG	C-N-CA	-5.25	113.64	120.67
12	O	124	ASP	N-CA-C	5.20	118.02	110.42
26	Q	97	VAL	N-CA-C	-5.19	104.39	110.05
1	2	1226	A	C2'-C3'-O3'	5.12	121.38	113.70
7	H	31	SER	N-CA-C	5.12	121.13	109.81
30	Z	71	ILE	N-CA-C	5.12	116.00	109.30
5	E	194	THR	N-CA-C	5.10	121.67	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	163	ASP	N-CA-C	5.09	117.49	111.33
1	2	782	U	P-O3'-C3'	5.08	127.82	120.20
14	V	82	VAL	N-CA-C	5.07	119.89	109.34
28	T	52	GLY	CA-C-N	5.05	131.18	121.54
28	T	52	GLY	C-N-CA	5.05	131.18	121.54
24	M	110	GLY	CA-C-N	5.04	131.17	121.54
24	M	110	GLY	C-N-CA	5.04	131.17	121.54
1	2	75	U	C2-N1-C1'	5.01	132.73	117.70

There are no chirality outliers.

All (83) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	166	GLY	Peptide
2	A	3	LEU	Peptide
2	A	94	GLY	Peptide
3	B	147	ALA	Peptide
3	B	206	PRO	Peptide
4	C	144	TRP	Peptide
4	C	87	GLN	Peptide
4	C	90	THR	Peptide
4	C	91	ARG	Peptide
21	D	216	PRO	Peptide
21	D	219	ALA	Peptide
5	E	193	GLY	Peptide
5	E	194	THR	Peptide
22	F	125	THR	Peptide
22	F	127	GLN	Peptide
22	F	128	ASN	Peptide
22	F	44	ASN	Peptide
22	F	49	GLU	Peptide
22	F	56	ALA	Peptide
22	F	57	SER	Peptide
22	F	65	ARG	Peptide
6	G	148	SER	Peptide
7	H	131	PHE	Peptide
7	H	133	THR	Peptide
7	H	64	VAL	Peptide
7	H	97	ARG	Peptide
8	I	151	LYS	Peptide
8	I	8	ARG	Peptide
9	J	117	GLY	Peptide

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Mol	Chain	Res	Type	Group
9	J	161	THR	Peptide
9	J	162	SER	Peptide
9	J	163	PRO	Peptide
9	J	98	ALA	Peptide
9	J	99	LEU	Peptide
23	K	53	GLY	Peptide
23	K	86	ILE	Peptide
23	K	87	VAL	Peptide
24	M	105	LYS	Peptide
24	M	108	ARG	Peptide
24	M	111	ASN	Peptide
24	M	129	GLU	Peptide
24	M	130	THR	Peptide
24	M	41	LEU	Peptide
24	M	84	ASN	Peptide
24	M	89	ILE	Peptide
11	N	137	PRO	Peptide
11	N	21	ASN	Peptide
11	N	22	ALA	Peptide
11	N	24	ALA	Peptide
12	O	123	SER	Peptide
25	P	11	VAL	Peptide
25	P	124	THR	Peptide
26	Q	13	LYS	Peptide
26	Q	40	GLU	Peptide
26	Q	58	ASP	Peptide
13	R	23	LYS	Peptide
13	R	87	GLU	Peptide
27	S	62	THR	Peptide
27	S	90	ASN	Peptide
27	S	91	ASP	Peptide
28	T	30	VAL	Peptide
28	T	52	GLY	Peptide
29	U	54	GLY	Peptide
29	U	94	GLU	Peptide
14	V	50	TYR	Peptide
14	V	79	LEU	Peptide
14	V	80	LYS	Peptide
14	V	81	ASN	Peptide
15	W	29	PRO	Peptide
15	W	82	LYS	Peptide
16	X	137	LYS	Peptide

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Mol	Chain	Res	Type	Group
16	X	88	PRO	Peptide
16	X	96	VAL	Peptide
17	Y	33	ALA	Peptide
17	Y	36	SER	Peptide
30	Z	43	ASP	Peptide
30	Z	54	VAL	Peptide
30	Z	93	SER	Peptide
32	f	119	ARG	Peptide
32	f	138	ARG	Peptide
32	f	143	LYS	Peptide
32	f	147	VAL	Peptide
33	g	73	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37285	0	18766	523	0
2	A	1577	0	1567	25	0
3	B	918	0	987	29	0
4	C	1635	0	1722	27	0
5	E	2068	0	2154	22	0
6	G	1799	0	1879	38	0
7	H	1481	0	1572	29	0
8	I	1489	0	1525	38	0
9	J	1494	0	1573	28	0
10	L	1213	0	1257	22	0
11	N	1192	0	1255	16	0
12	O	141	0	155	4	0
13	R	926	0	930	26	0
14	V	684	0	672	19	0
15	W	1021	0	1060	22	0
16	X	1121	0	1196	22	0
17	Y	1073	0	1132	13	0
18	b	610	0	633	10	0
19	d	442	0	432	9	0
20	e	475	0	525	10	0
21	D	1734	0	1817	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	F	1609	0	1675	49	0
23	K	772	0	727	21	0
24	M	890	0	887	24	0
25	P	977	0	1002	29	0
26	Q	1105	0	1166	39	0
27	S	1192	0	1222	39	0
28	T	1112	0	1124	35	0
29	U	792	0	851	22	0
30	Z	563	0	603	12	0
31	c	497	0	535	14	0
32	f	397	0	399	17	0
33	g	2437	0	2386	73	0
All	All	72721	0	55386	1125	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 9.

