



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 11:29 AM UTC

PDB ID : 8ZDD / pdb_00008zdd
EMDB ID : EMD-39958
Title : Cryo-EM structure of the human ubiquitylated pre-40S ribosome with R1OK3
(without NOB1)
Authors : Huang, Z.; Wang, M.; Li, Y.; Beckmann, R.; Cheng, J.
Deposited on : 2024-05-01
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
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

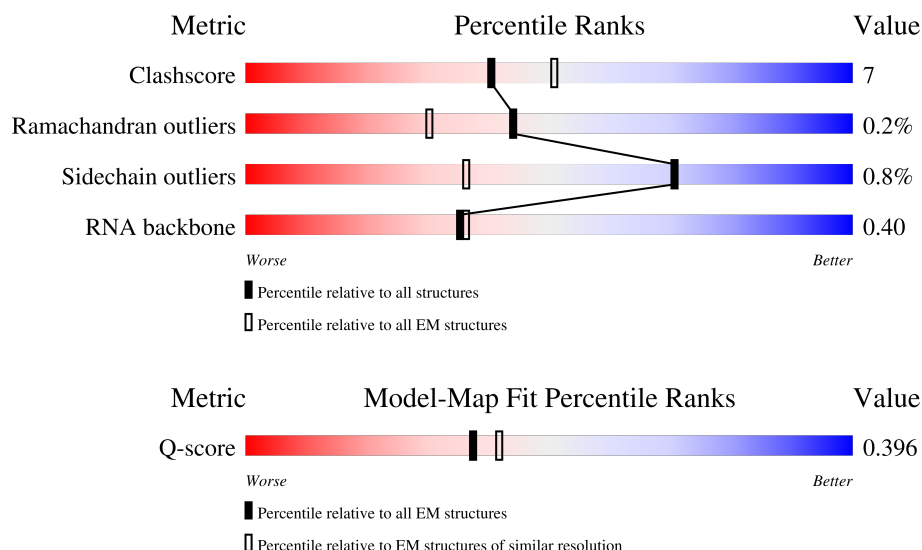
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	1873	
2	R	135	
3	A	295	

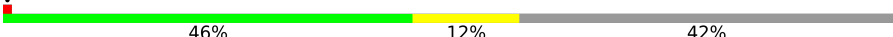
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Mol	Chain	Length	Quality of chain
4	B	264	
5	C	293	
6	E	263	
7	G	249	
8	H	194	
9	I	208	
10	J	194	
11	L	158	
12	N	151	
13	O	151	
14	V	83	
15	W	130	
16	X	143	
17	Y	133	
18	b	84	
19	x	252	
20	u	804	
21	t	475	
22	d	56	
23	D	243	
24	F	204	
25	K	165	
26	M	132	
27	P	145	
28	Q	146	

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Mol	Chain	Length	Quality of chain
29	S	152	
30	T	145	
31	U	119	
32	Z	125	
33	c	69	
34	g	317	
35	p	519	
36	i	76	
36	j	76	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 81515 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1652	Total	C	N	O	P	0	0
			35283	15748	6344	11540	1651		

- Molecule 2 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	122	Total	C	N	O	S	0	0
			990	621	184	182	3		

- Molecule 3 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	216	Total	C	N	O	S	0	0
			1705	1083	299	315	8		

- Molecule 4 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	218	Total	C	N	O	S	0	0
			1690	1094	289	297	10		

- Molecule 6 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 7 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 8 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	186	Total	C	N	O	S	0	0
			1501	957	276	267	1		

- Molecule 9 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 10 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 11 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 12 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 13 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	135	Total	C	N	O	S	0	0
			1009	618	198	187	6		

- Molecule 14 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 15 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 16 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 17 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 18 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 19 is a protein called RNA-binding protein PNO1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	x	178	Total	C	N	O	0	0
			880	524	178	178		

- Molecule 20 is a protein called Pre-rRNA-processing protein TSR1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	u	615	Total	C	N	O	S	0	0
			4954	3179	885	866	24		

- Molecule 21 is a protein called Protein LTV1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	t	61	Total	C	N	O	0	0
			517	316	107	94		

- Molecule 22 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	d	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 23 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	D	225	Total	C	N	O	S	0	0
			1752	1117	315	313	7		

- Molecule 24 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	F	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 25 is a protein called Small ribosomal subunit protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	K	95	Total	C	N	O	S	0	0
			800	522	142	131	5		

- Molecule 26 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	M	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 27 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	P	120	Total	C	N	O	S	0	0
			984	625	184	168	7		

- Molecule 28 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Q	139	Total	C	N	O	S	0	0
			1109	704	210	192	3		

- Molecule 29 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	S	143	Total	C	N	O	S	0	0
			1184	743	240	200	1		

- Molecule 30 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	T	144	Total	C	N	O	S	0	0
			1122	703	217	199	3		

- Molecule 31 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	U	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 32 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 33 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 34 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 35 is a protein called Serine/threonine-protein kinase RIO3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	p	389	Total	C	N	O	S	0	0
			2419	1468	462	483	6		

- Molecule 36 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	i	73	Total	C	N	O	0	0
			361	215	73	73		
36	j	73	Total	C	N	O	0	0
			361	215	73	73		

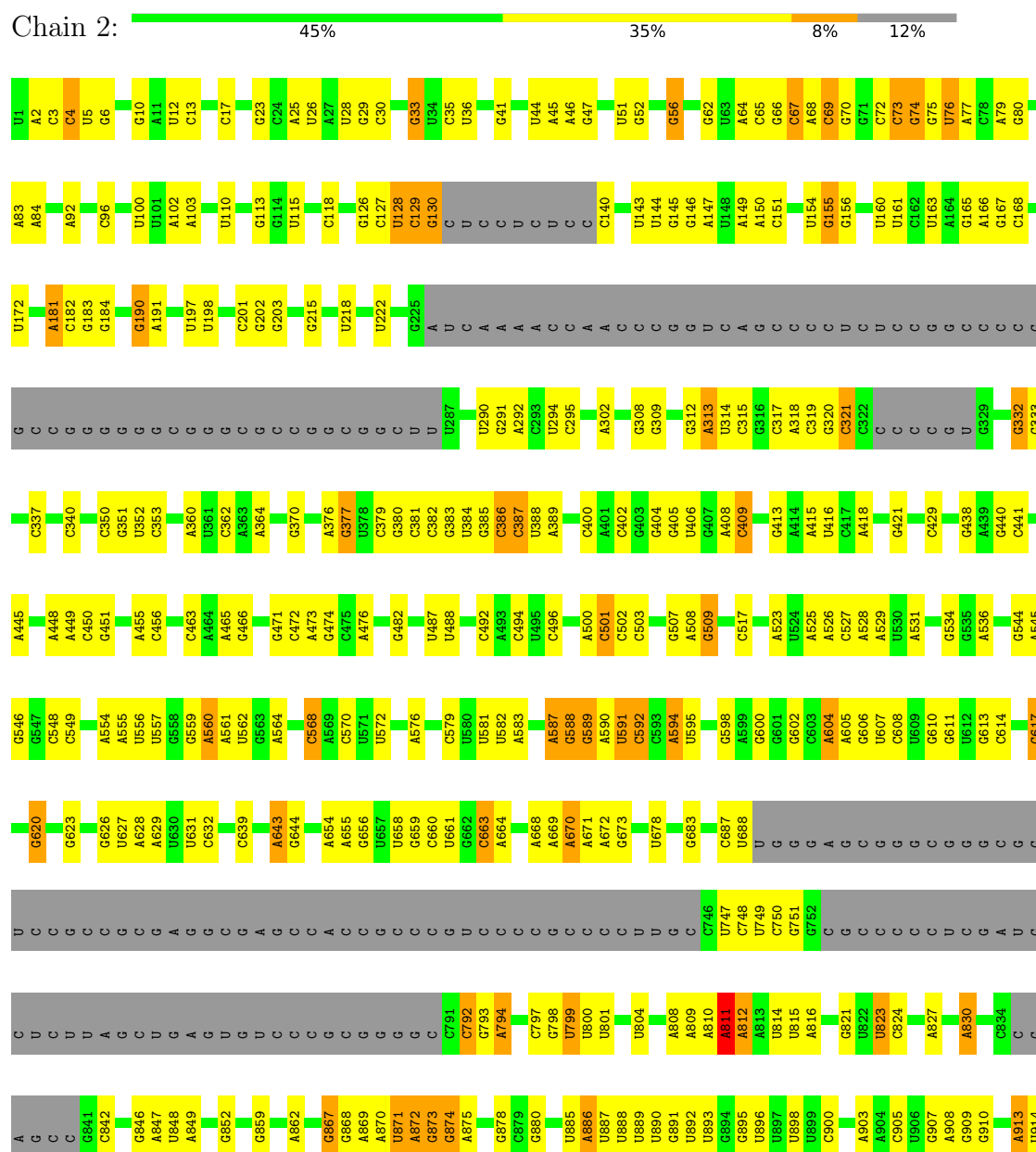
- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

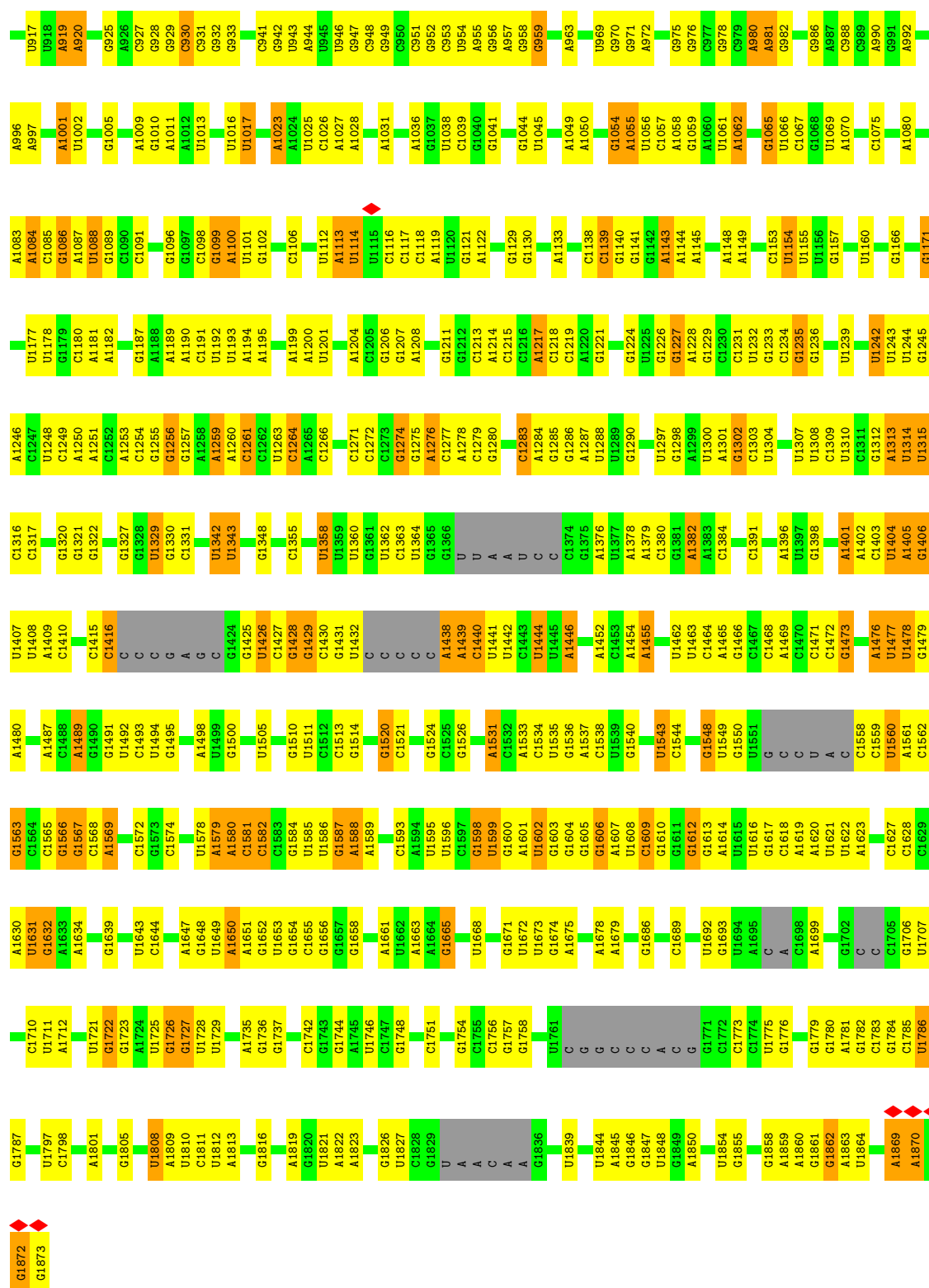
Mol	Chain	Residues	Atoms		AltConf
37	d	1	Total	Zn	0
			1	1	

3 Residue-property plots

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

• Molecule 1: 18S rRNA

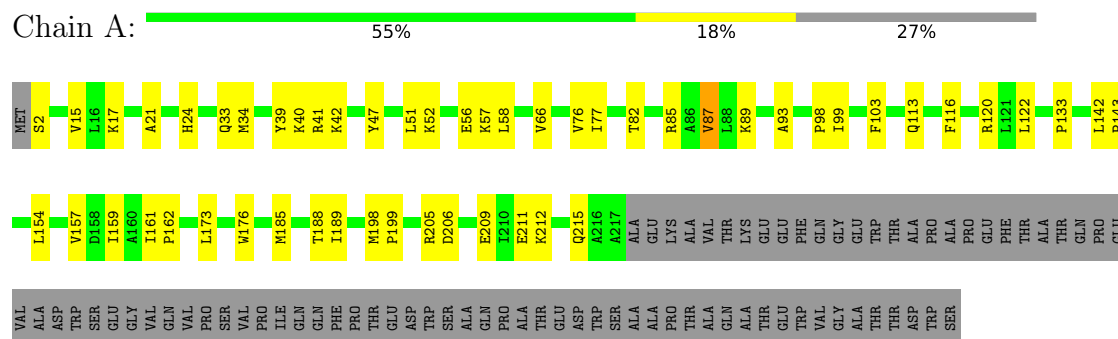




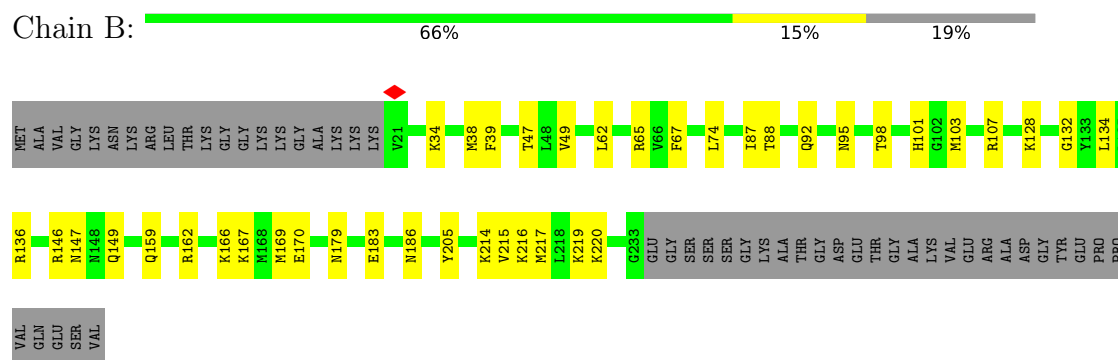
- Molecule 2: Small ribosomal subunit protein eS17

Chain R:

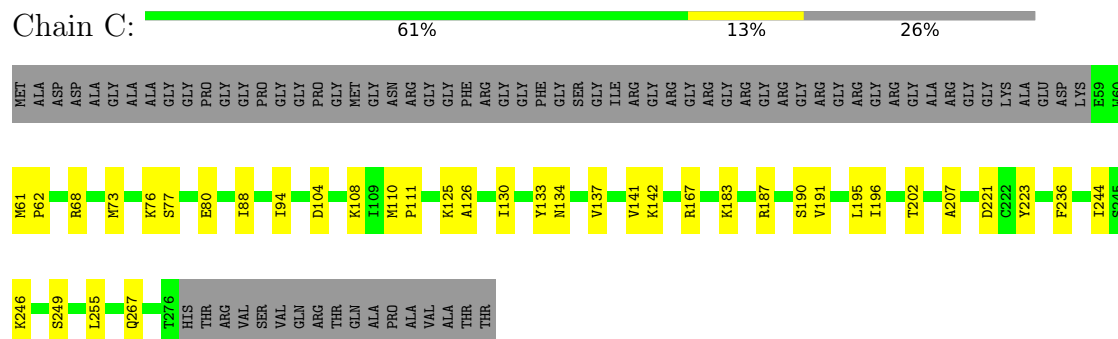
- Molecule 3: Small ribosomal subunit protein uS2



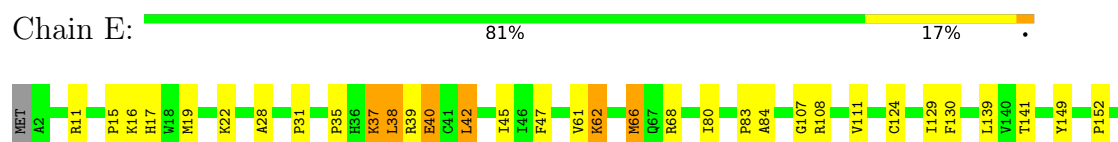
- Molecule 4: Small ribosomal subunit protein eS1



- Molecule 5: Small ribosomal subunit protein uS5

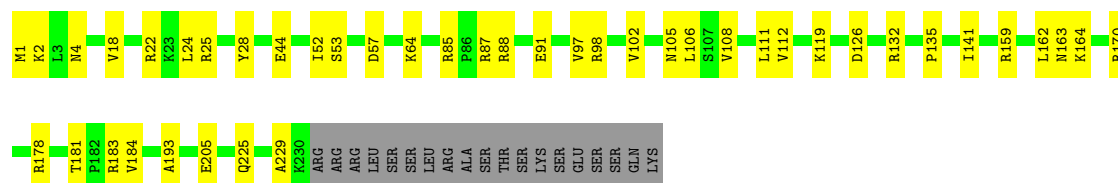
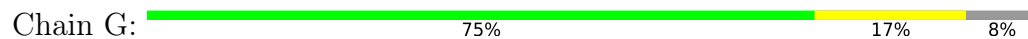


- Molecule 6: Small ribosomal subunit protein eS4, X isoform

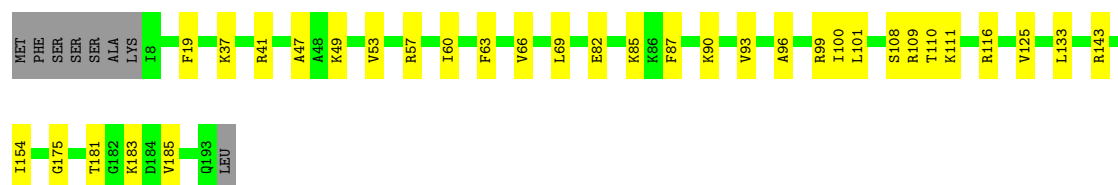
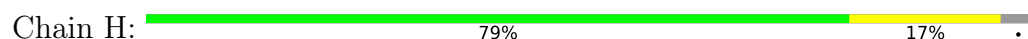




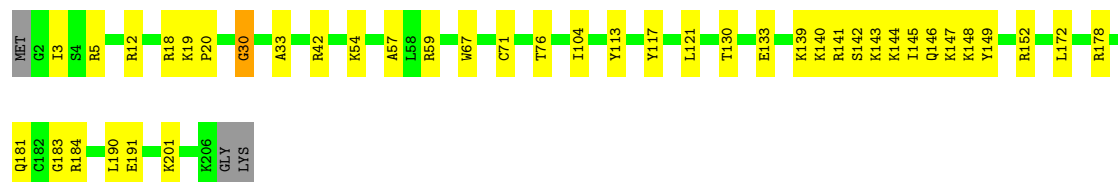
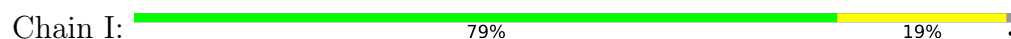
- Molecule 7: Small ribosomal subunit protein eS6



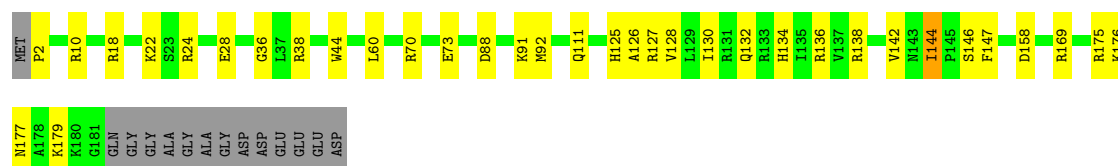
- Molecule 8: Small ribosomal subunit protein eS7



- Molecule 9: Small ribosomal subunit protein eS8



- Molecule 10: Small ribosomal subunit protein uS4



- Molecule 11: Small ribosomal subunit protein uS17





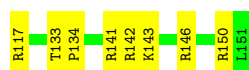
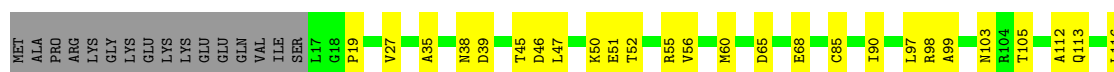
- Molecule 12: Small ribosomal subunit protein uS15

Chain N: 81% 17% .



- Molecule 13: Small ribosomal subunit protein uS11

Chain O: 67% 23% 11%



- Molecule 14: Small ribosomal subunit protein eS21

Chain V: 80% 19% .



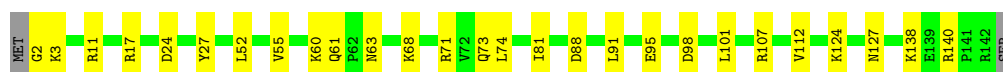
- Molecule 15: Small ribosomal subunit protein uS8

Chain W: 78% 21% ..



- Molecule 16: Small ribosomal subunit protein uS12

Chain X: 80% 19% .



