



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 06:34 AM UTC

PDB ID : 8ZDB / pdb_00008zdb
EMDB ID : EMD-39956
Title : Cryo-EM structure of the human ubiquitylated 40S ribosome with R1OK3
Authors : Huang, Z.; Wang, M.; Li, Y.; Beckmann, R.; Cheng, J.
Deposited on : 2024-05-01
Resolution : 3.60 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:

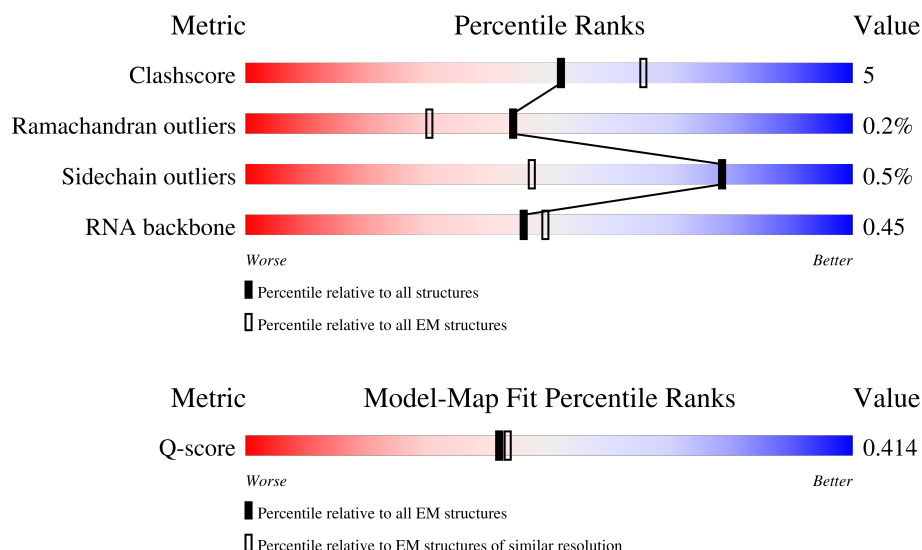
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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

Mol	Chain	Length	Quality of chain
1	2	1869	
2	A	295	
3	B	264	

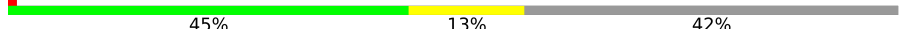
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Mol	Chain	Length	Quality of chain
4	C	293	
5	E	263	
6	G	249	
7	H	194	
8	I	208	
9	J	194	
10	L	158	
11	N	151	
12	O	151	
13	V	83	
14	W	130	
15	X	143	
16	Y	133	
17	a	115	
18	b	84	
19	d	56	
20	e	59	
21	h	25	
22	D	243	
23	F	204	
24	K	165	
25	M	132	
26	P	145	
27	Q	146	
28	R	135	

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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	f	156	
34	i	156	
34	j	156	
35	g	317	
36	p	519	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 77772 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	1665	Total	C	N	O	P	0	0
			35552	15869	6386	11632	1665		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	206	Total	C	N	O	S	0	0
			1624	1035	287	294	8		

- Molecule 3 is a protein called Small ribosomal subunit protein eS1.

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

- Molecule 4 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 5 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 6 is a protein called Small ribosomal subunit protein eS6.

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

- Molecule 7 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 8 is a protein called Small ribosomal subunit protein eS8.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 12 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	126	Total	C	N	O	S	0	0
			948	580	188	174	6		

- Molecule 13 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 16 is a protein called Small ribosomal subunit protein eS24.

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

- Molecule 17 is a protein called Small ribosomal subunit protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	101	Total	C	N	O	S	0	0
			814	507	170	132	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 Small ribosomal subunit protein uS14.

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

- Molecule 20 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	e	46	Total	C	N	O	S	0	0
			368	223	83	61	1		

- Molecule 21 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	h	24	Total	C	N	O	S	0	0
			231	140	63	26	2		

- Molecule 22 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 23 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	F	180	Total	C	N	O	S	0	0
			1427	894	266	260	7		

- Molecule 24 is a protein called Small ribosomal subunit protein eS10.

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

- Molecule 25 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 26 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 27 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 28 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	R	132	Total	C	N	O	S	0	0
			1066	669	199	194	4		

- 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 Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	29	Total	C	N	O		0	0
			248	162	51	35			
34	i	73	Total	C	N	O	S	0	0
			582	368	99	114	1		
34	j	73	Total	C	N	O	S	0	0
			574	364	99	110	1		

- Molecule 35 is a protein called Small ribosomal subunit protein RACK1.

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

- Molecule 36 is a protein called Serine/threonine-protein kinase RIO3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	p	342	Total	C	N	O	S	0	0
			2796	1767	497	510	22		

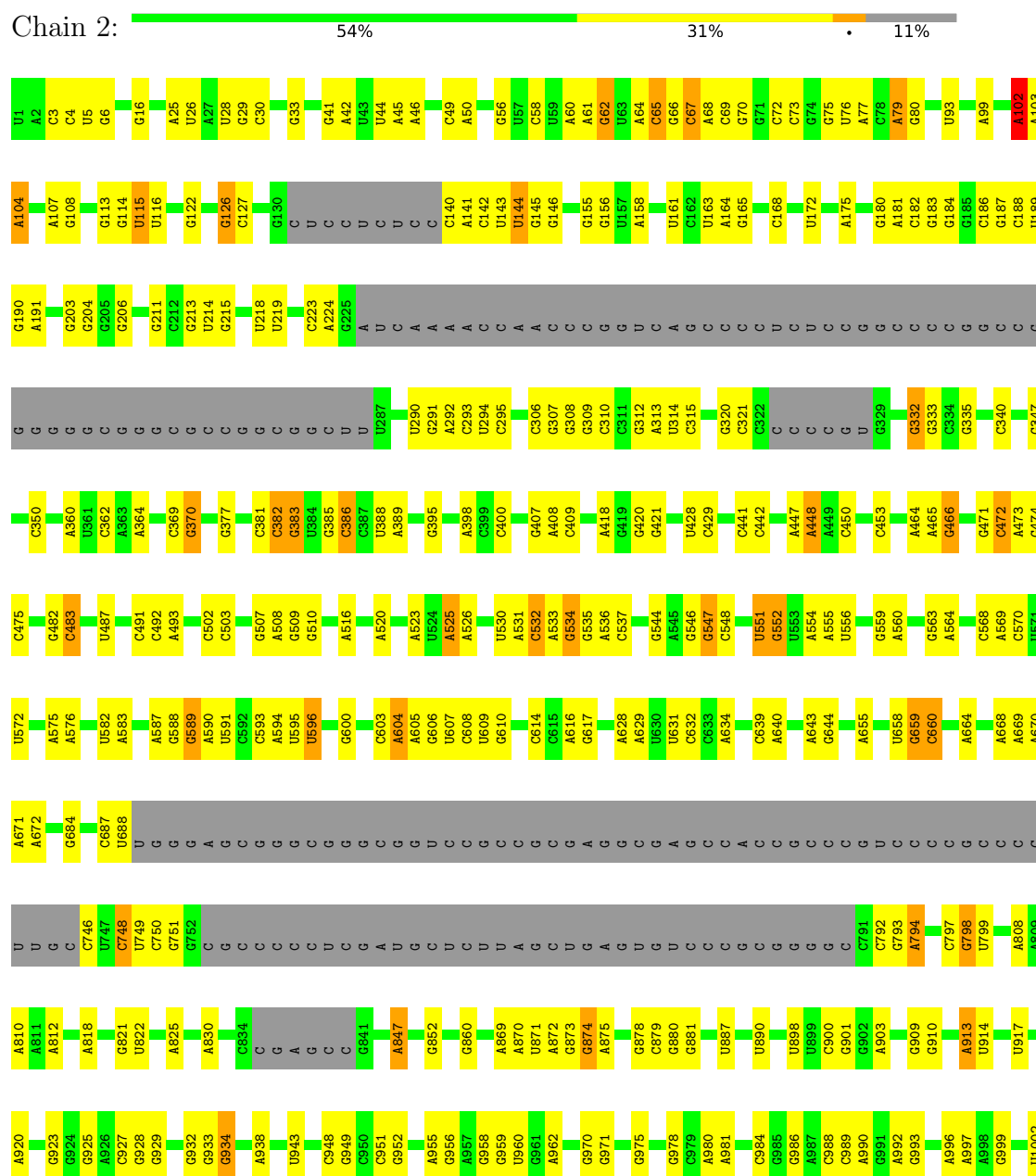
- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

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



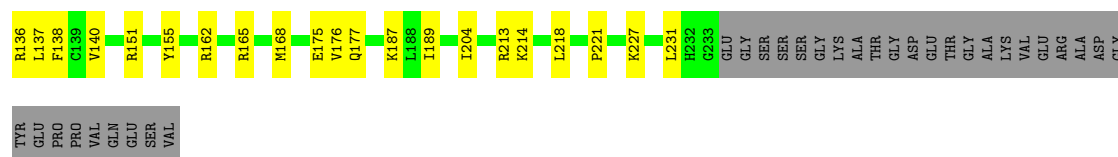


App Type	Percentage
Mobile app for a business	61%
Mobile app for a social media app	9%
Mobile app for a personal use	30%

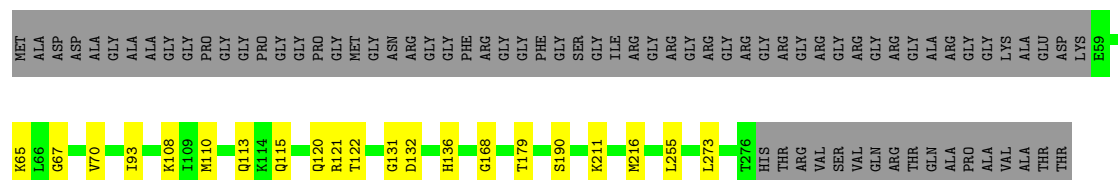


Response	Percentage
U.S. is responsible	65%
U.S. is not responsible	16%
Unsure	19%





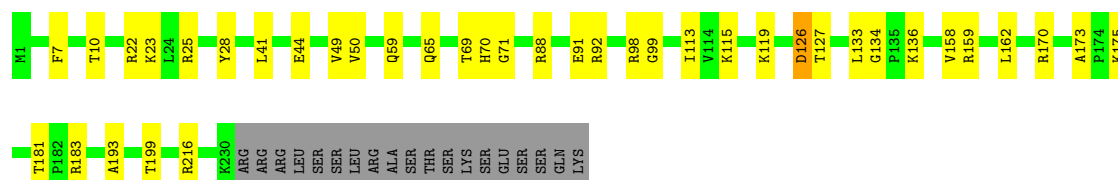
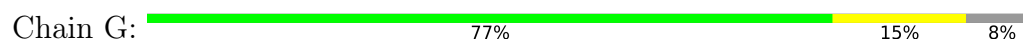
- Molecule 4: Small ribosomal subunit protein uS5



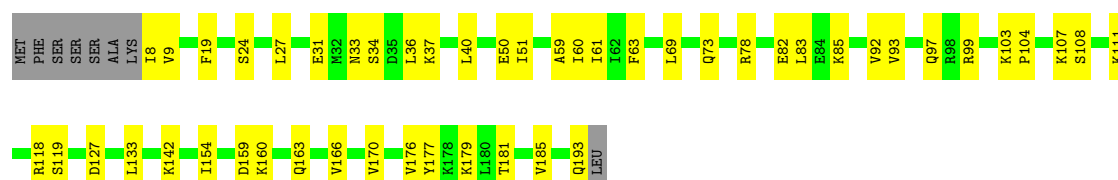
- Molecule 5: Small ribosomal subunit protein eS4, X isoform



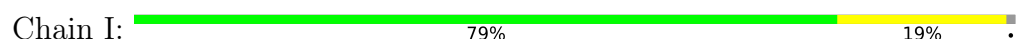
- Molecule 6: Small ribosomal subunit protein eS6



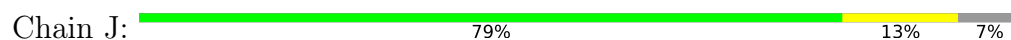
- Molecule 7: Small ribosomal subunit protein eS7



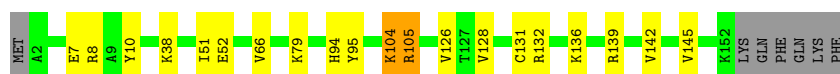
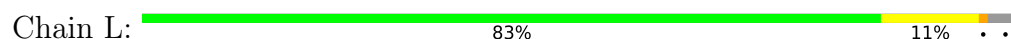
- Molecule 8: Small ribosomal subunit protein eS8



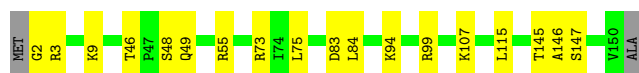
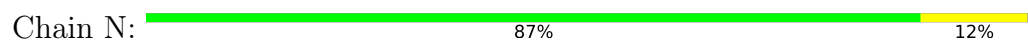
- Molecule 9: Small ribosomal subunit protein uS4



- Molecule 10: Small ribosomal subunit protein uS17



- Molecule 11: Small ribosomal subunit protein uS15



- Molecule 12: Small ribosomal subunit protein uS11



- Molecule 13: Small ribosomal subunit protein eS21



- Molecule 14: Small ribosomal subunit protein uS8



- Molecule 15: Small ribosomal subunit protein uS12

Chain X:  84% 15% .



- Molecule 16: Small ribosomal subunit protein eS24

Chain Y:  79% 14% 7%



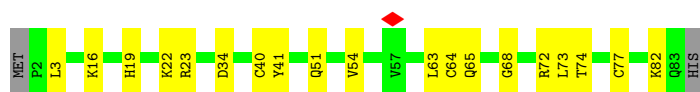
- Molecule 17: Small ribosomal subunit protein eS26

Chain a:  67% 19% . 12%



- Molecule 18: Small ribosomal subunit protein eS27

Chain b:  75% 23% .



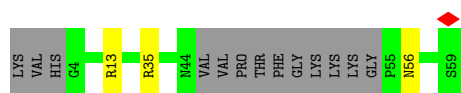
- Molecule 19: Small ribosomal subunit protein uS14

Chain d:  75% 23% .