All (1125) 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)
1:2:1047:G:H1	1:2:1071:U:H3	1.04	1.04
1:2:567:A:H62	1:2:576:G:N2	1.61	0.99
1:2:996:U:H3	1:2:1008:G:H1	1.00	0.98
1:2:1170:G:H1	1:2:1469:A:N6	1.62	0.98
1:2:875:G:H1	1:2:952:A:H61	1.05	0.94
1:2:1335:U:H3	1:2:1416:G:H1	1.01	0.94
1:2:567:A:N6	1:2:576:G:H21	1.65	0.92
1:2:40:A:H62	1:2:467:G:H21	1.11	0.90
6:G:161:GLU:HA	6:G:169:TYR:O	1.71	0.90
1:2:480:G:H1	1:2:508:U:H3	1.17	0.89
1:2:875:G:H1	1:2:952:A:N6	1.71	0.87
1:2:1499:G:H1	1:2:1508:U:H3	1.20	0.87
1:2:629:U:O2	1:2:970:A:N6	2.08	0.87
1:2:273:G:H1	1:2:283:U:H3	1.22	0.86
1:2:887:A:H2	1:2:925:G:H1	1.19	0.86
1:2:1639:C:N4	1:2:1765:A:C2	2.44	0.86
30:Z:89:ILE:HA	30:Z:102:THR:O	1.78	0.84
32:f:133:ALA:O	32:f:139:LEU:HA	1.77	0.83
1:2:1175:U:H3	1:2:1464:G:H1	1.22	0.82
1:2:1170:G:H1	1:2:1469:A:H61	0.86	0.82
4:C:85:PRO:HA	4:C:97:ARG:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:567:A:H62	1:2:576:G:H21	0.83	0.81
29:U:67:THR:O	29:U:80:GLU:HB3	1.80	0.80
1:2:1278:G:H1	1:2:1430:U:H3	1.27	0.79
1:2:40:A:H62	1:2:467:G:N2	1.80	0.79
1:2:1642:G:N2	1:2:1759:C:O2	2.15	0.79
25:P:56:PHE:O	25:P:60:LEU:HB2	1.84	0.78
23:K:72:GLY:O	23:K:76:LEU:HB2	1.84	0.78
1:2:1639:C:C4	1:2:1765:A:N1	2.51	0.78
21:D:172:THR:HA	21:D:184:ILE:O	1.84	0.78
1:2:1034:C:HO2'	15:W:2:THR:N	1.84	0.76
24:M:131:ASP:O	24:M:135:MET:HB2	1.85	0.76
33:g:89:LEU:HB2	33:g:103:PHE:HB2	1.68	0.75
1:2:1639:C:C4	1:2:1765:A:C2	2.75	0.74
1:2:1174:C:H42	1:2:1465:C:H42	1.36	0.73
21:D:169:ASP:O	21:D:187:LYS:HA	1.88	0.73
1:2:1145:U:H2'	4:C:91:ARG:HB2	1.71	0.73
1:2:863:A:H62	1:2:964:U:H3	1.37	0.72
1:2:765:G:H22	9:J:82:ARG:HE	1.37	0.72
1:2:1639:C:N3	1:2:1765:A:C6	2.57	0.72
1:2:196:G:N7	8:I:141:ARG:NH2	2.38	0.70
27:S:107:SER:O	27:S:110:ARG:HB3	1.93	0.69
22:F:51:VAL:HG21	22:F:130:ILE:HG23	1.73	0.68
29:U:57:ARG:HA	29:U:89:ARG:HG3	1.75	0.68
3:B:202:LYS:HA	3:B:206:PRO:HA	1.75	0.68
1:2:1729:C:HO2'	8:I:2:GLY:N	1.91	0.68
9:J:110:GLN:HE22	9:J:126:ARG:HB2	1.57	0.68
16:X:57:LEU:O	16:X:70:LYS:HA	1.94	0.67
1:2:647:G:H22	1:2:687:G:H1	1.41	0.67
32:f:139:LEU:HD13	32:f:152:ALA:H	1.59	0.67
1:2:227:U:H3	1:2:834:G:H1	1.40	0.67
3:B:191:GLU:HB2	3:B:194:ASN:HB2	1.76	0.67
15:W:31:SER:H	15:W:34:ILE:HD12	1.59	0.67
1:2:862:A:N7	11:N:64:ARG:NH1	2.42	0.67
2:A:82:GLY:O	2:A:85:ALA:HB3	1.95	0.67
1:2:7:G:N7	4:C:205:ARG:NH1	2.44	0.66
14:V:74:GLN:HA	14:V:79:LEU:HB2	1.78	0.66
1:2:1656:U:H3	1:2:1745:G:H22	1.41	0.66
21:D:172:THR:HG22	21:D:185:LYS:HG2	1.77	0.66
33:g:250:TYR:HB3	33:g:265:LEU:HB2	1.77	0.66
24:M:31:VAL:HG22	24:M:133:LEU:HG	1.78	0.65
1:2:40:A:N6	1:2:467:G:H21	1.91	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:45:VAL:HG21	4:C:68:ILE:HG23	1.77	0.65
33:g:260:ILE:HB	33:g:274:LEU:HB2	1.79	0.65
29:U:52:LYS:HA	29:U:92:ASP:O	1.97	0.65
1:2:1639:C:C2	1:2:1765:A:N6	2.64	0.65
33:g:131:ILE:HB	33:g:144:LEU:HB2	1.77	0.65
1:2:1663:G:H1	1:2:1738:U:H3	1.42	0.65
2:A:41:ARG:HG3	13:R:105:GLN:HE21	1.61	0.65
7:H:61:PHE:HA	7:H:93:LEU:O	1.97	0.65
21:D:72:LEU:HD23	23:K:20:VAL:HG13	1.79	0.65
1:2:23:G:H1	1:2:602:U:H3	1.43	0.64
6:G:159:ARG:HG2	6:G:172:ALA:HB2	1.79	0.64
1:2:1245:G:N2	1:2:1250:U:O4	2.30	0.64
1:2:1564:U:OP1	28:T:38:LYS:NZ	2.31	0.64
26:Q:50:GLU:OE1	26:Q:82:ARG:NH2	2.30	0.64
1:2:655:G:H4'	1:2:656:G:H5'	1.78	0.64
1:2:1235:C:N3	32:f:138:ARG:NH1	2.45	0.64
22:F:124:LEU:HD11	30:Z:59:TYR:HB2	1.80	0.64
33:g:123:ILE:HG21	33:g:169:ILE:HG21	1.79	0.64
1:2:162:A:H3'	1:2:163:G:H21	1.61	0.64
21:D:40:ARG:HG2	29:U:110:PRO:HB3	1.80	0.64
23:K:58:GLN:O	23:K:64:TYR:HA	1.97	0.64
1:2:237:C:H5''	1:2:238:U:H5'	1.80	0.63
2:A:41:ARG:HB3	2:A:45:VAL:HG23	1.80	0.63
22:F:57:SER:HA	22:F:59:VAL:H	1.63	0.63
18:b:73:LEU:HB3	18:b:77:THR:HG21	1.80	0.63
22:F:92:ARG:NH2	22:F:169:ASN:OD1	2.32	0.63
1:2:1548:G:OP1	25:P:18:ARG:NH2	2.31	0.63
1:2:1663:G:N2	1:2:1738:U:O2	2.29	0.63
1:2:1775:U:H3	1:2:1786:G:H1	1.45	0.63
4:C:38:VAL:HG13	4:C:39:THR:HG23	1.80	0.63
1:2:1610:G:N7	26:Q:14:LYS:NZ	2.44	0.63
10:L:21:ASN:HD22	10:L:31:THR:HA	1.63	0.63
19:d:20:GLN:HB2	19:d:25:SER:HA	1.80	0.63
1:2:65:A:H2	1:2:84:A:H62	1.47	0.63
8:I:57:ALA:HB2	8:I:177:GLY:HA2	1.79	0.63
24:M:46:ARG:HG3	32:f:103:LEU:HB2	1.81	0.63
11:N:119:GLU:O	11:N:123:HIS:ND1	2.31	0.62
20:e:49:LEU:HD12	20:e:51:ASN:HB3	1.80	0.62
1:2:763:G:OP2	9:J:79:ARG:NH2	2.32	0.62
1:2:1319:A:OP2	13:R:67:ARG:NH2	2.32	0.62
24:M:131:ASP:O	24:M:135:MET:CB	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:867:G:H1	1:2:961:U:H3	1.45	0.62
28:T:15:ILE:HD11	28:T:63:ARG:HE	1.63	0.62
33:g:74:THR:HG22	33:g:115:ILE:HG21	1.81	0.62
22:F:51:VAL:HG22	22:F:131:GLN:HB2	1.81	0.62
1:2:717:C:N4	1:2:720:G:N2	2.47	0.62
1:2:885:G:N2	1:2:928:U:O2	2.32	0.62
11:N:72:MET:HE1	11:N:82:PRO:HD2	1.82	0.62
22:F:117:THR:HG21	22:F:194:LEU:HD12	1.81	0.62
1:2:594:A:OP2	9:J:37:LYS:NZ	2.33	0.62
1:2:1278:G:N2	1:2:1430:U:O2	2.30	0.62
3:B:190:PRO:HG2	3:B:192:VAL:HG23	1.82	0.62
1:2:1482:C:N4	1:2:1525:A:OP2	2.33	0.61
32:f:123:ASN:HD22	32:f:124:PRO:HD2	1.65	0.61
9:J:113:VAL:HG12	9:J:119:ALA:HB2	1.81	0.61
1:2:385:A:H5''	8:I:22:ARG:HB3	1.82	0.61
7:H:64:VAL:HG22	7:H:94:ALA:HB1	1.82	0.61
1:2:565:C:H1'	16:X:66:SER:HB3	1.81	0.61
1:2:1174:C:O2'	1:2:1196:A:N6	2.34	0.61
24:M:63:VAL:HG11	24:M:94:ALA:HA	1.83	0.61
1:2:1278:G:OP1	21:D:185:LYS:NZ	2.34	0.61
1:2:1639:C:C2	1:2:1765:A:C6	2.89	0.61
24:M:60:VAL:HG23	24:M:87:PRO:HG2	1.83	0.61
25:P:60:LEU:HA	25:P:76:VAL:HG21	1.83	0.61
1:2:812:A:H4'	1:2:813:U:H3'	1.82	0.61
15:W:24:GLN:HA	15:W:63:VAL:O	2.00	0.61
33:g:136:ILE:HG13	33:g:137:LYS:HG2	1.83	0.61
1:2:179:A:N1	6:G:202:ARG:NH1	2.46	0.60
1:2:1335:U:O2	1:2:1416:G:N2	2.27	0.60
1:2:639:U:H5''	7:H:101:LYS:HB2	1.82	0.60
27:S:83:ALA:HA	27:S:86:LEU:HD13	1.83	0.60
1:2:322:G:O2'	8:I:10:LYS:NZ	2.34	0.60
1:2:1674:C:OP1	6:G:92:ARG:NH2	2.35	0.60
33:g:216:LYS:HA	33:g:239:GLU:HG3	1.82	0.60
15:W:25:VAL:O	15:W:62:VAL:HA	2.02	0.60
22:F:29:ILE:HB	22:F:34:GLN:HE21	1.66	0.60
3:B:198:GLU:O	3:B:202:LYS:HB2	2.01	0.60
9:J:62:ARG:O	9:J:69:ARG:NH1	2.34	0.60
24:M:62:LEU:HD22	24:M:88:LEU:HD11	1.84	0.60
1:2:477:A:O2'	20:e:33:ARG:NH2	2.35	0.60
1:2:1149:G:H1	1:2:1628:U:H3	1.47	0.60
1:2:1605:G:O2'	29:U:64:LYS:NZ	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:140:VAL:HB	15:W:52:TYR:HB3	1.84	0.60
33:g:112:SER:HB3	33:g:125:GLY:H	1.67	0.60
1:2:511:A:H5''	9:J:172:VAL:HG13	1.83	0.60
26:Q:39:VAL:HG12	26:Q:41:PRO:HD2	1.83	0.60
33:g:48:THR:H	33:g:55:GLY:HA2	1.67	0.60
1:2:1317:C:O2'	1:2:1400:A:N3	2.34	0.60
5:E:15:PRO:HB3	5:E:39:ARG:HD3	1.82	0.60
6:G:142:ARG:HG2	6:G:147:LEU:HB2	1.83	0.59
1:2:152:U:O4	17:Y:124:ARG:NH2	2.35	0.59
1:2:863:A:N6	1:2:964:U:H3	2.00	0.59
1:2:1163:A:N3	1:2:1613:U:O2'	2.33	0.59
1:2:1166:A:H5'	22:F:104:ASN:HD21	1.66	0.59
1:2:1729:C:O2'	8:I:2:GLY:N	2.35	0.59
8:I:116:HIS:O	8:I:146:ARG:NH1	2.36	0.59
1:2:72:A:N7	6:G:169:TYR:OH	2.30	0.59
1:2:142:G:H22	1:2:173:A:H2	1.50	0.59
1:2:177:U:O2	6:G:191:ARG:NH1	2.35	0.59
33:g:150:TRP:HB2	33:g:174:ASN:HD22	1.67	0.59
1:2:1499:G:N2	1:2:1508:U:O2	2.31	0.59
25:P:44:ARG:NH1	25:P:82:ASN:O	2.36	0.59
15:W:26:LEU:HA	15:W:61:ILE:O	2.02	0.59
21:D:171:ALA:O	21:D:185:LYS:HA	2.03	0.59
29:U:25:THR:HB	29:U:115:GLU:HB2	1.85	0.59
1:2:861:U:OP2	11:N:64:ARG:NH2	2.36	0.59
21:D:137:VAL:HG22	21:D:151:LYS:HG3	1.85	0.59
1:2:330:G:OP2	8:I:172:ARG:NH1	2.36	0.58
1:2:1471:A:OP1	22:F:185:ARG:NH2	2.36	0.58
24:M:66:VAL:HG11	24:M:71:ILE:HD11	1.84	0.58
1:2:1594:G:OP2	1:2:1596:C:N4	2.36	0.58
15:W:23:ARG:NH1	15:W:66:ASN:O	2.34	0.58
25:P:98:ASN:ND2	25:P:121:ILE:O	2.37	0.58
1:2:1213:G:N2	1:2:1450:U:O2	2.34	0.58
1:2:1565:C:OP1	27:S:41:ARG:NH1	2.37	0.58
24:M:49:THR:HA	24:M:52:LEU:HB2	1.85	0.58
25:P:98:ASN:HB2	25:P:122:THR:HA	1.86	0.58
1:2:1158:C:H5''	1:2:1161:C:H41	1.68	0.58
21:D:72:LEU:HD22	23:K:65:TYR:HB3	1.85	0.58
28:T:118:PRO:HD2	28:T:123:ARG:HE	1.66	0.58
22:F:62:VAL:HG13	22:F:89:ILE:HG12	1.84	0.58
32:f:108:VAL:HA	32:f:114:VAL:HA	1.85	0.58
24:M:45:LEU:HD12	24:M:120:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:S:45:LEU:HD11	28:T:36:ILE:HG22	1.85	0.58
28:T:39:THR:HA	28:T:100:ILE:HG13	1.85	0.58
1:2:1210:C:H2'	1:2:1211:A:C8	2.39	0.57
1:2:1340:U:H3	26:Q:10:PHE:HE1	1.52	0.57
21:D:164:VAL:HG13	21:D:168:ILE:HD11	1.84	0.57
33:g:80:ALA:HB3	33:g:92:TRP:HB2	1.85	0.57
1:2:1453:G:H21	25:P:99:GLY:HA2	1.69	0.57
1:2:887:A:N1	1:2:925:G:O6	2.37	0.57
13:R:47:ARG:NH1	13:R:48:ASN:OD1	2.38	0.57
29:U:106:ILE:HG23	29:U:107:THR:HG23	1.86	0.57
1:2:936:G:OP1	1:2:1074:G:N2	2.32	0.57
1:2:1525:A:N3	1:2:1589:C:O2'	2.34	0.57
1:2:1204:A:N3	19:d:10:HIS:NE2	2.50	0.57
6:G:163:THR:HG22	6:G:168:THR:HG22	1.87	0.57
10:L:14:GLN:HB3	10:L:54:ILE:HG21	1.87	0.57
1:2:478:A:O2'	9:J:124:HIS:ND1	2.34	0.57
1:2:703:G:H2'	1:2:704:C:H2'	1.84	0.57
1:2:1500:C:H5''	28:T:102:ARG:HD2	1.86	0.57
1:2:877:G:H22	1:2:951:A:H2	1.52	0.57
1:2:1191:U:OP2	26:Q:143:ARG:NH2	2.38	0.57
1:2:1570:A:O2'	27:S:144:ARG:NH2	2.38	0.57
1:2:1633:A:H5''	1:2:1635:A:H5''	1.85	0.57
6:G:3:LEU:O	6:G:15:THR:HA	2.04	0.57
33:g:32:LEU:HD21	33:g:94:VAL:HG11	1.87	0.57
1:2:434:G:N1	1:2:437:A:OP2	2.37	0.57
1:2:1177:C:O2'	1:2:1194:A:N1	2.38	0.57
2:A:36:TYR:OH	2:A:56:LYS:NZ	2.37	0.57
10:L:23:PRO:O	10:L:26:LYS:NZ	2.35	0.57
21:D:175:VAL:HG13	21:D:182:LEU:HB2	1.86	0.57
1:2:1787:C:OP2	12:O:132:ARG:N	2.36	0.57
8:I:37:LYS:H	8:I:59:ARG:H	1.52	0.57
22:F:225:ARG:NH2	31:c:57:MET:SD	2.76	0.57
1:2:1496:U:HO2'	1:2:1519:U:HO2'	1.53	0.56
18:b:33:LEU:HB3	18:b:81:ARG:HG3	1.85	0.56
31:c:27:GLN:NE2	31:c:64:ARG:O	2.38	0.56
1:2:1452:U:OP1	19:d:10:HIS:ND1	2.38	0.56
26:Q:4:VAL:HB	26:Q:24:ALA:HB3	1.87	0.56
1:2:808:U:H2'	1:2:809:A:H8	1.71	0.56
1:2:1500:C:OP1	28:T:122:ARG:NH2	2.37	0.56
1:2:1572:G:H1'	22:F:185:ARG:HH12	1.70	0.56
7:H:102:PRO:HD3	7:H:112:ARG:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:17:ARG:O	9:J:23:ARG:NH2	2.38	0.56
30:Z:90:LYS:HE2	30:Z:104:ALA:HA	1.86	0.56
1:2:609:U:O2	16:X:19:ARG:NH2	2.38	0.56
1:2:1318:G:OP2	13:R:67:ARG:NH1	2.38	0.56
4:C:108:ASN:OD1	4:C:141:ARG:NH1	2.38	0.56
12:O:134:GLY:O	12:O:136:ARG:NH1	2.39	0.56
1:2:140:A:N6	1:2:281:G:OP1	2.39	0.56
1:2:1064:G:O2'	3:B:204:ILE:O	2.24	0.56
1:2:1175:U:O2	1:2:1464:G:N2	2.31	0.56
1:2:1295:G:H2'	1:2:1296:A:H8	1.70	0.56
6:G:91:GLU:OE2	6:G:93:LYS:NZ	2.39	0.56
27:S:36:LYS:HB2	27:S:102:ALA:HA	1.87	0.56
1:2:343:C:H2'	1:2:344:A:H8	1.70	0.56
1:2:1561:U:OP1	1:2:1599:C:O2'	2.23	0.56
1:2:332:U:OP1	8:I:56:ARG:NH2	2.38	0.56
4:C:146:THR:HG23	4:C:148:LEU:H	1.71	0.56
5:E:180:LEU:HA	5:E:194:THR:HA	1.86	0.56
18:b:56:CYS:SG	18:b:57:GLU:N	2.78	0.56
21:D:139:SER:O	21:D:182:LEU:HA	2.06	0.56
28:T:131:ASP:OD1	28:T:134:ARG:NH2	2.39	0.56
33:g:255:ALA:HB2	33:g:292:LEU:HD22	1.88	0.56
1:2:1195:C:N4	26:Q:143:ARG:O	2.39	0.56
1:2:1573:A:H4'	1:2:1574:G:H5'	1.88	0.56
16:X:102:VAL:HG12	16:X:127:VAL:HG12	1.88	0.56
18:b:40:CYS:SG	18:b:58:SER:OG	2.63	0.56
22:F:118:LEU:HD22	22:F:129:PRO:HB2	1.88	0.56
26:Q:60:PHE:HA	26:Q:63:ILE:HG13	1.89	0.56
1:2:1167:G:N2	1:2:1578:U:O2	2.39	0.55
13:R:55:THR:O	13:R:59:LYS:HB2	2.06	0.55
28:T:41:SER:OG	28:T:95:ASP:O	2.24	0.55
1:2:1566:U:H5''	27:S:39:GLY:H	1.71	0.55
23:K:58:GLN:HB3	23:K:65:TYR:HB2	1.88	0.55
26:Q:95:LYS:O	33:g:59:ARG:NH1	2.40	0.55
1:2:150:U:OP1	17:Y:123:LYS:NZ	2.38	0.55
1:2:1149:G:O2'	1:2:1151:A:OP1	2.24	0.55
8:I:42:ARG:HD3	8:I:59:ARG:HD2	1.89	0.55
10:L:128:CYS:SG	10:L:129:ARG:N	2.80	0.55
1:2:67:A:N6	1:2:83:G:O2'	2.39	0.55
1:2:143:G:OP2	6:G:139:ASN:ND2	2.39	0.55
1:2:1351:G:OP1	26:Q:66:ARG:NH2	2.39	0.55
8:I:110:ARG:NH1	8:I:160:PHE:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:32:LEU:O	24:M:36:LEU:HB2	2.06	0.55
1:2:505:A:N6	1:2:507:U:O4	2.36	0.55
1:2:1160:A:OP2	26:Q:142:TYR:OH	2.25	0.55
7:H:30:SER:HB2	7:H:34:LEU:HB2	1.88	0.55
7:H:133:THR:OG1	7:H:134:GLU:N	2.40	0.55
13:R:24:LEU:HG	13:R:34:LEU:HD22	1.87	0.55
21:D:136:VAL:HG22	21:D:186:VAL:HG22	1.89	0.55
23:K:21:VAL:HB	23:K:66:TYR:HB2	1.89	0.55
1:2:863:A:N7	1:2:964:U:O4	2.39	0.55
7:H:96:ARG:HD2	7:H:121:VAL:HG13	1.88	0.55
22:F:57:SER:OG	31:c:53:ILE:O	2.23	0.55
1:2:883:C:N3	1:2:945:U:O4	2.40	0.55
3:B:181:LEU:HA	3:B:184:LEU:HB3	1.89	0.55
33:g:117:LYS:HE2	33:g:159:ASN:H	1.72	0.55
1:2:621:A:HO2'	1:2:1106:U:HO2'	1.55	0.55
1:2:1054:U:H3	1:2:1065:A:H61	1.54	0.55
1:2:1132:A:H2'	1:2:1133:A:H8	1.72	0.55
22:F:149:VAL:HG23	31:c:67:ARG:H	1.72	0.55
25:P:68:PRO:HG2	25:P:71:GLU:HB2	1.87	0.55
1:2:1178:G:OP1	1:2:1190:C:N4	2.39	0.55
1:2:1382:A:H5''	29:U:60:THR:H	1.71	0.55
16:X:14:LYS:HE3	16:X:18:HIS:HE1	1.71	0.55
1:2:269:G:N7	6:G:186:ARG:NH2	2.56	0.54
22:F:82:PHE:O	22:F:86:GLN:NE2	2.39	0.54
1:2:1592:A:H2'	1:2:1593:A:H8	1.72	0.54
5:E:196:VAL:N	5:E:209:HIS:O	2.32	0.54
31:c:36:THR:OG1	31:c:37:SER:N	2.40	0.54
33:g:38:ARG:HA	33:g:67:ILE:HG23	1.89	0.54
1:2:1114:G:H22	1:2:1130:G:H2'	1.72	0.54
1:2:1542:G:N1	1:2:1568:C:O2	2.40	0.54
4:C:157:LYS:NZ	15:W:94:LEU:O	2.39	0.54
24:M:36:LEU:HG	24:M:102:GLY:HA2	1.89	0.54
16:X:90:ASP:O	16:X:136:TRP:NE1	2.39	0.54
33:g:19:TRP:HB2	33:g:38:ARG:HE	1.71	0.54
1:2:442:C:O2'	1:2:525:A:N1	2.37	0.54
1:2:1315:U:OP1	1:2:1328:G:N2	2.38	0.54
1:2:1347:U:O4	29:U:88:LYS:NZ	2.40	0.54
3:B:144:ARG:HB3	3:B:208:GLN:HB3	1.90	0.54
19:d:43:PHE:O	19:d:47:ALA:HB2	2.08	0.54
1:2:717:C:C4	1:2:720:G:N2	2.75	0.54
13:R:29:GLN:OE1	13:R:32:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:D:222:VAL:HG21	33:g:229:LYS:HA	1.90	0.54
25:P:118:GLU:HB3	27:S:122:HIS:H	1.73	0.54
33:g:33:LEU:HB3	33:g:45:TRP:HB2	1.90	0.54
1:2:886:U:O2'	12:O:121:VAL:O	2.23	0.54
1:2:1057:U:H1'	1:2:1058:U:H2'	1.88	0.54
3:B:144:ARG:NH2	3:B:207:LEU:O	2.37	0.54
33:g:33:LEU:HB2	33:g:47:LEU:HD11	1.90	0.54
1:2:1478:G:OP1	28:T:43:ASN:ND2	2.41	0.54
21:D:137:VAL:O	21:D:184:ILE:HA	2.07	0.54
28:T:4:VAL:HG11	28:T:137:ALA:HB2	1.90	0.54
33:g:289:ALA:HA	33:g:305:TYR:HA	1.90	0.54
4:C:116:LYS:HB2	4:C:131:ILE:HD12	1.89	0.54
1:2:1287:A:N1	1:2:1328:G:O2'	2.35	0.54
21:D:47:GLU:HA	21:D:85:VAL:O	2.08	0.54
1:2:688:G:H2'	1:2:689:G:H8	1.73	0.53
1:2:1470:C:H3'	1:2:1573:A:H62	1.73	0.53
1:2:1584:G:N2	1:2:1611:A:O5'	2.41	0.53
2:A:52:LYS:HE2	14:V:81:ASN:HB3	1.89	0.53
4:C:37:PRO:HG2	4:C:43:ARG:HG2	1.89	0.53
6:G:159:ARG:NH2	6:G:170:THR:O	2.41	0.53
9:J:109:LEU:HB2	9:J:146:PHE:HB3	1.89	0.53
1:2:480:G:O6	1:2:508:U:O4	2.25	0.53
25:P:110:GLU:HG2	27:S:118:LYS:HD3	1.89	0.53
26:Q:82:ARG:NH1	26:Q:114:ARG:O	2.38	0.53
24:M:59:LEU:HB3	24:M:123:VAL:HB	1.88	0.53
32:f:138:ARG:HD3	32:f:149:LYS:HG3	1.91	0.53
1:2:753:A:OP2	5:E:187:ARG:N	2.38	0.53
1:2:1182:U:N3	1:2:1185:U:OP2	2.40	0.53
1:2:1681:A:N6	1:2:1720:G:O2'	2.41	0.53
1:2:490:C:H41	1:2:498:G:H21	1.57	0.53
1:2:1243:G:OP1	25:P:59:LYS:NZ	2.36	0.53
1:2:1775:U:O2	1:2:1786:G:N2	2.34	0.53
7:H:112:ARG:NH2	7:H:117:THR:OG1	2.41	0.53
26:Q:58:ASP:OD1	26:Q:58:ASP:N	2.40	0.53
27:S:100:THR:HG21	27:S:108:LYS:HG3	1.91	0.53
33:g:7:LEU:HG	33:g:315:VAL:HG22	1.89	0.53
3:B:170:GLU:HG2	3:B:174:LYS:HE3	1.90	0.53
5:E:180:LEU:N	5:E:229:GLY:O	2.41	0.53
18:b:33:LEU:O	18:b:45:THR:HA	2.09	0.53
1:2:996:U:O2	1:2:1008:G:N2	2.36	0.53
21:D:28:GLU:OE2	21:D:65:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1284:C:OP2	1:2:1623:C:O2'	2.22	0.53
9:J:102:GLU:HA	9:J:105:LEU:HB2	1.90	0.53
16:X:58:GLY:HA2	16:X:70:LYS:HA	1.91	0.53
24:M:28:LEU:HD11	24:M:61:VAL:HG21	1.91	0.53
29:U:27:THR:HG23	29:U:113:ASP:HB3	1.91	0.53
1:2:17:C:O2'	1:2:1137:A:N1	2.42	0.53
1:2:887:A:H2	1:2:925:G:N1	1.98	0.53
1:2:1601:G:H22	28:T:88:VAL:HG22	1.74	0.53
11:N:56:ASP:OD2	18:b:52:THR:OG1	2.27	0.53
1:2:687:G:OP1	15:W:118:ARG:NH1	2.42	0.53
1:2:953:G:H2'	1:2:954:G:H8	1.74	0.53
2:A:66:ALA:HB2	14:V:37:ALA:HB2	1.91	0.53
14:V:71:ARG:HE	18:b:4:VAL:HG11	1.74	0.53
33:g:159:ASN:ND2	33:g:166:SER:O	2.42	0.53
1:2:564:G:OP1	20:e:13:LYS:NZ	2.42	0.52
1:2:1542:G:N2	1:2:1569:A:OP2	2.43	0.52
2:A:184:LEU:HD12	14:V:45:ALA:HB2	1.91	0.52
15:W:22:LYS:HD3	18:b:3:LEU:HD13	1.91	0.52
21:D:167:PHE:HD1	21:D:190:ARG:HE	1.54	0.52
22:F:25:LEU:HB2	26:Q:27:GLY:HA3	1.91	0.52
1:2:130:C:HO2'	1:2:137:U:H3	1.57	0.52
1:2:1253:U:O5'	24:M:46:ARG:NH2	2.41	0.52
1:2:1431:C:O4'	1:2:1436:A:N6	2.42	0.52
12:O:133:ARG:HH21	12:O:136:ARG:HG2	1.74	0.52
14:V:36:VAL:O	14:V:50:TYR:HA	2.09	0.52
22:F:133:VAL:HA	22:F:198:LEU:HD22	1.90	0.52
28:T:45:MET:HE3	28:T:46:PRO:HD2	1.90	0.52
1:2:335:U:O3'	10:L:129:ARG:NH1	2.42	0.52
1:2:740:A:OP1	10:L:43:LYS:NZ	2.41	0.52
1:2:1234:A:HO2'	32:f:140:TYR:HH	1.52	0.52
24:M:57:ALA:HB3	24:M:85:LYS:HZ1	1.74	0.52
1:2:844:A:H2'	1:2:845:G:C8	2.44	0.52
1:2:1572:G:O3'	22:F:185:ARG:NH2	2.42	0.52
2:A:103:THR:O	2:A:106:SER:OG	2.26	0.52
5:E:100:ARG:HH12	5:E:122:LYS:HA	1.75	0.52
24:M:41:LEU:HD22	24:M:121:VAL:HB	1.91	0.52
27:S:48:LYS:NZ	28:T:47:PRO:O	2.43	0.52
14:V:84:SER:H	14:V:87:ARG:HH21	1.57	0.52