- Molecule 17: Small ribosomal subunit protein eS24

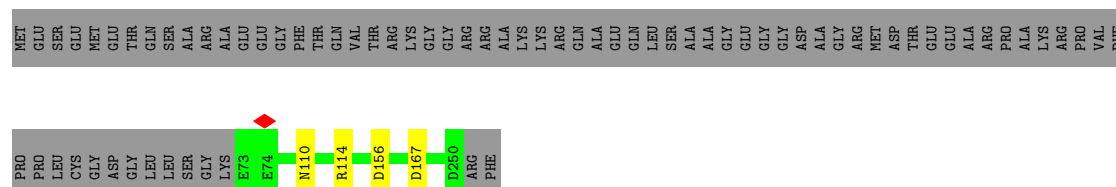
Chain Y: 74% 19% 7%



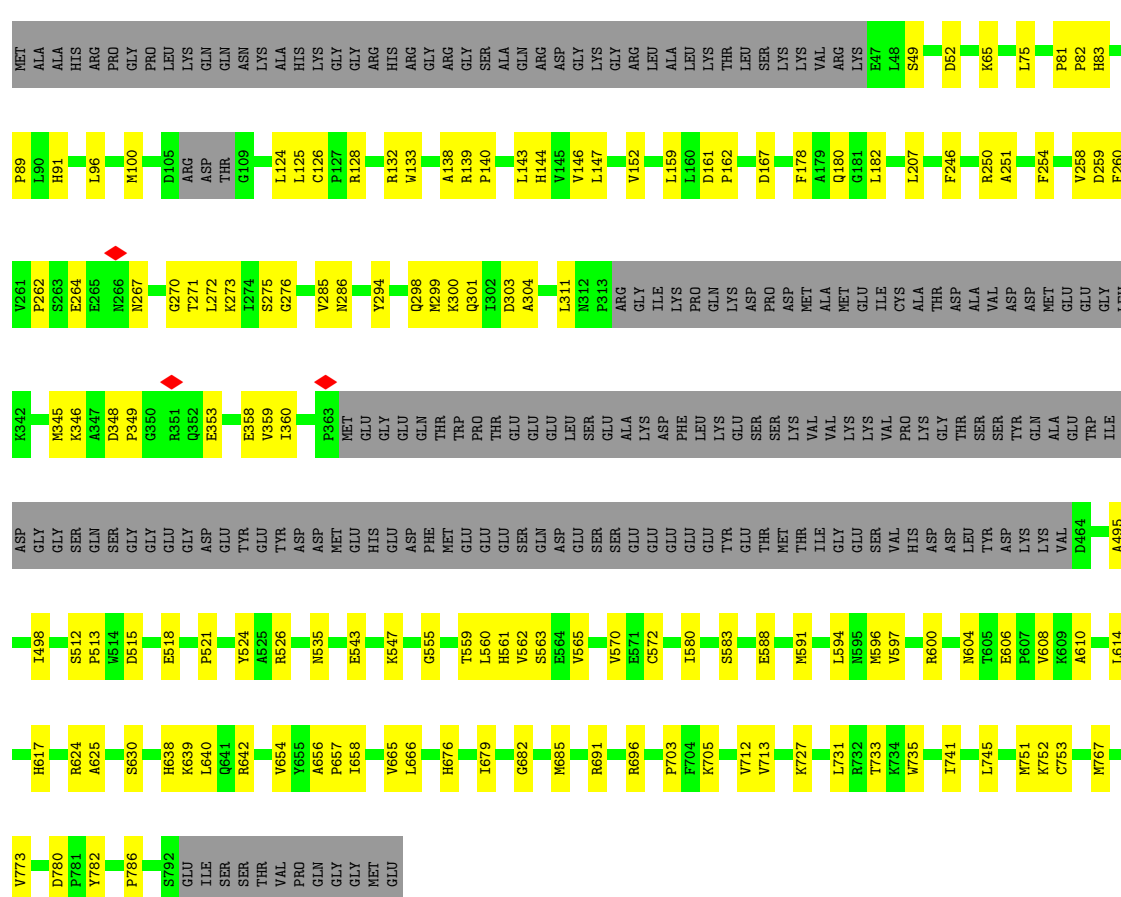
- Molecule 18: Small ribosomal subunit protein eS27



Chain x: 69% 29%



Chain u: 59% 17% 24%

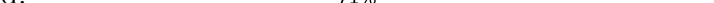


Chain t: 10% . 87%

[illegible]

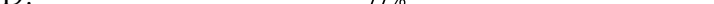
K431
K435
R441
K445
K453
L454
E455
Q459
E462
L466
V470
E471
G472
L473
K474
LEU

- Molecule 22: Small ribosomal subunit protein uS14

Chain d:  71% 27%

MET	G2	L6	S9	H10	P11	R12	G17	S20	N26	R27	H28	G29	K33	Y34	M38	C39	R40	I50	G51	D56
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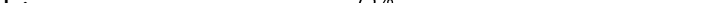
- Molecule 23: Small ribosomal subunit protein uS3

Chain D:  77% 13% • 7%

MET	V3	K8	I50	R54	R67	T70	V72	Q74	F79	A88	R94	Q101	R116	I126	V138	R146	G161	D162	P163	V164	I165	V166	V167	V172	I184	K185	I188	V192	D193	P194	K197	I198	G199	P200	K201	K202	D203
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L204	P205	K227	GLY	GLY	LYS	PRO	GLU	PRO	PRO	ALA	MET	PRO	GLN	PRO	VAL	PRO	THR	ALA
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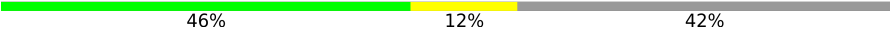
- Molecule 24: Small ribosomal subunit protein uS7

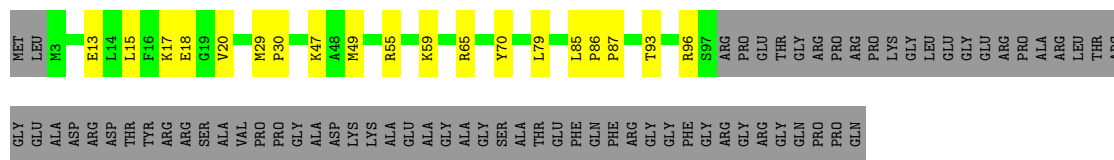
Chain F:  75% 16% • 7%

Met	THR	TRP	GLU	GLU	THR	ALA	PRO	ALA	VAL	ALA	GLU	PRO	D16	D27	I33	Q36	A40	V41	Y45	R55	Y56	R60	F61	R62	K63	I68	R71	H78	M79	G84	K85	K86	T89	I100	N107	T126	A131	N148
Met	THR	TRP	GLU	GLU	THR	ALA	PRO	ALA	VAL	ALA	GLU	PRO	D16	D27	I33	Q36	A40	V41	Y45	R55	Y56	R60	F61	R62	K63	I68	R71	H78	M79	G84	K85	K86	T89	I100	N107	T126	A131	N148

Category	Count
R159	1
A162	1
N165	1
I166	1
K167	1
T168	1
I169	1
A170	1
I178	1
K182	1
K201	1
R204	1

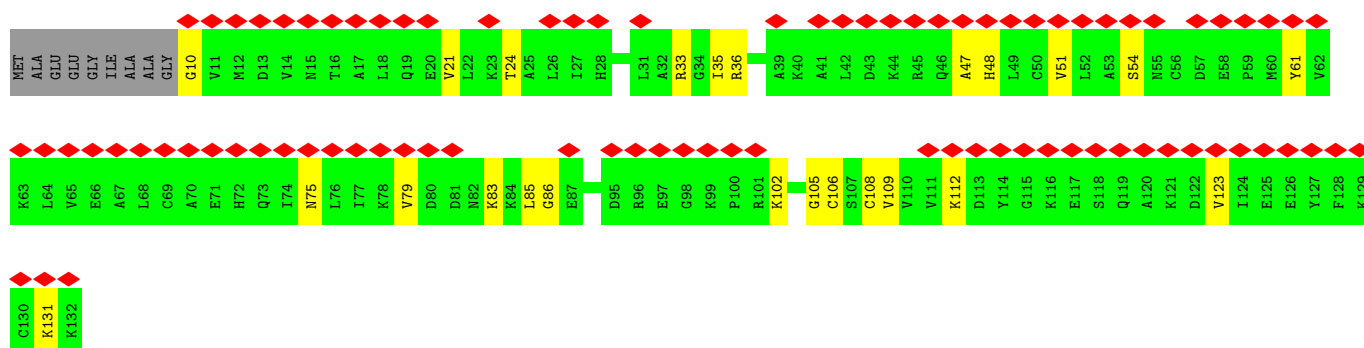
- Molecule 25: Small ribosomal subunit protein eS10

Chain K: 



- Molecule 26: Small ribosomal subunit protein eS12

Chain M: 



- Molecule 27: Small ribosomal subunit protein uS19

Chain P: 



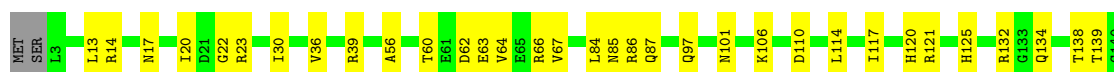
- Molecule 28: Small ribosomal subunit protein uS9

Chain Q: 



- Molecule 29: Small ribosomal subunit protein uS13

Chain S: 





MET ASP VAL GLY VAL ALA SER PRO GLU PRO GLY THR ALA ALA TRP GLY PRO SER LYS CYS TRP ALA TLE PRO GLN ASN THR TLE SER CYS SER LEU ALA ASP VAL MET SER GLN LEU LYS LYS GLU LEU GLN LEU GLU GLU ALA ALA VAL PHE PRO VAL ALA

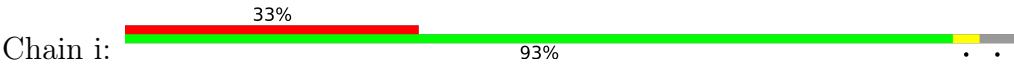
VAL ALA GLU VAL PRO PHE TLE THR GLU ASN ASP THR SER S76 Q95 R98 K101 D106 S107 K108 E129 D133 V134 Q136 D136 C171 M179 E180 V188 N200 R219 E222 E225 H226 S227 THR ALA GLU LYS V233 T237 E274

D275 E276 K277 E278 D279 S280 K281 V282 N287 E298 F299 R302 D303 K304 Y305 I306 K307 D308 D309 N320 P321 R322 K323 I324 W328 R338 R341 A342 G343 I344 P345 C346 P347 H364 K371 E374 V375 K376 L377 N378 S379 E380 E381 M382 K383 E384 A385 Y386 Q388

H391 L392 M393 R394 Q395 L396 Y397 H398 E399 C400 T401 L402 V403 H404 A405 D406 L407 S408 E409 Y410 W414 H415 A416 G417 K418 V419 Q426 S427 V428 E429 P430 T431 H432 P433 H434 G435 L436 E437 R441 D442 C443 V446 S447 Q448 F449 P450 Q451 K452 G453 V455 K456 E457 L459 S460

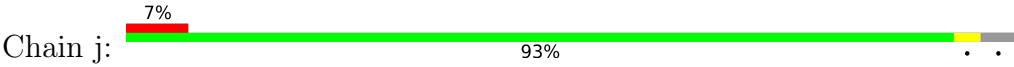
E461 R462 E463 L464 F465 M466 A467 V468 S469 GLY LEU ASN TLE THR ALA ASP ASN GLU ALA ASP PHE LEU ALA TLE GLU ALA A416 G417 K418 V419 Q426 S427 V428 E429 P430 T431 H432 P433 H434 G435 L436 E437 R441 D442 C443 V446 S447 Q448 F449 P450 Q451 K452 G453 V455 K456 E457 L459 S460

• Molecule 36: Ubiquitin



M1 D2 T9 G10 K11 T12 I13 T14 L15 E16 V17 P19 S20 D21 T22 P38 G53 R54 T55 L56 S57 D58 Y59 M60 I61 Q62 K63 E64 S65 L73 ARG GLY GLY

• Molecule 36: Ubiquitin



M1 S20 D21 T22 D52 G53 R54 T55 D58 L73 ARG GLY GLY

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34363	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 ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.366	Depositor
Minimum map value	-0.130	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	383.04, 383.04, 383.04	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.34	0/39452	0.48	3/61476 (0.0%)
2	R	0.35	0/1002	0.80	2/1345 (0.1%)
3	A	0.36	0/1742	0.64	0/2367
4	B	0.20	0/1756	0.47	0/2350
5	C	0.36	0/1726	0.65	2/2332 (0.1%)
6	E	0.54	0/2118	0.78	1/2849 (0.0%)
7	G	0.26	0/1885	0.55	0/2510
8	H	0.21	0/1524	0.48	0/2042
9	I	0.39	1/1711 (0.1%)	0.62	1/2282 (0.0%)
10	J	0.43	0/1524	0.63	1/2035 (0.0%)
11	L	0.41	0/1250	0.56	1/1673 (0.1%)
12	N	0.25	0/1226	0.44	0/1649
13	O	0.19	0/1022	0.48	0/1372
14	V	0.33	0/631	0.60	0/844
15	W	0.50	0/1051	0.79	4/1406 (0.3%)
16	X	0.41	0/1116	0.68	2/1490 (0.1%)
17	Y	0.40	0/1031	0.62	0/1370
18	b	0.27	0/653	0.56	0/876
19	x	0.15	0/879	0.46	0/1223
20	u	0.23	0/5076	0.52	0/6860
21	t	0.22	0/518	0.60	0/677
22	d	0.28	0/470	0.49	0/623
23	D	0.43	0/1780	0.74	1/2397 (0.0%)
24	F	0.31	0/1516	0.71	0/2037
25	K	0.28	0/824	0.66	0/1112
26	M	0.17	0/963	0.56	0/1291
27	P	0.24	0/1003	0.65	0/1341
28	Q	0.30	0/1126	0.71	0/1506
29	S	0.18	0/1202	0.52	0/1610
30	T	0.24	0/1142	0.63	0/1530
31	U	0.30	0/813	0.63	0/1092
32	Z	0.20	0/580	0.57	0/780

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.19	0/481	0.58	2/643 (0.3%)
34	g	0.20	0/2497	0.48	0/3399
35	p	0.26	0/2444	0.53	2/3338 (0.1%)
36	i	0.11	0/360	0.36	0/500
36	j	0.12	0/360	0.38	0/500
All	All	0.33	1/86454 (0.0%)	0.54	22/124727 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	I	0	1
24	F	0	1
30	T	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	30	GLY	C-N	-5.71	1.23	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	109	LEU	CA-C-N	7.33	135.54	121.54
2	R	109	LEU	C-N-CA	7.33	135.54	121.54
1	2	811	A	C2'-C3'-O3'	6.86	123.99	113.70
11	L	41	GLY	N-CA-C	6.33	119.84	112.50
33	c	36	ASP	CA-C-N	6.26	133.50	121.54
33	c	36	ASP	C-N-CA	6.26	133.50	121.54
5	C	133	TYR	CA-C-N	6.24	133.46	121.54
5	C	133	TYR	C-N-CA	6.24	133.46	121.54
9	I	20	PRO	N-CA-C	6.01	120.42	111.41
23	D	161	GLY	CA-C-O	-5.81	118.27	122.45
10	J	147	PHE	CA-CB-CG	5.62	119.42	113.80
6	E	130	PHE	CA-CB-CG	5.33	119.13	113.80
15	W	46	TYR	CA-C-N	-5.25	115.90	121.84
15	W	46	TYR	C-N-CA	-5.25	115.90	121.84
16	X	60	LYS	CA-C-N	5.20	134.50	121.80
16	X	60	LYS	C-N-CA	5.20	134.50	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	W	89	TRP	N-CA-C	-5.18	106.65	113.12
1	2	501	C	N1-C1'-C2'	5.16	119.74	112.00
1	2	409	C	C2'-C3'-O3'	-5.15	105.97	113.70
15	W	91	ASN	N-CA-C	-5.12	107.04	113.28
35	p	101	LYS	CA-C-N	-5.09	114.59	122.49
35	p	101	LYS	C-N-CA	-5.09	114.59	122.49

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	F	165	ASN	Peptide
9	I	140	LYS	Peptide
30	T	36	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	35283	0	17815	399	0
2	R	990	0	1037	19	0
3	A	1705	0	1706	41	0
4	B	1729	0	1803	29	0
5	C	1690	0	1777	24	0
6	E	2076	0	2177	27	0
7	G	1862	0	2018	30	0
8	H	1501	0	1593	20	0
9	I	1682	0	1769	30	0
10	J	1499	0	1618	28	0
11	L	1229	0	1302	25	0
12	N	1202	0	1289	17	0
13	O	1009	0	1034	29	0
14	V	625	0	628	13	0
15	W	1034	0	1080	15	0
16	X	1098	0	1167	21	0
17	Y	1014	0	1082	17	0
18	b	640	0	665	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	x	880	0	403	3	0
20	u	4954	0	5014	82	0
21	t	517	0	566	11	0
22	d	459	0	452	11	0
23	D	1752	0	1848	29	0
24	F	1495	0	1549	19	0
25	K	800	0	818	14	0
26	M	953	0	990	17	0
27	P	984	0	1028	23	0
28	Q	1109	0	1174	27	0
29	S	1184	0	1244	25	0
30	T	1122	0	1153	29	0
31	U	803	0	873	18	0
32	Z	574	0	627	12	0
33	c	479	0	507	13	0
34	g	2440	0	2396	48	0
35	p	2419	0	1696	15	0
36	i	361	0	155	1	0
36	j	361	0	155	1	0
37	d	1	0	0	0	0
All	All	81515	0	64208	991	0