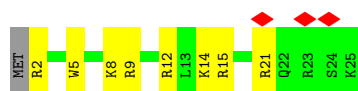
- Molecule 20: Small ribosomal subunit protein eS30

Chain e:  73% 5% 22%



- Molecule 21: Small ribosomal subunit protein eS32

Chain h:  12% 64% 32% .



- Molecule 22: Small ribosomal subunit protein uS3

- Molecule 23: Small ribosomal subunit protein uS7

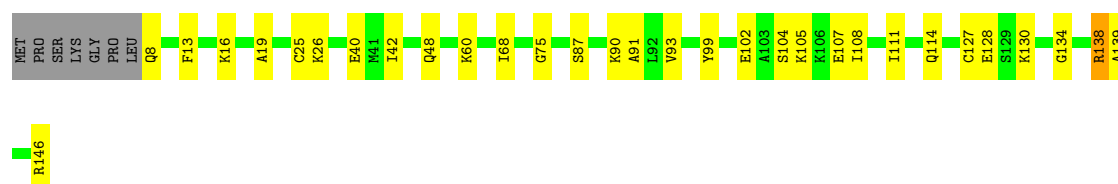
- Molecule 24: Small ribosomal subunit protein eS10

- Molecule 25: Small ribosomal subunit protein eS12

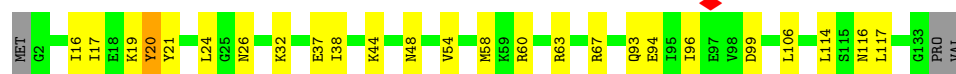
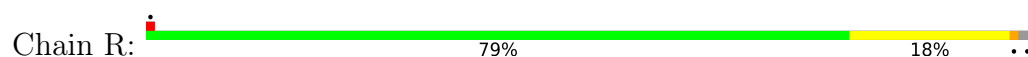
- Molecule 26: Small ribosomal subunit protein uS19

- Molecule 27: Small ribosomal subunit protein uS9

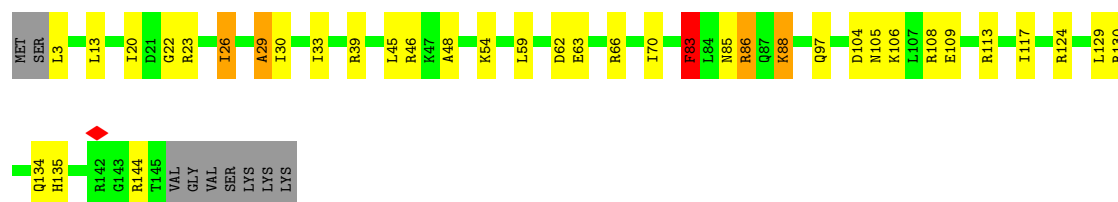




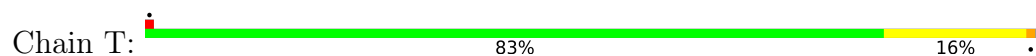
- Molecule 28: Small ribosomal subunit protein eS17



- Molecule 29: Small ribosomal subunit protein uS13



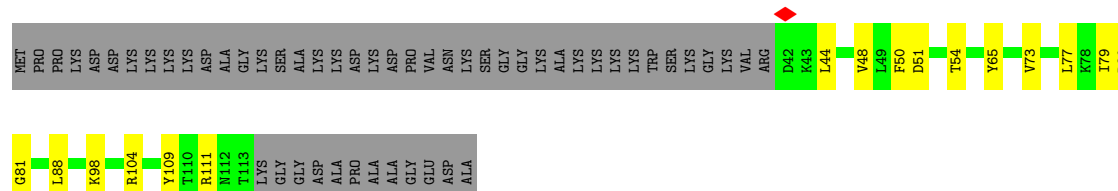
- Molecule 30: Small ribosomal subunit protein eS19



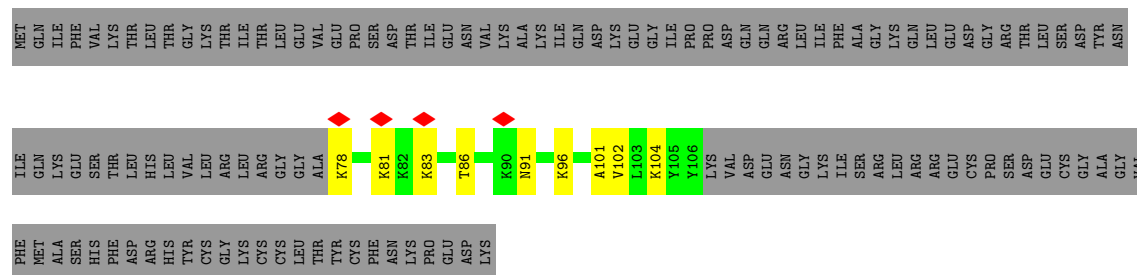
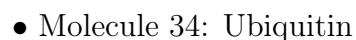
- Molecule 31: Small ribosomal subunit protein uS10



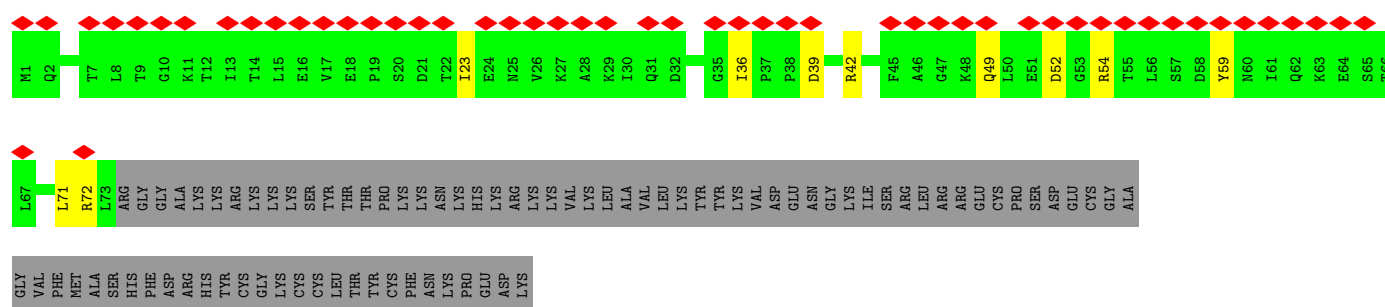
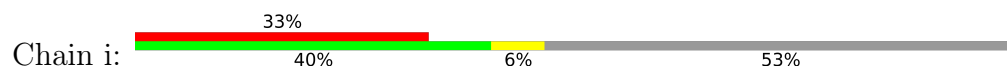
- Molecule 32: Small ribosomal subunit protein eS25



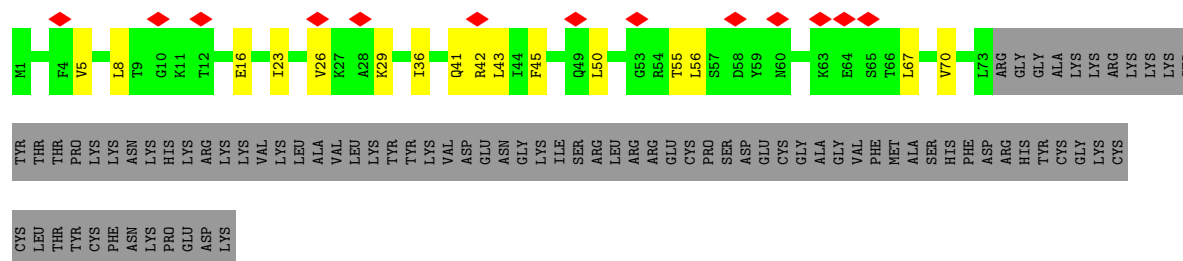
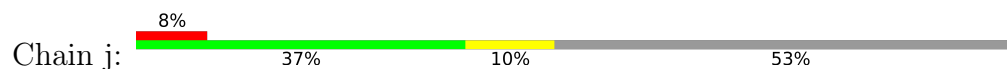
- Chain c:  75% 13% 12%



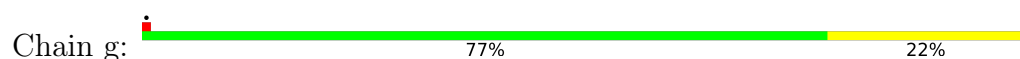
- Molecule 34: Ubiquitin

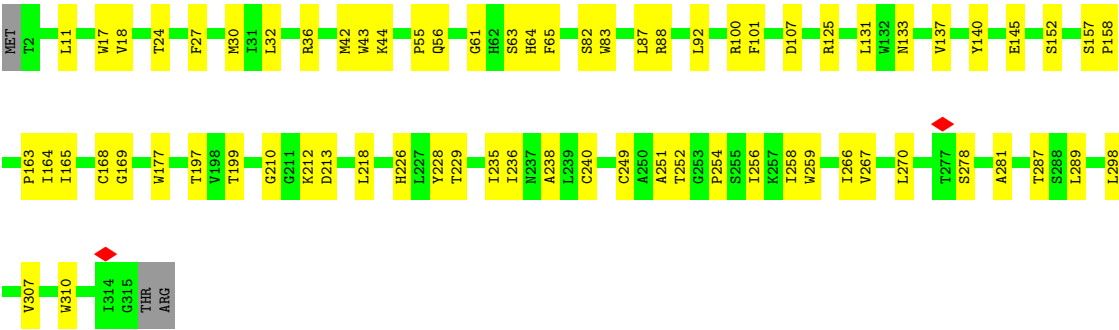


- Molecule 34: Ubiquitin

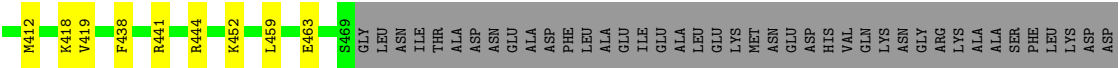
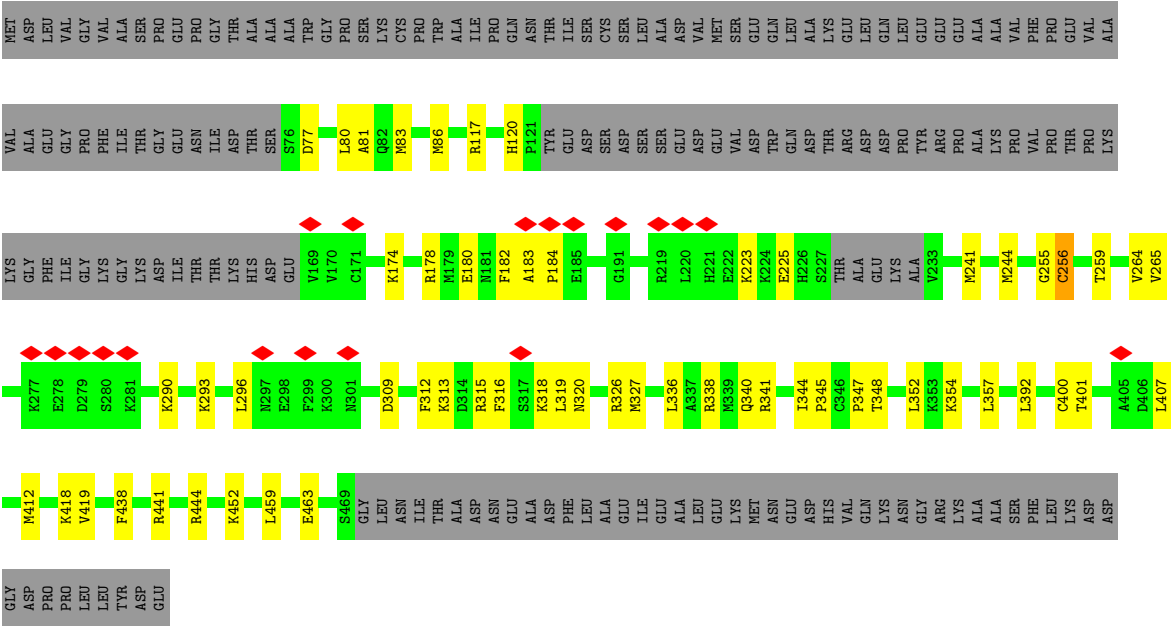


- Molecule 35: Small ribosomal subunit protein RACK1





• Molecule 36: Serine/threonine-protein kinase RIO3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20179	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.412	Depositor
Minimum map value	-0.253	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.24	0/39755	0.43	6/61954 (0.0%)
2	A	0.22	0/1661	0.54	1/2259 (0.0%)
3	B	0.20	0/1756	0.59	1/2350 (0.0%)
4	C	0.23	0/1726	0.55	0/2332
5	E	0.20	0/2118	0.52	0/2849
6	G	0.22	0/1885	0.60	0/2510
7	H	0.24	0/1524	0.63	0/2042
8	I	0.30	0/1711	0.65	0/2282
9	J	0.20	0/1524	0.52	0/2035
10	L	0.30	0/1250	0.61	1/1673 (0.1%)
11	N	0.18	0/1226	0.53	0/1649
12	O	0.28	0/960	0.61	0/1286
13	V	0.21	0/631	0.52	0/844
14	W	0.24	0/1051	0.57	0/1406
15	X	0.21	0/1116	0.61	0/1490
16	Y	0.19	0/1031	0.56	0/1370
17	a	0.57	0/828	0.91	3/1109 (0.3%)
18	b	0.23	0/653	0.64	0/876
19	d	0.25	0/470	0.64	0/623
20	e	0.20	0/370	0.59	0/482
21	h	0.15	0/232	0.48	0/295
22	D	0.23	0/1780	0.58	0/2397
23	F	0.22	0/1447	0.72	2/1944 (0.1%)
24	K	0.23	0/824	0.63	0/1112
25	M	0.24	0/963	0.64	0/1291
26	P	0.34	0/1003	0.71	0/1341
27	Q	0.32	0/1126	0.74	2/1506 (0.1%)
28	R	0.24	0/1080	0.71	2/1449 (0.1%)
29	S	0.46	0/1202	0.92	5/1610 (0.3%)
30	T	0.19	0/1142	0.56	2/1530 (0.1%)
31	U	0.21	0/813	0.59	0/1092
32	Z	0.22	0/580	0.70	2/780 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.21	0/481	0.62	0/643
34	f	0.36	0/251	0.68	1/326 (0.3%)
34	i	0.15	0/588	0.44	0/792
34	j	0.14	0/580	0.44	0/782
35	g	0.18	0/2497	0.50	1/3399 (0.0%)
36	p	0.22	0/2853	0.58	2/3824 (0.1%)
All	All	0.24	0/82688	0.52	31/119534 (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
14	W	0	1
23	F	0	1
All	All	0	2