1:2:398:G:OP2	8:I:47:ARG:NH1	2.38	0.52
1:2:838:G:O2'	10:L:26:LYS:O	2.27	0.52
1:2:939:A:OP1	11:N:114:ARG:NH2	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:11:ARG:NH1	5:E:21:ASP:OD1	2.42	0.52
5:E:36:HIS:NE2	5:E:88:ASP:OD2	2.40	0.52
33:g:109:ASP:HB2	33:g:127:ARG:HD2	1.92	0.52
1:2:1203:A:C2	1:2:1553:G:N2	2.73	0.52
22:F:49:GLU:O	22:F:51:VAL:N	2.43	0.52
1:2:992:A:OP2	1:2:1011:G:N1	2.32	0.52
1:2:1005:A:HO2'	1:2:1784:C:HO2'	1.57	0.52
5:E:31:PRO:HG3	5:E:43:PRO:HG3	1.90	0.52
9:J:108:ARG:HH21	9:J:144:PRO:HB2	1.75	0.52
4:C:165:VAL:HG11	4:C:210:THR:HA	1.90	0.52
13:R:115:LEU:HD13	13:R:116:LYS:H	1.74	0.52
27:S:132:ARG:HH12	27:S:145:ARG:HD3	1.73	0.52
1:2:271:A:H61	6:G:185:GLN:HE22	1.58	0.52
1:2:1147:A:N6	1:2:1630:U:O4	2.42	0.52
1:2:1173:C:H5'	1:2:1543:A:H4'	1.92	0.52
1:2:1441:C:O2'	1:2:1447:C:N4	2.42	0.52
1:2:1560:U:O2'	1:2:1599:C:O2	2.28	0.52
1:2:1638:G:O6	1:2:1766:A:C5	2.63	0.52
3:B:121:ILE:HG12	3:B:161:ILE:HG23	1.92	0.52
28:T:28:LEU:HD13	28:T:30:VAL:HG22	1.91	0.52
29:U:48:HIS:CE1	29:U:99:ILE:HG12	2.45	0.52
1:2:104:A:OP2	1:2:308:C:N4	2.31	0.51
31:c:8:THR:HB	31:c:56:LEU:HB2	1.91	0.51
1:2:5:U:H2'	1:2:6:G:H8	1.75	0.51
1:2:794:U:O2	1:2:795:U:N3	2.43	0.51
1:2:958:U:O2'	1:2:960:U:OP2	2.26	0.51
1:2:1056:U:O2'	3:B:202:LYS:NZ	2.43	0.51
1:2:1588:G:H1	1:2:1608:U:H3	1.57	0.51
1:2:1672:G:H2'	1:2:1673:G:C8	2.45	0.51
26:Q:58:ASP:O	26:Q:60:PHE:N	2.35	0.51
29:U:21:LYS:HA	29:U:94:GLU:HA	1.91	0.51
1:2:273:G:N2	1:2:283:U:O2	2.37	0.51
1:2:1546:G:N7	27:S:134:ARG:NH2	2.57	0.51
10:L:125:VAL:HG12	10:L:139:VAL:HA	1.92	0.51
1:2:1146:G:OP2	4:C:91:ARG:NH1	2.43	0.51
7:H:4:PRO:HA	7:H:7:LYS:HB2	1.92	0.51
1:2:460:A:H3'	1:2:461:G:H8	1.76	0.51
1:2:887:A:C2	1:2:925:G:N1	2.56	0.51
6:G:2:LYS:HB3	6:G:108:VAL:HG22	1.91	0.51
1:2:687:G:H4'	15:W:119:LYS:HG2	1.92	0.51
3:B:141:ALA:HB1	3:B:207:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1596:C:OP1	19:d:19:ARG:NH2	2.42	0.51
20:e:34:ALA:O	20:e:37:ARG:HB2	2.10	0.51
22:F:142:PRO:HD2	22:F:167:ARG:HG2	1.91	0.51
31:c:10:ALA:HA	31:c:32:PHE:HA	1.93	0.51
33:g:22:SER:HB3	33:g:36:ALA:HB3	1.91	0.51
1:2:1268:G:N2	1:2:1447:C:O2	2.39	0.51
28:T:27:LYS:HD3	28:T:111:ILE:HG23	1.93	0.51
1:2:1042:G:H2'	1:2:1043:A:H8	1.75	0.51
1:2:1295:G:H2'	1:2:1296:A:C8	2.46	0.51
10:L:92:HIS:O	10:L:100:TYR:HA	2.10	0.51
22:F:76:ARG:NH1	26:Q:121:SER:OG	2.43	0.51
28:T:7:ARG:HA	28:T:67:MET:HE2	1.92	0.51
29:U:65:ILE:HB	29:U:82:TYR:HB2	1.93	0.51
5:E:180:LEU:HD23	5:E:194:THR:HG22	1.93	0.51
32:f:140:TYR:OH	32:f:145:HIS:O	2.29	0.51
33:g:12:THR:HG22	33:g:311:ARG:HG2	1.92	0.51
1:2:996:U:O4	1:2:1008:G:O6	2.29	0.50
1:2:1300:A:C6	1:2:1301:U:H1'	2.47	0.50
1:2:1529:C:H1'	28:T:12:GLN:HE22	1.76	0.50
4:C:60:SER:OG	14:V:25:LYS:O	2.28	0.50
22:F:40:ILE:HG23	22:F:42:LEU:HB3	1.93	0.50
33:g:80:ALA:HB2	33:g:94:VAL:HG22	1.93	0.50
33:g:211:ILE:HB	33:g:223:TRP:HB2	1.93	0.50
1:2:931:C:O2'	3:B:118:GLN:O	2.27	0.50
3:B:168:ILE:HG12	3:B:197:ILE:HD12	1.94	0.50
33:g:211:ILE:O	33:g:222:LEU:HA	2.11	0.50
4:C:105:GLY:HA3	4:C:190:LEU:HB3	1.92	0.50
1:2:1390:U:OP2	13:R:49:LYS:NZ	2.40	0.50
1:2:1535:U:H5''	22:F:187:ILE:HD11	1.92	0.50
25:P:31:GLU:HA	25:P:34:VAL:HG22	1.92	0.50
33:g:28:GLY:N	33:g:75:ALA:O	2.38	0.50
1:2:246:G:N2	10:L:38:ALA:O	2.40	0.50
1:2:1277:G:H3'	1:2:1278:G:H8	1.76	0.50
1:2:1390:U:OP1	13:R:5:ARG:NH2	2.43	0.50
21:D:65:ARG:HD2	21:D:68:GLU:HB2	1.92	0.50
22:F:43:PHE:HB3	22:F:46:TRP:HB2	1.94	0.50
23:K:8:ARG:O	23:K:12:HIS:ND1	2.34	0.50
1:2:1173:C:O2'	1:2:1601:G:N1	2.43	0.50
1:2:1564:U:O2'	27:S:84:TRP:O	2.28	0.50
1:2:1682:U:O4	1:2:1720:G:N2	2.45	0.50
3:B:137:ILE:HD12	3:B:172:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:85:ILE:HG22	25:P:112:LEU:HD23	1.94	0.50
1:2:58:U:O2'	1:2:451:A:N3	2.42	0.50
1:2:870:C:H2'	1:2:871:G:H8	1.76	0.50
1:2:884:A:H2'	1:2:885:G:C8	2.46	0.50
13:R:17:ILE:HD11	13:R:57:LEU:HB3	1.92	0.50
19:d:30:LEU:HA	19:d:39:CYS:HA	1.94	0.50
25:P:44:ARG:HH12	25:P:82:ASN:HB2	1.75	0.50
1:2:766:U:H3	1:2:770:A:H62	1.59	0.50
1:2:1213:G:H1	1:2:1450:U:H3	1.59	0.50
4:C:54:GLU:O	4:C:58:LEU:HB2	2.11	0.50
23:K:10:LYS:HD3	23:K:36:ASP:HB3	1.93	0.50
25:P:127:ARG:HA	25:P:130:ARG:HH11	1.77	0.50
26:Q:32:ASN:HD21	26:Q:69:VAL:H	1.59	0.50
1:2:632:U:O2'	1:2:1103:U:OP1	2.29	0.50
1:2:1001:A:N6	1:2:1766:A:O2'	2.45	0.50
1:2:1534:G:OP2	30:Z:74:SER:OG	2.25	0.50
25:P:22:LEU:HA	25:P:25:LEU:HB2	1.94	0.50
1:2:126:A:N1	1:2:263:C:O2'	2.41	0.49
1:2:1272:U:O2	1:2:1438:G:O6	2.30	0.49
4:C:180:ALA:O	4:C:185:LYS:NZ	2.45	0.49
30:Z:88:ILE:O	30:Z:104:ALA:N	2.39	0.49
33:g:26:SER:HB2	33:g:73:LEU:HD13	1.94	0.49
1:2:252:U:H2'	1:2:253:A:H8	1.77	0.49
1:2:812:A:C8	1:2:858:G:N2	2.80	0.49
1:2:1501:C:OP2	28:T:102:ARG:NE	2.41	0.49
8:I:117:TYR:OH	8:I:149:SER:OG	2.26	0.49
15:W:89:TRP:HE3	15:W:93:LEU:HD21	1.77	0.49
28:T:62:ALA:HB1	28:T:132:LEU:HD11	1.94	0.49
29:U:53:LYS:HD3	29:U:92:ASP:HB2	1.93	0.49
1:2:592:A:O2'	1:2:596:C:OP1	2.30	0.49
1:2:705:U:H2'	1:2:706:A:C8	2.47	0.49
1:2:947:U:O3'	3:B:166:LYS:NZ	2.45	0.49
1:2:1041:G:H2'	1:2:1042:G:C8	2.47	0.49
1:2:1047:G:H2'	1:2:1048:G:C8	2.47	0.49
1:2:1605:G:H8	26:Q:127:LYS:HD2	1.77	0.49
7:H:82:GLU:OE2	7:H:165:LYS:NZ	2.36	0.49
28:T:9:VAL:HG21	28:T:136:ALA:HB1	1.95	0.49
1:2:561:G:H2'	1:2:562:G:H8	1.77	0.49
16:X:126:LYS:HG2	16:X:131:SER:HA	1.95	0.49
21:D:137:VAL:HB	21:D:185:LYS:HB2	1.93	0.49
27:S:123:ARG:HG3	27:S:133:VAL:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:g:248:ASN:ND2	33:g:297:ASP:O	2.46	0.49
1:2:114:C:HO2'	10:L:65:SER:HG	1.61	0.49
1:2:868:G:OP1	11:N:121:ARG:NH1	2.45	0.49
8:I:27:PHE:HB3	8:I:49:ARG:HH12	1.76	0.49
24:M:58:LEU:HD21	24:M:125:ASN:HA	1.93	0.49
33:g:178:VAL:HB	33:g:192:PHE:HB2	1.93	0.49
33:g:238:ASP:HB2	33:g:256:THR:HB	1.94	0.49
1:2:143:G:N7	6:G:177:ARG:NH2	2.59	0.49
1:2:1356:U:O2	1:2:1367:G:O6	2.30	0.49
17:Y:14:SER:HA	17:Y:21:LYS:HG3	1.94	0.49
1:2:406:U:H2'	1:2:407:A:C8	2.48	0.49
1:2:775:G:O6	1:2:785:U:O2	2.30	0.49
1:2:1181:U:O2'	25:P:126:VAL:O	2.29	0.49
1:2:1208:A:N1	1:2:1455:G:N2	2.60	0.49
1:2:1329:A:H3'	1:2:1330:G:H8	1.78	0.49
2:A:107:PHE:HB2	2:A:135:GLU:HG3	1.95	0.49
5:E:141:THR:OG1	5:E:143:ASP:OD1	2.27	0.49
13:R:35:CYS:HA	13:R:38:ILE:HG22	1.93	0.49
21:D:107:PHE:O	21:D:111:ASN:N	2.45	0.49
33:g:112:SER:HB2	33:g:153:GLN:HA	1.94	0.49
1:2:1323:C:H2'	1:2:1324:G:C8	2.48	0.49
1:2:1333:C:H5'	21:D:162:GLN:HG2	1.95	0.49
1:2:1475:A:H1'	1:2:1540:G:H5''	1.95	0.49
6:G:57:ASP:HA	6:G:106:LEU:HA	1.95	0.49
21:D:65:ARG:O	21:D:69:LEU:N	2.36	0.49
27:S:28:ILE:HD12	27:S:61:LEU:HG	1.95	0.49
1:2:976:G:H1	1:2:1023:A:HO2'	1.59	0.49
23:K:11:ILE:HD13	23:K:35:ILE:HG21	1.95	0.49
27:S:88:ARG:NE	27:S:91:ASP:OD1	2.45	0.49
1:2:149:C:O2'	6:G:132:ARG:NH1	2.44	0.49
1:2:152:U:OP2	17:Y:127:LYS:NZ	2.44	0.49
1:2:514:G:OP1	9:J:132:ARG:NH2	2.44	0.49
1:2:738:G:H2'	1:2:739:G:H8	1.78	0.49
1:2:1312:A:H2'	1:2:1313:A:C8	2.48	0.49
1:2:1366:U:O2'	28:T:7:ARG:NH1	2.43	0.49
10:L:109:VAL:HG21	10:L:125:VAL:HG11	1.95	0.49
33:g:180:ALA:HB3	33:g:190:ALA:HB3	1.95	0.49
22:F:27:THR:OG1	26:Q:29:ILE:N	2.41	0.48
28:T:7:ARG:HG2	28:T:67:MET:HG2	1.95	0.48
30:Z:60:VAL:HG23	30:Z:101:TYR:HB2	1.94	0.48
1:2:78:A:H2'	1:2:79:C:H6	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:d:21:CYS:HB3	19:d:26:SER:H	1.78	0.48
33:g:59:ARG:HD2	33:g:61:PHE:HE1	1.78	0.48
1:2:1220:C:H2'	1:2:1221:A:H8	1.77	0.48
1:2:1228:G:OP1	24:M:119:SER:OG	2.32	0.48
1:2:1482:C:N3	1:2:1525:A:N7	2.61	0.48
1:2:1570:A:OP2	1:2:1571:C:N4	2.45	0.48
33:g:36:ALA:HB2	33:g:71:CYS:HB3	1.95	0.48
1:2:992:A:O2'	1:2:1785:U:O2	2.22	0.48
1:2:1547:A:H2'	1:2:1548:G:C8	2.49	0.48
5:E:159:THR:HB	5:E:227:VAL:HG23	1.95	0.48
10:L:133:LYS:O	10:L:136:ARG:NH1	2.37	0.48
25:P:30:THR:HG23	25:P:86:VAL:HG21	1.95	0.48
26:Q:16:ALA:HB2	26:Q:72:GLY:HA3	1.95	0.48
27:S:14:ILE:HD11	27:S:21:ASN:HB3	1.94	0.48
28:T:16:ASN:OD1	28:T:56:LYS:NZ	2.46	0.48
33:g:51:ASP:N	33:g:51:ASP:OD1	2.46	0.48
33:g:154:VAL:O	33:g:155:ARG:NH1	2.43	0.48
1:2:523:G:O2'	1:2:529:A:N6	2.45	0.48
1:2:934:C:O2	1:2:1076:A:O2'	2.31	0.48
1:2:1146:G:H2'	1:2:1147:A:C8	2.48	0.48
1:2:1200:G:OP1	1:2:1595:U:O2'	2.32	0.48
1:2:1483:A:H4'	26:Q:71:GLY:HA2	1.95	0.48
21:D:106:LYS:HG3	21:D:175:VAL:HB	1.95	0.48
28:T:115:GLU:OE2	28:T:123:ARG:NH1	2.47	0.48
33:g:35:SER:OG	33:g:43:ILE:O	2.26	0.48
1:2:612:U:OP2	16:X:5:LYS:NZ	2.46	0.48
8:I:113:PHE:O	8:I:117:TYR:N	2.47	0.48
25:P:95:GLY:HA2	25:P:103:ASN:O	2.14	0.48
30:Z:49:ARG:O	30:Z:53:GLU:HB2	2.13	0.48
32:f:135:HIS:H	32:f:138:ARG:HB3	1.78	0.48
1:2:1027:A:OP1	1:2:1789:G:O2'	2.31	0.48
1:2:1483:A:N3	1:2:1607:G:O2'	2.39	0.48
7:H:46:ILE:HD11	7:H:58:LEU:HB3	1.93	0.48
14:V:84:SER:HB2	14:V:87:ARG:HE	1.79	0.48
22:F:76:ARG:HH11	26:Q:121:SER:H	1.62	0.48
26:Q:10:PHE:HA	26:Q:18:ALA:O	2.13	0.48
1:2:887:A:N1	1:2:925:G:C6	2.82	0.48
1:2:1609:U:H5''	26:Q:75:VAL:HB	1.95	0.48
1:2:1616:G:H4'	31:c:18:ARG:HG3	1.96	0.48
2:A:200:ASP:HB2	13:R:85:VAL:HG23	1.94	0.48
3:B:188:LEU:HD23	3:B:193:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:F:95:ASN:HA	22:F:98:MET:HE2	1.96	0.48
24:M:43:ARG:NH1	24:M:102:GLY:O	2.46	0.48
1:2:200:A:H2'	1:2:201:G:C8	2.49	0.48
1:2:406:U:H2'	1:2:407:A:H8	1.78	0.48
1:2:544:A:O2'	20:e:28:LYS:NZ	2.47	0.48
7:H:47:ARG:HB2	7:H:59:ALA:HB3	1.96	0.48
21:D:23:GLU:HB3	23:K:61:TRP:HE1	1.78	0.48
22:F:46:TRP:NE1	22:F:122:ASN:OD1	2.38	0.47
1:2:167:U:H1'	6:G:133:LEU:HD23	1.95	0.47
1:2:512:A:H2'	1:2:513:U:C6	2.49	0.47
1:2:803:A:C4	7:H:104:ARG:HG3	2.49	0.47
1:2:926:A:OP1	1:2:1016:C:O2'	2.31	0.47
9:J:101:VAL:O	9:J:104:PHE:HB2	2.14	0.47
14:V:62:ARG:HH12	15:W:20:THR:HB	1.77	0.47
30:Z:61:SER:H	30:Z:64:VAL:HB	1.79	0.47
1:2:405:C:O2'	6:G:92:ARG:O	2.32	0.47
7:H:166:LEU:O	7:H:169:PHE:HB2	2.13	0.47
8:I:61:GLU:HG3	8:I:62:THR:HG23	1.97	0.47
9:J:23:ARG:NH1	9:J:27:GLU:OE2	2.47	0.47
13:R:41:ILE:HD12	13:R:47:ARG:HG2	1.95	0.47
1:2:683:C:H2'	1:2:684:A:H8	1.80	0.47
1:2:1592:A:H2'	1:2:1593:A:C8	2.48	0.47
1:2:1639:C:H1'	1:2:1640:C:H5	1.78	0.47
8:I:36:THR:OG1	8:I:96:LEU:O	2.33	0.47
15:W:103:ILE:HA	15:W:112:ASP:HA	1.96	0.47
25:P:108:ARG:HB2	25:P:111:MET:HG3	1.96	0.47
1:2:925:G:H2'	1:2:926:A:C8	2.49	0.47
7:H:162:ILE:HG22	7:H:165:LYS:HD2	1.97	0.47
1:2:396:G:N1	1:2:399:A:OP2	2.48	0.47
1:2:478:A:O5'	20:e:33:ARG:NH2	2.47	0.47
1:2:1459:C:OP1	27:S:126:ARG:NH1	2.47	0.47
1:2:1793:G:H1'	1:2:1794:A:H2'	1.97	0.47
21:D:116:ARG:HG2	21:D:152:PHE:HE1	1.79	0.47
26:Q:42:GLU:HG3	26:Q:45:ARG:HH12	1.80	0.47
1:2:707:A:N1	1:2:730:G:N2	2.62	0.47
1:2:1122:G:N2	1:2:1125:A:OP2	2.39	0.47
1:2:1347:U:H5	29:U:23:ARG:HH21	1.62	0.47
1:2:1638:G:C6	1:2:1766:A:N7	2.83	0.47
1:2:1734:U:H2'	1:2:1735:U:H6	1.79	0.47
8:I:76:THR:HG22	8:I:108:PRO:HG2	1.97	0.47
17:Y:20:ARG:HD2	17:Y:74:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:D:173:ARG:HB2	21:D:184:ILE:HB	1.97	0.47
27:S:75:ASN:HB3	27:S:78:HIS:HB2	1.97	0.47
32:f:139:LEU:HB2	32:f:151:ASN:HA	1.96	0.47
1:2:1099:U:O4	4:C:168:ARG:NH1	2.43	0.47
23:K:29:GLN:OE1	23:K:39:ASN:ND2	2.38	0.47
30:Z:41:ILE:HD12	30:Z:41:ILE:HA	1.83	0.47
33:g:300:THR:HA	33:g:313:TRP:O	2.14	0.47
1:2:778:G:H1	17:Y:10:ARG:HG2	1.80	0.47
1:2:822:U:H2'	1:2:823:G:N3	2.30	0.47
1:2:868:G:H2'	1:2:869:A:H8	1.79	0.47
1:2:885:G:OP1	3:B:136:ARG:NH1	2.48	0.47
1:2:1032:G:O6	1:2:1103:U:O2	2.33	0.47
4:C:142:GLY:N	4:C:153:SER:O	2.48	0.47
6:G:98:ARG:HH21	6:G:99:GLY:H	1.63	0.47
30:Z:54:VAL:HG13	30:Z:57:TYR:HB2	1.97	0.47
1:2:1638:G:H1'	1:2:1767:G:H1	1.80	0.47
6:G:57:ASP:HA	6:G:107:ALA:H	1.80	0.47
1:2:369:A:O2'	1:2:371:G:OP2	2.26	0.46
1:2:1435:G:N7	23:K:25:LYS:NZ	2.57	0.46
1:2:1665:U:H2'	1:2:1666:U:H6	1.80	0.46
5:E:44:LEU:HG	5:E:82:TYR:HB3	1.98	0.46
7:H:6:ALA:HA	7:H:9:LEU:HB3	1.96	0.46
8:I:113:PHE:HE2	8:I:119:GLN:HB2	1.81	0.46
28:T:76:LEU:HD22	28:T:80:TYR:HE2	1.80	0.46
1:2:1482:C:OP2	1:2:1521:G:N2	2.38	0.46
3:B:140:ILE:HB	3:B:213:ARG:HD3	1.97	0.46
17:Y:22:GLN:HB3	17:Y:74:LEU:HD23	1.96	0.46
22:F:89:ILE:HA	22:F:92:ARG:HB2	1.97	0.46
28:T:37:VAL:HG21	28:T:100:ILE:HD11	1.96	0.46
29:U:28:SER:HB3	29:U:34:LEU:HB2	1.96	0.46
33:g:21:THR:OG1	33:g:68:VAL:O	2.33	0.46
33:g:239:GLU:HB3	33:g:257:ALA:HB2	1.97	0.46
2:A:52:LYS:HD3	14:V:82:VAL:HG22	1.97	0.46
8:I:117:TYR:HB3	8:I:119:GLN:HG2	1.98	0.46
32:f:107:LYS:HE3	32:f:117:LEU:HD11	1.98	0.46
1:2:123:G:OP1	5:E:77:ARG:NH2	2.40	0.46
1:2:168:A:OP1	6:G:140:ASN:ND2	2.45	0.46
1:2:984:G:O6	1:2:1017:U:O2	2.32	0.46
1:2:1569:A:H2'	1:2:1570:A:H8	1.81	0.46
26:Q:94:GLN:HB2	26:Q:102:LYS:HG3	1.97	0.46
31:c:13:ILE:HD13	31:c:31:GLU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:848:C:H2'	1:2:849:C:C2	2.51	0.46
1:2:1443:U:H5''	1:2:1444:A:H5'	1.97	0.46
1:2:1477:G:H2'	1:2:1478:G:C8	2.50	0.46
8:I:11:ARG:NH1	8:I:15:GLY:O	2.47	0.46
8:I:84:HIS:NE2	8:I:97:THR:OG1	2.49	0.46
15:W:15:ASN:HD21	15:W:71:LYS:HA	1.79	0.46
26:Q:60:PHE:HE1	26:Q:89:LEU:HD13	1.81	0.46
1:2:114:C:O2'	10:L:65:SER:OG	2.31	0.46
1:2:922:G:H2'	1:2:923:A:H8	1.81	0.46
13:R:19:ARG:HD3	21:D:210:GLU:HA	1.97	0.46
24:M:135:MET:O	24:M:139:HIS:HB2	2.16	0.46
1:2:307:G:OP1	10:L:103:ARG:NH1	2.48	0.46
1:2:591:A:OP1	20:e:43:ARG:NH2	2.49	0.46
1:2:877:G:O4'	1:2:937:C:O2'	2.30	0.46
33:g:249:ARG:HD2	33:g:251:TRP:CD2	2.51	0.46
1:2:1026:A:N3	1:2:1790:A:O2'	2.46	0.46
1:2:1068:C:H2'	1:2:1069:A:C8	2.51	0.46
13:R:55:THR:O	13:R:59:LYS:CB	2.63	0.46
32:f:109:ASP:HB2	32:f:113:LYS:HG3	1.97	0.46
32:f:132:LEU:HA	32:f:140:TYR:O	2.16	0.46
33:g:133:VAL:HB	33:g:142:ALA:HB3	1.98	0.46
1:2:561:G:H2'	1:2:562:G:C8	2.50	0.46
1:2:1066:C:O2'	3:B:148:ASN:O	2.34	0.46
1:2:1227:A:H5'	1:2:1228:G:C8	2.51	0.46
1:2:1339:C:O2'	1:2:1341:A:N6	2.39	0.46
1:2:1655:A:H61	1:2:1746:A:H2	1.64	0.46
1:2:1759:C:H2'	1:2:1760:G:C8	2.51	0.46
8:I:39:GLY:HA2	8:I:61:GLU:HB3	1.97	0.46
10:L:36:LYS:NZ	10:L:64:VAL:O	2.36	0.46
1:2:283:U:H5''	6:G:188:ARG:HD3	1.98	0.46
1:2:1387:G:O2'	1:2:1411:A:N6	2.43	0.46
1:2:1605:G:C8	26:Q:127:LYS:HD2	2.51	0.46
7:H:49:ILE:HD11	7:H:172:VAL:HG22	1.98	0.46
16:X:16:ARG:HE	16:X:20:ARG:HH12	1.64	0.46
29:U:44:ASN:O	29:U:48:HIS:NE2	2.49	0.46
1:2:392:G:OP1	8:I:2:GLY:N	2.50	0.45
4:C:53:ILE:HD11	4:C:73:LEU:HB2	1.98	0.45
21:D:37:VAL:HA	21:D:49:ILE:O	2.15	0.45
22:F:144:GLU:OE1	22:F:225:ARG:NH2	2.49	0.45
30:Z:70:LYS:HB3	30:Z:71:ILE:H	1.64	0.45
1:2:24:U:OP1	9:J:10:LYS:NZ	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:311:U:OP1	16:X:24:TRP:NE1	2.45	0.45
9:J:77:ILE:HD11	9:J:93:LEU:HB2	1.97	0.45
21:D:202:LEU:HB3	21:D:204:ASP:H	1.80	0.45
1:2:1567:U:H5''	27:S:37:GLY:H	1.82	0.45
9:J:110:GLN:NE2	9:J:122:VAL:O	2.49	0.45
21:D:11:LEU:HD12	29:U:86:ILE:HG12	1.99	0.45
22:F:29:ILE:HD13	26:Q:57:LEU:HD21	1.98	0.45
1:2:158:U:O2'	1:2:160:C:OP2	2.29	0.45
1:2:565:C:OP2	1:2:577:G:O2'	2.34	0.45
1:2:656:G:O2'	1:2:657:U:O4'	2.33	0.45
1:2:1042:G:H2'	1:2:1043:A:C8	2.51	0.45
1:2:1156:C:H2'	1:2:1157:A:C8	2.51	0.45
6:G:134:GLY:HA3	6:G:158:ILE:HG21	1.98	0.45
21:D:74:GLN:HA	21:D:79:TYR:HB2	1.97	0.45
25:P:55:GLY:HA2	25:P:58:LYS:HZ2	1.82	0.45
1:2:717:C:N3	1:2:720:G:C2	2.85	0.45
1:2:1087:A:H2'	1:2:1088:A:C8	2.52	0.45
1:2:1639:C:O2	1:2:1640:C:N4	2.39	0.45
22:F:88:PRO:HG2	22:F:91:GLU:HB3	1.98	0.45
33:g:273:ASP:OD2	33:g:275:ARG:NH1	2.49	0.45
1:2:513:U:H2'	1:2:514:G:C8	2.51	0.45
1:2:1064:G:H2'	1:2:1065:A:C8	2.51	0.45
1:2:1132:A:H2'	1:2:1133:A:C8	2.51	0.45
1:2:1213:G:O2'	1:2:1244:A:N6	2.50	0.45
1:2:1450:U:H2'	1:2:1451:C:C6	2.52	0.45
8:I:103:GLN:HE21	8:I:164:ARG:HB3	1.82	0.45
10:L:59:PRO:HB3	10:L:66:ILE:HD11	1.98	0.45
33:g:85:TRP:CD1	33:g:109:ASP:HB3	2.52	0.45
1:2:572:C:OP1	16:X:109:ARG:NH2	2.49	0.45
1:2:1569:A:H2'	1:2:1570:A:C8	2.52	0.45
1:2:1642:G:C2	1:2:1759:C:O2	2.69	0.45
2:A:79:ARG:NH2	2:A:164:ASN:O	2.49	0.45
7:H:172:VAL:O	7:H:176:LEU:N	2.50	0.45
14:V:67:ASP:HA	14:V:70:ASN:HD22	1.81	0.45
27:S:82:PRO:HB2	27:S:84:TRP:CD1	2.52	0.45
33:g:23:LEU:HD13	33:g:302:PHE:HB3	1.99	0.45
1:2:1787:C:H2'	1:2:1788:G:H8	1.82	0.45
2:A:18:LEU:HA	2:A:23:HIS:CD2	2.52	0.45
9:J:51:LYS:O	9:J:54:ARG:NH2	2.50	0.45
33:g:43:ILE:HA	33:g:59:ARG:O	2.16	0.45
1:2:343:C:H2'	1:2:344:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1240:U:N3	1:2:1243:G:OP2	2.45	0.45
1:2:1245:G:N1	1:2:1250:U:N3	2.64	0.45
6:G:88:ARG:HB3	6:G:91:GLU:HB2	1.99	0.45
16:X:61:SER:HB2	16:X:116:ASP:HB2	1.98	0.45
1:2:1022:C:H4'	1:2:1125:A:H61	1.82	0.45
1:2:1591:C:H2'	1:2:1592:A:C8	2.52	0.45
1:2:1787:C:H2'	1:2:1788:G:C8	2.52	0.45
7:H:137:GLY:HA3	7:H:153:LEU:HD12	1.99	0.45
16:X:6:PRO:HG3	16:X:14:LYS:HD3	1.99	0.45
1:2:29:U:H2'	1:2:30:G:C8	2.51	0.44
1:2:68:A:N6	6:G:132:ARG:O	2.49	0.44
1:2:513:U:OP1	9:J:133:HIS:NE2	2.50	0.44
1:2:1114:G:O2'	1:2:1130:G:O6	2.31	0.44
1:2:973:A:H2'	1:2:974:A:H8	1.83	0.44
1:2:1210:C:H2'	1:2:1211:A:H8	1.81	0.44
1:2:1251:U:H1'	1:2:1252:C:C6	2.52	0.44
1:2:1344:A:O2'	29:U:54:GLY:O	2.32	0.44