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

All (991) 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)
1:2:1455:A:H61	1:2:1471:C:N4	1.45	1.15
1:2:1455:A:N6	1:2:1471:C:H42	1.46	1.10
23:D:194:PRO:HA	23:D:201:LYS:HA	1.43	0.99
1:2:1206:G:H1	1:2:1692:U:H3	1.06	0.97
1:2:1244:U:H3	1:2:1255:G:H1	1.10	0.97
1:2:1710:C:H42	1:2:1823:A:N6	1.71	0.88
1:2:140:C:H42	1:2:313:A:H61	1.22	0.86
1:2:1091:C:HO2'	15:W:2:VAL:N	1.73	0.86
28:Q:8:GLN:N	28:Q:99:TYR:HH	1.78	0.82
1:2:1710:C:N4	1:2:1823:A:H61	1.80	0.79
20:u:617:HIS:HB2	20:u:666:LEU:HB2	1.67	0.77
20:u:258:VAL:HA	20:u:273:LYS:O	1.85	0.77
1:2:944:A:H61	1:2:982:G:H1	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:F:155:CYS:HB3	24:F:159:ARG:HH21	1.49	0.76
1:2:1652:G:H1	1:2:1672:U:H3	1.33	0.75
1:2:1710:C:N4	1:2:1823:A:N6	2.35	0.75
1:2:659:G:H21	16:X:17:ARG:HH22	1.36	0.74
1:2:928:G:H1	1:2:1013:U:H3	1.34	0.72
1:2:1069:U:H4'	21:t:430:ARG:HH22	1.52	0.72
1:2:1722:G:O6	1:2:1812:U:C2	2.41	0.72
23:D:138:VAL:HG12	23:D:184:ILE:HG22	1.70	0.72
1:2:1329:U:O4	1:2:1493:C:N3	2.22	0.72
27:P:28:MET:SD	27:P:32:GLN:NE2	2.62	0.72
1:2:76:U:H5'	7:G:159:ARG:HH22	1.54	0.71
1:2:1513:C:H2'	1:2:1514:G:H8	1.54	0.71
1:2:1227:G:H1	1:2:1531:A:H61	1.39	0.70
9:I:141:ARG:HH22	9:I:149:TYR:HB2	1.55	0.70
2:R:98:VAL:HG21	2:R:117:LEU:HD12	1.72	0.70
20:u:272:LEU:HB2	20:u:565:VAL:HG11	1.73	0.70
1:2:1533:A:N6	1:2:1602:U:N3	2.39	0.69
1:2:130:G:N1	1:2:181:A:N6	2.40	0.69
16:X:74:LEU:HG	16:X:81:ILE:HD13	1.75	0.69
1:2:1726:G:H1	1:2:1808:U:H3	1.41	0.69
1:2:1609:C:H42	1:2:1631:U:H3	1.41	0.68
20:u:727:LYS:HA	20:u:741:ILE:HD11	1.76	0.68
1:2:1566:G:N2	1:2:1569:A:C5	2.61	0.68
1:2:1313:A:H5''	26:M:33:ARG:HH22	1.58	0.68
4:B:38:MET:SD	4:B:186:ASN:ND2	2.67	0.68
1:2:925:G:H1	1:2:1017:U:H3	1.41	0.67
1:2:824:C:H1'	10:J:144:ILE:HG21	1.77	0.67
1:2:384:U:O4	9:I:5:ARG:NH2	2.27	0.67
1:2:1329:U:O4	1:2:1500:G:O6	2.11	0.67
1:2:867:G:H5'	11:L:149:ALA:HB1	1.75	0.67
1:2:957:A:H3'	1:2:958:G:H21	1.59	0.67
1:2:1261:C:O2	22:d:10:HIS:NE2	2.27	0.67
34:g:7:LEU:HB2	34:g:272:GLN:HE22	1.59	0.67
20:u:624:ARG:NH1	20:u:782:TYR:O	2.28	0.66
10:J:169:ARG:HE	10:J:175:ARG:HH21	1.41	0.66
1:2:1444:U:OP1	28:Q:15:ARG:NH2	2.29	0.66
20:u:625:ALA:HB1	20:u:654:VAL:HG21	1.76	0.66
4:B:128:LYS:HE2	4:B:132:GLY:HA2	1.76	0.66
7:G:85:ARG:HH12	17:Y:118:ARG:HD2	1.59	0.66
3:A:185:MET:HE1	14:V:39:VAL:HG12	1.78	0.66
13:O:97:LEU:HD11	13:O:112:ALA:HB1	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:17:LYS:HB3	3:A:173:LEU:HD11	1.77	0.66
4:B:103:MET:H	4:B:215:VAL:HB	1.60	0.65
30:T:76:THR:HG22	30:T:94:ARG:HB3	1.78	0.65
8:H:93:VAL:HG11	8:H:133:LEU:HD12	1.79	0.65
16:X:68:LYS:HB3	16:X:91:LEU:HD22	1.78	0.65
5:C:183:LYS:HA	5:C:195:LEU:O	1.97	0.65
30:T:101:ARG:HG2	30:T:105:GLN:HE22	1.59	0.65
34:g:245:ARG:HH12	34:g:312:VAL:HG21	1.60	0.65
2:R:74:GLN:HG3	2:R:78:ARG:HD2	1.78	0.65
1:2:572:U:OP2	17:Y:37:LYS:NZ	2.29	0.65
1:2:1567:G:H1'	30:T:37:VAL:HG21	1.79	0.65
3:A:113:GLN:HB3	3:A:116:PHE:HB2	1.78	0.65
18:b:34:ASP:HB3	18:b:82:LYS:HE3	1.79	0.65
1:2:617:G:H4'	16:X:88:ASP:HB3	1.79	0.64
1:2:1106:C:H5''	18:b:70:LYS:HG3	1.79	0.64
1:2:1599:U:H5''	32:Z:44:LEU:HD23	1.78	0.64
9:I:143:LYS:HA	9:I:146:GLN:HG2	1.79	0.64
17:Y:14:THR:HG22	17:Y:21:LYS:HG2	1.79	0.64
34:g:149:GLU:HG3	34:g:170:TRP:HB2	1.79	0.64
1:2:47:G:O2'	20:u:65:LYS:NZ	2.26	0.64
1:2:197:U:H3	1:2:202:G:H1	1.44	0.64
7:G:44:GLU:HG3	7:G:119:LYS:HE2	1.79	0.64
3:A:66:VAL:HG21	3:A:185:MET:HB2	1.80	0.64
34:g:46:THR:H	34:g:53:GLY:HA2	1.61	0.64
10:J:18:ARG:O	10:J:24:ARG:NH1	2.31	0.64
20:u:162:PRO:HA	20:u:207:LEU:HD11	1.78	0.64
34:g:24:THR:HG23	34:g:27:PHE:H	1.63	0.63
1:2:589:G:N2	1:2:591:U:O2	2.32	0.63
20:u:96:LEU:O	20:u:100:MET:HB2	1.97	0.63
1:2:1609:C:N3	1:2:1631:U:O2	2.31	0.63
20:u:260:PHE:HB2	20:u:570:VAL:HG21	1.80	0.63
34:g:31:ILE:HB	34:g:43:TRP:HB2	1.80	0.63
1:2:1455:A:N1	1:2:1471:C:N3	2.47	0.63
28:Q:97:GLN:HB2	28:Q:105:LYS:HD2	1.80	0.63
1:2:1548:G:OP1	31:U:62:ARG:NH2	2.31	0.63
1:2:1235:G:OP1	1:2:1246:A:N6	2.30	0.63
1:2:1396:A:O2'	1:2:1398:G:N7	2.31	0.63
1:2:1710:C:N3	1:2:1823:A:N1	2.46	0.63
2:R:74:GLN:NE2	2:R:79:GLU:OE2	2.32	0.63
7:G:22:ARG:HA	7:G:25:ARG:HG2	1.80	0.63
13:O:142:ARG:NH2	19:x:167:ASP:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:u:639:LYS:HD2	20:u:696:ARG:HD2	1.79	0.63
1:2:1154:U:OP2	5:C:187:ARG:NH2	2.31	0.63
1:2:64:A:H2	1:2:83:A:H62	1.47	0.63
5:C:108:LYS:HE3	5:C:110:MET:HB3	1.82	0.62
11:L:85:THR:HG22	11:L:112:HIS:HA	1.81	0.62
1:2:941:C:H2'	1:2:942:G:H8	1.63	0.62
24:F:201:LYS:HD3	24:F:204:ARG:HE	1.65	0.62
1:2:816:A:OP2	10:J:10:ARG:NH2	2.33	0.62
16:X:95:GLU:OE2	16:X:140:ARG:NH1	2.33	0.62
20:u:543:GLU:HA	20:u:547:LYS:HD3	1.81	0.62
1:2:151:C:H1'	7:G:132:ARG:HH22	1.65	0.62
8:H:37:LYS:HB3	8:H:41:ARG:HH21	1.65	0.62
8:H:101:LEU:O	8:H:116:ARG:NH1	2.32	0.62
13:O:39:ASP:HB3	13:O:68:GLU:HB3	1.82	0.61
1:2:944:A:N6	1:2:982:G:H1	1.97	0.61
1:2:948:C:H2'	1:2:949:G:H8	1.64	0.61
25:K:59:LYS:HB2	25:K:70:TYR:HB2	1.83	0.61
29:S:138:THR:HG23	29:S:139:THR:HG23	1.81	0.61
1:2:1533:A:N6	1:2:1602:U:C2	2.67	0.61
20:u:594:LEU:HD13	20:u:656:ALA:HB3	1.82	0.61
20:u:624:ARG:NH2	20:u:780:ASP:OD2	2.34	0.61
23:D:67:ARG:HE	25:K:96:ARG:HE	1.46	0.61
28:Q:16:LYS:HG2	28:Q:17:LYS:H	1.65	0.61
11:L:126:VAL:HG22	11:L:145:VAL:HG22	1.82	0.61
23:D:67:ARG:NH1	25:K:93:THR:O	2.34	0.61
1:2:1589:A:N3	1:2:1653:U:O2'	2.34	0.61
1:2:476:A:N3	1:2:488:U:O2'	2.32	0.61
1:2:1415:C:O2'	30:T:132:ASP:OD2	2.18	0.61
20:u:125:LEU:HD11	20:u:311:LEU:HA	1.82	0.61
20:u:705:LYS:HB2	20:u:712:VAL:HB	1.82	0.61
20:u:89:PRO:HG3	20:u:96:LEU:HB3	1.83	0.61
8:H:154:ILE:HB	8:H:185:VAL:HG22	1.82	0.60
24:F:126:THR:HG23	33:c:26:GLN:HE21	1.66	0.60
13:O:99:ALA:H	13:O:133:THR:HG22	1.65	0.60
1:2:1075:C:OP1	12:N:107:LYS:NZ	2.34	0.60
1:2:1428:G:O6	28:Q:73:LYS:NZ	2.34	0.60
20:u:180:GLN:HB3	20:u:666:LEU:HD11	1.83	0.60
1:2:379:C:OP2	9:I:181:GLN:NE2	2.33	0.60
1:2:604:A:N3	1:2:639:C:O2'	2.32	0.60
6:E:11:ARG:HA	6:E:28:ALA:HB2	1.82	0.60
29:S:39:ARG:HH22	30:T:37:VAL:HA	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D:116:ARG:NH1	35:p:180:GLU:O	2.34	0.60
33:c:43:ILE:HG22	33:c:65:ALA:HB3	1.84	0.60
34:g:107:ASP:HB2	34:g:125:ARG:HD2	1.84	0.60
1:2:380:G:O6	9:I:178:ARG:NH1	2.35	0.60
34:g:87:LEU:HB3	34:g:101:PHE:HB2	1.82	0.60
1:2:1854:U:H2'	1:2:1855:G:H8	1.65	0.60
28:Q:47:LEU:HD21	28:Q:78:VAL:HG23	1.84	0.60
5:C:196:ILE:HB	5:C:223:TYR:HB2	1.84	0.59
1:2:560:A:OP2	10:J:177:ASN:ND2	2.31	0.59
1:2:1580:A:C8	31:U:56:MET:HE1	2.37	0.59
3:A:52:LYS:NZ	14:V:82:ASN:O	2.35	0.59
7:G:162:LEU:HB3	7:G:170:ARG:HB3	1.84	0.59
1:2:678:U:OP2	1:2:1026:C:N4	2.35	0.59
1:2:943:U:H2'	1:2:944:A:C8	2.38	0.59
34:g:152:SER:OG	34:g:168:CYS:SG	2.60	0.59
1:2:943:U:H2'	1:2:944:A:H8	1.68	0.59
29:S:138:THR:HA	29:S:141:ARG:HH21	1.68	0.59
13:O:85:CYS:HB2	13:O:90:ILE:HB	1.84	0.59
30:T:9:VAL:O	30:T:11:GLN:NE2	2.35	0.59
5:C:125:LYS:HA	5:C:142:LYS:O	2.02	0.58
9:I:130:THR:HG23	9:I:133:GLU:H	1.69	0.58
34:g:258:ILE:O	34:g:267:VAL:N	2.36	0.58
1:2:952:G:H21	13:O:52:THR:HG21	1.68	0.58
1:2:953:C:O2	13:O:55:ARG:NH1	2.35	0.58
1:2:959:G:HO2'	1:2:1065:G:HO2'	1.49	0.58
1:2:1726:G:H2'	1:2:1727:G:H8	1.68	0.58
6:E:152:PRO:O	6:E:155:LYS:NZ	2.36	0.58
20:u:138:ALA:HB1	20:u:146:VAL:HG22	1.85	0.58
20:u:521:PRO:HD2	20:u:524:TYR:HD2	1.68	0.58
20:u:298:GLN:NE2	20:u:353:GLU:OE2	2.36	0.58
22:d:17:GLY:O	22:d:27:ARG:NH2	2.36	0.58
26:M:51:VAL:HB	26:M:109:VAL:HB	1.86	0.58
1:2:1025:U:O3'	1:2:1089:G:N2	2.37	0.58
1:2:1244:U:H2'	1:2:1245:G:H8	1.67	0.58
4:B:65:ARG:NH2	13:O:46:ASP:OD2	2.35	0.58
9:I:172:LEU:HB3	9:I:190:LEU:HD12	1.86	0.58
9:I:191:GLU:O	11:L:19:ASN:ND2	2.36	0.58
17:Y:110:ARG:NH1	17:Y:114:MET:SD	2.77	0.58
1:2:748:C:H42	1:2:794:A:H61	1.50	0.58
20:u:124:LEU:HB3	20:u:133:TRP:HB2	1.85	0.58
1:2:959:G:OP2	13:O:38:ASN:ND2	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:5:VAL:HA	17:Y:28:LEU:O	2.04	0.58
5:C:137:VAL:HG11	5:C:244:ILE:HD12	1.86	0.58
1:2:1380:C:O2'	3:A:113:GLN:OE1	2.20	0.58
29:S:13:LEU:HB2	29:S:20:ILE:HB	1.86	0.58
1:2:1038:U:O2'	1:2:1180:C:N3	2.35	0.57
9:I:67:TRP:O	9:I:71:CYS:N	2.37	0.57
20:u:91:HIS:HA	20:u:167:ASP:HB2	1.86	0.57
1:2:1217:A:OP2	28:Q:145:TYR:OH	2.22	0.57
28:Q:42:ILE:O	28:Q:48:GLN:NE2	2.38	0.57
1:2:1039:C:H5''	21:t:435:LYS:HE3	1.86	0.57
1:2:1722:G:O6	1:2:1812:U:O2	2.22	0.57
1:2:928:G:H2'	1:2:929:G:C8	2.39	0.57
1:2:1054:G:H2'	1:2:1055:A:H8	1.69	0.57
12:N:63:VAL:HG21	12:N:71:ILE:HD11	1.85	0.57
23:D:74:GLN:NE2	23:D:79:PHE:O	2.38	0.57
20:u:264:GLU:OE1	20:u:267:ASN:ND2	2.38	0.57
1:2:67:C:H41	7:G:163:ASN:HA	1.70	0.57
1:2:678:U:OP1	12:N:127:ARG:NH2	2.37	0.57
20:u:600:ARG:NH2	20:u:606:GLU:O	2.33	0.57
32:Z:48:VAL:HG22	32:Z:80:ARG:HG3	1.87	0.57
1:2:814:U:OP1	6:E:22:LYS:NZ	2.38	0.57
3:A:21:ALA:HB2	3:A:173:LEU:HD13	1.85	0.57
3:A:142:LEU:O	14:V:60:ARG:NH2	2.37	0.57
7:G:88:ARG:HB2	7:G:91:GLU:HG2	1.87	0.57
20:u:294:TYR:HH	20:u:572:CYS:HG	1.51	0.57
1:2:976:G:N3	13:O:50:LYS:NZ	2.53	0.57
1:2:1279:C:H2'	1:2:1280:G:H8	1.70	0.57
27:P:44:ARG:NH1	27:P:82:ASP:O	2.38	0.57
33:c:13:ARG:HB2	33:c:33:GLU:HB3	1.87	0.57
1:2:1274:G:H5'	25:K:47:LYS:HE2	1.86	0.56
30:T:98:SER:OG	30:T:101:ARG:NH2	2.38	0.56
1:2:886:A:H1'	1:2:900:C:H42	1.70	0.56
17:Y:41:ARG:NH2	17:Y:52:PRO:O	2.38	0.56
1:2:1489:A:N3	23:D:146:ARG:NH1	2.53	0.56
1:2:1650:A:H3'	1:2:1651:A:H8	1.71	0.56
4:B:34:LYS:NZ	4:B:95:ASN:OD1	2.38	0.56
4:B:136:ARG:HB3	4:B:216:LYS:HB2	1.87	0.56
18:b:49:HIS:HD2	18:b:70:LYS:HA	1.68	0.56
29:S:30:ILE:HG22	29:S:36:VAL:HG11	1.86	0.56
1:2:594:A:H61	1:2:643:A:H5''	1.69	0.56
1:2:975:G:OP1	13:O:98:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Z:68:ILE:HB	32:Z:109:TYR:HB2	1.85	0.56
5:C:126:ALA:O	5:C:141:VAL:HA	2.05	0.56
1:2:4:C:H1'	10:J:18:ARG:HH22	1.70	0.56
1:2:1263:U:H4'	22:d:27:ARG:HD3	1.87	0.56
1:2:1549:U:OP2	23:D:8:LYS:NZ	2.38	0.56
3:A:120:ARG:NH2	5:C:267:GLN:OE1	2.39	0.56
23:D:172:VAL:HG22	23:D:185:LYS:HG2	1.87	0.56
26:M:86:GLY:HA3	26:M:105:GLY:HA2	1.88	0.56
1:2:35:C:H5''	1:2:579:C:H5''	1.87	0.56
1:2:1614:A:OP2	27:P:42:ARG:NH2	2.39	0.56
6:E:45:ILE:HG13	6:E:61:VAL:HG21	1.88	0.56
1:2:1013:U:OP1	1:2:1129:G:O2'	2.24	0.56
3:A:157:VAL:O	14:V:65:SER:OG	2.24	0.56
4:B:134:LEU:HB3	4:B:219:LYS:HB3	1.87	0.56
24:F:165:ASN:O	24:F:167:LYS:N	2.39	0.56
1:2:568:C:H42	1:2:582:U:H3	1.53	0.56
2:R:102:THR:HA	2:R:105:MET:HG2	1.87	0.56
3:A:41:ARG:HA	3:A:47:TYR:HA	1.87	0.56
13:O:103:ASN:ND2	13:O:141:ARG:O	2.35	0.56
20:u:81:PRO:HB3	20:u:555:GLY:HA2	1.88	0.56
19:x:110:ASN:O	19:x:114:ARG:N	2.39	0.55
24:F:56:TYR:HA	24:F:62:ARG:HG2	1.88	0.55
34:g:11:LEU:HB2	34:g:307:VAL:HB	1.88	0.55
1:2:1036:A:N3	1:2:1844:U:O2'	2.39	0.55
1:2:1312:G:O2'	26:M:33:ARG:NH1	2.39	0.55
1:2:1329:U:C4	1:2:1493:C:N3	2.74	0.55
1:2:1384:C:OP1	35:p:108:LYS:NZ	2.35	0.55
1:2:1608:U:OP1	29:S:134:GLN:NE2	2.39	0.55
20:u:259:ASP:HB2	20:u:273:LYS:HB2	1.87	0.55
1:2:804:U:OP1	15:W:82:GLN:NE2	2.39	0.55
1:2:1050:A:OP1	1:2:1846:G:N2	2.39	0.55
1:2:1538:C:OP1	30:T:84:ARG:NH2	2.39	0.55
9:I:54:LYS:HD3	9:I:181:GLN:HG2	1.87	0.55
11:L:68:ILE:HG21	11:L:143:LEU:HD11	1.89	0.55
20:u:271:THR:HA	20:u:562:VAL:O	2.06	0.55
20:u:733:THR:HG22	20:u:735:TRP:H	1.70	0.55
34:g:57:ARG:NH1	34:g:94:THR:O	2.39	0.55
2:R:58:MET:HG2	2:R:61:ILE:HD12	1.88	0.55
7:G:98:ARG:NH1	7:G:105:ASN:OD1	2.39	0.55
8:H:69:LEU:HD22	8:H:96:ALA:HB2	1.88	0.55
34:g:30:MET:HE1	34:g:44:LYS:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:986:G:OP1	1:2:1001:A:O2'	2.23	0.55
1:2:1536:G:H2'	1:2:1537:A:H8	1.72	0.55
3:A:188:THR:HG23	3:A:189:ILE:HG13	1.89	0.55
12:N:25:TRP:O	12:N:27:LYS:NZ	2.38	0.55
13:O:105:THR:OG1	13:O:150:ARG:NH2	2.40	0.55
1:2:1391:C:O3'	31:U:83:ARG:NH2	2.35	0.55
20:u:143:LEU:O	20:u:147:LEU:HB2	2.07	0.55
20:u:251:ALA:HB3	20:u:583:SER:HB2	1.88	0.55
33:c:16:LYS:H	33:c:31:ARG:HB3	1.72	0.55
1:2:523:A:OP2	10:J:127:ARG:NH2	2.34	0.55
13:O:45:THR:HG22	13:O:52:THR:HG22	1.88	0.55
29:S:121:ARG:O	29:S:125:HIS:ND1	2.40	0.55
1:2:5:U:H2'	1:2:6:G:H8	1.72	0.55
1:2:1581:C:H5'	1:2:1582:C:H5	1.72	0.55
11:L:80:MET:HG2	11:L:86:ILE:HG22	1.88	0.55
20:u:604:ASN:HD22	20:u:679:ILE:HG13	1.72	0.55
1:2:1562:C:H5''	30:T:71:GLY:HA3	1.89	0.54
20:u:745:LEU:HB2	20:u:752:LYS:HE2	1.89	0.54
30:T:64:LEU:HD13	30:T:113:VAL:HG11	1.88	0.54
1:2:1416:C:H5'	30:T:133:ARG:HH12	1.72	0.54
15:W:44:HIS:NE2	15:W:112:ASP:OD2	2.40	0.54
4:B:217:MET:HE2	4:B:220:LYS:HG2	1.88	0.54
24:F:178:ILE:HG22	24:F:182:LYS:HE2	1.89	0.54
26:M:75:ASN:HD21	26:M:131:LYS:HD3	1.73	0.54
1:2:1160:U:O4	16:X:2:GLY:N	2.40	0.54
1:2:1427:C:H2'	1:2:1429:G:H8	1.73	0.54
17:Y:25:ILE:HG21	17:Y:40:ILE:HD11	1.88	0.54
29:S:22:GLY:O	29:S:23:ARG:NH1	2.40	0.54
23:D:194:PRO:HA	23:D:201:LYS:CA	2.28	0.54
1:2:1360:U:O2'	1:2:1379:A:OP2	2.24	0.54
4:B:88:THR:HA	4:B:98:THR:HA	1.90	0.54
9:I:191:GLU:HB2	11:L:19:ASN:HD22	1.71	0.54
10:J:28:GLU:OE2	10:J:44:TRP:NE1	2.36	0.54
28:Q:48:GLN:O	28:Q:52:LEU:N	2.40	0.54
1:2:154:U:O2	7:G:4:ASN:ND2	2.40	0.54
1:2:582:U:H1'	17:Y:33:ALA:HB2	1.90	0.54
1:2:1606:G:H22	1:2:1632:G:H2'	1.72	0.54
1:2:1858:G:OP2	13:O:146:ARG:NH2	2.32	0.54
1:2:1598:G:H2'	32:Z:81:GLY:H	1.73	0.54
1:2:1277:C:H5''	25:K:55:ARG:HE	1.71	0.53
1:2:1678:A:OP2	24:F:63:LYS:NZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:57:ASP:HA	7:G:106:LEU:HA	1.90	0.53
23:D:192:TRP:HD1	23:D:203:PRO:HA	1.73	0.53
26:M:83:LYS:HA	26:M:105:GLY:HA3	1.89	0.53
1:2:1217:A:H2'	1:2:1218:C:H6	1.73	0.53
1:2:1513:C:H2'	1:2:1514:G:C8	2.41	0.53
1:2:1565:C:OP2	30:T:101:ARG:NH1	2.32	0.53
12:N:99:ARG:NH1	12:N:141:TYR:OH	2.41	0.53
20:u:300:LYS:HD3	20:u:563:SER:HB3	1.90	0.53
31:U:27:ARG:HH21	31:U:82:MET:HE3	1.71	0.53
8:H:109:ARG:HD3	8:H:111:LYS:HG3	1.91	0.53
1:2:1726:G:H2'	1:2:1727:G:C8	2.43	0.53
1:2:1748:G:H1	1:2:1786:U:H3	1.57	0.53
11:L:104:LYS:O	16:X:11:ARG:NH2	2.41	0.53
18:b:42:LYS:NZ	18:b:56:CYS:SG	2.75	0.53
1:2:1588:A:H2'	1:2:1589:A:C8	2.43	0.53
1:2:1606:G:H5'	30:T:86:GLY:HA2	1.89	0.53
3:A:56:GLU:HG2	14:V:79:VAL:HG13	1.91	0.53
1:2:1101:U:H2'	1:2:1102:G:H8	1.72	0.53
3:A:2:SER:N	3:A:56:GLU:OE2	2.42	0.53
10:J:60:LEU:HD22	10:J:70:ARG:HA	1.91	0.53
23:D:8:LYS:HG2	31:U:61:LEU:HD21	1.90	0.53
29:S:60:THR:OG1	29:S:62:ASP:OD1	2.26	0.53
33:c:29:GLN:NE2	33:c:45:ASN:OD1	2.41	0.53
35:p:179:MET:HE3	35:p:188:VAL:HG13	1.91	0.53
1:2:76:U:OP1	7:G:159:ARG:NH1	2.42	0.53
6:E:149:TYR:HD2	7:G:205:GLU:HB3	1.73	0.53
10:J:136:ARG:HE	10:J:158:ASP:HB3	1.73	0.53
11:L:7:GLU:OE2	11:L:11:GLN:NE2	2.42	0.53
18:b:62:VAL:HG11	18:b:65:GLN:HE21	1.74	0.53
20:u:630:SER:HB2	20:u:691:ARG:HH22	1.73	0.53
25:K:13:GLU:HB3	25:K:17:LYS:HZ1	1.73	0.53
34:g:149:GLU:OE2	34:g:171:ASP:N	2.39	0.53
1:2:145:G:H2'	1:2:146:G:C8	2.44	0.53
7:G:85:ARG:O	7:G:87:ARG:NH1	2.42	0.53
14:V:71:ARG:HH12	15:W:23:ARG:HG3	1.71	0.53
20:u:640:LEU:HD22	20:u:773:VAL:HG11	1.90	0.53
1:2:1302:G:O6	1:2:1307:U:O4	2.27	0.53
18:b:36:LYS:HE2	18:b:41:TYR:HA	1.90	0.53
30:T:113:VAL:HG22	30:T:123:LEU:HA	1.90	0.53
9:I:149:TYR:HA	9:I:152:ARG:HD3	1.89	0.52
12:N:101:HIS:NE2	12:N:108:ASP:OD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:u:49:SER:O	20:u:52:ASP:N	2.31	0.52