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	F	175	ASP	N-CA-C	-8.85	104.53	114.62
17	a	78	ALA	N-CA-C	-8.24	103.16	113.55
36	p	182	PHE	CA-C-N	8.17	131.75	120.39
36	p	182	PHE	C-N-CA	8.17	131.75	120.39
23	F	94	LYS	N-CA-C	-7.52	105.27	114.75
1	2	1605	G	C4'-C3'-O3'	-7.35	101.98	113.00
1	2	1302	G	C2'-C3'-O3'	7.24	120.36	109.50
1	2	1601	A	C2'-C3'-O3'	7.20	120.30	109.50
17	a	28	ARG	CB-CA-C	-7.02	97.94	109.53
10	L	95	TYR	CB-CA-C	-6.28	100.84	110.26
28	R	19	LYS	CA-C-N	6.23	133.44	121.54
28	R	19	LYS	C-N-CA	6.23	133.44	121.54
17	a	26	CYS	CA-C-O	-6.07	114.07	120.63
29	S	83	PHE	N-CA-C	-6.06	105.81	112.72
1	2	102	A	C2'-C3'-O3'	6.02	118.53	109.50
27	Q	42	ILE	CA-C-N	5.88	129.67	120.97
27	Q	42	ILE	C-N-CA	5.88	129.67	120.97
3	B	108	ASP	N-CA-C	-5.81	106.73	113.88
29	S	29	ALA	N-CA-C	-5.60	105.56	112.90
34	f	91	ASN	N-CA-C	5.56	117.25	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S	85	ASN	CB-CA-C	-5.49	99.49	110.42
1	2	1531	A	P-O3'-C3'	5.42	128.33	120.20
1	2	547	G	P-O3'-C3'	5.36	128.25	120.20
2	A	44	ASP	N-CA-C	-5.36	108.00	114.75
29	S	22	GLY	CA-C-N	-5.32	114.12	122.95
29	S	22	GLY	C-N-CA	-5.32	114.12	122.95
32	Z	65	TYR	CA-C-N	5.32	131.69	121.54
32	Z	65	TYR	C-N-CA	5.32	131.69	121.54
30	T	87	VAL	CA-C-N	5.18	129.31	121.03
30	T	87	VAL	C-N-CA	5.18	129.31	121.03
35	g	145	GLU	CA-CB-CG	5.03	124.16	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	F	93	VAL	Peptide
14	W	28	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	35552	0	17949	259	0
2	A	1624	0	1634	17	0
3	B	1729	0	1803	26	0
4	C	1690	0	1777	13	0
5	E	2076	0	2177	17	0
6	G	1862	0	2018	29	0
7	H	1501	0	1593	33	0
8	I	1682	0	1769	28	0
9	J	1499	0	1618	19	0
10	L	1229	0	1302	11	0
11	N	1202	0	1289	13	0
12	O	948	0	976	20	0
13	V	625	0	628	6	0
14	W	1034	0	1080	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	X	1098	0	1167	14	0
16	Y	1014	0	1082	11	0
17	a	814	0	864	15	0
18	b	640	0	665	13	0
19	d	459	0	451	18	0
20	e	368	0	401	3	0
21	h	231	0	277	8	0
22	D	1752	0	1848	26	0
23	F	1427	0	1471	22	0
24	K	800	0	818	14	0
25	M	953	0	990	15	0
26	P	984	0	1028	22	0
27	Q	1109	0	1174	21	0
28	R	1066	0	1116	15	0
29	S	1184	0	1244	23	0
30	T	1122	0	1153	19	0
31	U	803	0	873	15	0
32	Z	574	0	627	13	0
33	c	479	0	507	6	0
34	f	248	0	298	6	0
34	i	582	0	610	5	0
34	j	574	0	602	9	0
35	g	2440	0	2396	40	0
36	p	2796	0	2785	39	0
37	a	1	0	0	0	0
37	d	1	0	0	0	0
All	All	77772	0	62060	741	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (741) 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)
7:H:50:GLU:HA	7:H:59:ALA:O	1.33	1.28
1:2:525:A:N6	1:2:589:G:H1	1.55	1.03
1:2:1729:U:H3	1:2:1805:G:H1	1.01	0.98
27:Q:8:GLN:N	27:Q:99:TYR:HH	1.62	0.97
1:2:1652:G:H1	1:2:1672:U:H3	0.93	0.90
1:2:525:A:H62	1:2:589:G:H1	1.22	0.87
1:2:140:C:H42	1:2:313:A:H61	1.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:525:A:N6	1:2:589:G:N1	2.29	0.79
35:g:226:HIS:HE2	35:g:229:THR:HG1	1.35	0.75
1:2:1705:C:H42	1:2:1830:U:H3	1.32	0.74
1:2:70:G:N1	1:2:79:A:N6	2.36	0.74
1:2:1537:A:H62	32:Z:104:ARG:HH21	1.37	0.72
1:2:684:G:C6	1:2:1021:U:N3	2.57	0.72
7:H:50:GLU:CA	7:H:59:ALA:O	2.27	0.72
22:D:23:GLU:HB3	24:K:64:TRP:HE1	1.53	0.71
1:2:164:A:H3'	1:2:165:G:H21	1.56	0.71
30:T:11:GLN:HB3	30:T:62:ARG:HH12	1.55	0.71
36:p:312:PHE:O	36:p:316:PHE:HB2	1.90	0.70
1:2:928:G:H1	1:2:1013:U:H3	1.37	0.69
1:2:1657:G:H1	1:2:1667:U:H3	1.38	0.69
1:2:1665:G:H22	30:T:87:VAL:HG22	1.57	0.69
22:D:101:GLN:HE22	22:D:122:VAL:HB	1.58	0.68
1:2:604:A:OP1	9:J:22:LYS:NZ	2.27	0.68
17:a:87:ARG:NH1	17:a:91:ALA:O	2.27	0.68
13:V:40:ASP:OD1	13:V:47:ASN:ND2	2.27	0.67
30:T:65:TYR:HA	30:T:123:LEU:HD21	1.77	0.67
1:2:1236:G:H21	1:2:1522:A:H62	1.42	0.66
1:2:1653:U:H3	1:2:1671:G:H1	1.43	0.66
35:g:44:LYS:HG2	35:g:56:GLN:HB2	1.77	0.66
7:H:36:LEU:HD21	7:H:78:ARG:HE	1.60	0.65
1:2:1227:G:H1	1:2:1531:A:H61	1.44	0.65
29:S:13:LEU:HB2	29:S:20:ILE:HB	1.79	0.64
30:T:104:LEU:HD23	30:T:121:ARG:HG3	1.80	0.64
1:2:1757:G:O6	1:2:1776:G:C6	2.50	0.64
6:G:49:VAL:HB	6:G:115:LYS:HB3	1.79	0.64
7:H:51:ILE:HG12	7:H:179:LYS:HG2	1.79	0.63
23:F:70:GLU:O	23:F:74:ASN:HB2	1.99	0.63
35:g:107:ASP:HB2	35:g:125:ARG:HD2	1.80	0.63
1:2:127:C:N3	5:E:134:LYS:NZ	2.46	0.62
1:2:1399:C:OP1	35:g:100:ARG:NH1	2.31	0.62
26:P:50:ARG:HD3	26:P:51:ARG:H	1.63	0.62
23:F:121:PRO:HG3	23:F:193:LYS:HG2	1.81	0.62
7:H:127:ASP:OD1	7:H:142:LYS:NZ	2.31	0.62
35:g:87:LEU:HB2	35:g:101:PHE:HB2	1.82	0.62
1:2:1679:A:H2'	23:F:60:ARG:HD2	1.82	0.62
1:2:1705:C:N4	1:2:1830:U:H3	1.98	0.61
11:N:55:ARG:NH2	18:b:51:GLN:OE1	2.33	0.61
19:d:21:CYS:O	24:K:65:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:684:G:O6	1:2:1021:U:N3	2.33	0.61
1:2:975:G:H21	12:O:50:LYS:HA	1.66	0.61
1:2:1033:G:N1	1:2:1080:A:O2'	2.33	0.61
1:2:748:C:H42	1:2:794:A:H61	1.49	0.61
16:Y:104:ARG:HA	16:Y:107:ARG:HH21	1.66	0.60
34:i:36:ILE:HG21	34:i:71:LEU:HD22	1.83	0.60
36:p:336:LEU:HD11	36:p:347:PRO:HD2	1.81	0.60
1:2:659:G:H21	15:X:17:ARG:HH22	1.50	0.60
1:2:1451:G:N7	28:R:44:LYS:NZ	2.48	0.60
1:2:1569:A:OP1	30:T:97:LYS:NZ	2.33	0.60
9:J:136:ARG:NH1	9:J:138:ARG:O	2.34	0.60
1:2:70:G:H1	1:2:79:A:N6	1.99	0.60
1:2:65:C:N4	6:G:134:GLY:O	2.34	0.60
1:2:1263:U:H4'	19:d:27:ARG:HE	1.67	0.60
2:A:33:GLN:HB3	2:A:154:LEU:HD12	1.83	0.60
1:2:1619:A:H4'	26:P:44:ARG:HH12	1.67	0.60
1:2:1650:A:H5''	27:Q:139:ALA:HB2	1.84	0.60
2:A:25:LEU:O	2:A:164:ASN:ND2	2.34	0.60
25:M:86:GLY:HA3	25:M:105:GLY:HA2	1.83	0.60
34:j:42:ARG:HB3	34:j:70:VAL:HB	1.83	0.60
1:2:448:A:H5''	8:I:25:ARG:HA	1.82	0.60
1:2:847:A:OP1	5:E:108:ARG:NH2	2.35	0.60
1:2:993:G:OP1	1:2:1131:G:N2	2.34	0.60
35:g:218:LEU:HB2	35:g:228:TYR:HB2	1.84	0.59
9:J:110:LEU:HB2	9:J:147:PHE:HB3	1.84	0.59
36:p:338:ARG:HA	36:p:341:ARG:HE	1.67	0.59
1:2:1495:G:HO2'	19:d:24:CYS:HG	1.51	0.59
1:2:1121:G:O2'	3:B:204:ILE:O	2.20	0.59
23:F:28:VAL:O	23:F:42:LYS:NZ	2.36	0.59
1:2:1740:C:H5''	8:I:58:LEU:HD21	1.85	0.59
6:G:88:ARG:HB2	6:G:91:GLU:HG3	1.84	0.59
27:Q:130:LYS:NZ	27:Q:134:GLY:O	2.36	0.59
1:2:1130:G:OP2	1:2:1130:G:N2	2.32	0.59
12:O:99:ALA:H	12:O:133:THR:HG22	1.68	0.59
1:2:1284:A:HO2'	25:M:106:CYS:HG	1.46	0.58
23:F:41:VAL:H	23:F:45:TYR:HB2	1.68	0.58
25:M:51:VAL:HB	25:M:109:VAL:HB	1.85	0.58
21:h:12:ARG:HG2	21:h:15:ARG:HH21	1.68	0.58
23:F:44:LYS:NZ	27:Q:114:GLN:O	2.36	0.58
3:B:136:ARG:HB2	3:B:218:LEU:HD11	1.86	0.58
5:E:191:ARG:HH11	5:E:245:ARG:HB3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:S:86:ARG:HG2	29:S:106:LYS:HE3	1.86	0.58
7:H:9:VAL:HG23	7:H:24:SER:HB3	1.84	0.58
35:g:152:SER:HG	35:g:168:CYS:HG	1.52	0.58
33:c:12:ALA:HB2	33:c:58:LEU:HD11	1.85	0.58
35:g:258:ILE:O	35:g:267:VAL:N	2.37	0.58
1:2:959:G:OP1	12:O:104:ARG:NH2	2.36	0.58
3:B:83:LYS:NZ	12:O:130:GLU:OE2	2.37	0.58
35:g:298:LEU:HB2	35:g:310:TRP:HB2	1.85	0.57
1:2:928:G:O6	1:2:1013:U:O4	2.22	0.57
1:2:1277:C:H2'	1:2:1278:A:H8	1.69	0.57
1:2:1507:G:N2	34:f:86:THR:OG1	2.37	0.57
15:X:52:LEU:HD11	15:X:73:GLN:HB2	1.86	0.57
22:D:74:GLN:NE2	22:D:79:PHE:O	2.35	0.57
5:E:87:MET:HE1	5:E:236:ILE:HD13	1.85	0.57
28:R:60:ARG:HH21	28:R:63:ARG:HH21	1.52	0.57
2:A:113:GLN:HB3	2:A:116:PHE:HB2	1.87	0.57
6:G:44:GLU:HA	6:G:119:LYS:HE2	1.86	0.57
25:M:61:TYR:OH	25:M:108:CYS:SG	2.62	0.56
3:B:92:GLN:HG2	3:B:97:LEU:HD11	1.86	0.56
1:2:30:C:O2'	1:2:596:U:OP1	2.23	0.56
1:2:984:C:O2'	12:O:138:ASP:OD2	2.24	0.56
1:2:1786:U:H2'	1:2:1787:G:H8	1.70	0.56
35:g:251:ALA:HB2	35:g:289:LEU:HD22	1.88	0.56
36:p:412:MET:HE2	36:p:419:VAL:HG12	1.86	0.56
1:2:1864:U:OP2	17:a:4:LYS:NZ	2.38	0.56
1:2:1581:C:H5'	1:2:1582:C:H5	1.70	0.56
8:I:72:CYS:HG	8:I:112:TRP:CG	2.24	0.56
17:a:44:ILE:HD12	17:a:65:PRO:HB2	1.88	0.56
1:2:466:G:O2'	6:G:59:GLN:NE2	2.38	0.56
3:B:63:LYS:NZ	3:B:89:GLU:O	2.39	0.56
31:U:56:MET:HE3	31:U:57:PRO:HD2	1.87	0.56
1:2:874:G:H2'	1:2:875:A:H8	1.71	0.56
1:2:1495:G:O2'	19:d:24:CYS:SG	2.60	0.56
9:J:18:ARG:O	9:J:24:ARG:NH2	2.38	0.56
8:I:34:ALA:HB2	8:I:56:ARG:HD2	1.88	0.56
22:D:44:THR:HG22	22:D:45:ARG:HD2	1.87	0.56
22:D:22:ASN:HD21	22:D:37:VAL:HB	1.70	0.55
6:G:159:ARG:HG2	6:G:173:ALA:HB2	1.89	0.55
9:J:63:LEU:O	9:J:70:ARG:NH1	2.39	0.55
14:W:28:ARG:HG2	14:W:29:PRO:HD3	1.87	0.55
3:B:62:LEU:HA	3:B:65:ARG:HE	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:P:44:ARG:HD3	26:P:84:ILE:HD11	1.87	0.55
5:E:137:PRO:HG2	5:E:150:PRO:HD2	1.89	0.55
13:V:64:GLU:HG3	18:b:3:LEU:HD13	1.89	0.55
16:Y:41:ARG:NH2	16:Y:52:PRO:O	2.39	0.55
22:D:38:GLU:HB3	22:D:49:ILE:HB	1.89	0.55
27:Q:19:ALA:HB2	27:Q:75:GLY:HA3	1.88	0.55
36:p:174:LYS:HG2	36:p:178:ARG:HE	1.70	0.55
1:2:572:U:OP2	16:Y:37:LYS:NZ	2.38	0.55
1:2:16:G:H21	1:2:1195:A:H62	1.55	0.54
1:2:1415:C:O2'	30:T:132:ASP:OD2	2.22	0.54
8:I:3:ILE:O	8:I:30:GLY:N	2.40	0.54
29:S:46:ARG:HH21	30:T:35:ASP:HA	1.72	0.54
35:g:11:LEU:HB2	35:g:307:VAL:HB	1.88	0.54
1:2:370:G:O3'	8:I:10:LYS:NZ	2.39	0.54
16:Y:34:THR:HG1	16:Y:62:THR:HG1	1.54	0.54
12:O:30:VAL:HG12	12:O:94:HIS:HB2	1.88	0.54
22:D:40:ARG:HE	22:D:47:GLU:HG2	1.72	0.54
24:K:29:MET:HE3	24:K:30:PRO:HD2	1.88	0.54
2:A:2:SER:N	2:A:56:GLU:OE1	2.40	0.54
18:b:40:CYS:SG	18:b:41:TYR:N	2.80	0.54
29:S:26:ILE:HB	29:S:45:LEU:HD21	1.88	0.54
34:i:23:ILE:HB	34:i:52:ASP:HA	1.89	0.54
1:2:1701:C:OP2	36:p:320:ASN:ND2	2.33	0.54
12:O:53:ILE:HG23	12:O:88:LEU:HD23	1.89	0.54
12:O:113:GLN:HE22	17:a:45:VAL:HA	1.73	0.54
22:D:62:LYS:NZ	24:K:93:THR:O	2.40	0.54
2:A:76:VAL:HG12	2:A:123:VAL:HB	1.89	0.54
36:p:338:ARG:NH2	36:p:401:THR:OG1	2.41	0.54
17:a:11:ALA:H	17:a:33:ASP:HB2	1.73	0.54
29:S:30:ILE:HD12	29:S:33:ILE:HD13	1.90	0.54
36:p:77:ASP:HA	36:p:80:LEU:HD12	1.89	0.54
1:2:1741:U:OP1	8:I:42:ARG:NH1	2.41	0.54
7:H:31:GLU:HG2	7:H:40:LEU:HB3	1.90	0.53
23:F:144:LEU:O	23:F:148:ASN:ND2	2.41	0.53
1:2:1156:U:OP1	14:W:71:LYS:NZ	2.41	0.53
1:2:1416:C:O3'	30:T:133:ARG:NH2	2.40	0.53
6:G:22:ARG:HA	6:G:25:ARG:HG2	1.89	0.53
27:Q:8:GLN:N	27:Q:99:TYR:OH	2.36	0.53
31:U:61:LEU:HB2	31:U:82:MET:HB3	1.90	0.53
36:p:83:MET:HA	36:p:86:MET:HG2	1.89	0.53
1:2:1513:C:H2'	1:2:1514:G:H8	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:143:PRO:HG3	13:V:32:ILE:HG23	1.90	0.53
11:N:99:ARG:HH11	11:N:115:LEU:HD21	1.73	0.53
35:g:61:GLY:O	35:g:88:ARG:NH1	2.41	0.53
3:B:165:ARG:HA	3:B:168:MET:HB2	1.90	0.53
14:W:11:LEU:HD12	14:W:74:VAL:HB	1.90	0.53
22:D:117:ARG:NH2	36:p:180:GLU:O	2.42	0.53
1:2:616:A:OP1	15:X:68:LYS:NZ	2.42	0.53
1:2:634:A:OP1	20:e:13:ARG:NH1	2.39	0.53
14:W:3:ARG:HD3	14:W:6:VAL:HG12	1.90	0.53
28:R:17:ILE:HD11	28:R:54:VAL:HG13	1.91	0.53
32:Z:73:VAL:HG13	32:Z:77:LEU:HD12	1.91	0.53
1:2:115:U:OP1	1:2:382:C:O2'	2.27	0.52
1:2:986:G:OP2	1:2:988:C:N4	2.42	0.52
31:U:62:ARG:HG2	31:U:81:GLN:HG2	1.91	0.52
1:2:1447:G:OP1	31:U:87:ARG:NH2	2.43	0.52
7:H:8:ILE:HG21	7:H:27:LEU:HD23	1.90	0.52
26:P:51:ARG:HA	26:P:54:HIS:HB2	1.91	0.52
16:Y:21:LYS:HB2	16:Y:75:ILE:HB	1.90	0.52
17:a:100:ARG:O	17:a:100:ARG:NH1	2.43	0.52
1:2:1841:C:H3'	21:h:2:ARG:HE	1.75	0.52
22:D:35:SER:HB2	22:D:100:ALA:HB2	1.91	0.52
6:G:10:THR:OG1	6:G:127:THR:O	2.27	0.52
23:F:118:ASN:O	23:F:193:LYS:NZ	2.43	0.52
35:g:256:ILE:HB	35:g:270:LEU:HB2	1.90	0.52
1:2:508:A:H3'	1:2:509:G:H8	1.74	0.52
35:g:278:SER:HB3	35:g:281:ALA:HB3	1.92	0.52
1:2:1513:C:OP1	19:d:12:ARG:NH2	2.43	0.52
8:I:121:LEU:O	8:I:123:ARG:NH1	2.43	0.52
26:P:72:LYS:NZ	26:P:106:GLU:OE2	2.43	0.52
1:2:472:C:O2	1:2:475:C:N4	2.40	0.52
1:2:1542:C:OP1	30:T:63:HIS:NE2	2.43	0.52
1:2:1729:U:O4	1:2:1805:G:O6	2.28	0.52
2:A:157:VAL:O	13:V:65:SER:OG	2.24	0.52
24:K:49:MET:HE1	24:K:58:VAL:HG21	1.92	0.52
24:K:95:ARG:HG3	24:K:96:ARG:HG2	1.91	0.52
35:g:32:LEU:HD21	35:g:92:LEU:HD21	1.91	0.52
1:2:122:G:H21	5:E:146:THR:HG21	1.75	0.51
1:2:1083:A:N7	1:2:1841:C:O2'	2.37	0.51
1:2:1451:G:OP1	28:R:32:LYS:NZ	2.38	0.51
7:H:154:ILE:HB	7:H:185:VAL:HG12	1.92	0.51
1:2:1243:U:O2'	34:f:78:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:U:20:ILE:HG22	31:U:116:ILE:HA	1.92	0.51
1:2:1060:A:N3	1:2:1062:A:N6	2.58	0.51
4:C:113:GLN:HG2	4:C:122:THR:HG22	1.91	0.51
10:L:131:CYS:SG	10:L:132:ARG:N	2.83	0.51
28:R:93:GLN:HE21	28:R:96:ILE:HG22	1.74	0.51
1:2:568:C:H2'	1:2:569:A:C8	2.45	0.51
1:2:1239:U:H4'	26:P:124:LYS:HD3	1.93	0.51
35:g:199:THR:HG21	35:g:240:CYS:HA	1.92	0.51
9:J:170:PRO:O	9:J:175:ARG:NH2	2.43	0.51
29:S:54:LYS:HE2	29:S:59:LEU:HD22	1.93	0.51