1:2:1451:C:H2'	1:2:1452:U:C6	2.52	0.44
8:I:38:ILE:HD11	8:I:81:VAL:HG23	1.98	0.44
13:R:96:SER:HA	13:R:97:ASN:HA	1.71	0.44
21:D:65:ARG:HA	21:D:68:GLU:HB2	1.99	0.44
25:P:123:TYR:HD2	25:P:125:PRO:HA	1.82	0.44
29:U:35:GLU:HA	29:U:38:SER:HB3	1.99	0.44
30:Z:80:LEU:HD22	30:Z:101:TYR:HD2	1.83	0.44
1:2:388:G:OP2	1:2:423:G:O2'	2.34	0.44
1:2:884:A:H5''	3:B:136:ARG:NE	2.32	0.44
1:2:967:A:OP2	11:N:124:ARG:NH2	2.30	0.44
21:D:132:LYS:HB2	21:D:191:ASP:HA	1.98	0.44
27:S:86:LEU:HG	27:S:99:HIS:HB2	1.98	0.44
29:U:22:ILE:HG13	29:U:100:VAL:HG11	1.99	0.44
33:g:29:GLN:HG2	33:g:32:LEU:HB2	1.98	0.44
1:2:5:U:H2'	1:2:6:G:C8	2.51	0.44
1:2:686:C:H2'	1:2:687:G:C8	2.53	0.44
1:2:1311:U:O2'	1:2:1313:A:N7	2.40	0.44
1:2:1556:A:H4'	1:2:1557:U:H5'	1.99	0.44
1:2:1645:G:H22	1:2:1756:A:H2	1.63	0.44
1:2:1746:A:H2'	1:2:1747:G:C8	2.53	0.44
22:F:225:ARG:HB2	31:c:61:ARG:HD2	1.98	0.44
1:2:85:A:N3	1:2:148:A:O2'	2.44	0.44
1:2:340:U:H2'	1:2:341:A:H8	1.83	0.44
1:2:753:A:H4'	5:E:221:ARG:HH12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:875:G:N2	1:2:952:A:N1	2.53	0.44
1:2:1557:U:OP2	1:2:1559:A:O2'	2.30	0.44
2:A:155:PHE:O	14:V:60:ARG:NH1	2.51	0.44
6:G:98:ARG:HE	6:G:106:LEU:HD21	1.81	0.44
7:H:87:ASP:O	7:H:88:ARG:NH1	2.47	0.44
23:K:10:LYS:NZ	23:K:36:ASP:OD2	2.41	0.44
29:U:31:VAL:O	29:U:35:GLU:HB2	2.18	0.44
31:c:31:GLU:OE2	31:c:36:THR:OG1	2.36	0.44
1:2:567:A:OP1	16:X:70:LYS:NZ	2.51	0.44
1:2:925:G:H2'	1:2:926:A:H8	1.83	0.44
1:2:1158:C:H6	1:2:1158:C:H2'	1.63	0.44
1:2:1590:G:H2'	1:2:1591:C:C6	2.52	0.44
2:A:124:THR:HG22	2:A:174:TRP:HE1	1.83	0.44
4:C:103:VAL:HG22	4:C:113:LEU:HD23	2.00	0.44
10:L:17:PRO:HG3	10:L:63:LEU:HD11	2.00	0.44
22:F:92:ARG:HA	22:F:95:ASN:HD22	1.81	0.44
26:Q:34:SER:OG	28:T:7:ARG:O	2.23	0.44
27:S:42:TYR:HA	27:S:85:PHE:HE2	1.82	0.44
27:S:48:LYS:HG2	27:S:54:LEU:HD21	2.00	0.44
33:g:61:PHE:HZ	33:g:94:VAL:HA	1.81	0.44
1:2:354:C:H5''	8:I:16:ALA:HB2	1.99	0.44
1:2:1287:A:H4'	1:2:1288:G:H5'	2.00	0.44
1:2:1295:G:O6	1:2:1302:U:O4	2.36	0.44
1:2:1476:C:H2'	1:2:1477:G:C8	2.53	0.44
7:H:48:GLU:HG2	7:H:56:LYS:HD3	2.00	0.44
7:H:67:LEU:O	7:H:71:HIS:ND1	2.37	0.44
8:I:193:LEU:O	8:I:197:THR:OG1	2.31	0.44
13:R:6:THR:OG1	13:R:7:LYS:N	2.51	0.44
23:K:30:ALA:HA	23:K:38:LYS:HA	1.99	0.44
32:f:109:ASP:N	32:f:113:LYS:O	2.50	0.44
33:g:224:ASN:O	33:g:228:LYS:N	2.50	0.44
1:2:1228:G:OP2	24:M:45:LEU:N	2.45	0.44
1:2:1291:G:H2'	1:2:1292:G:H8	1.83	0.44
11:N:119:GLU:HA	11:N:122:ILE:HD12	2.00	0.44
17:Y:87:PRO:HD2	17:Y:90:ARG:HD2	1.98	0.44
22:F:88:PRO:O	22:F:92:ARG:N	2.41	0.44
22:F:93:LEU:HD12	22:F:114:ILE:HD11	2.00	0.44
22:F:162:VAL:HG23	31:c:45:LYS:HB3	2.00	0.44
1:2:804:A:C8	15:W:107:SER:HA	2.53	0.43
1:2:852:C:H2'	1:2:853:G:C8	2.52	0.43
13:R:14:LYS:HG3	13:R:69:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:W:66:ASN:ND2	15:W:68:ARG:HE	2.16	0.43
1:2:849:C:H2'	1:2:850:A:C8	2.53	0.43
1:2:870:C:H2'	1:2:871:G:C8	2.52	0.43
1:2:1120:U:H2'	1:2:1121:C:C6	2.53	0.43
14:V:27:ASP:OD1	14:V:27:ASP:N	2.49	0.43
25:P:18:ARG:HB2	25:P:36:LEU:HD12	2.01	0.43
27:S:104:ASN:O	27:S:107:SER:HB2	2.18	0.43
1:2:954:G:H2'	1:2:955:A:H8	1.83	0.43
1:2:1064:G:N2	3:B:146:GLN:HE22	2.16	0.43
1:2:1617:U:O2'	31:c:21:SER:O	2.31	0.43
1:2:1676:U:OP1	8:I:44:HIS:ND1	2.47	0.43
27:S:101:LEU:O	27:S:105:VAL:N	2.41	0.43
1:2:732:G:H8	1:2:734:A:H61	1.67	0.43
1:2:836:U:H2'	1:2:837:G:C8	2.53	0.43
1:2:1073:G:H4'	11:N:10:GLY:HA2	2.00	0.43
1:2:1203:A:H61	1:2:1553:G:H1'	1.83	0.43
1:2:1482:C:C4	1:2:1525:A:N7	2.86	0.43
3:B:139:ALA:HA	3:B:212:VAL:HA	2.00	0.43
8:I:159:GLN:HE22	8:I:189:LEU:HD11	1.83	0.43
9:J:83:VAL:O	9:J:107:ARG:NE	2.52	0.43
11:N:16:ILE:HG13	11:N:62:GLN:HE22	1.82	0.43
15:W:23:ARG:HG3	18:b:4:VAL:HB	2.01	0.43
15:W:92:ASN:HB2	15:W:93:LEU:HD23	2.01	0.43
33:g:23:LEU:HD22	33:g:33:LEU:HD11	2.00	0.43
1:2:816:G:H22	1:2:855:A:H2	1.67	0.43
1:2:1276:U:H2'	1:2:1277:G:H8	1.82	0.43
1:2:1638:G:N1	1:2:1766:A:C8	2.86	0.43
1:2:1459:C:OP2	27:S:138:THR:OG1	2.36	0.43
1:2:1650:U:H2'	1:2:1651:A:N3	2.34	0.43
2:A:26:ALA:HB3	2:A:149:LEU:HB2	2.00	0.43
5:E:19:LEU:HB2	5:E:51:ARG:HH22	1.84	0.43
7:H:11:GLN:HG3	7:H:13:PRO:HD2	1.99	0.43
9:J:57:ARG:HD3	9:J:97:LEU:HD21	2.01	0.43
10:L:38:ALA:HB1	10:L:66:ILE:HD12	2.00	0.43
13:R:16:LEU:O	13:R:20:TYR:HB2	2.19	0.43
21:D:135:GLU:O	21:D:186:VAL:HA	2.18	0.43
26:Q:42:GLU:HG3	26:Q:45:ARG:HH22	1.83	0.43
1:2:218:A:N1	1:2:844:A:H1'	2.34	0.43
1:2:1481:C:H5''	28:T:68:ARG:HH22	1.82	0.43
1:2:1570:A:H4'	27:S:144:ARG:HH22	1.84	0.43
9:J:62:ARG:HB2	9:J:69:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:S:26:ILE:O	27:S:58:ALA:N	2.51	0.43
33:g:282:SER:H	33:g:285:ALA:HB3	1.84	0.43
1:2:1219:A:C6	1:2:1265:G:H1'	2.54	0.43
1:2:1434:U:O2'	1:2:1436:A:OP1	2.34	0.43
8:I:50:GLY:O	8:I:52:ASN:ND2	2.51	0.43
9:J:100:LYS:HE3	9:J:102:GLU:HB2	2.01	0.43
11:N:5:HIS:CE1	11:N:121:ARG:HG3	2.54	0.43
16:X:59:ILE:HD13	20:e:4:VAL:HA	2.01	0.43
16:X:92:CYS:HG	16:X:136:TRP:CD1	2.36	0.43
19:d:29:GLY:O	19:d:40:ARG:N	2.51	0.43
25:P:22:LEU:HG	25:P:109:PRO:HB3	2.01	0.43
28:T:83:ALA:HB1	28:T:91:TYR:HB3	2.00	0.43
1:2:1234:A:O2'	32:f:140:TYR:OH	2.24	0.43
1:2:1311:U:H2'	1:2:1312:A:H3'	2.00	0.43
1:2:1374:C:H2'	1:2:1375:A:C8	2.54	0.43
1:2:1662:G:H2'	1:2:1663:G:C8	2.54	0.43
3:B:176:VAL:HG12	3:B:177:GLN:H	1.84	0.43
15:W:28:ARG:HD3	15:W:60:LYS:HE2	2.01	0.43
21:D:20:GLU:O	21:D:24:PHE:HB3	2.18	0.43
27:S:60:GLU:HB3	27:S:61:LEU:H	1.64	0.43
27:S:81:ILE:HA	27:S:82:PRO:HD3	1.83	0.43
33:g:229:LYS:HB3	33:g:230:ALA:H	1.69	0.43
1:2:1276:U:H2'	1:2:1277:G:C8	2.53	0.43
1:2:1398:U:H3'	1:2:1399:C:H4'	2.01	0.43
1:2:1587:A:O2'	22:F:104:ASN:ND2	2.48	0.43
2:A:58:VAL:O	2:A:62:ARG:HB2	2.18	0.43
4:C:116:LYS:HG2	4:C:127:ALA:HB3	2.00	0.43
10:L:81:HIS:CE1	10:L:82:ARG:HG3	2.54	0.43
1:2:76:A:N6	1:2:80:A:O2'	2.46	0.42
1:2:490:C:H41	1:2:498:G:N2	2.17	0.42
1:2:1357:A:H2'	1:2:1358:G:C8	2.54	0.42
2:A:18:LEU:HD23	2:A:23:HIS:CD2	2.54	0.42
7:H:74:GLN:O	7:H:78:THR:N	2.41	0.42
13:R:23:LYS:HB3	13:R:34:LEU:HD11	2.01	0.42
33:g:192:PHE:CE2	33:g:211:ILE:HD12	2.54	0.42
1:2:368:U:HO2'	1:2:603:U:HO2'	1.58	0.42
1:2:1145:U:C2	4:C:91:ARG:HD3	2.53	0.42
1:2:1414:U:H5''	13:R:3:ARG:HE	1.84	0.42
22:F:72:HIS:ND1	26:Q:79:TYR:OH	2.35	0.42
25:P:90:ILE:HD11	25:P:112:LEU:HD11	2.00	0.42
33:g:210:LEU:HA	33:g:223:TRP:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:3:U:H5'	4:C:179:VAL:HG12	2.01	0.42
1:2:502:U:H2'	1:2:503:G:H8	1.84	0.42
1:2:1193:A:C6	1:2:1282:U:H4'	2.54	0.42
1:2:1294:G:H4'	2:A:109:ASN:HA	2.01	0.42
1:2:1316:G:H5'	13:R:7:LYS:HB3	2.01	0.42
1:2:1401:A:OP1	13:R:56:HIS:NE2	2.47	0.42
1:2:1662:G:H2'	1:2:1663:G:H8	1.83	0.42
6:G:5:ILE:HA	6:G:111:LEU:O	2.19	0.42
22:F:84:LYS:O	22:F:92:ARG:NH1	2.52	0.42
33:g:132:LYS:HA	33:g:142:ALA:O	2.19	0.42
1:2:1347:U:H1'	1:2:1516:A:H2'	2.02	0.42
1:2:1453:G:H2'	1:2:1454:G:C8	2.55	0.42
1:2:1496:U:O2'	1:2:1519:U:O2'	2.28	0.42
1:2:1498:G:H5''	28:T:72:GLY:HA3	2.01	0.42
16:X:69:ARG:NH2	16:X:116:ASP:OD2	2.46	0.42
23:K:59:PHE:O	23:K:64:TYR:N	2.51	0.42
27:S:106:GLU:O	27:S:109:LEU:HB3	2.20	0.42
32:f:132:LEU:HB3	32:f:139:LEU:HB3	2.02	0.42
1:2:773:C:OP1	5:E:22:LYS:N	2.37	0.42
1:2:868:G:H1	1:2:960:U:H3	1.67	0.42
1:2:1344:A:N6	1:2:1377:U:O2'	2.52	0.42
26:Q:53:LEU:HD21	26:Q:57:LEU:HD12	2.01	0.42
1:2:812:A:C5	1:2:858:G:C2	3.07	0.42
1:2:1478:G:H3'	1:2:1479:A:H8	1.83	0.42
1:2:1511:U:H2'	1:2:1512:G:C8	2.55	0.42
2:A:118:PRO:HG2	2:A:141:ILE:HD13	2.02	0.42
24:M:91:VAL:HG11	24:M:97:LEU:HD23	2.00	0.42
25:P:86:VAL:HG12	25:P:89:MET:HE3	2.02	0.42
26:Q:13:LYS:HG3	26:Q:14:LYS:H	1.84	0.42
33:g:7:LEU:HD22	33:g:274:LEU:HD11	2.01	0.42
33:g:91:LEU:O	33:g:100:TYR:N	2.40	0.42
1:2:127:G:N7	6:G:202:ARG:NH2	2.67	0.42
1:2:557:G:H5''	20:e:57:ASN:HB3	2.00	0.42
19:d:26:SER:OG	19:d:28:THR:O	2.38	0.42
33:g:147:HIS:NE2	33:g:171:SER:OG	2.42	0.42
1:2:724:C:O2'	1:2:725:U:O5'	2.36	0.42
1:2:1029:U:C2	1:2:1031:U:H5''	2.55	0.42
1:2:1277:G:H3'	1:2:1278:G:C8	2.54	0.42
4:C:222:TYR:OH	14:V:11:LEU:O	2.34	0.42
7:H:14:THR:OG1	7:H:15:GLU:OE1	2.36	0.42
11:N:99:ARG:NH2	11:N:119:GLU:OE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:29:HIS:ND1	17:Y:32:ARG:O	2.49	0.42
17:Y:42:GLU:HG2	17:Y:52:LYS:HE2	2.01	0.42
28:T:57:ARG:NH1	28:T:101:ASN:OD1	2.52	0.42
1:2:705:U:H2'	1:2:706:A:H8	1.84	0.42
1:2:1451:C:H2'	1:2:1452:U:H6	1.85	0.42
1:2:1610:G:H5''	22:F:107:LYS:HE3	2.00	0.42
3:B:171:ILE:HD12	3:B:197:ILE:HD13	2.01	0.42
6:G:52:ILE:HD13	6:G:102:VAL:HG21	2.01	0.42
8:I:67:TRP:HD1	8:I:70:GLU:HB2	1.85	0.42
22:F:37:GLN:HB3	26:Q:53:LEU:HD13	2.01	0.42
28:T:77:ASN:HA	28:T:96:ALA:HB3	2.02	0.42
1:2:878:G:H2'	1:2:879:G:C8	2.54	0.42
1:2:922:G:H2'	1:2:923:A:C8	2.54	0.42
1:2:1047:G:H2'	1:2:1048:G:H8	1.82	0.42
1:2:1776:A:H2'	1:2:1777:G:C8	2.54	0.42
1:2:1776:A:H2'	1:2:1777:G:H8	1.85	0.42
22:F:198:LEU:O	22:F:202:ALA:HB2	2.20	0.42
23:K:32:HIS:CE1	23:K:42:VAL:HG21	2.55	0.42
25:P:77:ARG:HD3	25:P:102:PHE:CD2	2.55	0.42
31:c:14:LYS:HB2	31:c:29:ARG:HB3	2.01	0.42
33:g:82:SER:O	33:g:89:LEU:HA	2.18	0.42
1:2:954:G:H2'	1:2:955:A:C8	2.55	0.41
1:2:1217:A:H4'	23:K:44:LYS:HD2	2.02	0.41
1:2:1545:A:H2'	1:2:1546:G:C8	2.55	0.41
4:C:153:SER:OG	4:C:154:LEU:N	2.53	0.41
9:J:109:LEU:HD12	9:J:129:ILE:HG12	2.02	0.41
21:D:176:LEU:HG	21:D:181:VAL:HG12	2.02	0.41
22:F:103:ASN:HA	22:F:106:LYS:HD2	2.00	0.41
1:2:393:C:H2'	1:2:394:C:C6	2.55	0.41
1:2:953:G:H2'	1:2:954:G:C8	2.54	0.41
1:2:972:G:O6	1:2:973:A:N6	2.53	0.41
1:2:1166:A:OP1	22:F:100:ASN:N	2.47	0.41
1:2:1537:C:N4	1:2:1571:C:OP2	2.52	0.41
2:A:200:ASP:HA	2:A:203:PHE:CD2	2.55	0.41
7:H:14:THR:HG1	7:H:15:GLU:H	1.67	0.41
9:J:172:VAL:HG23	9:J:175:ARG:HH21	1.83	0.41
22:F:102:ARG:O	22:F:106:LYS:NZ	2.43	0.41
23:K:42:VAL:O	23:K:46:LEU:HB2	2.21	0.41
26:Q:17:THR:OG1	26:Q:70:THR:OG1	2.38	0.41
27:S:92:ILE:HG23	27:S:93:THR:HG23	2.02	0.41
33:g:295:SER:OG	33:g:296:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:386:G:H2'	1:2:387:A:C8	2.56	0.41
1:2:489:C:N3	1:2:498:G:N2	2.69	0.41
1:2:546:U:H2'	1:2:547:U:C6	2.56	0.41
1:2:560:U:H2'	1:2:561:G:C8	2.56	0.41
1:2:996:U:H3'	1:2:997:G:H8	1.85	0.41
1:2:1393:C:H2'	1:2:1394:G:C8	2.56	0.41
1:2:1480:G:OP1	28:T:63:ARG:NH2	2.52	0.41
6:G:70:PRO:HD3	6:G:101:ILE:HD12	2.01	0.41
16:X:75:GLN:HB3	16:X:82:LYS:HG2	2.02	0.41
22:F:26:ALA:HB2	26:Q:26:LYS:HG3	2.03	0.41
1:2:639:U:H1'	1:2:640:U:C5	2.54	0.41
1:2:870:C:O2	18:b:51:GLN:NE2	2.54	0.41
1:2:1117:U:H2'	1:2:1118:G:C8	2.56	0.41
1:2:1657:U:H2'	1:2:1658:G:H8	1.85	0.41
2:A:89:PHE:O	2:A:93:THR:OG1	2.35	0.41
8:I:48:THR:OG1	8:I:52:ASN:O	2.34	0.41
21:D:64:ARG:HB3	21:D:65:ARG:H	1.63	0.41
27:S:16:ARG:HE	27:S:19:ASN:HA	1.85	0.41
27:S:18:LEU:HD13	27:S:18:LEU:HA	1.85	0.41
1:2:153:G:OP2	17:Y:131:ARG:NH1	2.54	0.41
1:2:1146:G:O4'	4:C:91:ARG:NE	2.52	0.41
1:2:1533:C:H4'	1:2:1539:G:C6	2.55	0.41
7:H:7:LYS:O	7:H:42:GLN:NE2	2.53	0.41
7:H:70:PHE:O	7:H:74:GLN:N	2.45	0.41
16:X:103:LEU:HB3	16:X:126:LYS:HB2	2.02	0.41
25:P:52:LYS:HG3	25:P:53:PRO:HD3	2.01	0.41
1:2:775:G:O6	1:2:785:U:C2	2.74	0.41
1:2:1552:U:OP2	25:P:43:ARG:NH2	2.52	0.41
1:2:1552:U:O2'	1:2:1597:A:N3	2.47	0.41
1:2:1566:U:OP1	27:S:42:TYR:N	2.48	0.41
2:A:76:ILE:HD13	2:A:98:ILE:HB	2.03	0.41
3:B:109:LYS:HG3	3:B:113:MET:HE3	2.03	0.41
3:B:171:ILE:HA	3:B:174:LYS:HZ1	1.85	0.41
10:L:57:LYS:HD2	10:L:131:ILE:HG23	2.02	0.41
21:D:21:LEU:HB3	21:D:37:VAL:HG21	2.03	0.41
1:2:31:C:O2'	1:2:547:U:OP1	2.37	0.41
1:2:94:U:OP2	5:E:3:ARG:NH2	2.47	0.41
1:2:393:C:H2'	1:2:394:C:H6	1.86	0.41
1:2:688:G:H2'	1:2:689:G:C8	2.55	0.41
1:2:762:A:P	9:J:79:ARG:HH22	2.43	0.41
1:2:1199:G:C2	1:2:1595:U:H4'	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1225:U:H3'	1:2:1226:A:H8	1.86	0.41
1:2:1415:U:H2'	1:2:1416:G:H8	1.86	0.41
1:2:1515:A:O2'	1:2:1518:C:N4	2.53	0.41
1:2:1660:A:H2'	1:2:1661:U:H6	1.86	0.41
14:V:3:ASN:OD1	14:V:7:GLN:HB3	2.21	0.41
14:V:38:LYS:HD2	14:V:49:GLU:HB3	2.03	0.41
23:K:54:TYR:HD1	23:K:71:GLU:HB3	1.85	0.41
27:S:48:LYS:HZ2	28:T:46:PRO:HB2	1.86	0.41
1:2:458:G:OP2	17:Y:105:ARG:NH1	2.47	0.41
1:2:794:U:O2'	1:2:795:U:O5'	2.35	0.41
1:2:1298:U:H2'	1:2:1299:G:H8	1.86	0.41
6:G:75:LEU:O	6:G:94:ARG:HA	2.21	0.41
6:G:148:SER:O	6:G:150:GLU:N	2.54	0.41
22:F:114:ILE:HD13	22:F:114:ILE:HA	1.88	0.41
23:K:1:MET:HE1	23:K:40:LEU:HD11	2.01	0.41
24:M:103:LEU:HD11	24:M:115:VAL:HG13	2.03	0.41
33:g:178:VAL:HG23	33:g:199:ILE:HD13	2.02	0.41
1:2:472:U:O2'	1:2:769:A:N3	2.50	0.41
1:2:868:G:H2'	1:2:869:A:C8	2.55	0.41
1:2:1064:G:H2'	1:2:1065:A:H8	1.86	0.41
1:2:1149:G:O6	1:2:1628:U:O4	2.39	0.41
1:2:1250:U:H2'	1:2:1251:U:C2	2.56	0.41
1:2:1714:A:H2'	1:2:1715:G:C8	2.56	0.41
8:I:12:SER:HB3	8:I:18:ARG:HE	1.85	0.41
26:Q:60:PHE:CE1	26:Q:89:LEU:HD13	2.55	0.41
27:S:88:ARG:NH2	27:S:112:ASP:OD2	2.54	0.41
33:g:38:ARG:HH11	33:g:67:ILE:HD13	1.86	0.41
33:g:123:ILE:HG22	33:g:133:VAL:HG22	2.02	0.41
1:2:144:U:H5	6:G:137:ARG:HH22	1.68	0.41
1:2:707:A:N6	1:2:708:C:N3	2.69	0.41
1:2:1007:C:H2'	1:2:1008:G:C8	2.56	0.41
1:2:1234:A:OP2	1:2:1245:G:O2'	2.37	0.41
1:2:1245:G:C2	1:2:1250:U:O4	2.73	0.41
1:2:1673:G:OP1	6:G:94:ARG:NH2	2.53	0.41
2:A:11:PRO:HG3	13:R:115:LEU:HD12	2.02	0.41
3:B:121:ILE:HD13	3:B:164:ILE:HG21	2.01	0.41
5:E:45:ILE:HG13	5:E:61:VAL:HG21	2.02	0.41
5:E:195:ILE:HA	5:E:210:ILE:HD13	2.03	0.41
8:I:8:ARG:HD2	8:I:8:ARG:HA	1.62	0.41
8:I:29:LEU:HD21	8:I:31:ARG:HG3	2.02	0.41
23:K:7:ASP:O	23:K:11:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:g:211:ILE:HG13	33:g:225:LEU:HB2	2.02	0.41
1:2:478:A:H5''	20:e:37:ARG:NH1	2.36	0.40
1:2:1106:U:H2'	1:2:1107:G:H8	1.86	0.40
2:A:173:ILE:O	2:A:177:LEU:HB2	2.21	0.40
4:C:58:LEU:HA	14:V:12:TYR:HE1	1.86	0.40
10:L:123:VAL:HG23	10:L:142:VAL:HA	2.03	0.40
13:R:19:ARG:HD2	21:D:208:ILE:HG22	2.02	0.40
21:D:132:LYS:HB3	21:D:189:MET:HG3	2.03	0.40
1:2:808:U:H2'	1:2:809:A:C8	2.53	0.40
1:2:878:G:H2'	1:2:879:G:H8	1.86	0.40
1:2:1587:A:H2'	1:2:1588:G:C8	2.55	0.40
5:E:159:THR:HG22	5:E:173:ILE:HB	2.02	0.40
6:G:71:THR:N	6:G:98:ARG:HH22	2.20	0.40
14:V:37:ALA:HB1	14:V:45:ALA:HB1	2.03	0.40
33:g:13:LEU:HB2	33:g:310:ILE:HB	2.03	0.40
1:2:255:U:H2'	1:2:256:A:C8	2.57	0.40
1:2:961:U:H5''	11:N:71:ILE:HD12	2.03	0.40
1:2:1048:G:H2'	1:2:1049:U:H6	1.86	0.40
5:E:94:ALA:HB1	17:Y:16:PRO:HB2	2.02	0.40
8:I:83:TYR:HB3	8:I:101:ILE:HB	2.03	0.40
9:J:99:LEU:HD13	9:J:99:LEU:HA	1.88	0.40
21:D:142:LEU:HD13	21:D:179:GLN:HB3	2.02	0.40
1:2:804:A:N7	15:W:107:SER:HA	2.37	0.40
1:2:1623:C:H2'	1:2:1624:C:C6	2.55	0.40
3:B:201:THR:HG21	3:B:207:LEU:HD22	2.02	0.40
15:W:27:ILE:HG12	15:W:61:ILE:HB	2.03	0.40
33:g:122:ILE:HD11	33:g:136:ILE:HG22	2.04	0.40
1:2:609:U:H1'	16:X:19:ARG:NH2	2.36	0.40
1:2:706:A:N6	1:2:731:C:O2'	2.52	0.40
1:2:863:A:N6	1:2:964:U:C2	2.86	0.40
6:G:98:ARG:HH21	6:G:99:GLY:N	2.19	0.40
11:N:4:MET:HG2	11:N:5:HIS:CD2	2.56	0.40
11:N:56:ASP:OD1	11:N:57:ALA:N	2.55	0.40
16:X:95:PHE:HE2	16:X:136:TRP:HA	1.87	0.40
21:D:38:GLU:HG2	21:D:49:ILE:HB	2.03	0.40
26:Q:125:GLU:HA	26:Q:126:PRO:HD3	1.87	0.40
33:g:68:VAL:HA	33:g:84:SER:HA	2.04	0.40
33:g:299:GLN:NE2	33:g:315:VAL:O	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	204/252 (81%)	160 (78%)	42 (21%)	2 (1%)	12	43
3	B	111/255 (44%)	93 (84%)	15 (14%)	3 (3%)	4	27
4	C	215/254 (85%)	194 (90%)	20 (9%)	1 (0%)	24	57
5	E	258/261 (99%)	235 (91%)	22 (8%)	1 (0%)	30	62
6	G	224/236 (95%)	204 (91%)	15 (7%)	5 (2%)	5	30
7	H	182/190 (96%)	146 (80%)	29 (16%)	7 (4%)	2	21
8	I	184/200 (92%)	157 (85%)	25 (14%)	2 (1%)	11	41
9	J	183/197 (93%)	164 (90%)	17 (9%)	2 (1%)	11	41
10	L	153/156 (98%)	139 (91%)	14 (9%)	0	100	100
11	N	148/151 (98%)	136 (92%)	9 (6%)	3 (2%)	6	32
12	O	16/137 (12%)	13 (81%)	3 (19%)	0	100	100
13	R	116/136 (85%)	103 (89%)	11 (10%)	2 (2%)	7	34
14	V	85/87 (98%)	64 (75%)	19 (22%)	2 (2%)	4	29
15	W	127/130 (98%)	111 (87%)	16 (13%)	0	100	100
16	X	142/145 (98%)	115 (81%)	25 (18%)	2 (1%)	9	37
17	Y	132/135 (98%)	121 (92%)	11 (8%)	0	100	100
18	b	79/82 (96%)	66 (84%)	12 (15%)	1 (1%)	9	38
19	d	51/56 (91%)	48 (94%)	3 (6%)	0	100	100
20	e	58/63 (92%)	53 (91%)	5 (9%)	0	100	100
21	D	221/240 (92%)	203 (92%)	16 (7%)	2 (1%)	14	45
22	F	204/225 (91%)	177 (87%)	25 (12%)	2 (1%)	12	43
23	K	94/105 (90%)	76 (81%)	17 (18%)	1 (1%)	11	41
24	M	122/143 (85%)	88 (72%)	28 (23%)	6 (5%)	1	17
25	P	122/142 (86%)	101 (83%)	19 (16%)	2 (2%)	7	35
26	Q	139/143 (97%)	125 (90%)	11 (8%)	3 (2%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	S	143/146 (98%)	119 (83%)	21 (15%)	3 (2%)	5	31
28	T	141/144 (98%)	125 (89%)	16 (11%)	0	100	100
29	U	90/121 (74%)	83 (92%)	6 (7%)	1 (1%)	11	41
30	Z	68/108 (63%)	58 (85%)	9 (13%)	1 (2%)	8	36
31	c	61/67 (91%)	55 (90%)	6 (10%)	0	100	100
32	f	49/152 (32%)	37 (76%)	11 (22%)	1 (2%)	6	32
33	g	316/319 (99%)	285 (90%)	31 (10%)	0	100	100
All	All	4438/5178 (86%)	3854 (87%)	529 (12%)	55 (1%)	13	40