25:K:15:LEU:HD13	25:K:49:MET:HE1	1.90	0.52
1:2:913:A:H2	8:H:99:ARG:H	1.56	0.52
1:2:1712:A:OP1	20:u:535:ASN:ND2	2.42	0.52
9:I:178:ARG:NH1	9:I:181:GLN:OE1	2.42	0.52
24:F:168:THR:HG22	24:F:170:ALA:H	1.74	0.52
30:T:39:LEU:HG	30:T:56:ARG:HE	1.75	0.52
1:2:317:C:OP2	7:G:183:ARG:NH1	2.35	0.52
14:V:32:ILE:O	14:V:54:ALA:HA	2.09	0.52
34:g:40:ILE:HB	34:g:59:LEU:HB2	1.90	0.52
8:H:100:ILE:HG22	8:H:125:VAL:HG21	1.92	0.52
28:Q:85:ARG:HE	28:Q:119:LEU:HD23	1.74	0.52
1:2:1533:A:N6	1:2:1602:U:H3	2.07	0.52
3:A:143:PRO:HG3	14:V:32:ILE:HG23	1.91	0.52
27:P:37:TYR:HB3	27:P:41:GLN:HB2	1.90	0.52
1:2:526:A:O2'	10:J:125:HIS:ND1	2.38	0.52
1:2:959:G:H1	13:O:65:ASP:HB3	1.73	0.52
10:J:36:GLY:O	10:J:111:GLN:NE2	2.32	0.52
1:2:150:A:OP1	17:Y:118:ARG:NH2	2.42	0.52
1:2:1839:U:C2	1:2:1862:G:C2	2.98	0.52
2:R:105:MET:HE1	3:A:39:TYR:HD2	1.75	0.52
16:X:52:LEU:HD11	16:X:73:GLN:HB2	1.90	0.52
29:S:17:ASN:OD1	29:S:101:ASN:ND2	2.43	0.52
1:2:617:G:OP2	16:X:68:LYS:NZ	2.32	0.52
4:B:65:ARG:NH2	13:O:51:GLU:OE1	2.43	0.52
20:u:731:LEU:HD23	20:u:767:MET:HB2	1.92	0.52
27:P:83:MET:HB3	27:P:116:LEU:HD12	1.92	0.52
34:g:259:TRP:HA	34:g:266:ILE:HA	1.92	0.52
23:D:54:ARG:NH1	35:p:136:ASP:OD2	2.43	0.51
31:U:27:ARG:HE	31:U:82:MET:HE3	1.75	0.51
36:j:22:THR:HA	36:j:55:THR:HA	1.91	0.51
4:B:65:ARG:HG2	13:O:50:LYS:HG3	1.93	0.51
20:u:89:PRO:HA	20:u:159:LEU:HB2	1.92	0.51
29:S:84:LEU:O	29:S:87:GLN:NE2	2.42	0.51
34:g:98:THR:HG22	34:g:99:ARG:HG2	1.92	0.51
1:2:980:A:H2'	1:2:981:A:C8	2.45	0.51
1:2:1023:A:OP2	12:N:124:ARG:NH1	2.42	0.51
11:L:23:VAL:HG12	11:L:25:LEU:H	1.76	0.51
20:u:299:MET:HG3	20:u:560:LEU:HD23	1.92	0.51
27:P:81:ARG:HB3	27:P:117:GLY:HA3	1.92	0.51
34:g:298:LEU:HB2	34:g:310:TRP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:941:C:H2'	1:2:942:G:C8	2.44	0.51
1:2:1536:G:H2'	1:2:1537:A:C8	2.45	0.51
1:2:1847:G:OP1	21:t:441:ARG:NE	2.43	0.51
20:u:262:PRO:HA	20:u:270:GLY:HA3	1.92	0.51
34:g:67:SER:H	34:g:82:SER:HA	1.75	0.51
34:g:129:ILE:HD11	34:g:151:VAL:HG11	1.92	0.51
1:2:1779:G:H2'	1:2:1780:G:C8	2.46	0.51
8:H:53:VAL:O	8:H:57:ARG:HB3	2.10	0.51
12:N:103:GLU:O	12:N:106:ARG:NH1	2.43	0.51
20:u:298:GLN:NE2	20:u:299:MET:O	2.44	0.51
24:F:162:ALA:HB1	24:F:169:ILE:HG12	1.91	0.51
1:2:1228:A:H2'	1:2:1229:G:C8	2.46	0.51
1:2:1297:U:H1'	1:2:1301:A:H62	1.76	0.51
1:2:1707:U:H3	1:2:1827:U:H3	1.59	0.51
1:2:1758:G:C2	1:2:1775:U:O2	2.64	0.51
23:D:94:ARG:NH1	35:p:133:ASP:OD1	2.43	0.51
5:C:191:VAL:HG11	5:C:236:PHE:HA	1.93	0.51
16:X:55:VAL:HG13	21:t:472:GLY:HA3	1.93	0.51
1:2:332:G:H5'	7:G:193:ALA:HB2	1.93	0.51
1:2:925:G:OP1	12:N:121:ARG:NH1	2.44	0.51
1:2:1038:U:H1'	1:2:1180:C:H42	1.76	0.51
1:2:1279:C:H2'	1:2:1280:G:C8	2.45	0.51
1:2:1550:G:H3'	1:2:1579:A:H61	1.76	0.51
1:2:1560:U:H2'	1:2:1561:A:H8	1.74	0.51
18:b:67:THR:OG1	18:b:70:LYS:O	2.26	0.51
21:t:455:GLU:OE2	21:t:459:GLN:NE2	2.44	0.51
1:2:190:G:OP2	9:I:149:TYR:OH	2.29	0.50
1:2:1329:U:O4	1:2:1493:C:C2	2.64	0.50
17:Y:5:VAL:HG12	17:Y:29:HIS:HB3	1.92	0.50
1:2:67:C:H5'	7:G:162:LEU:HD11	1.92	0.50
4:B:167:LYS:HA	4:B:170:GLU:HG2	1.93	0.50
5:C:88:ILE:HD13	5:C:94:ILE:HD11	1.92	0.50
6:E:107:GLY:HA2	6:E:189:LEU:HG	1.94	0.50
7:G:52:ILE:HA	7:G:111:LEU:HD23	1.92	0.50
11:L:119:ASP:O	11:L:147:LYS:NZ	2.45	0.50
1:2:51:U:H2'	1:2:52:G:C8	2.46	0.50
1:2:1468:C:H2'	1:2:1469:A:H8	1.76	0.50
24:F:27:ASP:OD1	24:F:107:ASN:ND2	2.43	0.50
24:F:100:ILE:HA	24:F:178:ILE:HD11	1.93	0.50
1:2:1285:G:H5'	26:M:35:ILE:HB	1.94	0.50
20:u:275:SER:HB3	20:u:559:THR:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:84:A:N3	1:2:150:A:O2'	2.44	0.50
1:2:587:A:H5'	1:2:592:C:H41	1.77	0.50
1:2:1122:A:H4'	4:B:205:TYR:CD1	2.46	0.50
1:2:1605:G:OP1	30:T:84:ARG:NH1	2.42	0.50
7:G:135:PRO:HG2	7:G:141:ILE:HD13	1.92	0.50
4:B:67:PHE:HD1	13:O:47:LEU:HG	1.77	0.50
20:u:254:PHE:O	20:u:276:GLY:HA3	2.11	0.50
27:P:61:ARG:HH21	27:P:64:LYS:HD3	1.77	0.50
1:2:1130:G:N2	1:2:1130:G:OP2	2.45	0.50
23:D:70:THR:HA	23:D:73:VAL:HG12	1.94	0.50
1:2:70:G:O6	1:2:80:G:N1	2.44	0.50
1:2:383:G:H4'	11:L:132:ARG:HD2	1.94	0.50
1:2:1651:A:H2'	1:2:1652:G:H8	1.77	0.50
15:W:86:LEU:HD23	15:W:117:ARG:HE	1.76	0.50
15:W:105:THR:O	15:W:123:GLY:HA3	2.11	0.50
24:F:40:ALA:HB3	24:F:68:ILE:HB	1.93	0.50
34:g:218:LEU:HD23	34:g:228:TYR:HD2	1.77	0.50
12:N:87:ASP:OD1	12:N:88:LEU:N	2.45	0.49
23:D:116:ARG:HD3	35:p:188:VAL:HB	1.93	0.49
1:2:51:U:H2'	1:2:52:G:H8	1.77	0.49
1:2:197:U:O2	1:2:202:G:N2	2.37	0.49
1:2:1099:G:O2'	1:2:1100:A:O5'	2.30	0.49
13:O:98:ARG:HE	13:O:134:PRO:HD3	1.77	0.49
6:E:47:PHE:HE1	6:E:111:VAL:HG12	1.77	0.49
17:Y:10:ARG:NE	17:Y:26:ASP:OD2	2.40	0.49
5:C:255:LEU:HD22	14:V:13:VAL:HG13	1.94	0.49
13:O:117:ARG:NH1	19:x:156:ASP:O	2.45	0.49
20:u:286:ASN:ND2	20:u:348:ASP:OD1	2.46	0.49
20:u:630:SER:HB3	20:u:638:HIS:HB3	1.94	0.49
23:D:192:TRP:O	23:D:193:ASP:C	2.55	0.49
29:S:14:ARG:HH12	29:S:17:ASN:HA	1.77	0.49
35:p:95:GLN:OE1	35:p:98:ARG:NH1	2.45	0.49
1:2:871:U:H3'	1:2:872:A:H4'	1.95	0.49
1:2:1348:G:OP2	1:2:1348:G:N2	2.44	0.49
1:2:943:U:OP1	4:B:214:LYS:NZ	2.38	0.49
1:2:1329:U:C4	1:2:1500:G:O6	2.66	0.49
1:2:1382:A:O2'	35:p:106:ASP:OD2	2.28	0.49
1:2:1785:C:O2'	1:2:1786:U:O4'	2.31	0.49
3:A:76:VAL:HG12	3:A:87:VAL:HG22	1.94	0.49
5:C:110:MET:HE3	5:C:125:LYS:HD2	1.95	0.49
6:E:124:CYS:HB3	6:E:141:THR:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:u:596:MET:HG3	20:u:665:VAL:HG21	1.94	0.49
1:2:1513:C:OP1	22:d:12:ARG:NH1	2.46	0.49
34:g:152:SER:H	34:g:169:GLY:HA2	1.78	0.49
1:2:1401:A:H2'	1:2:1402:A:C8	2.48	0.49
1:2:1427:C:H2'	1:2:1429:G:C8	2.47	0.49
7:G:102:VAL:HG13	7:G:106:LEU:HD12	1.94	0.49
9:I:148:LYS:HG2	9:I:152:ARG:HD2	1.95	0.49
20:u:608:VAL:HG11	20:u:614:LEU:HD11	1.94	0.49
34:g:152:SER:N	34:g:168:CYS:O	2.46	0.49
34:g:245:ARG:NH1	34:g:295:GLY:O	2.46	0.49
1:2:1086:G:O2'	1:2:1088:U:OP2	2.28	0.49
1:2:1101:U:H2'	1:2:1102:G:C8	2.48	0.49
4:B:146:ARG:HB2	4:B:149:GLN:HB2	1.94	0.49
5:C:62:PRO:HG2	5:C:68:ARG:HG2	1.94	0.49
27:P:81:ARG:O	27:P:117:GLY:N	2.42	0.49
1:2:1869:A:H5''	1:2:1870:A:H2	1.78	0.49
7:G:181:THR:HB	7:G:184:VAL:HG23	1.95	0.49
9:I:113:TYR:HE1	9:I:117:TYR:HD2	1.60	0.49
1:2:218:U:O2	9:I:184:ARG:NH1	2.40	0.48
2:R:91:LEU:HD11	3:A:17:LYS:HA	1.94	0.48
9:I:42:ARG:HH12	9:I:59:ARG:HE	1.60	0.48
11:L:120:VAL:HG12	11:L:145:VAL:HG11	1.95	0.48
2:R:66:VAL:HB	2:R:69:ILE:HG12	1.95	0.48
4:B:65:ARG:HH21	13:O:50:LYS:HB2	1.78	0.48
1:2:5:U:H2'	1:2:6:G:C8	2.47	0.48
1:2:1473:G:N2	1:2:1476:A:OP2	2.44	0.48
4:B:179:ASN:HB3	4:B:183:GLU:HB2	1.96	0.48
24:F:55:ARG:HD3	28:Q:125:ARG:HD3	1.96	0.48
1:2:1213:C:H2'	1:2:1214:A:C8	2.48	0.48
1:2:1283:C:H41	26:M:102:LYS:HE2	1.79	0.48
1:2:1608:U:H5''	29:S:134:GLN:HE22	1.76	0.48
14:V:16:LYS:HG2	14:V:23:ILE:HD13	1.95	0.48
9:I:141:ARG:HH21	9:I:146:GLN:HA	1.78	0.48
28:Q:102:GLU:HA	28:Q:105:LYS:HB3	1.95	0.48
15:W:87:GLU:HA	15:W:90:GLN:HG2	1.95	0.48
1:2:874:G:H2'	1:2:875:A:H8	1.77	0.48
1:2:1113:A:OP1	1:2:1114:U:O2'	2.28	0.48
1:2:1256:G:N2	1:2:1658:G:O2'	2.47	0.48
1:2:1616:U:O4	27:P:40:ARG:NH1	2.47	0.48
9:I:3:ILE:O	9:I:30:GLY:N	2.37	0.48
20:u:767:MET:HE2	20:u:767:MET:HB3	1.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:g:238:ALA:H	34:g:251:ALA:HB3	1.78	0.48
1:2:383:G:O2'	11:L:133:PRO:O	2.29	0.48
1:2:1227:G:H1	1:2:1531:A:N6	2.09	0.48
7:G:1:MET:N	7:G:18:VAL:O	2.47	0.48
15:W:11:LEU:HD22	15:W:72:CYS:HB2	1.96	0.48
22:d:38:MET:HE1	22:d:50:ILE:HD11	1.96	0.48
10:J:176:LYS:HA	10:J:179:LYS:HE3	1.95	0.48
20:u:591:MET:HE1	20:u:657:PRO:HG3	1.94	0.48
1:2:1479:G:H5''	28:Q:138:ARG:HH22	1.77	0.48
1:2:1821:U:H2'	1:2:1822:A:C8	2.48	0.48
10:J:111:GLN:OE1	10:J:127:ARG:NH1	2.47	0.48
1:2:623:G:O6	16:X:63:ASN:ND2	2.46	0.47
1:2:792:C:H2'	1:2:793:G:H8	1.79	0.47
1:2:1239:U:H4'	27:P:124:LYS:HB2	1.95	0.47
20:u:358:GLU:HG2	20:u:359:VAL:HG13	1.96	0.47
27:P:111:MET:HE1	29:S:117:ILE:HA	1.96	0.47
32:Z:73:VAL:HG13	32:Z:77:LEU:HD12	1.96	0.47
1:2:1044:G:H2'	21:t:418:ARG:HH22	1.79	0.47
12:N:46:THR:HG23	12:N:49:GLN:H	1.79	0.47
20:u:703:PRO:HB3	20:u:713:VAL:HG22	1.97	0.47
31:U:18:HIS:ND1	31:U:19:ARG:HG3	2.29	0.47
31:U:32:LEU:HD21	31:U:87:ARG:HG3	1.95	0.47
34:g:64:HIS:CG	34:g:65:PHE:H	2.32	0.47
1:2:33:G:O2'	1:2:564:A:O2'	2.33	0.47
1:2:494:C:N4	1:2:509:G:H21	2.12	0.47
1:2:1404:U:OP1	31:U:21:ARG:NH2	2.48	0.47
1:2:1593:C:H4'	28:Q:45:ARG:HD2	1.96	0.47
6:E:62:LYS:HB2	6:E:62:LYS:HE2	1.48	0.47
1:2:1189:A:H2'	1:2:1190:A:H8	1.79	0.47
1:2:1473:G:N7	28:Q:117:ARG:NH2	2.62	0.47
3:A:209:GLU:HA	3:A:212:LYS:HG2	1.96	0.47
9:I:139:LYS:HE2	9:I:139:LYS:HB2	1.73	0.47
32:Z:69:THR:HG22	32:Z:71:ALA:H	1.79	0.47
34:g:89:LEU:HB3	34:g:99:ARG:HB2	1.96	0.47
34:g:239:LEU:HD23	34:g:250:ALA:HA	1.96	0.47
1:2:128:U:H5'	1:2:129:C:H5	1.78	0.47
1:2:155:G:H2'	1:2:156:G:H8	1.80	0.47
1:2:1228:A:O2'	1:2:1634:A:N3	2.42	0.47
1:2:1610:G:N2	29:S:85:ASN:O	2.46	0.47
3:A:76:VAL:O	3:A:98:PRO:HA	2.13	0.47
6:E:35:PRO:HD2	6:E:83:PRO:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:d:6:LEU:HA	22:d:9:SER:HB3	1.96	0.47
31:U:61:LEU:HB2	31:U:82:MET:HB3	1.95	0.47
1:2:588:G:OP2	1:2:588:G:N2	2.39	0.47
1:2:1244:U:H2'	1:2:1245:G:C8	2.49	0.47
3:A:85:ARG:HD2	3:A:205:ARG:HG2	1.95	0.47
34:g:106:LYS:HB3	34:g:125:ARG:HB2	1.95	0.47
34:g:256:ILE:HB	34:g:270:LEU:HB2	1.96	0.47
1:2:1531:A:H4'	1:2:1605:G:H4'	1.96	0.47
6:E:171:ASP:OD1	6:E:171:ASP:N	2.47	0.47
9:I:141:ARG:HG3	9:I:146:GLN:HE22	1.79	0.47
16:X:24:ASP:HB3	16:X:27:TYR:HB3	1.96	0.47
34:g:8:ARG:HB3	34:g:309:VAL:HG23	1.96	0.47
34:g:249:CYS:HA	34:g:258:ILE:HA	1.97	0.47
5:C:202:THR:HG22	5:C:221:ASP:HB2	1.95	0.47
20:u:610:ALA:HB2	20:u:642:ARG:HA	1.97	0.47
23:D:167:TYR:CE1	23:D:200:PRO:HG2	2.50	0.47
34:g:67:SER:HB3	34:g:83:TRP:CD1	2.50	0.47
1:2:928:G:N2	18:b:68:GLY:O	2.43	0.47
1:2:1665:G:C5	30:T:88:MET:HE1	2.50	0.47
11:L:49:GLU:HG2	11:L:116:CYS:HA	1.97	0.47
20:u:246:PHE:O	20:u:250:ARG:NH2	2.48	0.47
1:2:17:C:O2'	1:2:1194:A:N1	2.46	0.47
1:2:798:G:H4'	8:H:108:SER:HB2	1.95	0.47
26:M:21:VAL:O	26:M:24:THR:OG1	2.28	0.47
27:P:81:ARG:NH2	27:P:117:GLY:O	2.33	0.47
31:U:91:LEU:HD11	31:U:98:VAL:HG22	1.97	0.47
1:2:658:U:H1'	16:X:17:ARG:HH12	1.78	0.46
14:V:73:ALA:HB1	14:V:78:ILE:HB	1.97	0.46
33:c:44:ARG:NH1	33:c:60:GLU:O	2.48	0.46
1:2:1736:G:H2'	1:2:1737:G:H8	1.79	0.46
2:R:78:ARG:O	2:R:82:ASP:HB2	2.15	0.46
10:J:88:ASP:HB2	10:J:91:LYS:HG2	1.96	0.46
15:W:32:LYS:HA	15:W:32:LYS:HD3	1.63	0.46
1:2:931:C:H2'	1:2:932:G:C8	2.51	0.46
1:2:1016:U:O4	12:N:19:ARG:NH2	2.48	0.46
1:2:1171:G:O2'	1:2:1187:G:O6	2.29	0.46
13:O:56:VAL:HG13	13:O:60:MET:HG3	1.97	0.46
14:V:66:ASP:OD1	14:V:67:ASP:N	2.48	0.46
20:u:143:LEU:HD21	20:u:676:HIS:HB2	1.95	0.46
1:2:581:U:H4'	17:Y:66:GLY:HA2	1.97	0.46
3:A:206:ASP:O	3:A:209:GLU:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D:50:ILE:HB	23:D:88:ALA:HA	1.97	0.46
29:S:63:GLU:HG3	29:S:66:ARG:HH21	1.80	0.46
1:2:1313:A:H4'	1:2:1314:U:H5'	1.98	0.46
16:X:55:VAL:HG21	16:X:71:ARG:HG3	1.98	0.46
27:P:49:LEU:HD22	27:P:53:GLN:HG2	1.97	0.46
1:2:388:U:H2'	1:2:389:A:H8	1.80	0.46
1:2:1069:U:H2'	1:2:1070:A:C8	2.50	0.46
2:R:17:ILE:HG13	2:R:57:LEU:HD22	1.98	0.46
2:R:91:LEU:HD21	3:A:17:LYS:HG2	1.97	0.46
8:H:109:ARG:HG2	8:H:110:THR:H	1.81	0.46
32:Z:111:ARG:NH1	32:Z:113:THR:O	2.49	0.46
1:2:1255:G:H5''	1:2:1256:G:H5''	1.97	0.46
3:A:58:LEU:HD23	3:A:161:ILE:HD13	1.96	0.46
8:H:143:ARG:HG3	15:W:53:ILE:HA	1.96	0.46
11:L:135:SER:OG	11:L:136:LYS:N	2.48	0.46
12:N:2:GLY:HA2	12:N:9:LYS:HG2	1.98	0.46
26:M:54:SER:N	26:M:79:VAL:O	2.48	0.46
34:g:218:LEU:HB3	34:g:228:TYR:HB2	1.98	0.46
5:C:134:ASN:O	5:C:167:ARG:NH1	2.49	0.46
6:E:42:LEU:HD13	6:E:47:PHE:HB2	1.97	0.46
20:u:515:ASP:HB2	20:u:518:GLU:HB2	1.96	0.46
8:H:19:PHE:HZ	8:H:60:ILE:HG23	1.81	0.46
11:L:22:ARG:HE	11:L:27:GLU:HA	1.81	0.46
12:N:33:VAL:HG21	12:N:66:VAL:HG11	1.97	0.46
17:Y:83:LYS:HD3	17:Y:96:LEU:HD22	1.98	0.46
33:c:13:ARG:N	33:c:33:GLU:O	2.43	0.46
35:p:222:GLU:HA	35:p:225:GLU:HG2	1.97	0.46
1:2:130:G:H1	1:2:181:A:N6	2.14	0.46
1:2:1242:U:C2	1:2:1520:G:C6	3.04	0.46
1:2:1415:C:H5''	30:T:129:ARG:HG2	1.98	0.46
1:2:1595:U:H2'	1:2:1596:U:C6	2.51	0.46
10:J:22:LYS:NZ	35:p:171:CYS:SG	2.89	0.46
10:J:22:LYS:NZ	35:p:200:ASN:OD1	2.45	0.46
20:u:285:VAL:HG23	20:u:346:LYS:HZ3	1.80	0.46
1:2:130:G:O6	1:2:181:A:N1	2.49	0.45
1:2:1084:A:OP1	1:2:1858:G:O2'	2.34	0.45
1:2:1144:A:H5'	1:2:1355:C:H41	1.80	0.45
1:2:1543:U:OP2	30:T:62:ARG:NH2	2.35	0.45
18:b:38:PRO:HD3	18:b:77:CYS:HA	1.97	0.45
20:u:126:CYS:HB2	20:u:128:ARG:HE	1.80	0.45
1:2:545:A:H2'	1:2:546:G:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1491:G:N2	31:U:70:CYS:SG	2.79	0.45
1:2:1587:G:OP1	30:T:77:LYS:NZ	2.49	0.45
1:2:1620:A:OP1	27:P:115:TYR:OH	2.27	0.45
6:E:66:MET:HE2	6:E:66:MET:HB2	1.73	0.45
8:H:47:ALA:HB3	8:H:63:PHE:HB2	1.99	0.45
23:D:167:TYR:CE2	23:D:204:LEU:HG	2.51	0.45
28:Q:85:ARG:HH11	28:Q:85:ARG:HB3	1.80	0.45
1:2:1054:G:H2'	1:2:1055:A:C8	2.49	0.45
29:S:86:ARG:NH2	29:S:110:ASP:OD1	2.49	0.45
1:2:4:C:H4'	5:C:207:ALA:HB2	1.99	0.45
1:2:379:C:H5'	9:I:33:ALA:HA	1.98	0.45
1:2:656:G:H21	1:2:663:C:H5''	1.82	0.45
1:2:946:U:H2'	1:2:947:G:C8	2.51	0.45
1:2:1005:G:OP2	4:B:162:ARG:NH2	2.50	0.45
1:2:1277:C:H2'	1:2:1278:A:C8	2.51	0.45
1:2:1810:U:H2'	1:2:1811:C:C6	2.52	0.45
8:H:82:GLU:HA	8:H:85:LYS:HE2	1.97	0.45
9:I:142:SER:HB2	9:I:145:ILE:HD12	1.99	0.45
10:J:125:HIS:HA	10:J:128:VAL:HG12	1.98	0.45
16:X:101:LEU:HB3	16:X:124:LYS:HB2	1.98	0.45
20:u:358:GLU:HB2	20:u:591:MET:HE3	1.98	0.45
24:F:79:HIS:H	24:F:159:ARG:NH1	2.14	0.45
34:g:149:GLU:OE2	34:g:170:TRP:N	2.49	0.45
35:p:136:ASP:OD1	35:p:136:ASP:N	2.48	0.45
1:2:528:A:H2'	1:2:529:A:C8	2.51	0.45
1:2:913:A:H1'	8:H:66:VAL:HB	1.98	0.45
1:2:1226:G:N1	1:2:1639:G:OP2	2.37	0.45
1:2:1568:C:O2	1:2:1627:C:O2'	2.35	0.45
1:2:1614:A:P	27:P:42:ARG:HH22	2.40	0.45
6:E:162:ILE:HG22	6:E:169:ILE:HA	1.99	0.45
8:H:49:LYS:HD2	8:H:63:PHE:HE2	1.81	0.45
11:L:48:LYS:HD3	11:L:51:ILE:HD11	1.97	0.45
18:b:33:MET:HE3	18:b:48:SER:HA	1.98	0.45
34:g:17:TRP:HB2	34:g:36:ARG:HG3	1.98	0.45
5:C:73:MET:O	5:C:76:LYS:NZ	2.47	0.45
23:D:162:ASP:N	23:D:163:PRO:HD2	2.32	0.45
1:2:951:C:H2'	1:2:952:G:C8	2.52	0.45
1:2:1310:U:OP2	26:M:36:ARG:NH2	2.40	0.45
1:2:1808:U:O4	1:2:1809:A:N6	2.50	0.45
6:E:228:ILE:HG22	6:E:235:TRP:H	1.80	0.45
11:L:89:ARG:HE	11:L:106:HIS:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:P:118:GLU:CD	29:S:120:HIS:H	2.25	0.45
29:S:114:LEU:HD23	29:S:117:ILE:HD12	1.99	0.45
1:2:562:U:O2'	10:J:132:GLN:HG2	2.17	0.45
1:2:658:U:H1'	16:X:17:ARG:NH1	2.32	0.45
9:I:57:ALA:HB2	9:I:183:GLY:HA2	1.99	0.45
20:u:139:ARG:HD3	20:u:140:PRO:HD2	1.97	0.45
1:2:1287:A:O2'	1:2:1315:U:O2	2.33	0.45
1:2:1409:A:H2'	1:2:1410:C:C6	2.52	0.45
5:C:246:LYS:HA	5:C:249:SER:HB2	1.98	0.45
7:G:24:LEU:O	7:G:28:TYR:N	2.49	0.45
9:I:144:LYS:HA	9:I:147:LYS:HD3	1.99	0.45
12:N:91:LEU:HB3	12:N:122:ILE:HG12	1.98	0.45
1:2:1468:C:H2'	1:2:1469:A:C8	2.51	0.45
1:2:1628:C:OP1	30:T:38:LYS:NZ	2.50	0.45
7:G:2:LYS:HB2	7:G:108:VAL:HG22	1.98	0.45
15:W:101:PHE:HA	15:W:113:HIS:CE1	2.52	0.45
23:D:167:TYR:HE1	23:D:200:PRO:HG2	1.82	0.45
1:2:830:A:OP2	1:2:846:G:N2	2.50	0.44