1:2:1600:G:OP1	32:Z:44:LEU:HG	2.11	0.51
2:A:77:ILE:HD12	2:A:122:LEU:HD11	1.93	0.51
5:E:133:THR:HG22	5:E:134:LYS:HG3	1.92	0.51
15:X:24:ASP:HB3	15:X:27:TYR:HB3	1.93	0.51
36:p:309:ASP:O	36:p:313:LYS:N	2.42	0.51
1:2:928:G:H2'	1:2:929:G:C8	2.46	0.51
1:2:1012:A:OP1	11:N:3:ARG:NH1	2.43	0.51
1:2:1620:A:H8	26:P:40:ARG:HH22	1.58	0.51
5:E:11:ARG:HA	5:E:28:ALA:HB2	1.93	0.51
9:J:159:PHE:HE2	9:J:165:TYR:HB2	1.75	0.51
1:2:1415:C:H5''	30:T:129:ARG:HD3	1.93	0.51
4:C:108:LYS:HE3	4:C:110:MET:HB3	1.92	0.51
1:2:453:C:O2'	6:G:92:ARG:O	2.28	0.50
1:2:798:G:O2'	7:H:108:SER:OG	2.29	0.50
1:2:1792:G:H2'	1:2:1793:A:H8	1.76	0.50
4:C:65:LYS:HD2	4:C:273:LEU:HD13	1.93	0.50
11:N:83:ASP:OD1	11:N:84:LEU:N	2.40	0.50
1:2:1277:C:H2'	1:2:1278:A:C8	2.46	0.50
8:I:69:SER:OG	8:I:70:GLU:OE1	2.28	0.50
8:I:198:TYR:O	8:I:202:ILE:HG13	2.12	0.50
14:W:30:CYS:SG	14:W:31:SER:N	2.83	0.50
15:X:140:ARG:HD3	15:X:141:PRO:HD2	1.93	0.50
34:f:81:LYS:HE2	34:f:83:LYS:HD3	1.93	0.50
35:g:210:GLY:HA3	35:g:236:ILE:HD11	1.92	0.50
1:2:1719:A:N6	1:2:1814:G:O2'	2.44	0.50
7:H:33:ASN:OD1	7:H:34:SER:N	2.43	0.50
12:O:45:THR:OG1	12:O:51:GLU:O	2.25	0.50
1:2:62:G:O2'	1:2:172:U:OP1	2.29	0.50
1:2:1084:A:OP1	1:2:1858:G:O2'	2.28	0.50
8:I:83:TYR:HD2	8:I:101:ILE:HD13	1.76	0.50
28:R:37:GLU:HG3	28:R:38:ILE:HG13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:U:56:MET:HG3	31:U:86:LYS:HD2	1.92	0.50
32:Z:48:VAL:HG12	32:Z:80:ARG:HG3	1.93	0.50
34:j:5:VAL:HG22	34:j:67:LEU:HB2	1.94	0.50
1:2:144:U:H2'	1:2:145:G:H8	1.77	0.50
1:2:989:C:OP2	3:B:155:TYR:OH	2.27	0.50
23:F:190:ILE:HA	23:F:193:LYS:HE3	1.93	0.50
1:2:684:G:O6	1:2:1021:U:C2	2.64	0.50
1:2:1402:A:H1'	31:U:54:VAL:HG23	1.94	0.50
3:B:33:VAL:HG21	3:B:67:PHE:HE2	1.77	0.50
35:g:157:SER:OG	35:g:164:ILE:O	2.29	0.50
1:2:1864:U:H5'	17:a:79:ILE:HD11	1.93	0.50
5:E:100:ARG:O	5:E:112:HIS:HB3	2.12	0.50
7:H:93:VAL:HG21	7:H:133:LEU:HD12	1.93	0.50
19:d:3:HIS:C	19:d:5:GLN:N	2.70	0.50
19:d:3:HIS:C	19:d:5:GLN:H	2.19	0.50
29:S:105:ASN:HA	29:S:108:ARG:HE	1.76	0.50
1:2:1757:G:O6	1:2:1776:G:C5	2.65	0.50
22:D:114:ALA:HB1	22:D:117:ARG:HH21	1.76	0.50
30:T:112:MET:SD	30:T:126:GLN:NE2	2.84	0.50
36:p:326:ARG:HE	36:p:354:LYS:HB3	1.77	0.50
1:2:189:U:H2'	1:2:190:G:O4'	2.12	0.49
1:2:491:C:O2'	1:2:493:A:N7	2.43	0.49
1:2:1092:G:OP2	11:N:9:LYS:NZ	2.36	0.49
28:R:114:LEU:HB2	28:R:117:LEU:HD23	1.94	0.49
1:2:1259:A:N6	1:2:1519:U:OP1	2.44	0.49
6:G:70:HIS:O	6:G:98:ARG:NH1	2.45	0.49
27:Q:40:GLU:O	27:Q:48:GLN:NE2	2.44	0.49
27:Q:87:SER:O	27:Q:91:ALA:HB2	2.12	0.49
1:2:609:U:H2'	1:2:610:G:H8	1.77	0.49
1:2:913:A:OP2	7:H:99:ARG:NH2	2.45	0.49
6:G:25:ARG:HA	6:G:28:TYR:HD2	1.77	0.49
10:L:94:HIS:HB2	10:L:105:ARG:HD2	1.94	0.49
32:Z:51:ASP:OD1	32:Z:54:THR:OG1	2.28	0.49
1:2:1102:G:OP2	3:B:151:ARG:NH1	2.45	0.49
1:2:1341:C:H4'	1:2:1342:U:H5'	1.94	0.49
1:2:382:C:H2'	1:2:383:G:H8	1.77	0.49
1:2:1658:G:H5'	19:d:33:LYS:HZ2	1.77	0.49
34:i:54:ARG:HH21	34:i:59:TYR:HE1	1.59	0.49
1:2:1351:G:H1	1:2:1360:U:H3	1.59	0.49
12:O:44:VAL:HG13	12:O:53:ILE:HB	1.93	0.49
31:U:28:ASN:OD1	31:U:31:SER:OG	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:948:C:H2'	1:2:949:G:H8	1.78	0.49
1:2:1280:G:H2'	1:2:1281:G:H8	1.78	0.49
10:L:128:VAL:HG12	10:L:142:VAL:HA	1.95	0.49
28:R:16:ILE:HG22	28:R:24:LEU:HD21	1.94	0.49
1:2:1779:G:H2'	1:2:1780:G:C8	2.47	0.49
22:D:172:VAL:HG22	22:D:185:LYS:HG2	1.95	0.49
25:M:113:ASP:OD1	25:M:113:ASP:N	2.45	0.49
34:i:42:ARG:HH21	34:i:49:GLN:HE22	1.61	0.49
1:2:526:A:OP1	20:e:35:ARG:NH1	2.46	0.48
1:2:532:C:H2'	1:2:533:A:C8	2.48	0.48
8:I:91:VAL:HG21	8:I:205:ARG:HH12	1.78	0.48
19:d:3:HIS:HD1	19:d:5:GLN:HB2	1.78	0.48
6:G:181:THR:HG22	6:G:183:ARG:H	1.78	0.48
27:Q:13:PHE:O	27:Q:90:LYS:NZ	2.38	0.48
34:j:45:PHE:HB3	34:j:50:LEU:HD21	1.95	0.48
1:2:1698:C:H1'	36:p:223:LYS:HG3	1.93	0.48
7:H:103:LYS:HD2	7:H:104:PRO:HD2	1.95	0.48
8:I:143:LYS:O	8:I:143:LYS:NZ	2.46	0.48
19:d:41:GLN:HG2	31:U:69:PRO:HB3	1.94	0.48
29:S:113:ARG:O	29:S:117:ILE:HG12	2.14	0.48
1:2:5:U:H2'	1:2:6:G:H8	1.78	0.48
1:2:145:G:H2'	1:2:146:G:C8	2.48	0.48
1:2:658:U:N3	15:X:20:GLN:O	2.42	0.48
1:2:925:G:N2	11:N:48:SER:OG	2.46	0.48
1:2:1652:G:O6	1:2:1672:U:O4	2.31	0.48
5:E:131:VAL:HA	5:E:137:PRO:HA	1.96	0.48
7:H:37:LYS:HA	7:H:40:LEU:HB2	1.96	0.48
8:I:143:LYS:NZ	8:I:147:LYS:HB3	2.28	0.48
25:M:51:VAL:HG22	25:M:77:ILE:HB	1.95	0.48
18:b:16:LYS:HA	18:b:23:ARG:HH21	1.79	0.48
35:g:152:SER:H	35:g:169:GLY:HA2	1.79	0.48
1:2:1174:U:OP1	21:h:21:ARG:NH2	2.46	0.48
1:2:1711:U:H2'	1:2:1712:A:H8	1.79	0.48
4:C:131:GLY:HA3	4:C:216:MET:HB3	1.95	0.48
5:E:94:LYS:HD2	16:Y:16:ARG:HH21	1.79	0.48
6:G:50:VAL:HG22	6:G:113:ILE:HG12	1.96	0.48
23:F:197:GLU:OE1	23:F:201:LYS:NZ	2.28	0.48
34:i:39:ASP:O	34:i:72:ARG:NH1	2.45	0.48
1:2:1347:U:OP1	4:C:121:ARG:NH1	2.46	0.48
1:2:1598:G:H2'	32:Z:81:GLY:H	1.78	0.48
1:2:1842:C:OP2	21:h:2:ARG:NE	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:p:315:ARG:HE	36:p:327:MET:HE2	1.79	0.48
1:2:1005:G:OP2	3:B:162:ARG:NH2	2.47	0.48
1:2:1228:A:H2'	1:2:1229:G:H8	1.77	0.48
1:2:1410:C:H2'	1:2:1411:G:H8	1.79	0.48
7:H:111:LYS:HE2	7:H:111:LYS:HB3	1.74	0.48
16:Y:29:HIS:NE2	16:Y:69:THR:OG1	2.42	0.48
27:Q:102:GLU:HB2	27:Q:105:LYS:HE3	1.94	0.48
1:2:1398:G:H1'	35:g:63:SER:HB3	1.96	0.47
7:H:60:ILE:HD11	7:H:92:VAL:HG22	1.95	0.47
8:I:151:GLU:HA	8:I:154:LYS:NZ	2.29	0.47
31:U:27:ARG:HD3	31:U:82:MET:HE2	1.96	0.47
1:2:388:U:H2'	1:2:389:A:H8	1.79	0.47
1:2:551:U:H2'	1:2:552:G:C8	2.50	0.47
1:2:664:A:O2'	1:2:670:A:N1	2.43	0.47
1:2:909:G:H2'	1:2:910:G:H8	1.77	0.47
35:g:213:ASP:OD1	35:g:213:ASP:N	2.45	0.47
34:j:55:THR:OG1	34:j:56:LEU:N	2.47	0.47
1:2:1620:A:H8	26:P:40:ARG:NH2	2.12	0.47
26:P:111:MET:HG3	29:S:117:ILE:HG23	1.96	0.47
36:p:293:LYS:HD3	36:p:296:LEU:HD13	1.96	0.47
1:2:5:U:H2'	1:2:6:G:C8	2.49	0.47
1:2:420:G:O2'	1:2:660:C:N3	2.48	0.47
24:K:80:ARG:HG2	24:K:85:LEU:HD11	1.95	0.47
35:g:131:LEU:HD12	35:g:140:TYR:HB2	1.97	0.47
1:2:900:C:H2'	1:2:901:G:H8	1.78	0.47
1:2:1705:C:N3	1:2:1830:U:O2	2.47	0.47
30:T:141:ALA:HA	30:T:145:HIS:HD2	1.78	0.47
1:2:1119:A:O5'	18:b:72:ARG:NH1	2.46	0.47
23:F:40:ALA:H	23:F:68:ILE:HD11	1.79	0.47
1:2:1865:C:O5'	17:a:5:ARG:NH1	2.47	0.47
3:B:34:LYS:HA	3:B:43:ASN:HA	1.96	0.47
15:X:105:PHE:HD1	15:X:121:LYS:HB3	1.80	0.47
19:d:3:HIS:ND1	19:d:5:GLN:HB2	2.30	0.47
22:D:138:VAL:HG12	22:D:184:ILE:HG22	1.97	0.47
28:R:21:TYR:HE1	28:R:58:MET:HE1	1.79	0.47
29:S:20:ILE:HG23	29:S:29:ALA:HB1	1.95	0.47
9:J:164:PRO:HB3	9:J:170:PRO:HA	1.95	0.47
11:N:46:THR:OG1	11:N:49:GLN:OE1	2.27	0.47
26:P:132:GLY:C	36:p:255:GLY:HA2	2.40	0.47
1:2:684:G:O6	1:2:1021:U:C4	2.68	0.47
1:2:925:G:H1	1:2:1017:U:H3	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:144:ILE:HG22	9:J:146:SER:H	1.80	0.47
19:d:3:HIS:O	19:d:5:GLN:N	2.48	0.47
23:F:34:SER:HA	33:c:55:VAL:HG23	1.97	0.47
26:P:41:GLN:HG3	26:P:84:ILE:HD13	1.97	0.47
35:g:24:THR:HG23	35:g:27:PHE:H	1.79	0.47
1:2:1312:G:O2'	1:2:1313:A:H8	1.98	0.46
6:G:98:ARG:HD2	6:G:99:GLY:H	1.79	0.46
15:X:74:LEU:HD21	15:X:81:ILE:HD12	1.97	0.46
35:g:42:MET:O	35:g:56:GLN:N	2.30	0.46
1:2:1309:C:H41	34:f:96:LYS:NZ	2.14	0.46
29:S:3:LEU:HD12	32:Z:50:PHE:HE2	1.81	0.46
31:U:64:THR:HA	31:U:78:ASP:O	2.16	0.46
1:2:1722:G:O6	1:2:1812:U:O2	2.34	0.46
3:B:132:GLY:HA3	3:B:221:PRO:HG3	1.98	0.46
22:D:142:LEU:HB2	36:p:184:PRO:HG3	1.98	0.46
26:P:81:ARG:HB3	26:P:117:GLY:HA3	1.97	0.46
6:G:126:ASP:OD1	6:G:127:THR:N	2.43	0.46
6:G:134:GLY:HA3	6:G:158:VAL:HG11	1.97	0.46
35:g:249:CYS:HB3	35:g:258:ILE:HG23	1.96	0.46
4:C:255:LEU:HD21	13:V:14:PRO:HD2	1.98	0.46
29:S:39:ARG:NH1	29:S:83:PHE:HZ	2.14	0.46
36:p:318:LYS:NZ	36:p:319:LEU:O	2.48	0.46
3:B:72:ALA:HB3	12:O:128:ARG:HH22	1.81	0.46
15:X:71:ARG:HH21	15:X:80:LYS:HD2	1.80	0.46
21:h:14:LYS:HB3	21:h:14:LYS:HE2	1.82	0.46
36:p:340:GLN:HE22	36:p:348:THR:HG23	1.80	0.46
1:2:168:C:O2'	6:G:133:LEU:O	2.34	0.46
5:E:254:LYS:HB3	5:E:254:LYS:HE3	1.81	0.46
26:P:134:GLY:H	36:p:256:CYS:HB3	1.81	0.46
2:A:42:LYS:NZ	28:R:99:ASP:OD2	2.32	0.46
12:O:96:LYS:HD3	12:O:130:GLU:HB3	1.96	0.46
15:X:101:LEU:HD22	15:X:124:LYS:HE2	1.98	0.46
1:2:530:U:H2'	1:2:531:A:H8	1.79	0.46
1:2:980:A:H2'	1:2:981:A:C8	2.51	0.46
1:2:1076:G:OP2	11:N:107:LYS:NZ	2.44	0.46
1:2:1174:U:H2'	1:2:1175:G:H8	1.80	0.46
23:F:89:THR:HA	23:F:92:ILE:HD12	1.97	0.46
29:S:86:ARG:HD2	29:S:86:ARG:HA	1.47	0.46
36:p:345:PRO:HG2	36:p:418:LYS:HE2	1.98	0.46
1:2:1776:G:H2'	1:2:1777:G:H8	1.81	0.45
2:A:77:ILE:HG12	2:A:99:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:92:ILE:HG22	5:E:95:THR:H	1.81	0.45
27:Q:104:SER:HA	27:Q:107:GLU:HG2	1.99	0.45
33:c:32:VAL:HG11	33:c:44:ARG:HH22	1.82	0.45
1:2:509:G:H2'	1:2:510:G:C8	2.52	0.45
6:G:22:ARG:HG3	6:G:23:LYS:HD3	1.98	0.45
18:b:54:VAL:HG13	18:b:63:LEU:HB2	1.97	0.45
1:2:126:G:H8	6:G:199:THR:HG21	1.81	0.45
1:2:923:G:OP1	11:N:2:GLY:N	2.50	0.45
1:2:1301:A:H2'	1:2:1303:C:C6	2.51	0.45
1:2:1409:A:OP1	27:Q:26:LYS:NZ	2.35	0.45
8:I:143:LYS:HZ2	8:I:147:LYS:HB3	1.81	0.45
23:F:79:HIS:O	23:F:81:ARG:N	2.50	0.45
35:g:18:VAL:O	35:g:287:THR:OG1	2.27	0.45
35:g:30:MET:HA	35:g:43:TRP:O	2.16	0.45
1:2:525:A:H2'	1:2:526:A:C8	2.50	0.45
1:2:928:G:N2	18:b:68:GLY:O	2.46	0.45
19:d:23:VAL:HG22	24:K:64:TRP:CZ3	2.51	0.45
1:2:1415:C:OP1	30:T:129:ARG:NH1	2.50	0.45
1:2:1711:U:H2'	1:2:1712:A:C8	2.52	0.45
10:L:104:LYS:HB2	10:L:104:LYS:HE3	1.64	0.45
25:M:60:MET:HG2	25:M:63:LYS:HE3	1.99	0.45
27:Q:138:ARG:HA	27:Q:138:ARG:HD3	1.76	0.45
34:j:16:GLU:O	34:j:29:LYS:NZ	2.46	0.45
1:2:203:G:H2'	1:2:204:G:C8	2.52	0.45
1:2:628:A:OP1	22:D:145:GLN:NE2	2.50	0.45
1:2:1588:A:H2'	1:2:1589:A:C8	2.52	0.45
7:H:159:ASP:OD1	7:H:193:GLN:NE2	2.46	0.45
8:I:105:ASP:OD1	8:I:106:SER:N	2.48	0.45
10:L:136:LYS:O	10:L:139:ARG:NH2	2.50	0.45
31:U:24:LEU:HB2	31:U:87:ARG:HB2	1.99	0.45
3:B:140:VAL:HG12	3:B:213:ARG:HB3	1.98	0.45
30:T:28:LEU:HA	30:T:110:LEU:HD21	1.97	0.45
34:j:23:ILE:HG23	34:j:43:LEU:HD12	1.98	0.45
1:2:1245:G:O2'	1:2:1492:U:OP1	2.35	0.45
1:2:1289:U:H2'	1:2:1290:G:C8	2.52	0.45
1:2:1409:A:H2'	1:2:1410:C:C6	2.52	0.45
1:2:1545:A:H2'	1:2:1546:G:C8	2.52	0.45
7:H:82:GLU:HA	7:H:85:LYS:HG2	1.99	0.45
10:L:38:LYS:NZ	10:L:66:VAL:O	2.40	0.45
32:Z:88:LEU:HB3	32:Z:109:TYR:HE2	1.82	0.45
34:f:101:ALA:O	34:f:104:LYS:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:259:TRP:HA	35:g:266:ILE:HA	1.99	0.45
1:2:28:U:H2'	1:2:29:G:H8	1.81	0.45
1:2:520:A:O2'	1:2:825:A:N3	2.45	0.45
22:D:40:ARG:HB3	22:D:47:GLU:HB3	1.98	0.45
22:D:48:ILE:HB	22:D:86:LEU:HD23	1.99	0.45
23:F:175:ASP:O	23:F:179:ASN:ND2	2.50	0.45
1:2:1301:A:H4'	19:d:3:HIS:NE2	2.32	0.44
1:2:1464:C:H2'	1:2:1465:A:C8	2.52	0.44
1:2:1693:G:OP2	17:a:89:ARG:NH2	2.50	0.44
1:2:1808:U:H2'	1:2:1809:A:C8	2.52	0.44
8:I:67:TRP:CZ3	8:I:109:TYR:HB3	2.52	0.44
29:S:124:ARG:HD2	29:S:129:LEU:HB2	1.99	0.44
35:g:82:SER:OG	35:g:83:TRP:N	2.49	0.44
1:2:1232:U:H2'	1:2:1233:G:H8	1.83	0.44
1:2:1598:G:H3'	32:Z:80:ARG:NE	2.32	0.44
9:J:136:ARG:HD3	9:J:160:SER:HA	1.99	0.44
25:M:47:ALA:HA	25:M:112:LYS:HA	1.99	0.44
1:2:483:C:H5'	15:X:48:LYS:HE2	1.98	0.44
1:2:1396:A:O2'	1:2:1398:G:N7	2.45	0.44
27:Q:108:ILE:HA	27:Q:111:ILE:HG22	1.98	0.44
3:B:227:LYS:HE2	3:B:231:LEU:HD21	1.99	0.44
17:a:99:PRO:HA	17:a:102:ARG:HH11	1.82	0.44
22:D:50:ILE:HB	22:D:88:ALA:HA	1.99	0.44
22:D:150:MET:HE1	36:p:184:PRO:HA	1.99	0.44
28:R:94:GLU:HA	28:R:116:ASN:HD22	1.81	0.44
1:2:309:G:OP2	8:I:53:LYS:NZ	2.45	0.44
2:A:19:LEU:HD21	28:R:106:LEU:HD21	1.99	0.44
3:B:24:PRO:O	3:B:27:LYS:HG3	2.17	0.44
26:P:81:ARG:NH2	26:P:120:SER:O	2.51	0.44
9:J:81:LEU:HD23	9:J:84:ILE:HD11	2.00	0.44
12:O:78:ALA:HB1	12:O:119:LEU:HD22	1.99	0.44
15:X:101:LEU:HB3	15:X:124:LYS:HB2	1.99	0.44
26:P:61:ARG:O	26:P:65:LYS:NZ	2.30	0.44
35:g:36:ARG:HD2	35:g:65:PHE:HB3	1.99	0.44
1:2:1227:G:H1	1:2:1531:A:N6	2.12	0.44
9:J:21:GLU:OE2	9:J:23:SER:OG	2.36	0.44
1:2:67:C:H5''	6:G:162:LEU:HD11	1.99	0.44
1:2:818:A:OP1	9:J:80:ARG:NH1	2.47	0.44
1:2:927:C:H2'	1:2:928:G:H8	1.82	0.44
1:2:1013:U:OP1	1:2:1129:G:O2'	2.35	0.44
1:2:1264:C:N4	1:2:1518:C:N3	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:61:ILE:HG21	7:H:176:VAL:HG21	1.99	0.44
9:J:65:GLU:HG3	9:J:66:LYS:HG2	1.99	0.44
1:2:606:G:H5''	20:e:56:ASN:HB3	2.00	0.44
1:2:1232:U:H2'	1:2:1233:G:C8	2.53	0.44
36:p:259:THR:HG22	36:p:264:VAL:HG13	2.00	0.44