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	195	ILE
6	G	173	PRO
9	J	99	LEU
11	N	22	ALA
14	V	81	ASN
14	V	82	VAL
22	F	50	GLU
24	M	130	THR
24	M	131	ASP
26	Q	59	LYS
27	S	91	ASP
3	B	180	THR
3	B	206	PRO
3	B	207	LEU
6	G	149	LYS
7	H	155	ASP
8	I	22	ARG
9	J	98	ALA
13	R	24	LEU
16	X	97	ASP
21	D	65	ARG
30	Z	44	GLN
2	A	4	PRO
2	A	196	SER
4	C	40	LYS
6	G	68	LEU
7	H	133	THR
13	R	86	PRO

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Mol	Chain	Res	Type
24	M	126	TRP
25	P	12	PHE
25	P	125	PRO
26	Q	58	ASP
21	D	211	PRO
22	F	49	GLU
24	M	109	GLU
27	S	60	GLU
32	f	148	TYR
7	H	98	ILE
7	H	134	GLU
11	N	138	ASN
16	X	96	VAL
18	b	75	GLU
23	K	81	ASN
24	M	85	LYS
24	M	90	LYS
29	U	120	SER
6	G	67	VAL
6	G	174	LYS
27	S	92	ILE
7	H	65	PRO
8	I	152	ILE
7	H	132	PRO
11	N	23	PRO
26	Q	33	GLY
7	H	131	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	164/210 (78%)	162 (99%)	2 (1%)	63	72
3	B	104/224 (46%)	103 (99%)	1 (1%)	68	74
4	C	176/205 (86%)	176 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	221/222 (100%)	217 (98%)	4 (2%)	51	67
6	G	188/201 (94%)	186 (99%)	2 (1%)	65	73
7	H	165/170 (97%)	163 (99%)	2 (1%)	63	72
8	I	150/161 (93%)	150 (100%)	0	100	100
9	J	158/166 (95%)	155 (98%)	3 (2%)	50	66
10	L	129/137 (94%)	129 (100%)	0	100	100
11	N	127/128 (99%)	124 (98%)	3 (2%)	43	62
12	O	15/105 (14%)	15 (100%)	0	100	100
13	R	94/124 (76%)	91 (97%)	3 (3%)	34	56
14	V	74/74 (100%)	70 (95%)	4 (5%)	20	45
15	W	110/111 (99%)	108 (98%)	2 (2%)	51	67
16	X	119/120 (99%)	119 (100%)	0	100	100
17	Y	112/113 (99%)	110 (98%)	2 (2%)	51	67
18	b	70/71 (99%)	69 (99%)	1 (1%)	59	70
19	d	47/49 (96%)	46 (98%)	1 (2%)	47	64
20	e	51/54 (94%)	50 (98%)	1 (2%)	48	65
21	D	182/195 (93%)	178 (98%)	4 (2%)	45	63
22	F	173/191 (91%)	170 (98%)	3 (2%)	53	67
23	K	77/98 (79%)	76 (99%)	1 (1%)	61	71
24	M	88/119 (74%)	88 (100%)	0	100	100
25	P	101/118 (86%)	100 (99%)	1 (1%)	68	74
26	Q	117/119 (98%)	117 (100%)	0	100	100
27	S	128/129 (99%)	127 (99%)	1 (1%)	73	76
28	T	115/116 (99%)	112 (97%)	3 (3%)	40	60
29	U	93/114 (82%)	92 (99%)	1 (1%)	65	73
30	Z	61/89 (68%)	57 (93%)	4 (7%)	15	41
31	c	56/60 (93%)	56 (100%)	0	100	100
32	f	43/135 (32%)	41 (95%)	2 (5%)	23	48
33	g	259/262 (99%)	259 (100%)	0	100	100
All	All	3767/4390 (86%)	3716 (99%)	51 (1%)	57	70