1:2:1061:U:H5''	1:2:1062:A:H2	1.83	0.44
1:2:1477:U:H2'	1:2:1478:U:H5''	1.99	0.44
1:2:1622:U:H3	27:P:122:THR:HG22	1.83	0.44
18:b:14:GLU:HG3	18:b:17:ARG:HH12	1.82	0.44
25:K:15:LEU:HD23	25:K:79:LEU:HD11	1.98	0.44
1:2:69:C:OP2	7:G:164:LYS:NZ	2.35	0.44
1:2:1415:C:OP1	30:T:129:ARG:NH2	2.51	0.44
1:2:1472:C:O2	1:2:1476:A:N6	2.50	0.44
1:2:1655:C:OP1	30:T:92:PHE:N	2.50	0.44
1:2:1845:A:H2'	1:2:1846:G:C8	2.52	0.44
6:E:37:LYS:HB2	6:E:40:GLU:HG3	1.98	0.44
20:u:144:HIS:HB2	20:u:786:PRO:HD2	1.98	0.44
20:u:741:ILE:HA	20:u:753:CYS:HA	2.00	0.44
6:E:173:ILE:HG23	6:E:230:LYS:HD2	2.00	0.44
12:N:16:LEU:H	15:W:57:ARG:HH22	1.65	0.44
1:2:1607:A:N6	1:2:1632:G:O2'	2.50	0.44
1:2:1736:G:H2'	1:2:1737:G:C8	2.51	0.44
1:2:1781:A:H2'	1:2:1782:G:C8	2.53	0.44
33:c:9:ILE:HD12	33:c:59:LEU:HA	1.99	0.44
1:2:1139:C:H2'	1:2:1140:G:O4'	2.18	0.44
5:C:190:SER:O	5:C:190:SER:OG	2.30	0.44
8:H:53:VAL:HB	8:H:175:GLY:HA3	1.99	0.44
24:F:41:VAL:HG22	24:F:45:TYR:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1201:U:HO2'	1:2:1358:U:HO2'	1.62	0.44
1:2:1540:G:H4'	30:T:56:ARG:HH12	1.82	0.44
1:2:1786:U:H2'	1:2:1787:G:C8	2.52	0.44
4:B:92:GLN:HB2	4:B:95:ASN:HB2	1.99	0.44
6:E:17:HIS:HE1	6:E:39:ARG:O	2.01	0.44
8:H:181:THR:HG22	8:H:183:LYS:HG3	1.99	0.44
23:D:101:GLN:NE2	35:p:135:GLN:OE1	2.50	0.44
28:Q:47:LEU:HG	28:Q:81:ILE:HG21	1.99	0.44
28:Q:112:LEU:HD22	28:Q:119:LEU:HD13	1.99	0.44
1:2:402:C:OP1	9:I:12:ARG:NH1	2.45	0.44
1:2:1446:A:H5''	31:U:58:THR:HG23	1.99	0.44
2:R:89:SER:HB3	3:A:198:MET:SD	2.58	0.44
9:I:201:LYS:HD2	9:I:201:LYS:HA	1.86	0.44
22:d:33:LYS:HE2	22:d:34:TYR:CZ	2.52	0.44
1:2:1673:U:H5''	28:Q:78:VAL:HG12	1.99	0.44
16:X:98:ASP:OD2	16:X:140:ARG:NH2	2.50	0.44
33:c:12:ALA:HB3	33:c:56:LEU:HB2	1.99	0.44
34:g:213:ASP:OD1	34:g:213:ASP:N	2.49	0.44
1:2:1609:C:N4	1:2:1631:U:H3	2.11	0.44
5:C:61:MET:SD	5:C:61:MET:N	2.91	0.44
7:G:225:GLN:O	7:G:229:ALA:HB2	2.18	0.44
1:2:155:G:H2'	1:2:156:G:C8	2.53	0.43
3:A:40:LYS:NZ	3:A:41:ARG:O	2.47	0.43
16:X:107:ARG:HB2	16:X:112:VAL:HG22	2.00	0.43
29:S:84:LEU:HD22	29:S:97:GLN:HB2	2.00	0.43
33:c:13:ARG:HH11	33:c:55:VAL:HB	1.83	0.43
1:2:1192:U:H2'	1:2:1193:U:C6	2.53	0.43
3:A:99:ILE:HG21	3:A:103:PHE:HD1	1.82	0.43
20:u:597:VAL:HG23	20:u:685:MET:HB2	2.00	0.43
33:c:12:ALA:HB1	33:c:32:VAL:HG13	2.01	0.43
34:g:154:VAL:O	34:g:155:ARG:NH1	2.50	0.43
1:2:386:C:H2'	1:2:387:C:C6	2.54	0.43
1:2:570:C:O2'	17:Y:34:THR:O	2.30	0.43
3:A:34:MET:HE1	3:A:162:PRO:HB3	2.01	0.43
3:A:205:ARG:O	3:A:209:GLU:HB3	2.17	0.43
8:H:87:PHE:HB3	8:H:90:LYS:HE2	2.01	0.43
14:V:45:ARG:HD2	14:V:45:ARG:HA	1.85	0.43
21:t:416:GLN:O	21:t:430:ARG:NH2	2.51	0.43
24:F:167:LYS:HA	32:Z:71:ALA:HB1	2.00	0.43
27:P:44:ARG:HH12	27:P:82:ASP:C	2.25	0.43
1:2:388:U:H2'	1:2:389:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1439:A:H2'	1:2:1440:C:C6	2.54	0.43
1:2:1598:G:H5'	32:Z:80:ARG:HB3	2.00	0.43
1:2:1725:U:H2'	1:2:1726:G:H8	1.84	0.43
3:A:176:TRP:CG	3:A:199:PRO:HB3	2.52	0.43
10:J:60:LEU:HD11	10:J:73:GLU:HB3	2.01	0.43
13:O:19:PRO:HG2	13:O:27:VAL:HG21	2.00	0.43
20:u:304:ALA:HB3	20:u:345:MET:HE3	1.99	0.43
20:u:588:GLU:HA	20:u:658:ILE:HG23	1.99	0.43
25:K:29:MET:HA	25:K:30:PRO:HD3	1.76	0.43
1:2:1609:C:H3'	29:S:132:ARG:HH21	1.84	0.43
9:I:121:LEU:HD23	9:I:121:LEU:HA	1.90	0.43
11:L:57:ASP:OD1	11:L:57:ASP:N	2.51	0.43
25:K:85:LEU:HA	25:K:86:PRO:HD3	1.90	0.43
34:g:131:LEU:HD12	34:g:140:TYR:HB3	2.01	0.43
1:2:602:G:N2	1:2:620:G:O6	2.52	0.43
1:2:1277:C:H2'	1:2:1278:A:H8	1.84	0.43
1:2:1480:A:H4'	28:Q:131:LYS:HD3	2.01	0.43
6:E:129:ILE:HG12	6:E:139:LEU:HD22	2.00	0.43
10:J:144:ILE:HG23	10:J:146:SER:H	1.84	0.43
16:X:138:LYS:HE2	16:X:138:LYS:HB3	1.75	0.43
20:u:152:VAL:HG11	20:u:580:ILE:HG21	2.00	0.43
25:K:18:GLU:HG2	25:K:20:VAL:H	1.83	0.43
26:M:61:TYR:OH	26:M:108:CYS:SG	2.62	0.43
30:T:33:TRP:HE1	30:T:99:VAL:HG13	1.84	0.43
1:2:848:U:H2'	1:2:849:A:H8	1.83	0.43
1:2:867:G:H2'	1:2:868:G:C8	2.54	0.43
1:2:952:G:H2'	1:2:953:C:C6	2.53	0.43
1:2:1438:A:H3'	1:2:1439:A:H2	1.83	0.43
1:2:1643:U:H2'	1:2:1644:C:C6	2.53	0.43
1:2:1656:G:H1	1:2:1668:U:H3	1.66	0.43
4:B:39:PHE:HB3	4:B:74:LEU:HB3	2.01	0.43
5:C:110:MET:HA	5:C:111:PRO:HD3	1.89	0.43
6:E:211:LYS:HE3	6:E:215:GLY:HA2	2.01	0.43
15:W:26:LEU:HD11	15:W:60:LYS:HD3	1.99	0.43
1:2:28:U:H2'	1:2:29:G:H8	1.84	0.43
1:2:909:G:H2'	1:2:910:G:C8	2.54	0.43
1:2:946:U:H2'	1:2:947:G:H8	1.83	0.43
1:2:1549:U:O4	1:2:1584:G:O6	2.36	0.43
3:A:211:GLU:O	3:A:215:GLN:OE1	2.36	0.43
20:u:301:GLN:HB3	20:u:561:HIS:HB2	2.00	0.43
1:2:1066:U:OP2	13:O:143:LYS:NZ	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1405:A:H2'	1:2:1406:G:O4'	2.19	0.43
1:2:1479:G:H5''	28:Q:138:ARG:HH12	1.83	0.43
4:B:87:ILE:HG12	4:B:101:HIS:HB2	2.01	0.43
5:C:77:SER:OG	5:C:80:GLU:OE1	2.28	0.43
34:g:197:THR:HG21	34:g:239:LEU:H	1.84	0.43
1:2:1177:U:H2'	1:2:1178:U:C6	2.54	0.42
2:R:111:PHE:HD2	3:A:15:VAL:HG21	1.84	0.42
7:G:53:SER:HB2	7:G:112:VAL:HG23	2.01	0.42
10:J:142:VAL:HG12	10:J:144:ILE:H	1.83	0.42
25:K:86:PRO:HA	25:K:87:PRO:HD3	1.92	0.42
1:2:455:A:C6	1:2:456:C:N4	2.87	0.42
1:2:1228:A:H2'	1:2:1229:G:H8	1.84	0.42
1:2:1477:U:OP2	2:R:3:ARG:NH2	2.37	0.42
15:W:96:SER:OG	15:W:97:ARG:N	2.52	0.42
21:t:453:LYS:HB2	21:t:453:LYS:HE2	1.76	0.42
23:D:201:LYS:H	23:D:201:LYS:HG2	1.48	0.42
24:F:71:ARG:NH2	24:F:148:ASN:OD1	2.37	0.42
29:S:64:VAL:HA	29:S:67:VAL:HG22	2.02	0.42
1:2:56:G:OP1	17:Y:111:LYS:NZ	2.39	0.42
1:2:415:A:H2'	1:2:416:U:O4'	2.19	0.42
1:2:1248:U:H2'	1:2:1249:C:C6	2.55	0.42
1:2:1845:A:H2'	1:2:1846:G:H8	1.83	0.42
2:R:28:PHE:O	2:R:31:ASN:HB2	2.19	0.42
3:A:122:LEU:HD21	3:A:133:PRO:HB2	2.00	0.42
23:D:126:ILE:HD12	23:D:188:ILE:HG12	2.02	0.42
31:U:56:MET:HA	31:U:57:PRO:HD3	1.89	0.42
1:2:824:C:C2	10:J:144:ILE:HG12	2.54	0.42
1:2:862:A:C8	15:W:107:SER:HA	2.55	0.42
1:2:1181:A:H2'	1:2:1182:A:C8	2.54	0.42
1:2:1401:A:H2'	1:2:1402:A:H8	1.84	0.42
3:A:89:LYS:O	3:A:93:ALA:N	2.49	0.42
20:u:741:ILE:HG21	20:u:751:MET:HE2	2.00	0.42
1:2:1010:G:H2'	1:2:1011:A:C8	2.54	0.42
1:2:1069:U:H2'	1:2:1070:A:H8	1.85	0.42
1:2:1144:A:N3	1:2:1199:A:O2'	2.47	0.42
1:2:1189:A:H2'	1:2:1190:A:C8	2.55	0.42
2:R:24:LEU:HD22	2:R:54:VAL:HG11	2.01	0.42
3:A:33:GLN:HB3	3:A:154:LEU:HD12	2.00	0.42
13:O:113:GLN:HA	13:O:116:LEU:HG	2.01	0.42
18:b:49:HIS:CD2	18:b:70:LYS:HA	2.52	0.42
18:b:74:THR:OG1	18:b:77:CYS:SG	2.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:d:51:GLY:HA3	31:U:27:ARG:HH22	1.85	0.42
32:Z:66:LYS:NZ	32:Z:111:ARG:HH21	2.18	0.42
1:2:198:U:O2'	1:2:201:C:N4	2.52	0.42
1:2:1579:A:O2'	1:2:1582:C:N4	2.53	0.42
1:2:1581:C:H5'	1:2:1582:C:C5	2.52	0.42
4:B:49:VAL:HG11	4:B:62:LEU:HD23	2.02	0.42
4:B:159:GLN:OE1	4:B:162:ARG:NH1	2.51	0.42
29:S:22:GLY:HA2	29:S:56:ALA:HB3	2.01	0.42
30:T:23:LYS:HE3	30:T:23:LYS:HB3	1.92	0.42
35:p:219:ARG:O	35:p:222:GLU:HG2	2.19	0.42
1:2:455:A:O2'	1:2:1735:A:N3	2.40	0.42
1:2:1219:C:O2'	33:c:26:GLN:OE1	2.38	0.42
6:E:42:LEU:N	6:E:84:ALA:O	2.51	0.42
20:u:161:ASP:OD1	20:u:161:ASP:N	2.53	0.42
30:T:39:LEU:HG	30:T:56:ARG:HH21	1.85	0.42
1:2:320:G:H2'	1:2:321:C:C6	2.55	0.42
1:2:811:A:H2'	1:2:812:A:C8	2.54	0.42
1:2:1568:C:O2'	1:2:1627:C:H4'	2.20	0.42
1:2:1846:G:OP2	21:t:445:LYS:NZ	2.40	0.42
29:S:39:ARG:NH2	30:T:37:VAL:HA	2.34	0.42
1:2:10:G:H1	1:2:1201:U:H3	1.67	0.42
1:2:664:A:O2'	1:2:670:A:N1	2.50	0.42
1:2:996:A:H2'	1:2:997:A:C8	2.55	0.42
1:2:1144:A:H2'	1:2:1145:A:C8	2.55	0.42
1:2:1839:U:N3	1:2:1862:G:N1	2.68	0.42
5:C:104:ASP:HB3	5:C:130:ILE:HG22	2.00	0.42
13:O:46:ASP:OD1	13:O:46:ASP:N	2.50	0.42
21:t:462:GLU:O	21:t:466:LEU:HG	2.20	0.42
23:D:166:TYR:O	23:D:200:PRO:HG3	2.20	0.42
26:M:10:GLY:HA2	26:M:123:VAL:HG22	2.01	0.42
33:c:51:ARG:N	33:c:54:ASP:OD2	2.50	0.42
34:g:172:LYS:HB3	34:g:191:HIS:HB2	2.02	0.42
6:E:192:ILE:HD12	6:E:243:GLY:HA3	2.02	0.42
18:b:31:TYR:OH	18:b:70:LYS:NZ	2.46	0.42
34:g:249:CYS:HB3	34:g:258:ILE:HG23	2.01	0.42
1:2:591:U:O2'	1:2:592:C:H3'	2.20	0.41
1:2:1562:C:H2'	1:2:1563:G:H8	1.84	0.41
3:A:24:HIS:HB3	3:A:51:LEU:HD11	2.02	0.41
20:u:96:LEU:O	20:u:100:MET:CB	2.67	0.41
32:Z:42:ASP:OD1	32:Z:42:ASP:N	2.53	0.41
1:2:145:G:O6	7:G:178:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:656:G:N2	1:2:663:C:H5''	2.35	0.41
1:2:815:U:O4	1:2:816:A:N6	2.53	0.41
1:2:873:G:H1	11:L:152:LYS:HD2	1.84	0.41
1:2:1245:G:O2'	1:2:1492:U:OP1	2.29	0.41
1:2:1612:G:O5'	27:P:18:ARG:NH2	2.53	0.41
1:2:1786:U:H2'	1:2:1787:G:H8	1.85	0.41
3:A:185:MET:HB3	3:A:185:MET:HE3	1.65	0.41
22:d:29:GLY:O	22:d:40:ARG:N	2.41	0.41
28:Q:38:PRO:HD2	28:Q:41:MET:SD	2.61	0.41
30:T:70:ALA:HB1	30:T:74:SER:OG	2.20	0.41
34:g:212:LYS:HA	34:g:212:LYS:HD2	1.89	0.41
35:p:129:GLU:OE1	35:p:129:GLU:N	2.52	0.41
1:2:561:A:O2'	10:J:134:HIS:NE2	2.30	0.41
1:2:1143:A:H5'	5:C:190:SER:HB2	2.02	0.41
2:R:105:MET:HE1	3:A:39:TYR:CD2	2.55	0.41
3:A:57:LYS:HE2	3:A:159:ILE:HG23	2.02	0.41
20:u:178:PHE:CE1	20:u:182:LEU:HD11	2.55	0.41
32:Z:92:LEU:HD11	32:Z:109:TYR:HE1	1.85	0.41
1:2:222:U:H5''	11:L:17:PHE:CG	2.56	0.41
1:2:929:G:H2'	1:2:930:C:O4'	2.20	0.41
1:2:941:C:H5''	4:B:136:ARG:CZ	2.51	0.41
1:2:1259:A:H1'	1:2:1264:C:H41	1.85	0.41
20:u:207:LEU:HD23	20:u:207:LEU:HA	1.90	0.41
24:F:33:ILE:HA	24:F:36:GLN:HG2	2.02	0.41
1:2:523:A:OP2	10:J:38:ARG:NH1	2.52	0.41
1:2:528:A:H2'	1:2:529:A:H8	1.84	0.41
1:2:1191:C:H2'	1:2:1192:U:H6	1.85	0.41
1:2:1254:C:O5'	31:U:75:LYS:NZ	2.40	0.41
1:2:1613:G:P	27:P:42:ARG:HH21	2.43	0.41
1:2:1725:U:H2'	1:2:1726:G:C8	2.55	0.41
28:Q:50:LYS:O	28:Q:53:GLU:HB3	2.20	0.41
34:g:152:SER:HB3	34:g:170:TRP:CD1	2.56	0.41
1:2:1679:A:H2'	24:F:60:ARG:HD2	2.02	0.41
6:E:233:LYS:HD2	6:E:234:PRO:HD2	2.01	0.41
17:Y:83:LYS:HE3	17:Y:83:LYS:HB3	1.78	0.41
20:u:303:ASP:OD1	20:u:561:HIS:NE2	2.52	0.41
20:u:495:ALA:HB3	20:u:498:ILE:HD12	2.02	0.41
26:M:79:VAL:HG21	26:M:85:LEU:HD21	2.03	0.41
34:g:79:LEU:HD11	34:g:87:LEU:HG	2.02	0.41
1:2:919:A:H4'	1:2:920:A:H5''	2.02	0.41
1:2:1407:U:O3'	28:Q:71:ARG:NH1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1652:G:N2	1:2:1672:U:O2	2.39	0.41
10:J:92:MET:HE2	10:J:92:MET:HB3	1.81	0.41
11:L:13:GLN:NE2	11:L:36:TYR:O	2.53	0.41
20:u:75:LEU:HD21	20:u:83:HIS:ND1	2.36	0.41
23:D:192:TRP:CD1	23:D:203:PRO:HA	2.55	0.41
29:S:86:ARG:HH11	29:S:106:LYS:HD3	1.86	0.41
34:g:17:TRP:CE2	34:g:303:THR:HG23	2.55	0.41
1:2:823:U:H2'	1:2:824:C:H6	1.86	0.41
1:2:1070:A:H5''	21:t:431:LYS:HE2	2.03	0.41
1:2:1098:C:H2'	1:2:1099:G:C8	2.56	0.41
1:2:1872:G:OP1	4:B:147:ASN:ND2	2.49	0.41
7:G:126:ASP:OD1	7:G:126:ASP:N	2.53	0.41
9:I:76:THR:HG21	9:I:104:ILE:HD12	2.03	0.41
22:d:20:SER:OG	25:K:65:ARG:NH1	2.41	0.41
28:Q:41:MET:HE2	28:Q:41:MET:HB3	1.93	0.41
1:2:12:U:H2'	1:2:13:C:C6	2.56	0.41
1:2:118:C:H1'	1:2:445:A:C5	2.55	0.41
1:2:610:G:H2'	1:2:611:G:H8	1.86	0.41
1:2:808:A:H5''	6:E:219:ALA:O	2.20	0.41
1:2:1276:A:H61	1:2:1321:G:H1'	1.85	0.41
1:2:1290:G:N2	1:2:1310:U:H1'	2.35	0.41
1:2:1342:U:H4'	1:2:1343:U:O5'	2.21	0.41
1:2:1426:U:H2'	1:2:1427:C:C6	2.56	0.41
3:A:77:ILE:HG12	3:A:99:ILE:HB	2.03	0.41
6:E:16:LYS:HA	6:E:16:LYS:HD2	1.95	0.41
6:E:31:PRO:HD2	6:E:38:LEU:HD12	2.03	0.41
20:u:82:PRO:HB3	20:u:132:ARG:HD2	2.02	0.41
20:u:597:VAL:O	20:u:682:GLY:HA3	2.20	0.41
31:U:60:THR:OG1	31:U:62:ARG:NH2	2.53	0.41
1:2:747:U:H2'	1:2:748:C:C6	2.56	0.41
2:R:27:ASP:O	2:R:31:ASN:ND2	2.54	0.41
4:B:107:ARG:NH1	13:O:133:THR:H	2.19	0.41
4:B:166:LYS:HA	4:B:169:MET:HE2	2.03	0.41
20:u:360:ILE:HG22	20:u:526:ARG:HA	2.02	0.41
34:g:199:THR:HG21	34:g:240:CYS:HA	2.02	0.41
1:2:1284:A:O2'	26:M:106:CYS:SG	2.64	0.40
1:2:1797:U:H2'	1:2:1798:C:C6	2.55	0.40
2:R:95:ILE:HD11	2:R:118:GLN:HB2	2.03	0.40
3:A:42:LYS:HE3	3:A:42:LYS:HB2	1.85	0.40
6:E:19:MET:SD	6:E:108:ARG:HD2	2.61	0.40
10:J:126:ALA:O	10:J:130:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:35:ALA:HB2	13:O:112:ALA:HB2	2.03	0.40
20:u:286:ASN:HD21	20:u:349:PRO:HD2	1.86	0.40
26:M:48:HIS:ND1	26:M:112:LYS:O	2.35	0.40
34:g:125:ARG:HG2	34:g:150:TRP:CG	2.57	0.40
1:2:73:C:O2'	1:2:74:G:O4'	2.35	0.40
1:2:661:U:OP2	16:X:3:LYS:NZ	2.54	0.40
4:B:47:THR:HB	4:B:65:ARG:HH12	1.87	0.40
7:G:64:LYS:HB2	7:G:97:VAL:HG11	2.03	0.40
10:J:60:LEU:HD23	10:J:60:LEU:HA	1.91	0.40
12:N:91:LEU:HD23	12:N:91:LEU:HA	1.89	0.40
27:P:22:LEU:HA	27:P:22:LEU:HD23	1.91	0.40
27:P:23:ASP:HA	27:P:26:LEU:HD12	2.03	0.40
27:P:31:GLU:O	27:P:34:MET:HB3	2.21	0.40
28:Q:43:GLU:H	28:Q:43:GLU:HG3	1.66	0.40
1:2:352:U:H2'	1:2:353:C:C6	2.56	0.40
1:2:792:C:H2'	1:2:793:G:C8	2.56	0.40
1:2:799:U:H2'	1:2:800:U:C6	2.56	0.40
1:2:1408:U:P	28:Q:71:ARG:HH12	2.44	0.40
23:D:72:VAL:HA	25:K:20:VAL:HG11	2.03	0.40
31:U:35:VAL:HG11	31:U:107:GLU:HB2	2.02	0.40
1:2:376:A:H2'	1:2:377:G:O4'	2.21	0.40
1:2:1271:C:H2'	1:2:1272:C:C6	2.56	0.40
16:X:127:ASN:ND2	16:X:127:ASN:O	2.54	0.40
20:u:512:SER:HA	20:u:513:PRO:HD3	1.96	0.40
22:d:26:ASN:OD1	22:d:27:ARG:N	2.55	0.40
26:M:47:ALA:HA	26:M:112:LYS:HA	2.02	0.40
36:i:22:THR:HA	36:i:55:THR:HA	2.03	0.40
1:2:202:G:H2'	1:2:203:G:H8	1.85	0.40
1:2:527:C:H2'	1:2:528:A:H8	1.87	0.40
1:2:1562:C:H2'	1:2:1563:G:C8	2.56	0.40
1:2:1710:C:H2'	1:2:1711:U:C6	2.56	0.40
11:L:35:ARG:NH2	11:L:55:TYR:O	2.29	0.40
11:L:48:LYS:HD3	11:L:48:LYS:HA	1.98	0.40
17:Y:11:LYS:H	17:Y:11:LYS:HG3	1.66	0.40
23:D:163:PRO:HD3	23:D:205:PRO:HG2	2.02	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	R	120/135 (89%)	108 (90%)	11 (9%)	1 (1%)	16	48
3	A	214/295 (72%)	205 (96%)	9 (4%)	0	100	100
4	B	211/264 (80%)	203 (96%)	8 (4%)	0	100	100
5	C	216/293 (74%)	206 (95%)	10 (5%)	0	100	100
6	E	260/263 (99%)	246 (95%)	13 (5%)	1 (0%)	30	60
7	G	228/249 (92%)	220 (96%)	8 (4%)	0	100	100
8	H	184/194 (95%)	182 (99%)	2 (1%)	0	100	100
9	I	203/208 (98%)	197 (97%)	6 (3%)	0	100	100
10	J	178/194 (92%)	166 (93%)	11 (6%)	1 (1%)	21	52
11	L	149/158 (94%)	144 (97%)	5 (3%)	0	100	100
12	N	147/151 (97%)	142 (97%)	5 (3%)	0	100	100
13	O	133/151 (88%)	127 (96%)	6 (4%)	0	100	100
14	V	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
15	W	127/130 (98%)	125 (98%)	1 (1%)	1 (1%)	16	48
16	X	139/143 (97%)	134 (96%)	4 (3%)	1 (1%)	18	50
17	Y	122/133 (92%)	116 (95%)	6 (5%)	0	100	100
18	b	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
19	x	176/252 (70%)	171 (97%)	5 (3%)	0	100	100
20	u	607/804 (76%)	577 (95%)	30 (5%)	0	100	100
21	t	59/475 (12%)	55 (93%)	3 (5%)	1 (2%)	7	34
22	d	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
23	D	223/243 (92%)	214 (96%)	8 (4%)	1 (0%)	30	60
24	F	187/204 (92%)	172 (92%)	13 (7%)	2 (1%)	11	42
25	K	93/165 (56%)	87 (94%)	6 (6%)	0	100	100
26	M	121/132 (92%)	117 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	P	118/145 (81%)	118 (100%)	0	0	100	100
28	Q	137/146 (94%)	129 (94%)	8 (6%)	0	100	100
29	S	141/152 (93%)	130 (92%)	11 (8%)	0	100	100
30	T	142/145 (98%)	135 (95%)	7 (5%)	0	100	100
31	U	99/119 (83%)	95 (96%)	4 (4%)	0	100	100
32	Z	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
33	c	59/69 (86%)	55 (93%)	4 (7%)	0	100	100
34	g	312/317 (98%)	290 (93%)	22 (7%)	0	100	100
35	p	385/519 (74%)	368 (96%)	17 (4%)	0	100	100
36	i	71/76 (93%)	71 (100%)	0	0	100	100
36	j	71/76 (93%)	71 (100%)	0	0	100	100
All	All	5915/7348 (80%)	5651 (96%)	255 (4%)	9 (0%)	44	72