1:2:388:U:H2'	1:2:389:A:C8	2.53	0.43
4:C:115:GLN:NE2	4:C:120:GLN:OE1	2.51	0.43
7:H:36:LEU:HD11	7:H:78:ARG:HH21	1.83	0.43
12:O:75:MET:O	12:O:79:GLN:HG2	2.17	0.43
1:2:525:A:H2'	1:2:526:A:H8	1.84	0.43
1:2:980:A:H2'	1:2:981:A:H8	1.83	0.43
1:2:1415:C:H5''	30:T:129:ARG:HH11	1.83	0.43
3:B:127:VAL:HG11	3:B:176:VAL:HB	2.00	0.43
17:a:97:PRO:O	17:a:102:ARG:NH1	2.45	0.43
18:b:65:GLN:HE22	18:b:74:THR:HG22	1.82	0.43
26:P:110:GLU:HG2	29:S:113:ARG:HH12	1.83	0.43
35:g:43:TRP:HA	35:g:55:PRO:HA	1.99	0.43
1:2:386:C:H1'	8:I:5:ARG:HG2	2.00	0.43
1:2:1452:A:H5''	28:R:48:ASN:HD22	1.82	0.43
1:2:932:G:O2'	1:2:934:G:OP2	2.34	0.43
1:2:1628:C:H2'	1:2:1629:C:C6	2.53	0.43
3:B:71:LEU:HD21	3:B:189:ILE:HG23	2.00	0.43
12:O:84:ARG:HH12	12:O:88:LEU:HB2	1.82	0.43
22:D:51:LEU:HG	22:D:91:VAL:HG22	2.00	0.43
1:2:29:G:H2'	1:2:30:C:C6	2.54	0.43
1:2:534:G:H2'	1:2:535:G:C8	2.53	0.43
1:2:1249:C:OP2	1:2:1250:A:O2'	2.34	0.43
1:2:1542:C:H5''	30:T:62:ARG:NH2	2.34	0.43
10:L:51:ILE:HG13	10:L:52:GLU:HG3	2.01	0.43
26:P:24:GLN:O	26:P:28:MET:HG3	2.17	0.43
29:S:109:GLU:O	29:S:113:ARG:HB2	2.18	0.43
30:T:115:LYS:NZ	30:T:119:GLY:O	2.41	0.43
32:Z:88:LEU:HB3	32:Z:109:TYR:CE2	2.54	0.43
1:2:913:A:N6	7:H:119:SER:OG	2.51	0.43
2:A:140:VAL:HG23	2:A:142:LEU:HB2	2.00	0.43
4:C:132:ASP:HB3	4:C:136:HIS:HB2	2.01	0.43
13:V:17:CYS:HB2	13:V:56:CYS:HB3	2.00	0.43
3:B:38:MET:HE1	3:B:231:LEU:HD12	2.00	0.43
17:a:12:LYS:HE3	17:a:12:LYS:HB3	1.83	0.43
22:D:116:ARG:NH2	36:p:183:ALA:O	2.52	0.43
27:Q:87:SER:O	27:Q:91:ALA:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:S:48:ALA:HB2	29:S:70:ILE:HG13	2.01	0.43
36:p:338:ARG:NH2	36:p:400:CYS:O	2.52	0.43
36:p:459:LEU:HD13	36:p:463:GLU:HG3	2.01	0.43
1:2:1228:A:H2'	1:2:1229:G:C8	2.53	0.43
1:2:1279:C:H2'	1:2:1280:G:C8	2.54	0.43
1:2:1280:G:H2'	1:2:1281:G:C8	2.53	0.43
23:F:80:GLY:HA2	23:F:83:ASN:HB2	2.00	0.43
28:R:20:TYR:CE2	28:R:38:ILE:HG21	2.53	0.43
35:g:197:THR:HG21	35:g:238:ALA:HA	2.00	0.43
1:2:186:C:H2'	1:2:187:G:C8	2.54	0.43
1:2:1036:A:N3	1:2:1844:U:O2'	2.52	0.43
1:2:1456:G:H2'	1:2:1457:U:C6	2.53	0.43
25:M:32:ALA:HB1	25:M:37:GLU:HB3	2.01	0.43
27:Q:146:ARG:HE	36:p:293:LYS:HD2	1.84	0.43
1:2:951:C:H2'	1:2:952:G:C8	2.54	0.43
1:2:1391:C:O3'	31:U:83:ARG:NH2	2.51	0.43
19:d:10:HIS:HB3	19:d:12:ARG:HH21	1.84	0.43
23:F:161:ALA:O	23:F:165:ASN:ND2	2.51	0.43
35:g:44:LYS:HE3	35:g:56:GLN:HG2	2.00	0.43
36:p:265:VAL:HG22	36:p:290:LYS:HD2	2.01	0.43
1:2:395:G:OP2	10:L:79:LYS:NZ	2.51	0.42
1:2:1298:G:H1'	26:P:79:HIS:HB2	2.01	0.42
9:J:136:ARG:HG2	9:J:160:SER:H	1.84	0.42
15:X:53:GLU:HG3	15:X:71:ARG:HB3	2.01	0.42
25:M:93:LYS:HB3	25:M:101:ARG:HE	1.84	0.42
1:2:1083:A:O2'	1:2:1858:G:N2	2.44	0.42
1:2:1279:C:H2'	1:2:1280:G:H8	1.84	0.42
1:2:1522:A:P	29:S:144:ARG:HH21	2.41	0.42
1:2:1856:C:H2'	1:2:1857:G:C8	2.54	0.42
4:C:168:GLY:N	4:C:179:THR:O	2.41	0.42
7:H:63:PHE:HB3	7:H:97:GLN:HB2	2.01	0.42
16:Y:15:ASN:HB2	16:Y:20:ARG:HG3	2.02	0.42
24:K:21:MET:HG2	24:K:49:MET:HG3	2.02	0.42
27:Q:16:LYS:HA	27:Q:16:LYS:HD2	1.89	0.42
1:2:1598:G:H3'	32:Z:80:ARG:HE	1.83	0.42
4:C:67:GLY:HA2	4:C:70:VAL:HG12	2.02	0.42
4:C:70:VAL:HG11	4:C:93:ILE:HG23	2.01	0.42
4:C:211:LYS:HB2	4:C:211:LYS:HE3	1.79	0.42
11:N:73:ARG:HE	11:N:73:ARG:HB2	1.70	0.42
12:O:85:CYS:HB3	12:O:124:MET:HE3	2.02	0.42
16:Y:111:LYS:HA	16:Y:114:MET:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Q:60:LYS:HD2	27:Q:60:LYS:HA	1.86	0.42
29:S:130:ARG:NH2	29:S:134:GLN:OE1	2.52	0.42
31:U:22:ILE:HD13	31:U:91:LEU:HD23	2.00	0.42
36:p:407:LEU:HD11	36:p:412:MET:SD	2.59	0.42
36:p:418:LYS:HA	36:p:418:LYS:HD2	1.81	0.42
1:2:223:C:H2'	1:2:224:A:C8	2.54	0.42
1:2:1866:A:N6	17:a:84:VAL:HB	2.34	0.42
6:G:23:LYS:HG3	6:G:41:LEU:HA	2.00	0.42
6:G:136:LYS:NZ	6:G:175:LYS:O	2.37	0.42
8:I:168:GLN:HE21	8:I:168:GLN:C	2.27	0.42
27:Q:105:LYS:HA	27:Q:108:ILE:HG22	2.02	0.42
29:S:104:ASP:O	29:S:108:ARG:HG3	2.20	0.42
1:2:1489:A:N6	36:p:225:GLU:OE2	2.52	0.42
8:I:157:LYS:HB3	8:I:157:LYS:HE2	1.83	0.42
18:b:34:ASP:HB2	18:b:82:LYS:HE3	2.01	0.42
19:d:23:VAL:HG22	24:K:64:TRP:HZ3	1.84	0.42
25:M:53:ALA:HB2	25:M:85:LEU:HD12	2.02	0.42
1:2:1624:U:H2'	1:2:1625:U:O4'	2.20	0.42
5:E:151:ASP:OD1	6:G:216:ARG:NH2	2.52	0.42
8:I:57:ALA:HB2	8:I:183:GLY:HA2	2.02	0.42
25:M:21:VAL:O	25:M:24:THR:OG1	2.32	0.42
35:g:252:THR:HG22	35:g:254:PRO:HD2	2.01	0.42
36:p:452:LYS:HB3	36:p:452:LYS:HE3	1.84	0.42
1:2:913:A:H2	7:H:99:ARG:H	1.66	0.42
1:2:1050:A:H62	1:2:1068:G:H21	1.67	0.42
3:B:138:PHE:HD2	3:B:214:LYS:HB3	1.84	0.42
23:F:150:ALA:O	23:F:154:LEU:HG	2.20	0.42
35:g:165:ILE:HG13	35:g:177:TRP:HB2	2.01	0.42
36:p:117:ARG:HB3	36:p:120:HIS:HE2	1.85	0.42
34:j:36:ILE:O	34:j:41:GLN:NE2	2.51	0.42
1:2:1677:U:H2'	1:2:1678:A:H8	1.84	0.42
8:I:194:GLU:HG2	10:L:10:TYR:CE2	2.55	0.42
10:L:126:VAL:HG12	10:L:145:VAL:HG22	2.02	0.42
34:j:26:VAL:HG21	34:j:56:LEU:HD21	2.01	0.42
1:2:1098:C:H2'	1:2:1099:G:C8	2.55	0.42
1:2:1264:C:N3	1:2:1517:G:N1	2.67	0.42
1:2:1538:C:H5''	30:T:44:GLU:OE2	2.19	0.42
5:E:126:VAL:HG22	5:E:139:LEU:HD21	2.00	0.42
8:I:103:LEU:HD12	8:I:170:LYS:HB3	2.02	0.42
22:D:33:GLY:HA3	22:D:53:THR:HG22	2.02	0.42
35:g:17:TRP:H	35:g:36:ARG:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:133:ASN:HD22	35:g:137:VAL:HB	1.85	0.42
35:g:158:PRO:HA	35:g:163:PRO:HB3	2.02	0.42
36:p:81:ALA:HB3	34:j:8:LEU:HD21	2.02	0.42
1:2:1338:G:H4'	31:U:74:SER:H	1.85	0.42
1:2:1410:C:H2'	1:2:1411:G:C8	2.55	0.42
22:D:194:PRO:O	22:D:201:LYS:NZ	2.52	0.42
1:2:568:C:H2'	1:2:569:A:H8	1.84	0.41
1:2:1705:C:H2'	1:2:1706:G:C8	2.54	0.41
11:N:75:LEU:HD23	11:N:75:LEU:HA	1.89	0.41
36:p:438:PHE:HA	36:p:441:ARG:HG2	2.02	0.41
3:B:127:VAL:HG13	3:B:177:GLN:HG2	2.01	0.41
9:J:160:SER:O	9:J:163:SER:N	2.45	0.41
12:O:39:ASP:OD1	12:O:40:THR:N	2.53	0.41
21:h:8:LYS:HB3	21:h:8:LYS:HE2	1.90	0.41
24:K:23:ALA:O	24:K:66:HIS:ND1	2.52	0.41
27:Q:25:CYS:SG	27:Q:68:ILE:HG12	2.60	0.41
36:p:241:MET:HA	36:p:244:MET:HE2	2.02	0.41
2:A:104:THR:O	2:A:107:THR:OG1	2.31	0.41
2:A:118:GLU:HG3	4:C:65:LYS:HE2	2.03	0.41
6:G:25:ARG:HA	6:G:28:TYR:CD2	2.55	0.41
7:H:118:ARG:HD2	7:H:118:ARG:HA	1.91	0.41
12:O:101:GLY:HA2	12:O:106:LYS:HG3	2.02	0.41
18:b:73:LEU:HB3	18:b:77:CYS:HB2	2.02	0.41
23:F:51:HIS:HD2	23:F:86:LYS:HG2	1.85	0.41
26:P:31:GLU:O	26:P:34:MET:HB3	2.20	0.41
32:Z:98:LYS:NZ	32:Z:111:ARG:O	2.38	0.41
1:2:996:A:H2'	1:2:997:A:C8	2.55	0.41
1:2:1731:A:H2'	1:2:1732:G:H8	1.85	0.41
3:B:124:HIS:HA	3:B:137:LEU:O	2.20	0.41
3:B:175:GLU:HB3	3:B:187:LYS:HE2	2.02	0.41
7:H:166:VAL:O	7:H:170:VAL:HG13	2.20	0.41
9:J:151:LEU:HD23	9:J:151:LEU:HA	1.90	0.41
12:O:75:MET:HE2	12:O:75:MET:HB3	1.88	0.41
23:F:122:ARG:HG3	33:c:59:LEU:HD21	2.03	0.41
1:2:746:C:OP2	7:H:107:LYS:NZ	2.53	0.41
7:H:177:TYR:O	7:H:181:THR:OG1	2.26	0.41
26:P:60:LEU:HD13	26:P:89:MET:HG3	2.03	0.41
36:p:352:LEU:HD13	36:p:357:LEU:HD13	2.03	0.41
1:2:909:G:H2'	1:2:910:G:C8	2.54	0.41
1:2:1852:C:H5''	21:h:5:TRP:CZ3	2.55	0.41
22:D:116:ARG:HB2	22:D:117:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:M:36:ARG:HA	34:f:102:VAL:HG11	2.02	0.41
1:2:218:U:H2'	1:2:219:U:C6	2.56	0.41
1:2:1217:A:H2'	1:2:1218:C:C6	2.55	0.41
2:A:42:LYS:HE2	2:A:46:ILE:HB	2.02	0.41
8:I:91:VAL:HG23	8:I:92:ARG:HD3	2.02	0.41
22:D:135:GLU:HG2	22:D:153:VAL:HG12	2.01	0.41
23:F:153:LEU:HD23	23:F:189:ALA:HA	2.02	0.41
36:p:344:ILE:HG23	36:p:392:LEU:HD12	2.02	0.41
1:2:860:G:H21	14:W:107:SER:HB3	1.86	0.41
1:2:1513:C:H2'	1:2:1514:G:C8	2.53	0.41
1:2:1545:A:N3	1:2:1671:G:O2'	2.46	0.41
1:2:1670:C:H2'	1:2:1671:G:C8	2.55	0.41
9:J:18:ARG:HD3	9:J:18:ARG:HA	1.78	0.41
17:a:21:ILE:HD11	17:a:35:ALA:HB3	2.03	0.41
24:K:9:ILE:HD12	24:K:9:ILE:HA	1.97	0.41
28:R:67:ARG:H	28:R:67:ARG:HG3	1.69	0.41
36:p:441:ARG:HA	36:p:444:ARG:HG3	2.03	0.41
1:2:1010:G:H2'	1:2:1011:A:C8	2.55	0.41
1:2:1205:C:H2'	1:2:1206:G:H8	1.86	0.41
1:2:1297:U:O2'	1:2:1301:A:N6	2.54	0.41
1:2:1312:G:O6	25:M:36:ARG:HB3	2.21	0.41
2:A:57:LYS:HA	2:A:57:LYS:HD2	1.88	0.41
5:E:197:ASN:HB3	5:E:209:HIS:HB2	2.03	0.41
6:G:65:GLN:HE21	6:G:65:GLN:HB2	1.70	0.41
7:H:83:LEU:HB3	7:H:92:VAL:HG21	2.02	0.41
24:K:14:LEU:HA	24:K:17:LYS:HG2	2.03	0.41
25:M:33:ARG:HD3	25:M:89:VAL:HG11	2.02	0.41
33:c:44:ARG:HA	33:c:65:ALA:HB2	2.03	0.41
35:g:212:LYS:HA	35:g:235:ILE:HG12	2.03	0.41
1:2:158:A:N6	1:2:466:G:O6	2.54	0.41
1:2:441:C:H2'	1:2:442:C:C6	2.56	0.41
1:2:1232:U:OP1	29:S:135:HIS:NE2	2.54	0.41
1:2:1281:G:H2'	1:2:1282:A:H8	1.86	0.41
2:A:182:VAL:O	2:A:186:ARG:HG3	2.21	0.41
10:L:7:GLU:HG3	10:L:8:ARG:H	1.85	0.41
11:N:94:LYS:HB2	11:N:94:LYS:HE3	1.82	0.41
18:b:74:THR:OG1	18:b:77:CYS:SG	2.75	0.41
1:2:332:G:H5'	6:G:193:ALA:HB2	2.03	0.40
1:2:575:A:OP2	16:Y:93:ARG:NH2	2.52	0.40
6:G:69:THR:HG22	6:G:71:GLY:H	1.85	0.40
7:H:160:LYS:HB2	7:H:160:LYS:HE3	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:56:ARG:HD3	8:I:56:ARG:HA	1.95	0.40
16:Y:54:VAL:HG22	16:Y:76:TYR:HB2	2.03	0.40
32:Z:79:ILE:HG22	32:Z:80:ARG:O	2.21	0.40
33:c:22:GLY:HA2	33:c:68:LEU:HB2	2.03	0.40
35:g:64:HIS:CG	35:g:65:PHE:H	2.38	0.40
1:2:1226:G:N1	1:2:1639:G:OP2	2.42	0.40
1:2:1599:U:C4	23:F:166:ILE:HD13	2.56	0.40
8:I:151:GLU:HA	8:I:154:LYS:HZ2	1.86	0.40
15:X:63:ASN:ND2	15:X:114:ASP:OD2	2.51	0.40
18:b:19:HIS:HB3	18:b:22:LYS:HG3	2.03	0.40
19:d:10:HIS:HA	19:d:11:PRO:HD3	1.97	0.40
29:S:66:ARG:O	29:S:70:ILE:HG12	2.22	0.40
30:T:73:GLY:O	30:T:94:ARG:NH2	2.55	0.40
1:2:1773:C:H2'	1:2:1774:C:C6	2.56	0.40
3:B:33:VAL:HG21	3:B:67:PHE:CE2	2.57	0.40
3:B:62:LEU:HD23	3:B:91:VAL:HG11	2.03	0.40
5:E:122:LYS:HG2	5:E:164:LEU:HG	2.04	0.40
6:G:7:PHE:CD2	6:G:10:THR:HG22	2.57	0.40
7:H:69:LEU:O	7:H:73:GLN:HB2	2.21	0.40
17:a:28:ARG:HE	17:a:28:ARG:HB3	1.62	0.40
18:b:64:CYS:HB3	18:b:73:LEU:HD23	2.02	0.40
22:D:167:TYR:OH	22:D:202:LYS:O	2.34	0.40
26:P:81:ARG:NH2	26:P:117:GLY:O	2.54	0.40
1:2:102:A:H5'	1:2:104:A:C4	2.56	0.40
1:2:107:A:H2'	1:2:108:G:C8	2.56	0.40
1:2:1391:C:H4'	19:d:55:LEU:HD13	2.04	0.40
1:2:1851:A:P	21:h:9:ARG:HH21	2.44	0.40
7:H:19:PHE:HZ	7:H:60:ILE:HG22	1.86	0.40
12:O:151:LEU:HD12	12:O:151:LEU:HA	1.94	0.40
26:P:86:LEU:H	26:P:89:MET:HE2	1.86	0.40
27:Q:90:LYS:HA	27:Q:93:VAL:HB	2.03	0.40
1:2:1274:G:C5	24:K:43:LEU:HD11	2.57	0.40
6:G:162:LEU:HD23	6:G:170:ARG:HD2	2.03	0.40
7:H:160:LYS:HA	7:H:163:GLN:HB2	2.04	0.40
9:J:159:PHE:CE2	9:J:165:TYR:HB2	2.56	0.40
11:N:145:THR:O	11:N:147:SER:N	2.55	0.40
29:S:62:ASP:OD1	29:S:63:GLU:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	204/295 (69%)	189 (93%)	15 (7%)	0	100	100
3	B	211/264 (80%)	200 (95%)	11 (5%)	0	100	100
4	C	216/293 (74%)	201 (93%)	14 (6%)	1 (0%)	24	57
5	E	260/263 (99%)	248 (95%)	12 (5%)	0	100	100
6	G	228/249 (92%)	216 (95%)	11 (5%)	1 (0%)	30	61
7	H	184/194 (95%)	175 (95%)	9 (5%)	0	100	100
8	I	203/208 (98%)	190 (94%)	13 (6%)	0	100	100
9	J	178/194 (92%)	168 (94%)	10 (6%)	0	100	100
10	L	149/158 (94%)	142 (95%)	7 (5%)	0	100	100
11	N	147/151 (97%)	142 (97%)	4 (3%)	1 (1%)	18	51
12	O	124/151 (82%)	117 (94%)	6 (5%)	1 (1%)	16	49
13	V	80/83 (96%)	77 (96%)	3 (4%)	0	100	100
14	W	127/130 (98%)	123 (97%)	3 (2%)	1 (1%)	16	49
15	X	139/143 (97%)	125 (90%)	14 (10%)	0	100	100
16	Y	122/133 (92%)	118 (97%)	4 (3%)	0	100	100
17	a	99/115 (86%)	92 (93%)	6 (6%)	1 (1%)	12	45
18	b	80/84 (95%)	76 (95%)	4 (5%)	0	100	100
19	d	53/56 (95%)	52 (98%)	0	1 (2%)	6	33
20	e	42/59 (71%)	40 (95%)	2 (5%)	0	100	100
21	h	22/25 (88%)	22 (100%)	0	0	100	100
22	D	223/243 (92%)	217 (97%)	6 (3%)	0	100	100
23	F	176/204 (86%)	153 (87%)	20 (11%)	3 (2%)	7	35
24	K	93/165 (56%)	90 (97%)	3 (3%)	0	100	100
25	M	121/132 (92%)	115 (95%)	6 (5%)	0	100	100
26	P	118/145 (81%)	115 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	Q	137/146 (94%)	125 (91%)	12 (9%)	0	100	100
28	R	130/135 (96%)	118 (91%)	11 (8%)	1 (1%)	16	49
29	S	141/152 (93%)	131 (93%)	9 (6%)	1 (1%)	18	51
30	T	142/145 (98%)	140 (99%)	2 (1%)	0	100	100
31	U	99/119 (83%)	95 (96%)	4 (4%)	0	100	100
32	Z	70/125 (56%)	67 (96%)	3 (4%)	0	100	100
33	c	59/69 (86%)	55 (93%)	4 (7%)	0	100	100
34	f	27/156 (17%)	22 (82%)	5 (18%)	0	100	100
34	i	71/156 (46%)	70 (99%)	1 (1%)	0	100	100
34	j	71/156 (46%)	70 (99%)	1 (1%)	0	100	100
35	g	312/317 (98%)	293 (94%)	19 (6%)	0	100	100
36	p	336/519 (65%)	318 (95%)	18 (5%)	0	100	100
All	All	5194/6332 (82%)	4907 (94%)	275 (5%)	12 (0%)	44	72