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	133	ILE
2	A	177	LEU
3	B	207	LEU
5	E	180	LEU
5	E	181	VAL
5	E	206	ASP
5	E	236	ILE
6	G	68	LEU
6	G	170	THR
7	H	38	LEU
7	H	64	VAL
9	J	99	LEU
9	J	109	LEU
9	J	134	ILE
11	N	50	ILE
11	N	60	VAL
11	N	125	LEU
13	R	44	LYS
13	R	46	LEU
13	R	115	LEU
14	V	8	LEU
14	V	32	VAL
14	V	69	LEU
14	V	82	VAL
15	W	93	LEU
15	W	103	ILE
17	Y	17	LEU
17	Y	35	VAL
18	b	4	VAL
19	d	28	THR
20	e	33	ARG
21	D	4	LEU
21	D	158	ILE
21	D	175	VAL
21	D	222	VAL
22	F	84	LYS
22	F	93	LEU
22	F	194	LEU
23	K	40	LEU
25	P	36	LEU
27	S	119	ILE
28	T	28	LEU
28	T	114	VAL

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Mol	Chain	Res	Type
28	T	135	ILE
29	U	20	ILE
30	Z	40	VAL
30	Z	42	LEU
30	Z	69	LEU
30	Z	78	ILE
32	f	108	VAL
32	f	123	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	23	HIS
2	A	30	GLN
2	A	49	ASN
2	A	109	ASN
3	B	118	GLN
3	B	208	GLN
6	G	119	GLN
6	G	190	GLN
6	G	201	GLN
7	H	11	GLN
7	H	29	ASN
7	H	42	GLN
7	H	180	GLN
8	I	32	GLN
8	I	64	ASN
8	I	88	ASN
8	I	103	GLN
8	I	159	GLN
9	J	38	ASN
9	J	74	ASN
9	J	110	GLN
9	J	112	GLN
9	J	155	HIS
10	L	106	ASN
10	L	138	ASN
11	N	5	HIS
11	N	36	GLN
11	N	58	HIS
11	N	62	GLN
13	R	105	GLN

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Mol	Chain	Res	Type
14	V	70	ASN
15	W	15	ASN
15	W	80	ASN
16	X	63	GLN
16	X	79	ASN
17	Y	34	ASN
17	Y	77	ASN
17	Y	106	GLN
19	d	48	ASN
19	d	53	ASN
20	e	17	GLN
21	D	67	ASN
21	D	111	ASN
21	D	162	GLN
22	F	34	GLN
22	F	104	ASN
22	F	139	ASN
24	M	80	ASN
24	M	125	ASN
24	M	142	GLN
25	P	103	ASN
26	Q	94	GLN
27	S	75	ASN
28	T	43	ASN
28	T	129	GLN
30	Z	37	GLN
30	Z	95	HIS
30	Z	98	GLN
32	f	123	ASN
33	g	69	GLN
33	g	182	ASN
33	g	187	GLN
33	g	237	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1743/1800 (96%)	627 (35%)	49 (2%)

All (627) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	14	C
1	2	20	G
1	2	23	G
1	2	24	U
1	2	25	C
1	2	26	A
1	2	27	U
1	2	34	G
1	2	42	G
1	2	43	A
1	2	45	U
1	2	46	A
1	2	47	A
1	2	50	C
1	2	57	G
1	2	60	U
1	2	68	A
1	2	69	G
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	77	U
1	2	100	A
1	2	104	A
1	2	105	A
1	2	114	C
1	2	115	G
1	2	126	A
1	2	127	G
1	2	128	U
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	137	U
1	2	138	A
1	2	139	C
1	2	140	A

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Mol	Chain	Res	Type
1	2	141	U
1	2	144	U
1	2	145	A
1	2	146	U
1	2	153	G
1	2	158	U
1	2	159	U
1	2	176	C
1	2	178	U
1	2	179	A
1	2	183	U
1	2	185	U
1	2	186	C
1	2	187	G
1	2	188	A
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U
1	2	194	U
1	2	195	G
1	2	196	G
1	2	197	A
1	2	198	A
1	2	200	A
1	2	201	G
1	2	202	A
1	2	212	U
1	2	215	A
1	2	218	A
1	2	219	A
1	2	223	U
1	2	226	A
1	2	229	U
1	2	231	U
1	2	233	C
1	2	234	G
1	2	236	A
1	2	238	U
1	2	239	C
1	2	240	U
1	2	241	U

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Mol	Chain	Res	Type
1	2	244	A
1	2	250	C
1	2	257	A
1	2	261	U
1	2	265	A
1	2	271	A
1	2	272	U
1	2	275	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	282	C
1	2	288	A
1	2	299	A
1	2	301	A
1	2	309	C
1	2	314	C
1	2	316	A
1	2	320	U
1	2	321	C
1	2	322	G
1	2	331	A
1	2	332	U
1	2	333	A
1	2	337	G
1	2	338	C
1	2	352	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	369	A
1	2	380	U
1	2	381	C
1	2	391	A
1	2	400	A
1	2	401	A
1	2	402	C
1	2	404	G
1	2	416	A
1	2	417	A

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Mol	Chain	Res	Type
1	2	418	G
1	2	419	G
1	2	421	A
1	2	424	C
1	2	425	A
1	2	426	G
1	2	434	G
1	2	435	C
1	2	439	U
1	2	444	C
1	2	448	C
1	2	452	A
1	2	453	U
1	2	454	U
1	2	464	A
1	2	468	A
1	2	469	C
1	2	475	A
1	2	477	A
1	2	478	A
1	2	481	A
1	2	484	C
1	2	485	A
1	2	486	G
1	2	487	G
1	2	490	C
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	497	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	501	U
1	2	502	U
1	2	504	U
1	2	505	A
1	2	506	A
1	2	507	U
1	2	510	G
1	2	511	A

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Mol	Chain	Res	Type
1	2	513	U
1	2	514	G
1	2	515	A
1	2	519	C
1	2	524	U
1	2	529	A
1	2	532	U
1	2	534	A
1	2	538	A
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	544	A
1	2	545	A
1	2	548	G
1	2	551	G
1	2	555	A
1	2	556	A
1	2	557	G
1	2	558	U
1	2	559	C
1	2	564	G
1	2	565	C
1	2	568	G
1	2	570	A
1	2	571	G
1	2	574	G
1	2	579	A
1	2	580	A
1	2	581	U
1	2	582	U
1	2	585	A
1	2	594	A
1	2	595	G
1	2	606	A
1	2	609	U
1	2	611	U
1	2	619	A
1	2	620	A
1	2	621	A

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Mol	Chain	Res	Type
1	2	622	A
1	2	623	A
1	2	624	G
1	2	634	G
1	2	635	A
1	2	639	U
1	2	648	G
1	2	649	U
1	2	650	U
1	2	652	G
1	2	653	C
1	2	654	C
1	2	655	G
1	2	656	G
1	2	658	C
1	2	677	G
1	2	679	U
1	2	680	U
1	2	684	A
1	2	685	A
1	2	686	C
1	2	687	G
1	2	691	C
1	2	694	U
1	2	695	U
1	2	696	C
1	2	697	C
1	2	698	U
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	706	A
1	2	707	A
1	2	708	C
1	2	709	C
1	2	710	U
1	2	712	G
1	2	714	G
1	2	717	C
1	2	718	U
1	2	719	U

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Mol	Chain	Res	Type
1	2	720	G
1	2	721	U
1	2	722	G
1	2	723	G
1	2	725	U
1	2	727	U
1	2	729	G
1	2	730	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	735	C
1	2	737	A
1	2	738	G
1	2	740	A
1	2	741	C
1	2	742	U
1	2	743	U
1	2	744	U
1	2	745	U
1	2	752	A
1	2	753	A
1	2	754	A
1	2	755	A
1	2	756	A
1	2	766	U
1	2	774	A
1	2	775	G
1	2	778	G
1	2	780	A
1	2	781	U
1	2	782	U
1	2	783	G
1	2	784	C
1	2	787	G
1	2	789	A
1	2	794	U
1	2	795	U
1	2	803	A
1	2	807	A
1	2	808	U

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Mol	Chain	Res	Type
1	2	811	A
1	2	812	A
1	2	813	U
1	2	814	A
1	2	815	G
1	2	818	C
1	2	820	U
1	2	821	U
1	2	822	U
1	2	823	G
1	2	824	G
1	2	826	U
1	2	827	C
1	2	829	A
1	2	830	U
1	2	831	U
1	2	841	U
1	2	843	U
1	2	844	A
1	2	845	G
1	2	846	G
1	2	850	A
1	2	856	A
1	2	863	A
1	2	876	G
1	2	877	G
1	2	879	G
1	2	904	G
1	2	908	U
1	2	909	U
1	2	912	U
1	2	932	U
1	2	933	A
1	2	934	C
1	2	935	U
1	2	940	A
1	2	942	G
1	2	944	A
1	2	953	G
1	2	960	U
1	2	961	U
1	2	966	A

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Mol	Chain	Res	Type
1	2	973	A
1	2	977	A
1	2	990	C
1	2	992	A
1	2	993	A
1	2	996	U
1	2	997	G
1	2	998	A
1	2	1004	U
1	2	1005	A
1	2	1007	C
1	2	1011	G
1	2	1026	A
1	2	1028	C
1	2	1029	U
1	2	1030	A
1	2	1031	U
1	2	1032	G
1	2	1036	A
1	2	1039	A
1	2	1040	G
1	2	1051	G
1	2	1052	U
1	2	1053	G
1	2	1058	U
1	2	1060	U
1	2	1061	A
1	2	1064	G
1	2	1072	C
1	2	1074	G
1	2	1075	C
1	2	1076	A
1	2	1078	C
1	2	1081	A
1	2	1082	C
1	2	1091	A
1	2	1092	A
1	2	1094	G
1	2	1096	C
1	2	1097	U
1	2	1098	U
1	2	1100	G

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Mol	Chain	Res	Type
1	2	1138	A
1	2	1143	A
1	2	1145	U
1	2	1147	A
1	2	1150	G
1	2	1151	A
1	2	1154	G
1	2	1155	G
1	2	1156	C
1	2	1158	C
1	2	1160	A
1	2	1161	C
1	2	1162	C
1	2	1163	A
1	2	1166	A
1	2	1167	G
1	2	1170	G
1	2	1171	A
1	2	1172	G
1	2	1174	C
1	2	1176	G
1	2	1185	U
1	2	1186	U
1	2	1191	U
1	2	1193	A
1	2	1194	A
1	2	1196	A
1	2	1197	C
1	2	1199	G
1	2	1200	G
1	2	1201	G
1	2	1202	A
1	2	1203	A
1	2	1207	C
1	2	1212	G
1	2	1213	G
1	2	1214	U
1	2	1217	A
1	2	1218	G
1	2	1226	A
1	2	1227	A
1	2	1228	G

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Mol	Chain	Res	Type
1	2	1229	G
1	2	1230	A
1	2	1233	G
1	2	1244	A
1	2	1245	G
1	2	1246	C
1	2	1247	U
1	2	1251	U
1	2	1254	U
1	2	1257	U
1	2	1258	U
1	2	1259	U
1	2	1260	U
1	2	1263	G
1	2	1265	G
1	2	1276	U
1	2	1284	C
1	2	1286	U
1	2	1297	G
1	2	1303	U
1	2	1305	U
1	2	1306	C
1	2	1312	A
1	2	1314	U
1	2	1315	U
1	2	1316	G
1	2	1319	A
1	2	1320	U
1	2	1321	A
1	2	1322	A
1	2	1323	C
1	2	1325	A
1	2	1327	C
1	2	1336	A
1	2	1337	A
1	2	1338	C
1	2	1339	C
1	2	1340	U
1	2	1341	A
1	2	1344	A
1	2	1345	A
1	2	1347	U

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Mol	Chain	Res	Type
1	2	1348	A
1	2	1349	G
1	2	1354	G
1	2	1355	C
1	2	1361	U
1	2	1363	U
1	2	1364	G
1	2	1367	G
1	2	1368	G
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1382	A
1	2	1385	G
1	2	1388	A
1	2	1390	U
1	2	1391	A
1	2	1392	U
1	2	1395	G
1	2	1396	U
1	2	1398	U
1	2	1399	C
1	2	1400	A
1	2	1412	G
1	2	1413	U
1	2	1415	U
1	2	1418	G
1	2	1421	A
1	2	1422	A
1	2	1423	U
1	2	1427	A
1	2	1428	G
1	2	1431	C
1	2	1432	U
1	2	1433	G
1	2	1437	U
1	2	1438	G
1	2	1439	C
1	2	1446	A
1	2	1448	G
1	2	1456	C
1	2	1457	C

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Mol	Chain	Res	Type
1	2	1458	G
1	2	1459	C
1	2	1464	G
1	2	1466	G
1	2	1469	A
1	2	1470	C
1	2	1473	U
1	2	1474	G
1	2	1475	A
1	2	1478	G
1	2	1479	A
1	2	1482	C
1	2	1486	G
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1496	U
1	2	1504	G
1	2	1506	G
1	2	1510	U
1	2	1515	A
1	2	1516	A
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1530	C
1	2	1531	G
1	2	1532	U
1	2	1535	U
1	2	1536	G
1	2	1537	C
1	2	1538	U
1	2	1539	G
1	2	1540	G
1	2	1542	G
1	2	1543	A
1	2	1548	G
1	2	1557	U
1	2	1559	A
1	2	1560	U
1	2	1561	U

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Mol	Chain	Res	Type
1	2	1568	C
1	2	1569	A
1	2	1574	G
1	2	1577	A
1	2	1584	G
1	2	1593	A
1	2	1601	G
1	2	1611	A
1	2	1614	A
1	2	1616	G
1	2	1631	A
1	2	1632	C
1	2	1634	C
1	2	1635	A
1	2	1636	C
1	2	1637	C
1	2	1638	G
1	2	1640	C
1	2	1641	C
1	2	1649	G
1	2	1651	A
1	2	1652	C
1	2	1653	C
1	2	1654	G
1	2	1656	U
1	2	1657	U
1	2	1658	G
1	2	1659	A
1	2	1660	A
1	2	1661	U
1	2	1663	G
1	2	1665	U
1	2	1666	U
1	2	1680	G
1	2	1682	U
1	2	1683	C
1	2	1684	U
1	2	1712	A
1	2	1713	G
1	2	1715	G
1	2	1716	C
1	2	1717	G

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Mol	Chain	Res	Type
1	2	1731	A
1	2	1735	U
1	2	1736	G
1	2	1738	U
1	2	1739	C
1	2	1741	U
1	2	1742	U
1	2	1743	U
1	2	1744	A
1	2	1745	G
1	2	1748	G
1	2	1749	A
1	2	1750	A
1	2	1752	U
1	2	1753	A
1	2	1754	A
1	2	1755	A
1	2	1757	G
1	2	1758	U
1	2	1760	G
1	2	1761	U
1	2	1762	A
1	2	1763	A
1	2	1765	A
1	2	1766	A
1	2	1767	G
1	2	1769	U
1	2	1770	U
1	2	1771	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1790	A
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1796	C
1	2	1797	A

All (49) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	2	25	C
1	2	45	U
1	2	68	A
1	2	73	U
1	2	131	C
1	2	139	C
1	2	158	U
1	2	187	G
1	2	217	A
1	2	218	A
1	2	240	U
1	2	278	U
1	2	280	U
1	2	417	A
1	2	484	C
1	2	497	G
1	2	499	U
1	2	501	U
1	2	503	G
1	2	512	A
1	2	555	A
1	2	558	U
1	2	685	A
1	2	720	G
1	2	721	U
1	2	755	A
1	2	779	U
1	2	781	U
1	2	782	U
1	2	783	G
1	2	794	U
1	2	829	A
1	2	1051	G
1	2	1081	A
1	2	1196	A
1	2	1226	A
1	2	1244	A
1	2	1250	U
1	2	1296	A
1	2	1344	A
1	2	1370	U

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Mol	Chain	Res	Type
1	2	1481	C
1	2	1568	C
1	2	1573	A
1	2	1615	C
1	2	1630	U
1	2	1650	U
1	2	1652	C
1	2	1734	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	2
29	U	2
4	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	839:U	O3'	840:U	P	4.31
1	2	1654:G	O3'	1655:A	P	4.14

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	84:MET	C	85:ARG	N	3.97
1	U	61:LYS	C	62:VAL	N	3.80
1	C	225:LEU	C	226:THR	N	1.20

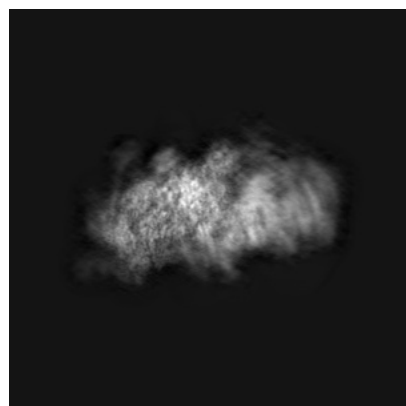
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4793. These allow visual inspection of the internal detail of the map and identification of artifacts.