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	X	61	GLN
23	D	194	PRO
24	F	166	ILE
10	J	138	ARG
15	W	5	ASN
6	E	68	ARG
2	R	42	PRO
24	F	84	GLY
21	t	470	VAL

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	R	110/122 (90%)	107 (97%)	3 (3%)	39	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	180/243 (74%)	178 (99%)	2 (1%)	65	73
4	B	194/231 (84%)	194 (100%)	0	100	100
5	C	184/225 (82%)	184 (100%)	0	100	100
6	E	224/225 (100%)	215 (96%)	9 (4%)	28	52
7	G	200/218 (92%)	200 (100%)	0	100	100
8	H	167/174 (96%)	167 (100%)	0	100	100
9	I	178/180 (99%)	176 (99%)	2 (1%)	65	73
10	J	160/168 (95%)	158 (99%)	2 (1%)	61	71
11	L	135/142 (95%)	135 (100%)	0	100	100
12	N	130/131 (99%)	130 (100%)	0	100	100
13	O	105/119 (88%)	105 (100%)	0	100	100
14	V	66/67 (98%)	66 (100%)	0	100	100
15	W	112/113 (99%)	110 (98%)	2 (2%)	51	67
16	X	113/115 (98%)	113 (100%)	0	100	100
17	Y	108/115 (94%)	105 (97%)	3 (3%)	38	58
18	b	74/76 (97%)	74 (100%)	0	100	100
20	u	539/705 (76%)	539 (100%)	0	100	100
21	t	56/434 (13%)	56 (100%)	0	100	100
22	d	48/49 (98%)	48 (100%)	0	100	100
23	D	189/202 (94%)	181 (96%)	8 (4%)	26	51
24	F	159/170 (94%)	154 (97%)	5 (3%)	35	57
25	K	86/136 (63%)	86 (100%)	0	100	100
26	M	104/108 (96%)	104 (100%)	0	100	100
27	P	107/130 (82%)	107 (100%)	0	100	100
28	Q	115/121 (95%)	115 (100%)	0	100	100
29	S	124/132 (94%)	124 (100%)	0	100	100
30	T	114/115 (99%)	113 (99%)	1 (1%)	70	75
31	U	93/107 (87%)	93 (100%)	0	100	100
32	Z	64/103 (62%)	64 (100%)	0	100	100
33	c	54/62 (87%)	54 (100%)	0	100	100
34	g	272/275 (99%)	272 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	p	136/454 (30%)	136 (100%)	0	100	100
All	All	4700/5967 (79%)	4663 (99%)	37 (1%)	70	76

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	R	43	SER
2	R	45	LYS
2	R	47	ARG
3	A	82	THR
3	A	87	VAL
6	E	15	PRO
6	E	37	LYS
6	E	38	LEU
6	E	40	GLU
6	E	42	LEU
6	E	62	LYS
6	E	66	MET
6	E	80	ILE
6	E	204	SER
9	I	18	ARG
9	I	19	LYS
10	J	2	PRO
10	J	144	ILE
15	W	32	LYS
15	W	33	VAL
17	Y	104	ARG
17	Y	107	ARG
17	Y	108	LYS
23	D	164	VAL
23	D	192	TRP
23	D	193	ASP
23	D	197	LYS
23	D	198	ILE
23	D	201	LYS
23	D	202	LYS
23	D	204	LEU
24	F	78	MET
24	F	79	HIS
24	F	86	LYS
24	F	89	THR
24	F	159	ARG

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Mol	Chain	Res	Type
30	T	51	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	81	ASN
3	A	131	HIS
4	B	124	HIS
4	B	177	GLN
4	B	186	ASN
5	C	120	GLN
5	C	136	HIS
6	E	161	GLN
7	G	56	ASN
7	G	187	HIS
7	G	197	GLN
8	H	33	ASN
8	H	73	GLN
9	I	22	HIS
9	I	52	ASN
10	J	27	GLN
11	L	83	GLN
11	L	100	ASN
11	L	112	HIS
13	O	83	GLN
14	V	49	GLN
15	W	92	ASN
16	X	127	ASN
17	Y	85	ASN
17	Y	89	HIS
18	b	9	HIS
18	b	49	HIS
20	u	114	ASN
20	u	286	ASN
20	u	632	HIS
20	u	702	HIS
20	u	719	ASN
24	F	82	ASN
24	F	118	ASN
27	P	41	GLN
27	P	104	GLN
28	Q	86	GLN

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Mol	Chain	Res	Type
29	S	134	GLN
30	T	83	GLN
30	T	91	HIS
30	T	126	GLN
33	c	26	GLN
33	c	29	GLN
33	c	45	ASN
34	g	56	GLN
34	g	237	ASN
35	p	181	ASN
35	p	209	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1639/1873 (87%)	481 (29%)	35 (2%)

All (481) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	C
1	2	4	C
1	2	23	G
1	2	25	A
1	2	26	U
1	2	30	C
1	2	33	G
1	2	36	U
1	2	41	G
1	2	44	U
1	2	45	A
1	2	46	A
1	2	56	G
1	2	62	G
1	2	65	C
1	2	66	G
1	2	67	C
1	2	68	A
1	2	69	C
1	2	72	C

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Mol	Chain	Res	Type
1	2	73	C
1	2	74	G
1	2	75	G
1	2	76	U
1	2	77	A
1	2	79	A
1	2	92	A
1	2	96	C
1	2	100	U
1	2	103	A
1	2	110	U
1	2	113	G
1	2	115	U
1	2	126	G
1	2	127	C
1	2	128	U
1	2	129	C
1	2	130	G
1	2	143	U
1	2	144	U
1	2	147	A
1	2	149	A
1	2	155	G
1	2	160	U
1	2	161	U
1	2	163	U
1	2	165	G
1	2	166	A
1	2	167	G
1	2	168	C
1	2	172	U
1	2	181	A
1	2	182	C
1	2	183	G
1	2	184	G
1	2	190	G
1	2	191	A
1	2	215	G
1	2	290	U
1	2	291	G
1	2	292	A
1	2	294	U

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Mol	Chain	Res	Type
1	2	295	C
1	2	302	A
1	2	308	G
1	2	309	G
1	2	312	G
1	2	313	A
1	2	315	C
1	2	318	A
1	2	319	C
1	2	321	C
1	2	332	G
1	2	333	G
1	2	337	C
1	2	340	C
1	2	350	C
1	2	351	G
1	2	360	A
1	2	362	C
1	2	364	A
1	2	370	G
1	2	377	G
1	2	381	C
1	2	382	C
1	2	385	G
1	2	386	C
1	2	387	C
1	2	400	C
1	2	404	G
1	2	405	G
1	2	406	U
1	2	408	A
1	2	409	C
1	2	413	G
1	2	418	A
1	2	421	G
1	2	429	C
1	2	438	G
1	2	441	C
1	2	448	A
1	2	449	A
1	2	450	C
1	2	451	G

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Mol	Chain	Res	Type
1	2	463	C
1	2	466	G
1	2	471	G
1	2	472	C
1	2	473	A
1	2	474	G
1	2	482	G
1	2	487	U
1	2	492	C
1	2	496	C
1	2	500	A
1	2	501	C
1	2	502	C
1	2	503	C
1	2	507	G
1	2	508	A
1	2	509	G
1	2	517	C
1	2	525	A
1	2	531	A
1	2	534	G
1	2	536	A
1	2	544	G
1	2	548	C
1	2	549	C
1	2	555	A
1	2	556	U
1	2	557	U
1	2	559	G
1	2	560	A
1	2	568	C
1	2	576	A
1	2	583	A
1	2	587	A
1	2	588	G
1	2	589	G
1	2	590	A
1	2	591	U
1	2	592	C
1	2	594	A
1	2	595	U
1	2	598	G

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Mol	Chain	Res	Type
1	2	600	G
1	2	605	A
1	2	606	G
1	2	607	U
1	2	608	C
1	2	613	G
1	2	614	C
1	2	617	G
1	2	620	G
1	2	626	G
1	2	627	U
1	2	628	A
1	2	629	A
1	2	632	C
1	2	643	A
1	2	644	G
1	2	654	A
1	2	655	A
1	2	660	C
1	2	663	C
1	2	668	A
1	2	669	A
1	2	670	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	683	G
1	2	687	C
1	2	688	U
1	2	749	U
1	2	750	C
1	2	751	G
1	2	792	C
1	2	794	A
1	2	797	C
1	2	799	U
1	2	801	U
1	2	809	A
1	2	810	A
1	2	812	A
1	2	821	G
1	2	823	U

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Mol	Chain	Res	Type
1	2	827	A
1	2	830	A
1	2	842	C
1	2	847	A
1	2	852	G
1	2	859	G
1	2	867	G
1	2	869	A
1	2	870	A
1	2	871	U
1	2	872	A
1	2	873	G
1	2	874	G
1	2	878	G
1	2	880	G
1	2	885	U
1	2	886	A
1	2	887	U
1	2	888	U
1	2	889	U
1	2	890	U
1	2	891	G
1	2	892	U
1	2	893	U
1	2	895	G
1	2	896	U
1	2	898	U
1	2	903	A
1	2	905	C
1	2	907	G
1	2	908	A
1	2	913	A
1	2	914	U
1	2	917	U
1	2	919	A
1	2	920	A
1	2	927	C
1	2	930	C
1	2	933	G
1	2	954	U
1	2	955	A
1	2	956	G

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Mol	Chain	Res	Type
1	2	959	G
1	2	963	A
1	2	969	U
1	2	970	G
1	2	971	G
1	2	972	A
1	2	978	G
1	2	981	A
1	2	988	C
1	2	990	A
1	2	992	A
1	2	1001	A
1	2	1002	U
1	2	1009	A
1	2	1017	U
1	2	1023	A
1	2	1027	A
1	2	1028	A
1	2	1031	A
1	2	1041	G
1	2	1045	U
1	2	1049	A
1	2	1054	G
1	2	1055	A
1	2	1056	U
1	2	1057	C
1	2	1058	A
1	2	1059	G
1	2	1062	A
1	2	1065	G
1	2	1067	C
1	2	1080	A
1	2	1083	A
1	2	1084	A
1	2	1085	C
1	2	1086	G
1	2	1087	A
1	2	1088	U
1	2	1096	G
1	2	1099	G
1	2	1100	A
1	2	1112	U

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Mol	Chain	Res	Type
1	2	1113	A
1	2	1114	U
1	2	1116	C
1	2	1117	C
1	2	1118	C
1	2	1119	A
1	2	1121	G
1	2	1133	A
1	2	1138	C
1	2	1139	C
1	2	1141	G
1	2	1143	A
1	2	1148	A
1	2	1149	A
1	2	1153	C
1	2	1154	U
1	2	1155	U
1	2	1157	G
1	2	1166	G
1	2	1171	G
1	2	1195	A
1	2	1200	A
1	2	1204	A
1	2	1207	G
1	2	1208	A
1	2	1211	G
1	2	1215	C
1	2	1217	A
1	2	1221	G
1	2	1224	G
1	2	1227	G
1	2	1232	U
1	2	1233	G
1	2	1234	C
1	2	1235	G
1	2	1236	G
1	2	1242	U
1	2	1243	U
1	2	1250	A
1	2	1251	A
1	2	1253	A
1	2	1257	G

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Mol	Chain	Res	Type
1	2	1259	A
1	2	1260	A
1	2	1261	C
1	2	1264	C
1	2	1266	C
1	2	1274	G
1	2	1275	G
1	2	1276	A
1	2	1283	C
1	2	1286	G
1	2	1288	U
1	2	1298	G
1	2	1300	U
1	2	1302	G
1	2	1303	C
1	2	1304	U
1	2	1308	U
1	2	1309	C
1	2	1313	A
1	2	1314	U
1	2	1315	U
1	2	1317	C
1	2	1320	G
1	2	1322	G
1	2	1327	G
1	2	1329	U
1	2	1331	C
1	2	1343	U
1	2	1358	U
1	2	1362	U
1	2	1363	C
1	2	1364	U
1	2	1376	A
1	2	1378	A
1	2	1382	A
1	2	1401	A
1	2	1404	U
1	2	1405	A
1	2	1406	G
1	2	1416	C
1	2	1426	U
1	2	1428	G

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Mol	Chain	Res	Type
1	2	1429	G
1	2	1430	C
1	2	1431	G
1	2	1432	U
1	2	1439	A
1	2	1441	U
1	2	1442	U
1	2	1444	U
1	2	1446	A
1	2	1452	A
1	2	1454	A
1	2	1455	A
1	2	1462	U
1	2	1463	U
1	2	1465	A
1	2	1466	G
1	2	1473	G
1	2	1476	A
1	2	1477	U
1	2	1478	U
1	2	1487	A
1	2	1489	A
1	2	1494	U
1	2	1495	G
1	2	1498	A
1	2	1505	U
1	2	1510	G
1	2	1511	U
1	2	1520	G
1	2	1521	C
1	2	1524	G
1	2	1526	G
1	2	1531	A
1	2	1535	U
1	2	1543	U
1	2	1544	C
1	2	1548	G
1	2	1559	C
1	2	1560	U
1	2	1563	G
1	2	1566	G
1	2	1567	G

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Mol	Chain	Res	Type
1	2	1569	A
1	2	1572	C
1	2	1574	C
1	2	1578	U
1	2	1579	A
1	2	1580	A
1	2	1581	C
1	2	1582	C
1	2	1585	U
1	2	1586	U
1	2	1587	G
1	2	1588	A
1	2	1598	G
1	2	1599	U
1	2	1600	G
1	2	1601	A
1	2	1602	U
1	2	1603	G
1	2	1604	G
1	2	1606	G
1	2	1609	C
1	2	1612	G
1	2	1617	G
1	2	1618	C
1	2	1619	A
1	2	1621	U
1	2	1623	A
1	2	1630	A
1	2	1631	U
1	2	1632	G
1	2	1647	A
1	2	1649	U
1	2	1650	A
1	2	1654	G
1	2	1661	A
1	2	1663	A
1	2	1665	G
1	2	1671	G
1	2	1674	G
1	2	1675	A
1	2	1686	G
1	2	1689	C

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Mol	Chain	Res	Type
1	2	1693	G
1	2	1699	A
1	2	1706	G
1	2	1721	U
1	2	1722	G
1	2	1723	G
1	2	1727	G
1	2	1728	U
1	2	1729	U
1	2	1742	C
1	2	1744	G
1	2	1746	U
1	2	1751	C
1	2	1754	G
1	2	1756	C
1	2	1757	G
1	2	1773	C
1	2	1776	G
1	2	1783	C
1	2	1784	G
1	2	1786	U
1	2	1801	A
1	2	1805	G
1	2	1808	U
1	2	1813	A
1	2	1816	G
1	2	1819	A
1	2	1826	G
1	2	1848	U
1	2	1850	A
1	2	1859	A
1	2	1860	A
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1864	U
1	2	1869	A
1	2	1870	A
1	2	1872	G
1	2	1873	G

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	102	A
1	2	143	U
1	2	291	G
1	2	314	U
1	2	332	G
1	2	440	G
1	2	465	A
1	2	473	A
1	2	554	A
1	2	604	A
1	2	631	U
1	2	811	A
1	2	870	A
1	2	980	A
1	2	1231	C
1	2	1256	G
1	2	1302	G
1	2	1308	U
1	2	1316	C
1	2	1330	G
1	2	1342	U
1	2	1403	C
1	2	1425	G
1	2	1430	C
1	2	1438	A
1	2	1440	C
1	2	1464	C
1	2	1494	U
1	2	1534	C
1	2	1558	C
1	2	1585	U
1	2	1601	A
1	2	1648	G
1	2	1649	U
1	2	1726	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

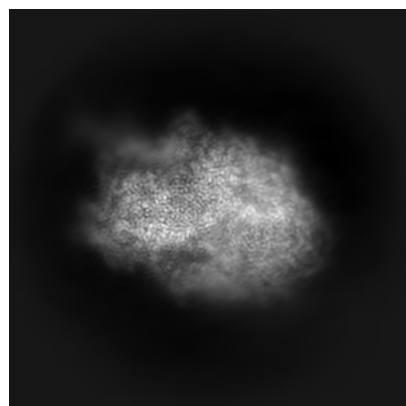
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39958. These allow visual inspection of the internal detail of the map and identification of artifacts.