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	190	SER
6	G	126	ASP
11	N	146	ALA
28	R	20	TYR
17	a	27	ALA
19	d	4	GLN
23	F	80	GLY
23	F	42	LYS
12	O	149	ARG
29	S	88	LYS
23	F	41	VAL
14	W	29	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	172/243 (71%)	172 (100%)	0	100	100
3	B	194/231 (84%)	194 (100%)	0	100	100
4	C	184/225 (82%)	184 (100%)	0	100	100
5	E	224/225 (100%)	224 (100%)	0	100	100
6	G	200/218 (92%)	200 (100%)	0	100	100
7	H	167/174 (96%)	167 (100%)	0	100	100
8	I	178/180 (99%)	174 (98%)	4 (2%)	45	65
9	J	160/168 (95%)	160 (100%)	0	100	100
10	L	135/142 (95%)	133 (98%)	2 (2%)	57	70
11	N	130/131 (99%)	130 (100%)	0	100	100
12	O	99/119 (83%)	98 (99%)	1 (1%)	68	75
13	V	66/67 (98%)	66 (100%)	0	100	100
14	W	112/113 (99%)	112 (100%)	0	100	100
15	X	113/115 (98%)	113 (100%)	0	100	100
16	Y	108/115 (94%)	108 (100%)	0	100	100
17	a	88/98 (90%)	86 (98%)	2 (2%)	44	64
18	b	74/76 (97%)	74 (100%)	0	100	100
19	d	48/49 (98%)	48 (100%)	0	100	100
20	e	37/48 (77%)	37 (100%)	0	100	100
21	h	23/24 (96%)	23 (100%)	0	100	100
22	D	189/202 (94%)	189 (100%)	0	100	100
23	F	153/170 (90%)	153 (100%)	0	100	100
24	K	86/136 (63%)	86 (100%)	0	100	100
25	M	104/108 (96%)	103 (99%)	1 (1%)	68	75
26	P	107/130 (82%)	107 (100%)	0	100	100
27	Q	115/121 (95%)	112 (97%)	3 (3%)	40	62
28	R	118/122 (97%)	117 (99%)	1 (1%)	73	77
29	S	124/132 (94%)	118 (95%)	6 (5%)	23	50
30	T	114/115 (99%)	114 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	f	27/140 (19%)	27 (100%)	0	100	100
34	i	67/140 (48%)	67 (100%)	0	100	100
34	j	65/140 (46%)	65 (100%)	0	100	100
35	g	272/275 (99%)	272 (100%)	0	100	100
36	p	308/454 (68%)	307 (100%)	1 (0%)	86	83
All	All	4572/5418 (84%)	4551 (100%)	21 (0%)	78	80