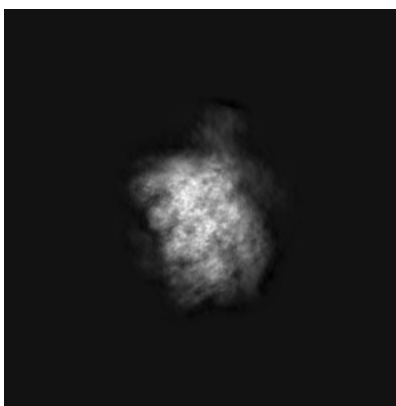
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

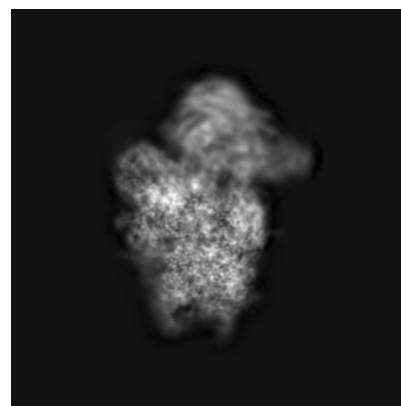
6.1.1 Primary map



X

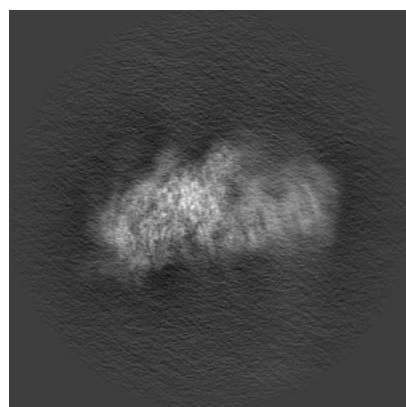


Y

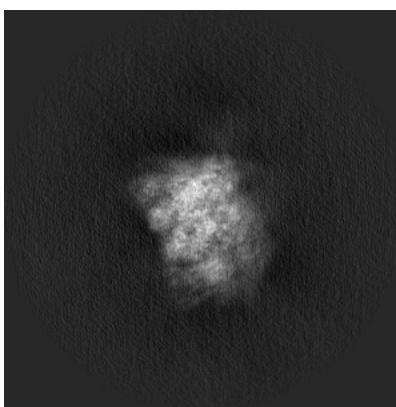


Z

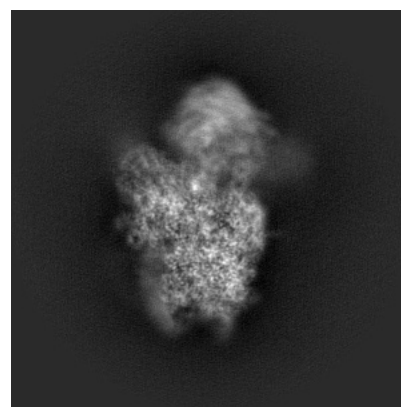
6.1.2 Raw map



X



Y

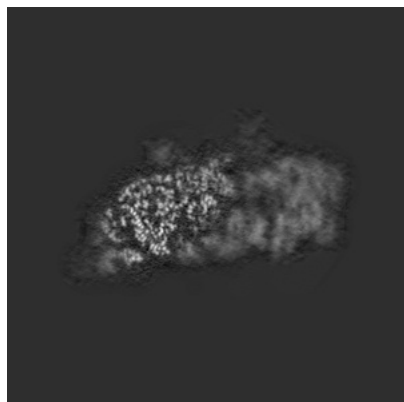


Z

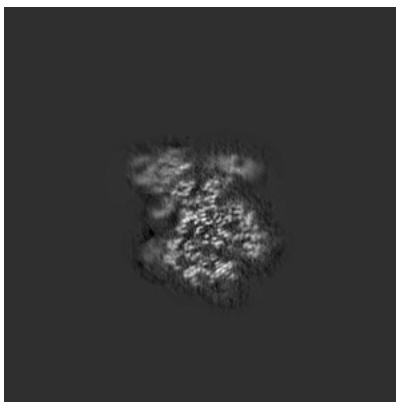
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

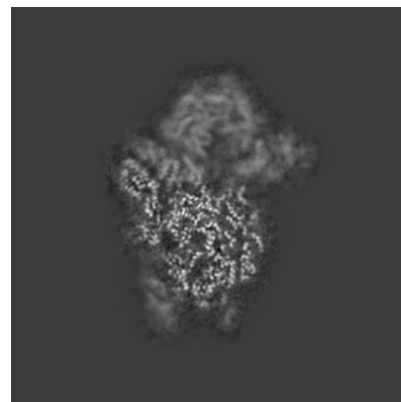
6.2.1 Primary map



X Index: 192

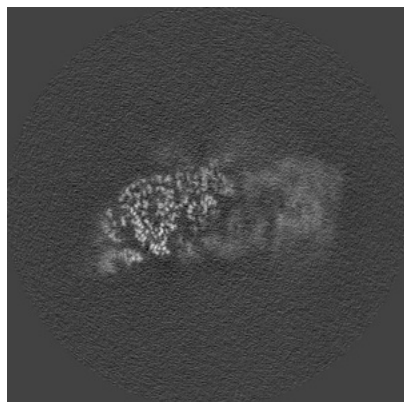


Y Index: 192

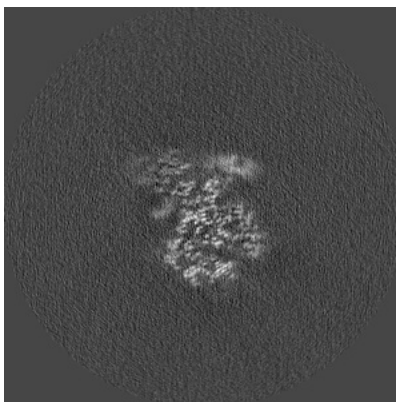


Z Index: 192

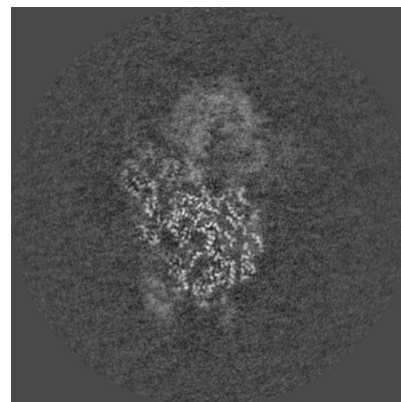
6.2.2 Raw map



X Index: 192



Y Index: 192

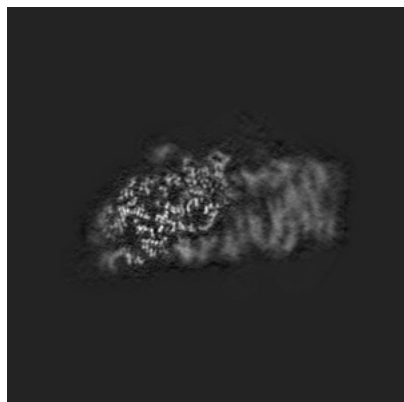


Z Index: 192

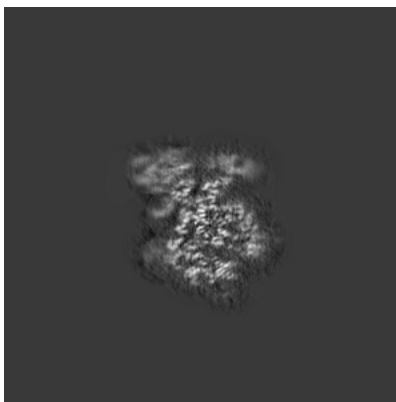
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

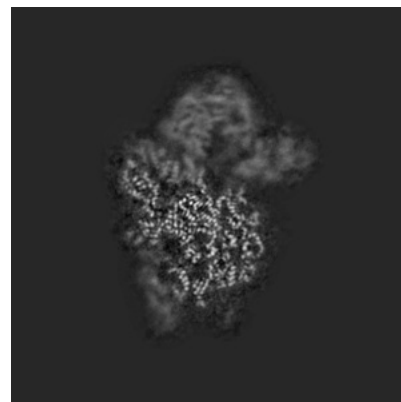
6.3.1 Primary map



X Index: 188

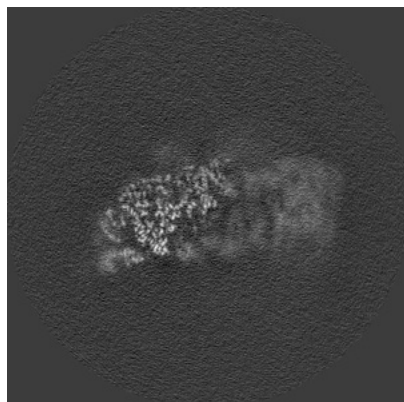


Y Index: 191

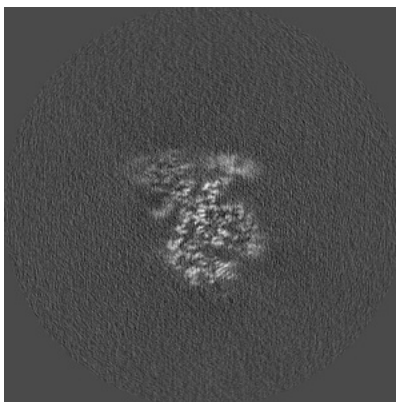


Z Index: 194

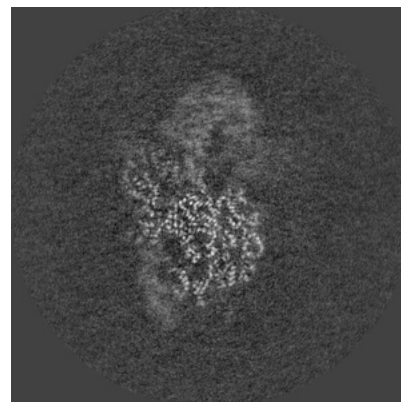
6.3.2 Raw map



X Index: 191



Y Index: 191

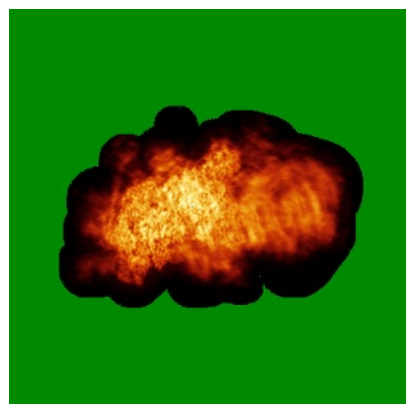


Z Index: 194

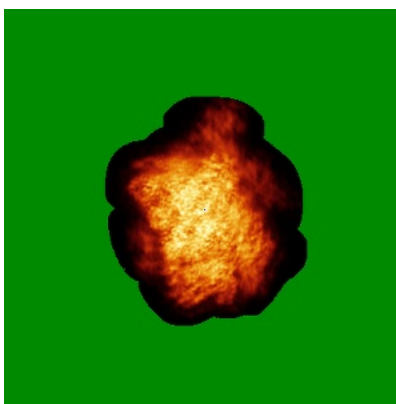
The images above show the largest variance slices of the map in three orthogonal directions.

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

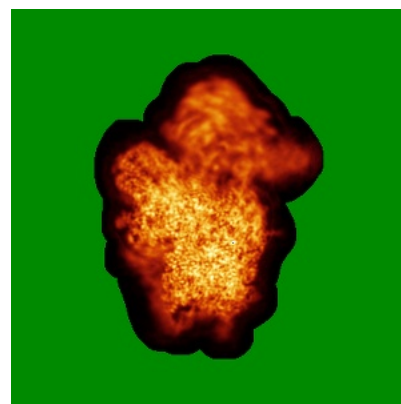
6.4.1 Primary map



X

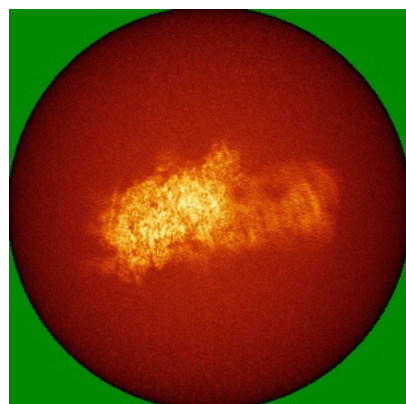


Y

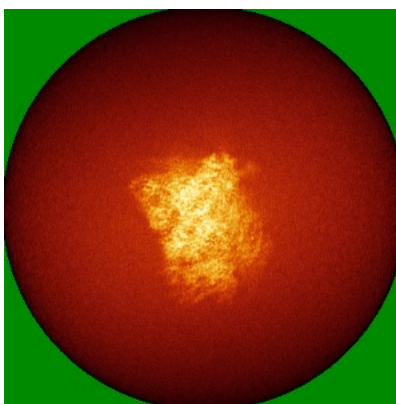


Z

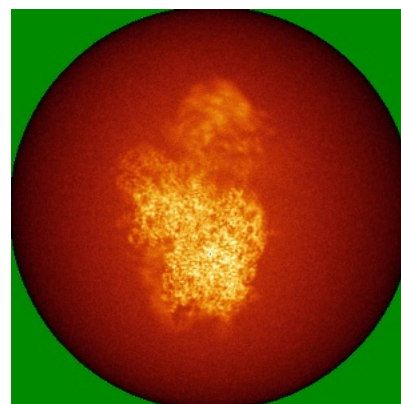
6.4.2 Raw map



X



Y



Z

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

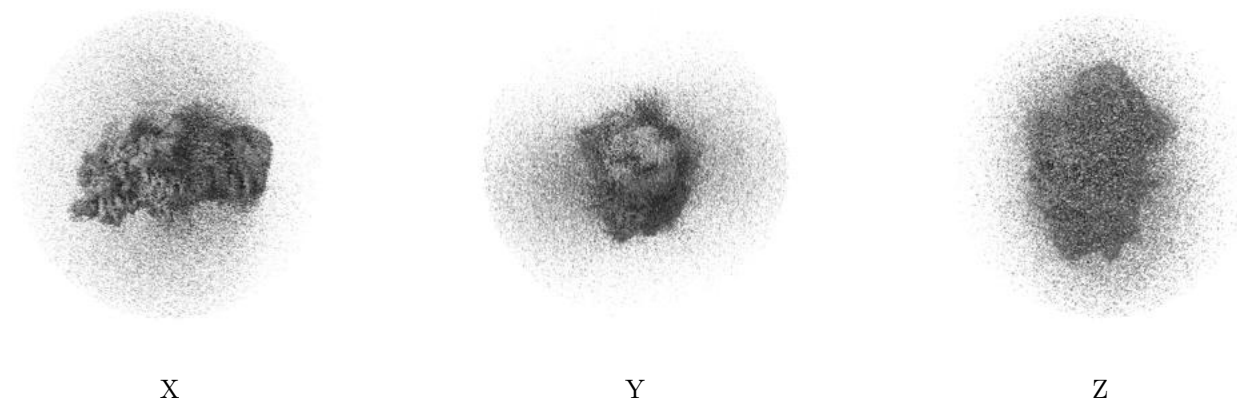
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

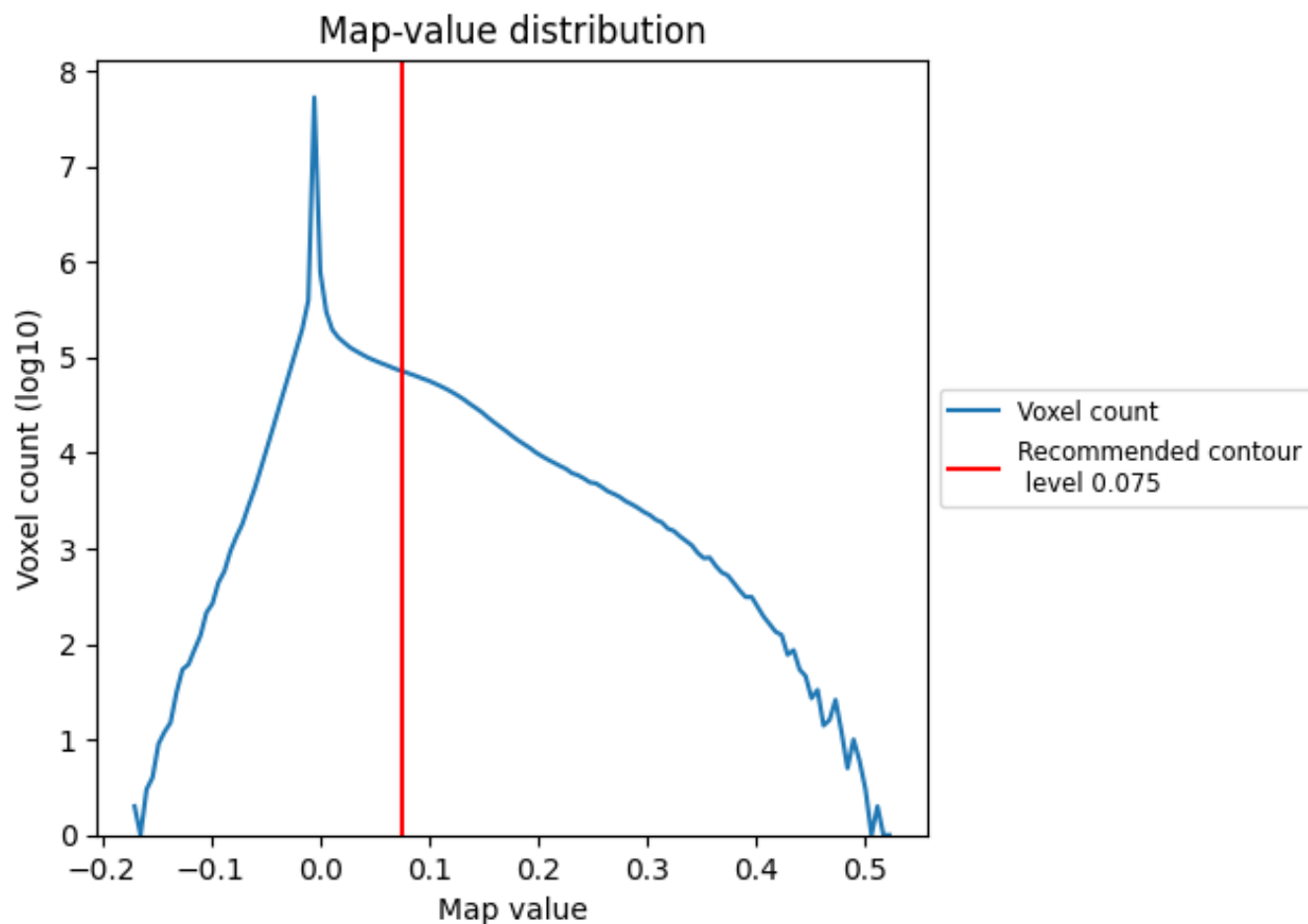
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