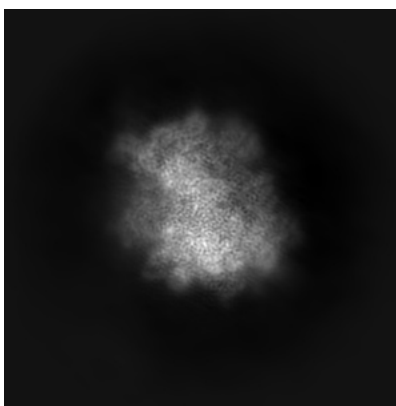
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

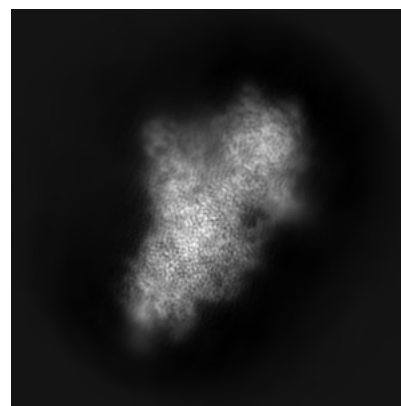
6.1.1 Primary map



X

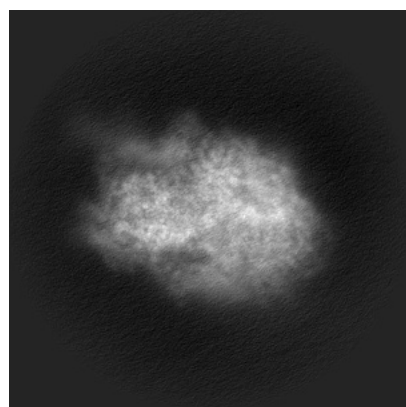


Y

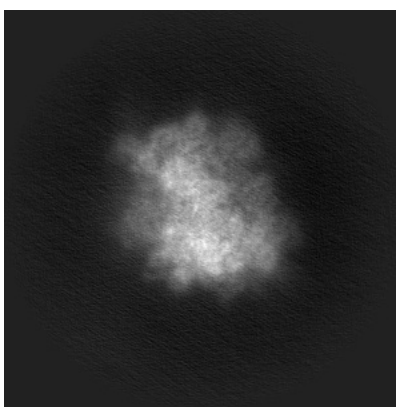


Z

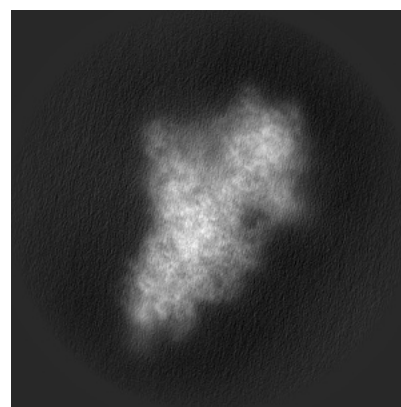
6.1.2 Raw map



X



Y

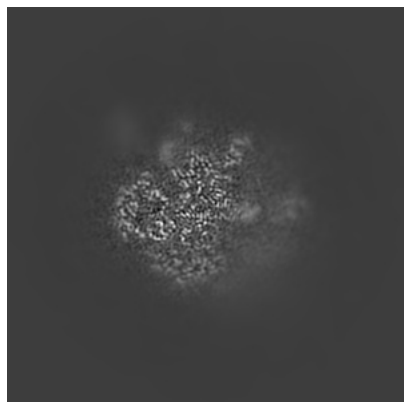


Z

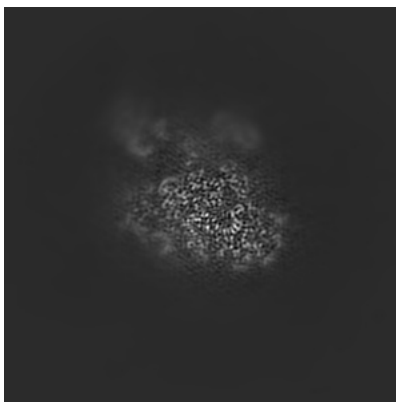
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

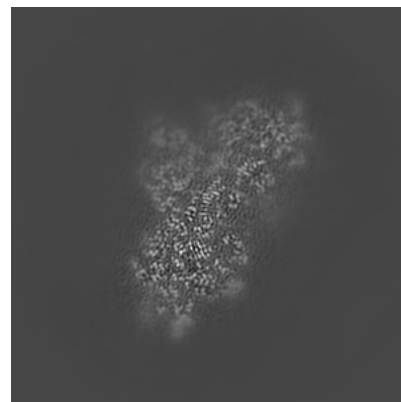
6.2.1 Primary map



X Index: 180

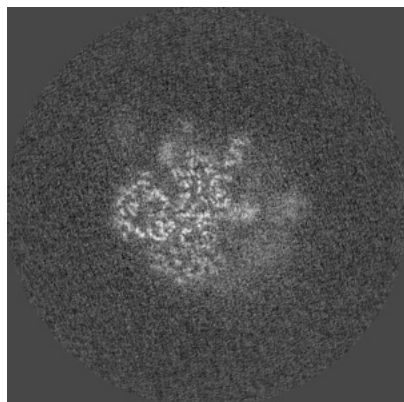


Y Index: 180

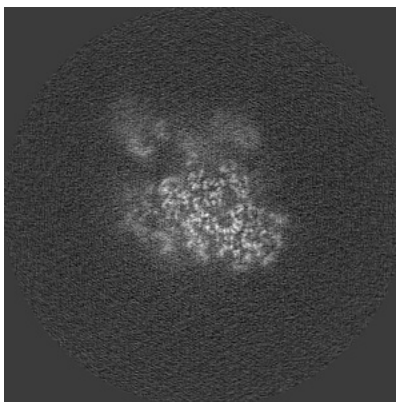


Z Index: 180

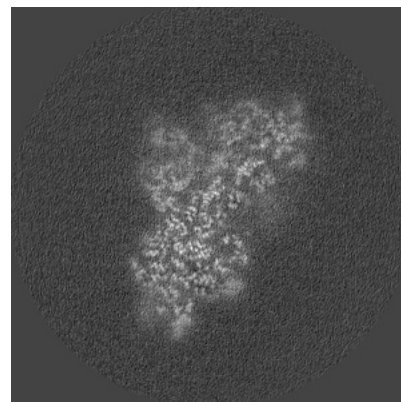
6.2.2 Raw map



X Index: 180



Y Index: 180

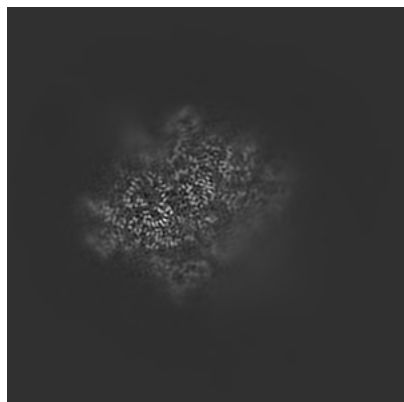


Z Index: 180

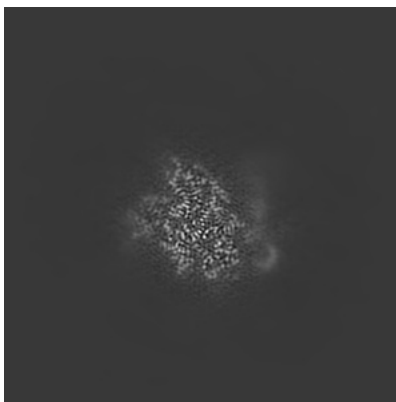
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

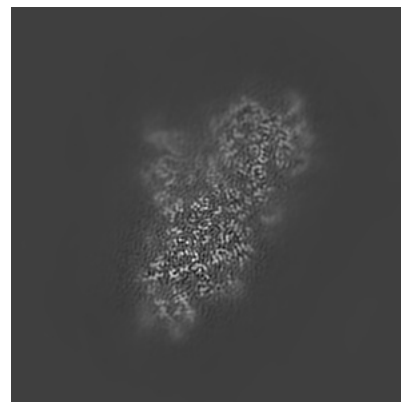
6.3.1 Primary map



X Index: 158

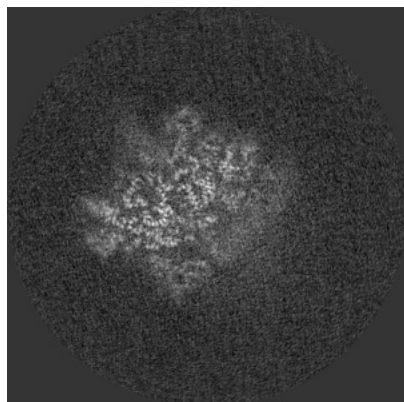


Y Index: 139

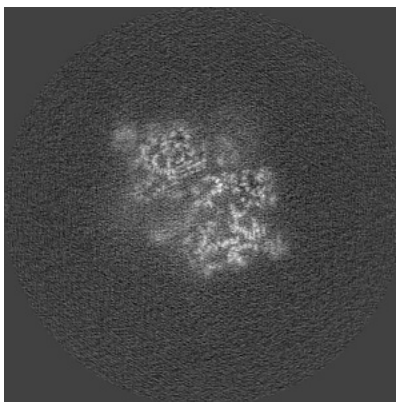


Z Index: 175

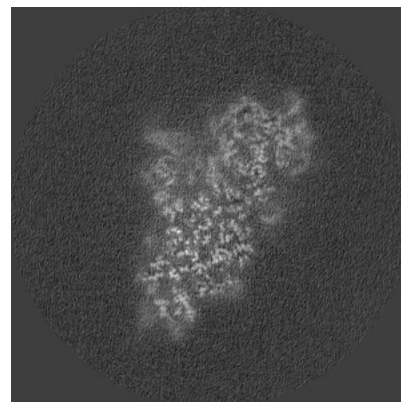
6.3.2 Raw map



X Index: 158



Y Index: 200

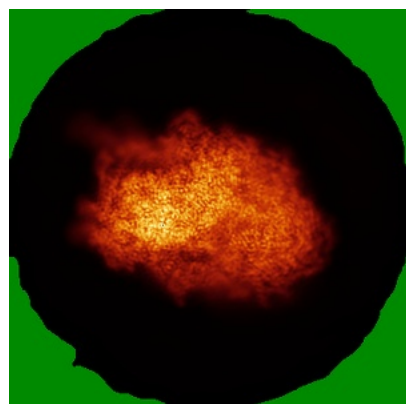


Z Index: 175

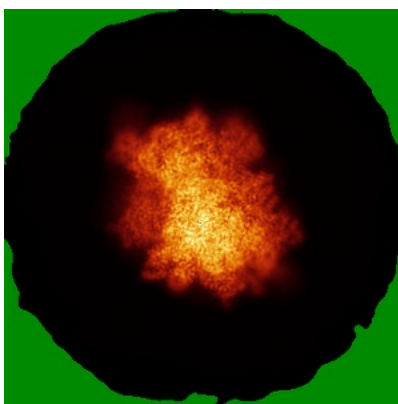
The images above show the largest variance slices of the map in three orthogonal directions.

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

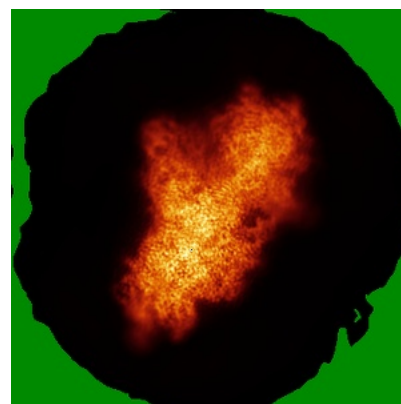
6.4.1 Primary map



X

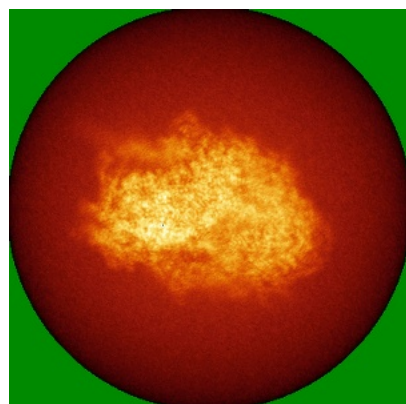


Y

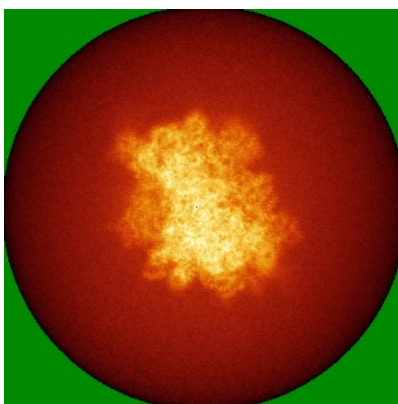


Z

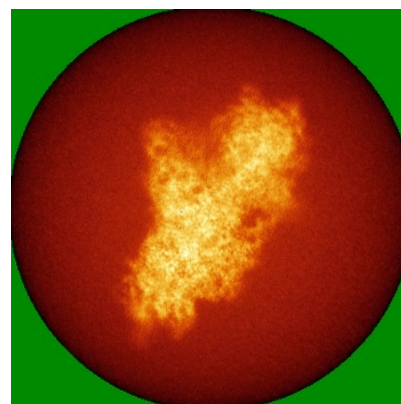
6.4.2 Raw map



X



Y

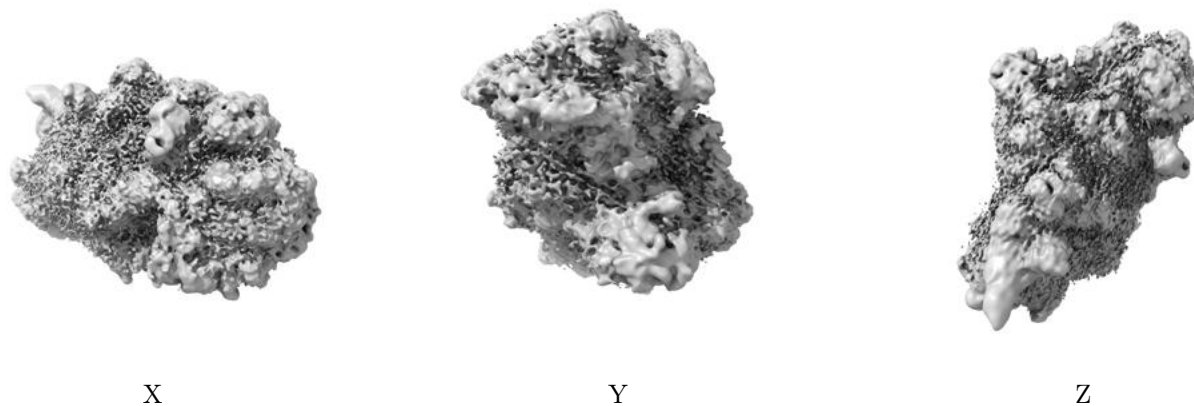


Z

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.

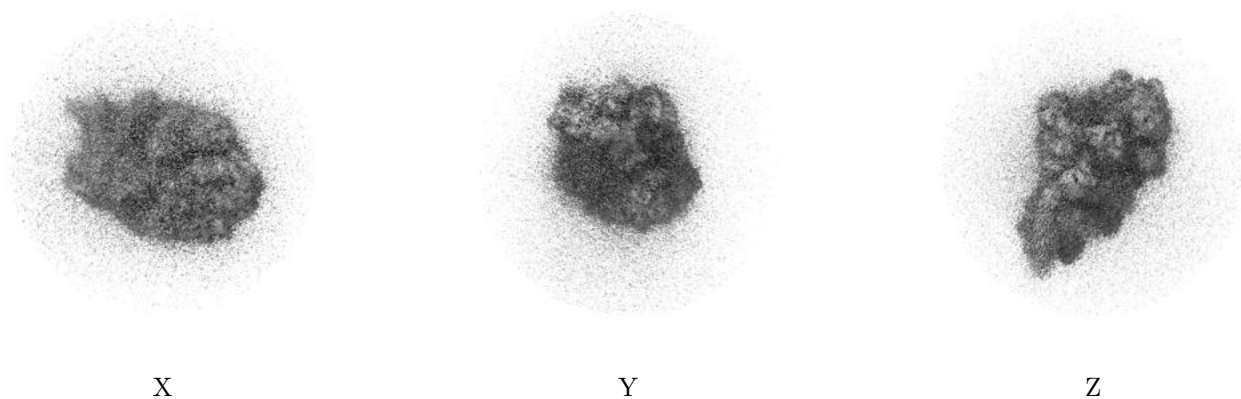
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

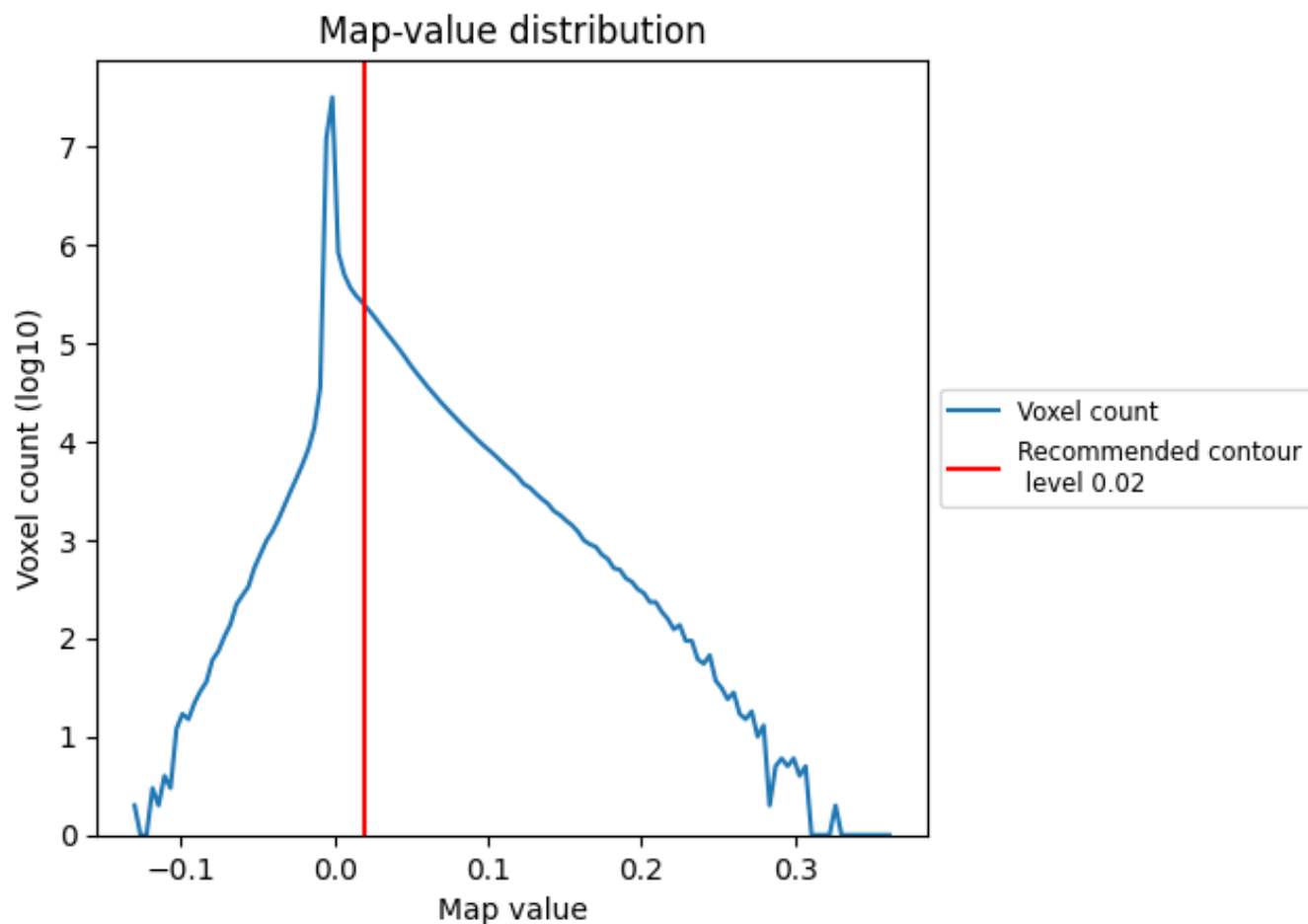
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