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	I	129	LEU
8	I	130	THR
8	I	135	GLU
8	I	151	GLU
10	L	104	LYS
10	L	105	ARG
12	O	150	ARG
17	a	19	GLN
17	a	26	CYS
25	M	36	ARG
27	Q	127	CYS
27	Q	128	GLU
27	Q	138	ARG
28	R	26	ASN
29	S	23	ARG
29	S	26	ILE
29	S	83	PHE
29	S	86	ARG
29	S	88	LYS
29	S	97	GLN
36	p	256	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	36	GLN
3	B	118	GLN
3	B	158	HIS
3	B	159	GLN

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Mol	Chain	Res	Type
4	C	115	GLN
4	C	120	GLN
5	E	36	HIS
6	G	163	ASN
7	H	25	GLN
7	H	97	GLN
7	H	126	HIS
7	H	165	ASN
8	I	52	ASN
8	I	138	ASN
8	I	168	GLN
10	L	18	GLN
11	N	105	ASN
14	W	56	HIS
15	X	97	ASN
17	a	19	GLN
17	a	25	ASN
17	a	86	ASN
18	b	9	HIS
19	d	4	GLN
19	d	5	GLN
19	d	37	ASN
22	D	22	ASN
22	D	101	GLN
23	F	101	HIS
25	M	28	HIS
25	M	72	HIS
26	P	114	HIS
28	R	48	ASN
28	R	93	GLN
29	S	10	GLN
29	S	11	HIS
29	S	42	HIS
34	f	93	HIS
35	g	56	GLN
35	g	133	ASN
35	g	237	ASN
36	p	175	ASN
36	p	201	HIS
36	p	209	HIS
36	p	267	HIS
36	p	366	GLN