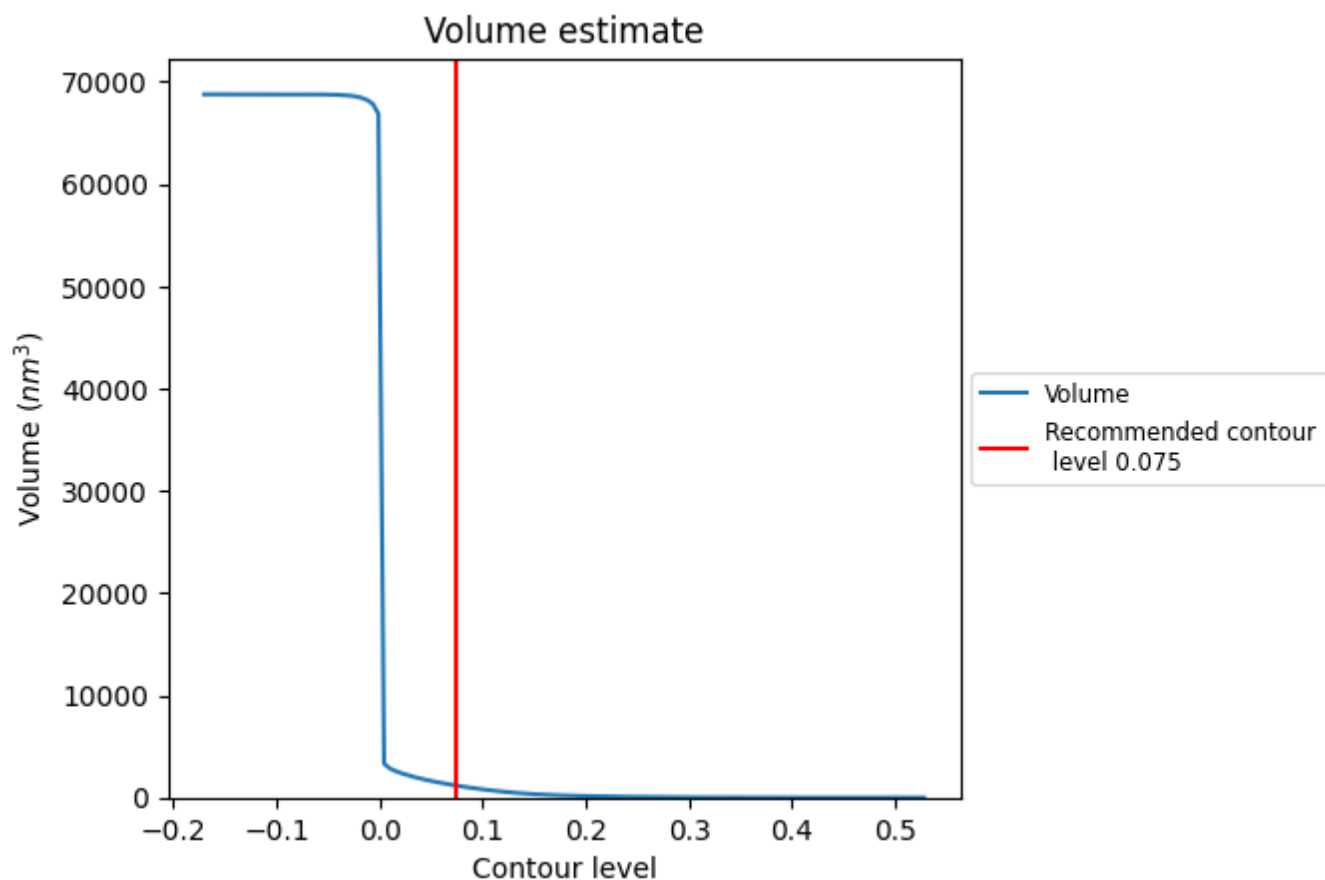
This section contains the results of statistical analysis of the map.

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.

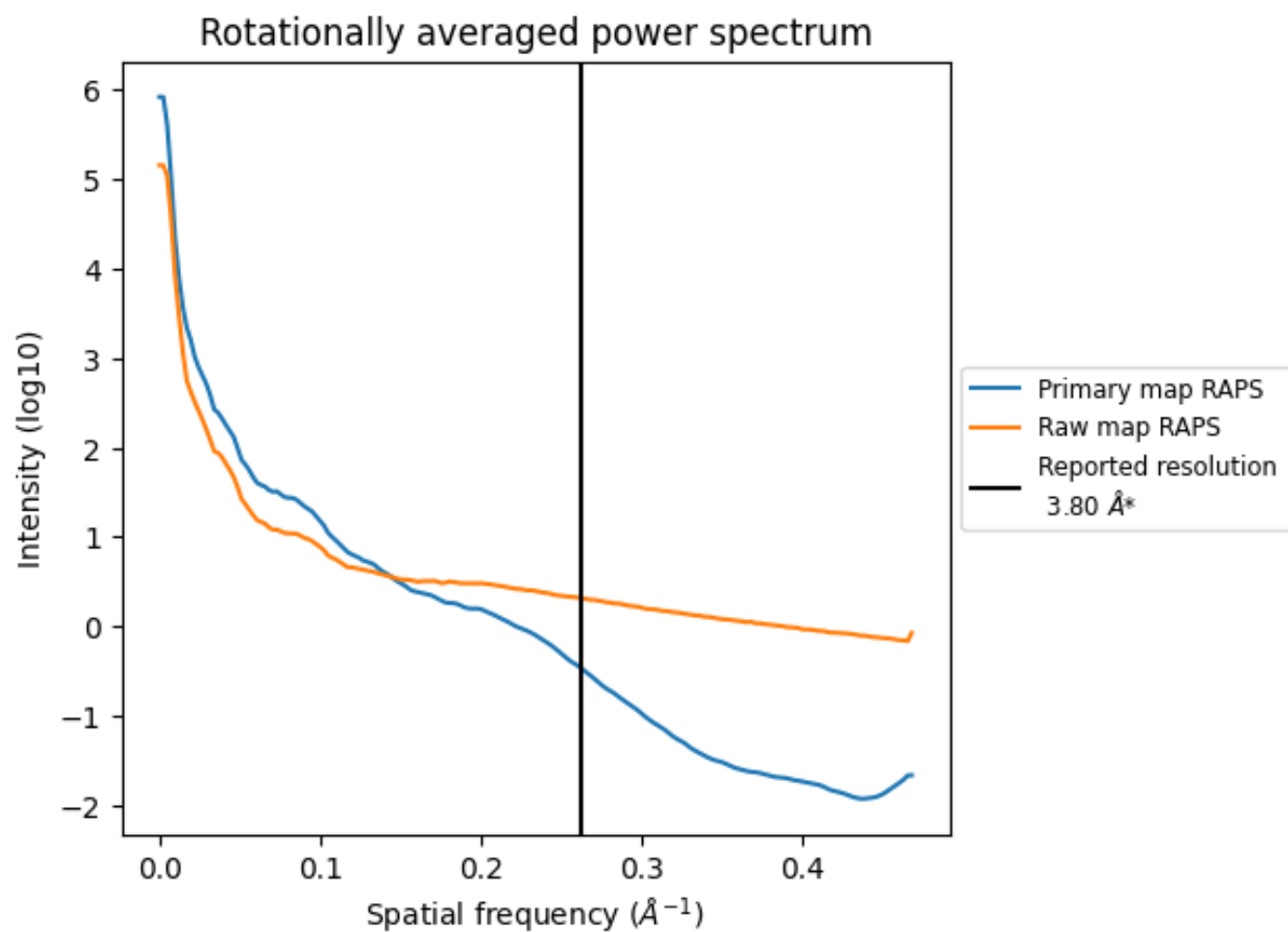
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1165 nm³; this corresponds to an approximate mass of 1053 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 ⓘ

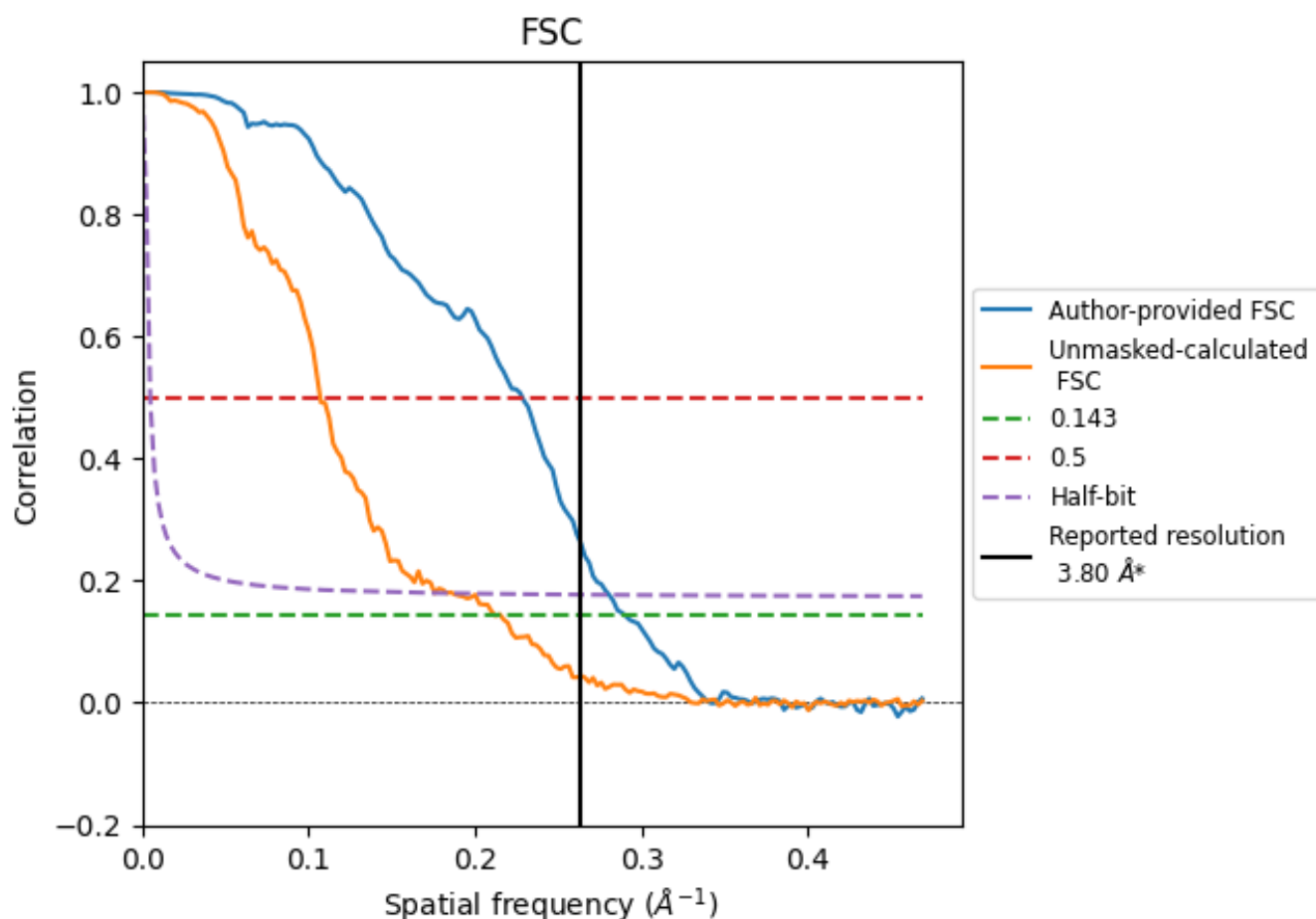


*Reported resolution corresponds to spatial frequency of $0.263 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

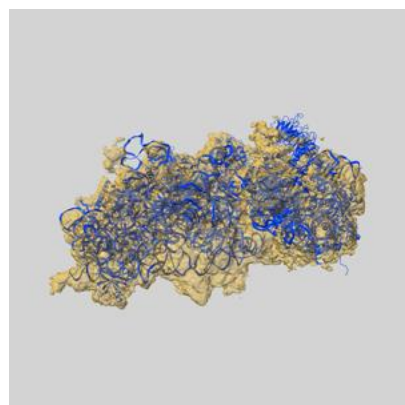
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.45	4.38	3.57
Unmasked-calculated*	4.71	9.35	5.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.71 differs from the reported value 3.8 by more than 10 %

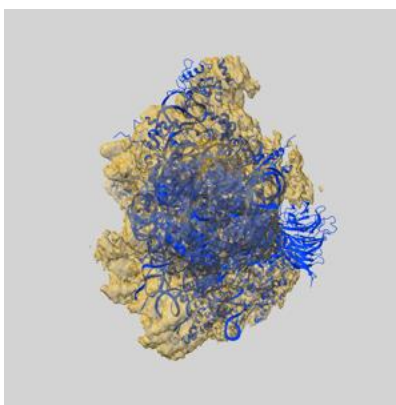
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4793 and PDB model 6RBE. Per-residue inclusion information can be found in section 3 on page 10.

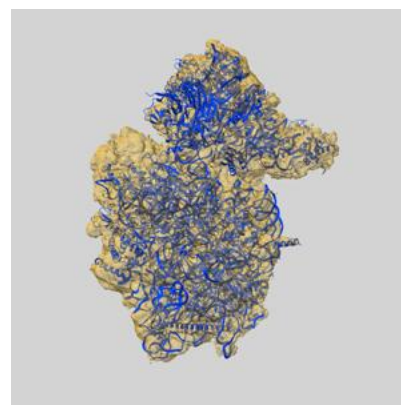
9.1 Map-model overlay [i](#)



X



Y



Z

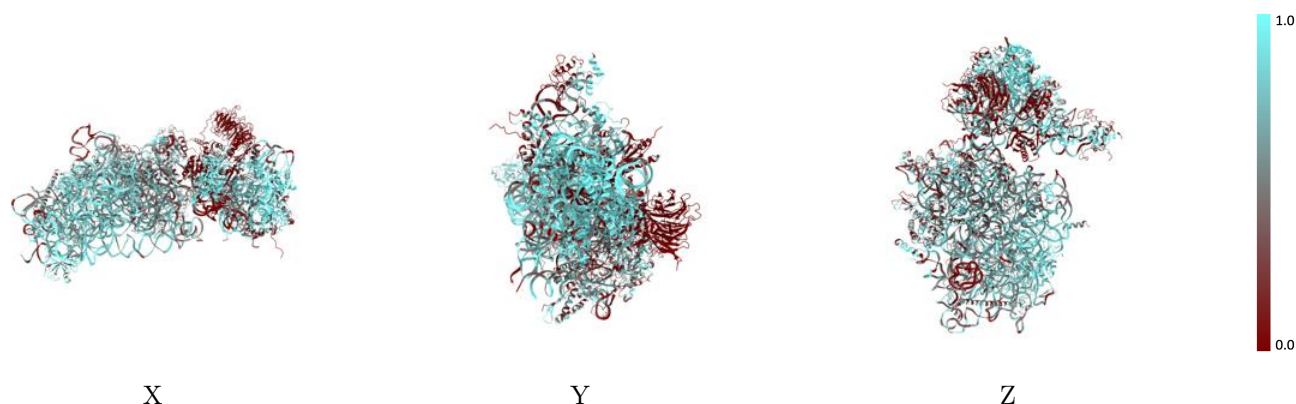
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



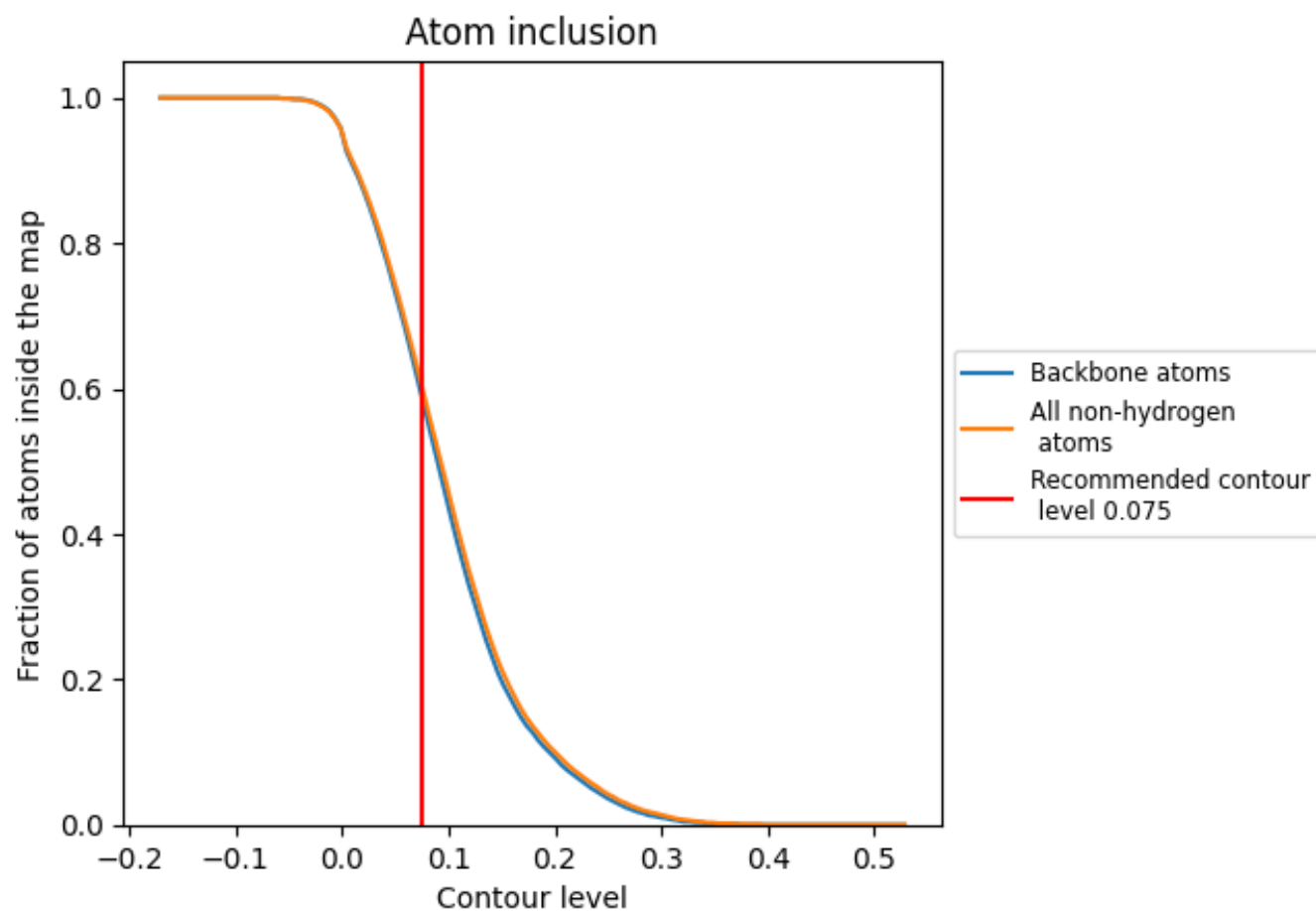
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 60% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6040	 0.0190
2	 0.6670	 0.0320
A	 0.5710	 -0.0250
B	 0.4790	 -0.0530
C	 0.5450	 -0.0190
D	 0.3010	 0.0160
E	 0.6850	 -0.0010
F	 0.7180	 0.0120
G	 0.6840	 0.0400
H	 0.5500	 0.0020
I	 0.5800	 -0.0250
J	 0.7120	 0.0250
K	 0.6610	 0.0130
L	 0.5190	 -0.0230
M	 0.5170	 -0.0000
N	 0.5940	 0.0000
O	 0.4660	 -0.0060
P	 0.5220	 -0.0130
Q	 0.6020	 0.0280
R	 0.3980	 0.0140
S	 0.5970	 0.0280
T	 0.8820	 0.0340
U	 0.1330	 0.0070
V	 0.6600	 0.0020
W	 0.6370	 -0.0260
X	 0.6200	 -0.0390
Y	 0.8250	 0.1970
Z	 0.5230	 -0.0290
b	 0.4810	 0.0290
c	 0.4760	 0.0590
d	 0.6050	 0.0310
e	 0.3660	 -0.0290
f	 0.0750	 -0.0000
g	 0.0030	 -0.0210