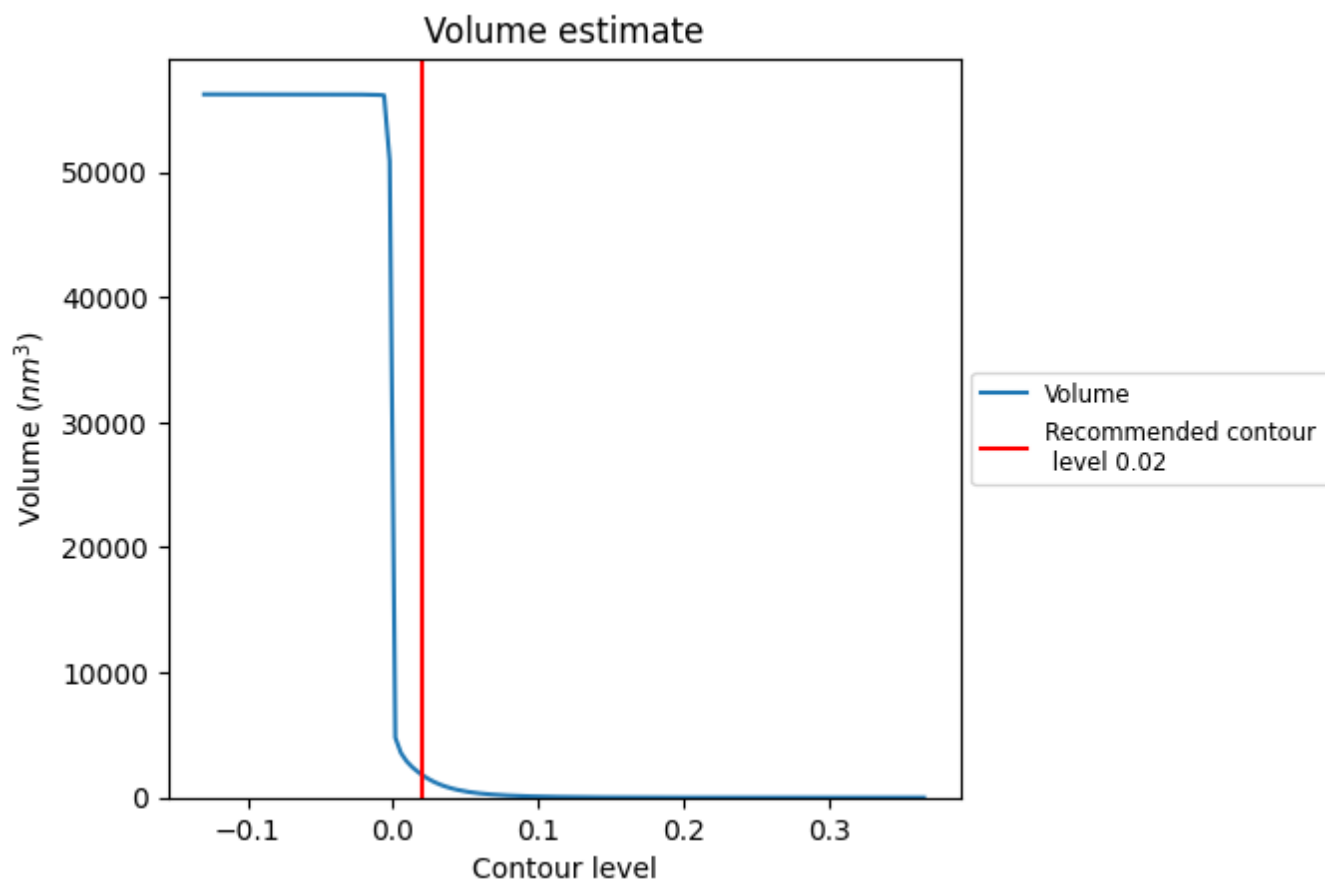
This section contains the results of statistical analysis of the map.

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.

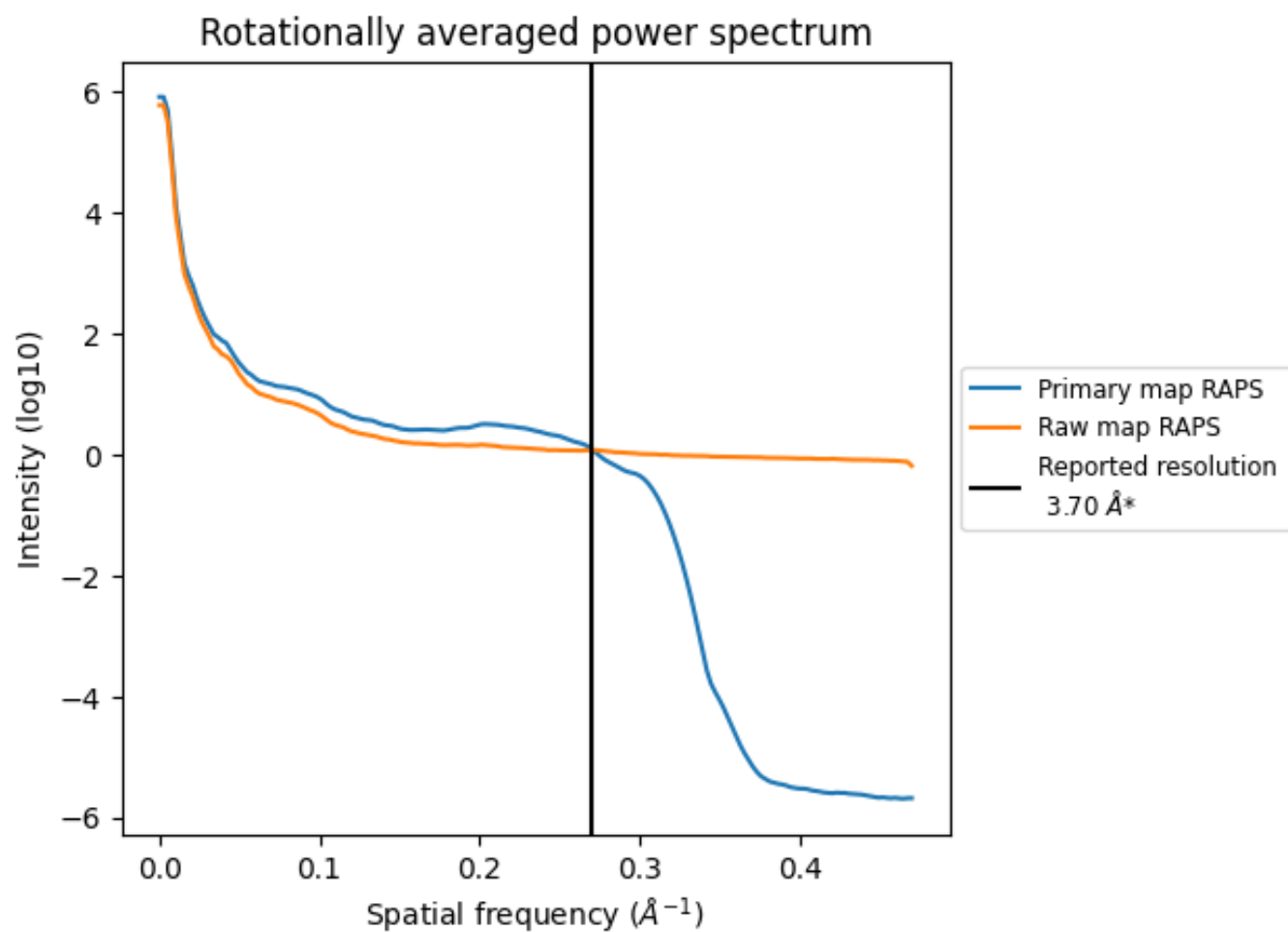
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1820 nm³; this corresponds to an approximate mass of 1644 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 ⓘ

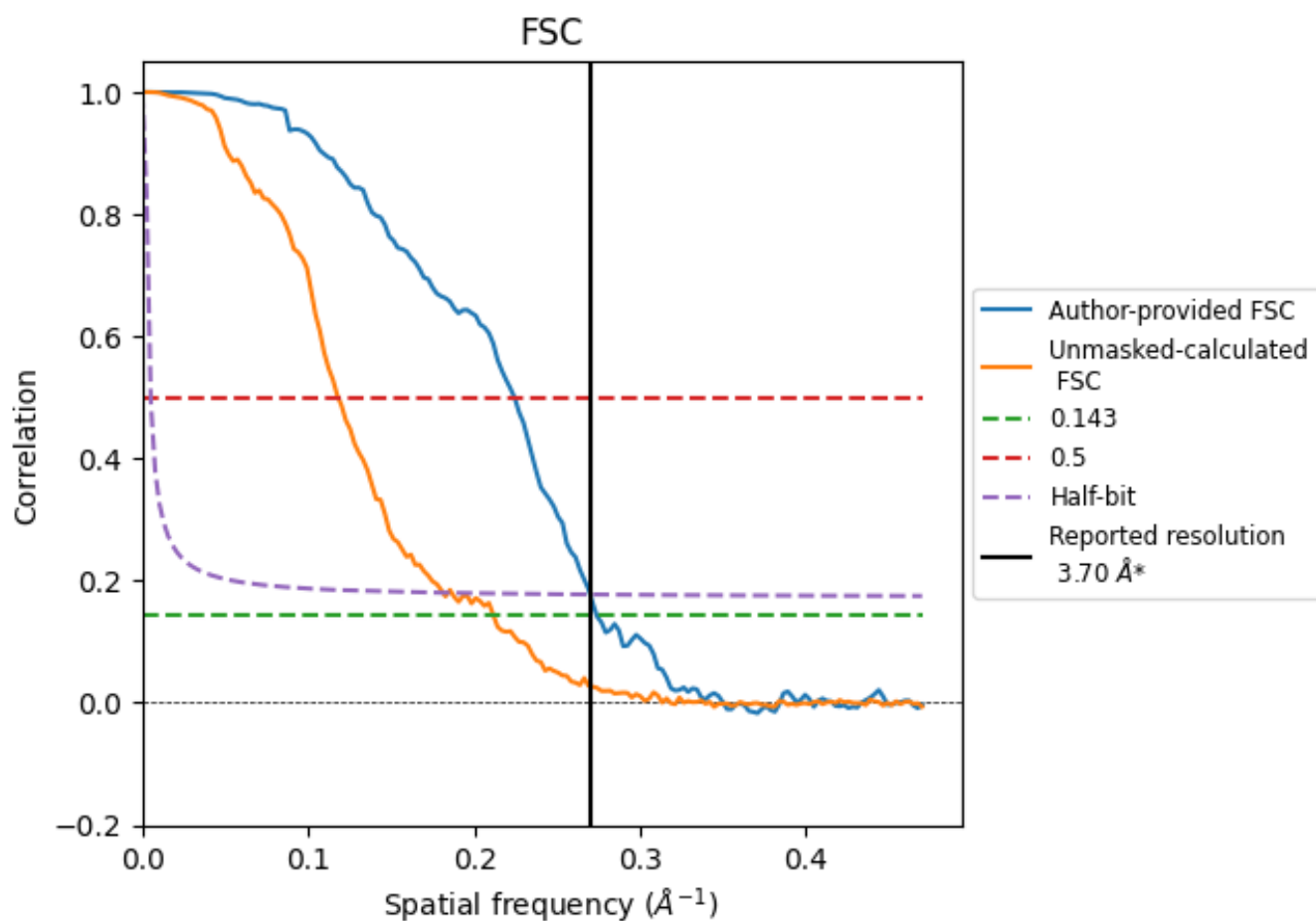


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

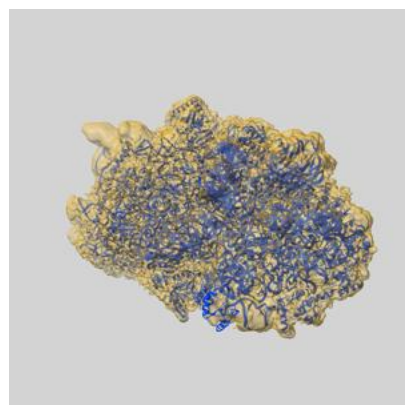
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.65	4.46	3.71
Unmasked-calculated*	4.73	8.47	5.52

*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 4.73 differs from the reported value 3.7 by more than 10 %

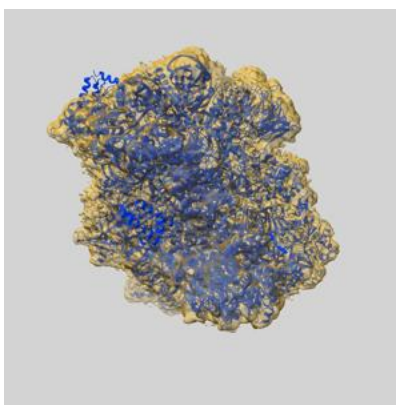
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39958 and PDB model 8ZDD. Per-residue inclusion information can be found in section 3 on page 11.

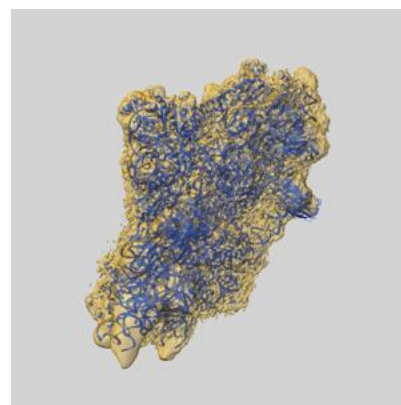
9.1 Map-model overlay [i](#)



X



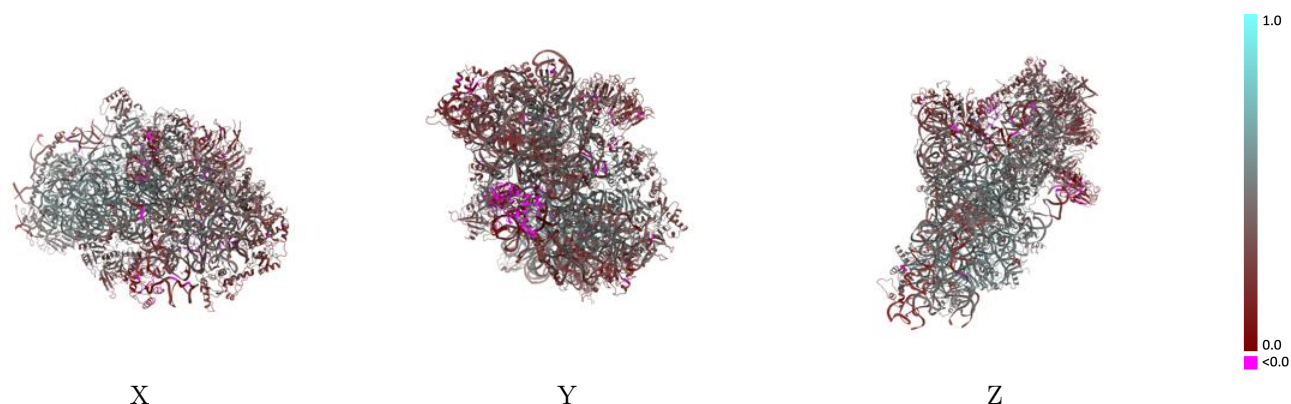
Y



Z

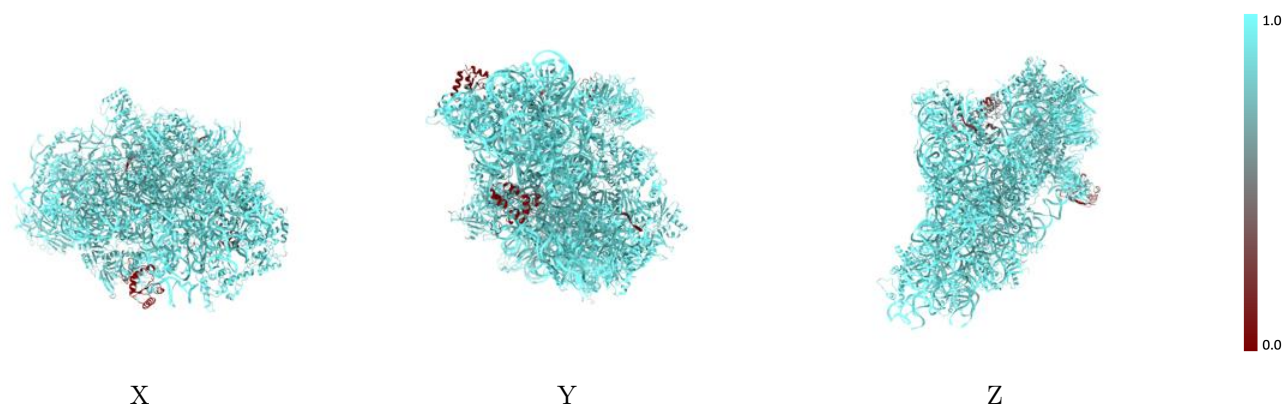
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



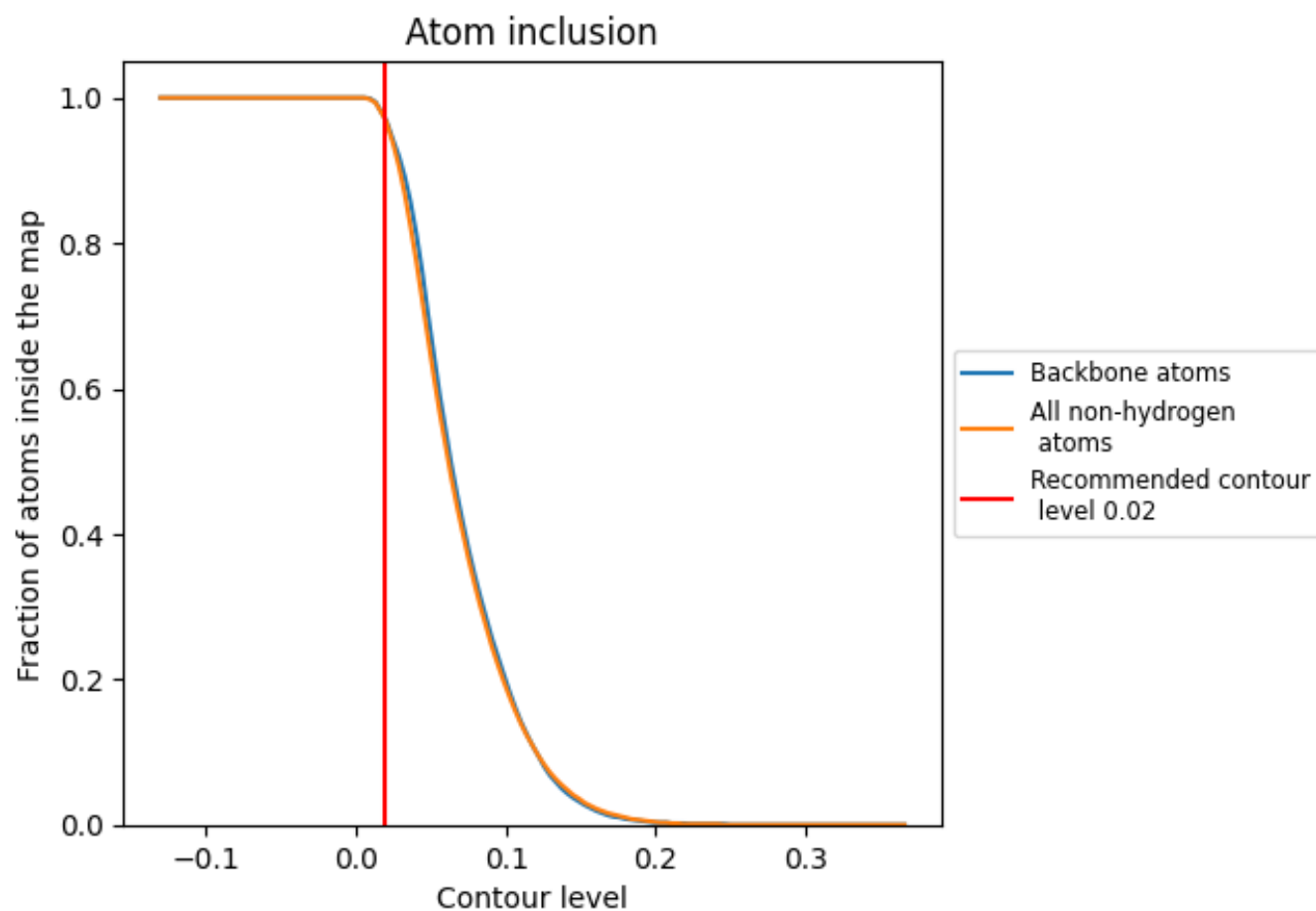
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9690	 0.3960
2	 0.9940	 0.4210
A	 0.9760	 0.4250
B	 0.9680	 0.3040
C	 0.9930	 0.4880
D	 0.9750	 0.4110
E	 0.9910	 0.5260
F	 0.9820	 0.3260
G	 0.9820	 0.4180
H	 0.9720	 0.3670
I	 0.9850	 0.4560
J	 0.9950	 0.5070
K	 0.9820	 0.3210
L	 0.9870	 0.5040
M	 0.2480	 0.1020
N	 0.9920	 0.4390
O	 0.9710	 0.2950
P	 0.9680	 0.3050
Q	 0.9940	 0.3940
R	 0.9760	 0.3600
S	 0.9410	 0.2630
T	 0.9730	 0.3440
U	 0.9860	 0.3820
V	 0.9900	 0.4580
W	 0.9940	 0.5350
X	 0.9940	 0.5100
Y	 0.9990	 0.5150
Z	 0.8840	 0.2090
b	 0.9830	 0.4010
c	 0.9850	 0.2780
d	 0.9820	 0.4130
g	 0.9700	 0.2910
i	 0.6340	 0.1600
j	 0.9090	 0.1550
p	 0.7840	 0.2150



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Chain	Atom inclusion	Q-score
t	 0.9800	 0.3410
u	 0.9700	 0.3780
x	 0.9920	 0.3560