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Mol	Chain	Res	Type
34	j	49	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1654/1869 (88%)	418 (25%)	40 (2%)

All (418) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	C
1	2	4	C
1	2	25	A
1	2	26	U
1	2	33	G
1	2	41	G
1	2	42	A
1	2	44	U
1	2	45	A
1	2	46	A
1	2	49	C
1	2	50	A
1	2	56	G
1	2	58	C
1	2	61	A
1	2	62	G
1	2	64	A
1	2	65	C
1	2	66	G
1	2	67	C
1	2	68	A
1	2	69	C
1	2	72	C
1	2	73	C
1	2	75	G
1	2	76	U
1	2	77	A
1	2	79	A
1	2	80	G
1	2	93	U
1	2	99	A

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Mol	Chain	Res	Type
1	2	103	A
1	2	104	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	116	U
1	2	126	G
1	2	141	A
1	2	142	C
1	2	143	U
1	2	144	U
1	2	155	G
1	2	156	G
1	2	161	U
1	2	163	U
1	2	175	A
1	2	181	A
1	2	182	C
1	2	183	G
1	2	184	G
1	2	188	C
1	2	191	A
1	2	206	G
1	2	211	G
1	2	213	G
1	2	214	U
1	2	215	G
1	2	290	U
1	2	291	G
1	2	292	A
1	2	293	C
1	2	294	U
1	2	295	C
1	2	306	C
1	2	307	G
1	2	308	G
1	2	310	C
1	2	312	G
1	2	315	C
1	2	320	G
1	2	321	C
1	2	332	G

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Mol	Chain	Res	Type
1	2	333	G
1	2	335	G
1	2	340	C
1	2	347	G
1	2	350	C
1	2	360	A
1	2	362	C
1	2	364	A
1	2	369	C
1	2	370	G
1	2	377	G
1	2	381	C
1	2	383	G
1	2	385	G
1	2	386	C
1	2	398	A
1	2	400	C
1	2	407	G
1	2	408	A
1	2	409	C
1	2	418	A
1	2	421	G
1	2	428	U
1	2	429	C
1	2	447	A
1	2	448	A
1	2	450	C
1	2	464	A
1	2	465	A
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	483	C
1	2	487	U
1	2	492	C
1	2	502	C
1	2	503	C
1	2	507	G
1	2	516	A

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Mol	Chain	Res	Type
1	2	523	A
1	2	525	A
1	2	532	C
1	2	534	G
1	2	536	A
1	2	537	C
1	2	544	G
1	2	546	G
1	2	548	C
1	2	551	U
1	2	552	G
1	2	554	A
1	2	555	A
1	2	556	U
1	2	559	G
1	2	560	A
1	2	563	G
1	2	564	A
1	2	570	C
1	2	576	A
1	2	582	U
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	593	C
1	2	595	U
1	2	596	U
1	2	600	G
1	2	603	C
1	2	604	A
1	2	605	A
1	2	607	U
1	2	608	C
1	2	614	C
1	2	617	G
1	2	629	A
1	2	631	U
1	2	632	C
1	2	639	C

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Mol	Chain	Res	Type
1	2	640	A
1	2	643	A
1	2	644	G
1	2	655	A
1	2	659	G
1	2	660	C
1	2	668	A
1	2	669	A
1	2	671	A
1	2	672	A
1	2	687	C
1	2	688	U
1	2	748	C
1	2	749	U
1	2	750	C
1	2	751	G
1	2	792	C
1	2	793	G
1	2	794	A
1	2	798	G
1	2	799	U
1	2	808	A
1	2	810	A
1	2	812	A
1	2	821	G
1	2	822	U
1	2	830	A
1	2	847	A
1	2	852	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	879	C
1	2	880	G
1	2	881	G
1	2	887	U
1	2	890	U
1	2	898	U

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Mol	Chain	Res	Type
1	2	903	A
1	2	913	A
1	2	914	U
1	2	917	U
1	2	920	A
1	2	933	G
1	2	934	G
1	2	938	A
1	2	943	U
1	2	955	A
1	2	956	G
1	2	958	G
1	2	960	U
1	2	962	A
1	2	970	G
1	2	971	G
1	2	978	G
1	2	990	A
1	2	992	A
1	2	999	G
1	2	1002	U
1	2	1009	A
1	2	1015	U
1	2	1017	U
1	2	1023	A
1	2	1030	A
1	2	1041	G
1	2	1042	A
1	2	1045	U
1	2	1047	C
1	2	1049	A
1	2	1053	C
1	2	1059	G
1	2	1061	U
1	2	1062	A
1	2	1083	A
1	2	1084	A
1	2	1085	C
1	2	1089	G
1	2	1096	G
1	2	1114	U
1	2	1115	U

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Mol	Chain	Res	Type
1	2	1116	C
1	2	1118	C
1	2	1119	A
1	2	1120	U
1	2	1123	C
1	2	1126	G
1	2	1133	A
1	2	1136	U
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	1150	A
1	2	1153	C
1	2	1154	U
1	2	1157	G
1	2	1171	G
1	2	1195	A
1	2	1199	A
1	2	1207	G
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	1239	U
1	2	1242	U
1	2	1243	U
1	2	1251	A
1	2	1256	G
1	2	1257	G
1	2	1259	A
1	2	1260	A
1	2	1271	C
1	2	1274	G
1	2	1275	G
1	2	1283	C
1	2	1284	A
1	2	1285	G

Continued on next page...

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Mol	Chain	Res	Type
1	2	1286	G
1	2	1288	U
1	2	1291	A
1	2	1301	A
1	2	1302	G
1	2	1303	C
1	2	1309	C
1	2	1312	G
1	2	1313	A
1	2	1314	U
1	2	1315	U
1	2	1317	C
1	2	1322	G
1	2	1324	G
1	2	1330	G
1	2	1331	C
1	2	1343	U
1	2	1348	G
1	2	1358	U
1	2	1363	C
1	2	1371	U
1	2	1372	U
1	2	1373	C
1	2	1378	A
1	2	1401	A
1	2	1404	U
1	2	1426	U
1	2	1429	G
1	2	1431	G
1	2	1432	U
1	2	1441	U
1	2	1442	U
1	2	1446	A
1	2	1450	G
1	2	1454	A
1	2	1463	U
1	2	1464	C
1	2	1465	A
1	2	1466	G
1	2	1473	G
1	2	1476	A
1	2	1477	U

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Mol	Chain	Res	Type
1	2	1489	A
1	2	1490	G
1	2	1493	C
1	2	1494	U
1	2	1495	G
1	2	1505	U
1	2	1509	U
1	2	1512	C
1	2	1517	G
1	2	1520	G
1	2	1521	C
1	2	1522	A
1	2	1531	A
1	2	1533	A
1	2	1534	C
1	2	1535	U
1	2	1536	G
1	2	1544	C
1	2	1559	C
1	2	1560	U
1	2	1563	G
1	2	1566	G
1	2	1567	G
1	2	1569	A
1	2	1570	G
1	2	1572	C
1	2	1579	A
1	2	1580	A
1	2	1581	C
1	2	1584	G
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	1613	G
1	2	1617	G
1	2	1618	C

Continued on next page...

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Mol	Chain	Res	Type
1	2	1621	U
1	2	1623	A
1	2	1629	C
1	2	1648	G
1	2	1649	U
1	2	1654	G
1	2	1663	A
1	2	1665	G
1	2	1675	A
1	2	1680	G
1	2	1683	C
1	2	1695	A
1	2	1698	C
1	2	1699	A
1	2	1721	U
1	2	1722	G
1	2	1728	U
1	2	1729	U
1	2	1742	C
1	2	1744	G
1	2	1748	G
1	2	1753	C
1	2	1778	C
1	2	1782	G
1	2	1783	C
1	2	1785	C
1	2	1786	U
1	2	1799	G
1	2	1819	A
1	2	1822	A
1	2	1825	A
1	2	1826	G
1	2	1829	G
1	2	1831	A
1	2	1835	A
1	2	1836	G
1	2	1838	U
1	2	1839	U
1	2	1849	G
1	2	1850	A
1	2	1851	A
1	2	1852	C

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Mol	Chain	Res	Type
1	2	1853	C
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1864	U
1	2	1865	C
1	2	1867	U
1	2	1868	U
1	2	1869	A

All (40) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	60	A
1	2	65	C
1	2	102	A
1	2	114	G
1	2	143	U
1	2	180	G
1	2	291	G
1	2	314	U
1	2	332	G
1	2	382	C
1	2	465	A
1	2	547	G
1	2	554	A
1	2	594	A
1	2	604	A
1	2	750	C
1	2	793	G
1	2	797	C
1	2	870	A
1	2	1148	A
1	2	1274	G
1	2	1302	G
1	2	1316	C
1	2	1330	G
1	2	1342	U
1	2	1403	C
1	2	1425	G
1	2	1431	G
1	2	1440	C

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Mol	Chain	Res	Type
1	2	1464	C
1	2	1511	U
1	2	1520	G
1	2	1534	C
1	2	1585	U
1	2	1587	G
1	2	1599	U
1	2	1601	A
1	2	1620	A
1	2	1648	G
1	2	1838	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are 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.

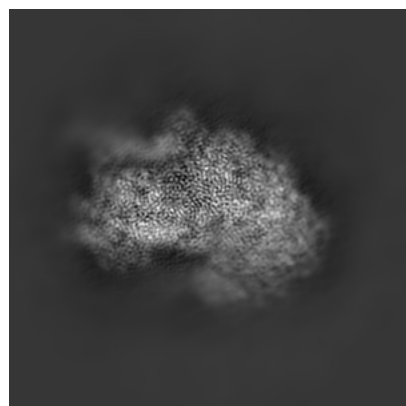
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39956. These allow visual inspection of the internal detail of the map and identification of artifacts.

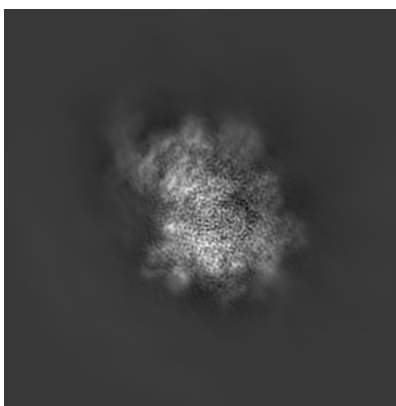
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

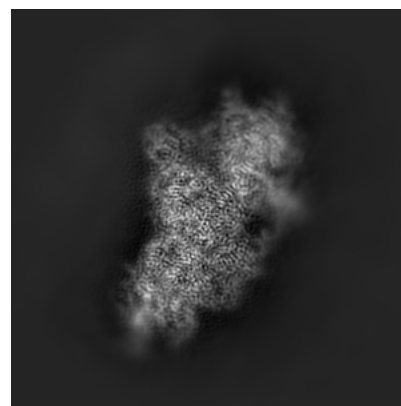
6.1.1 Primary map



X

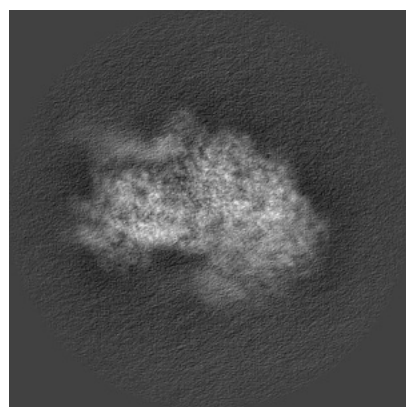


Y

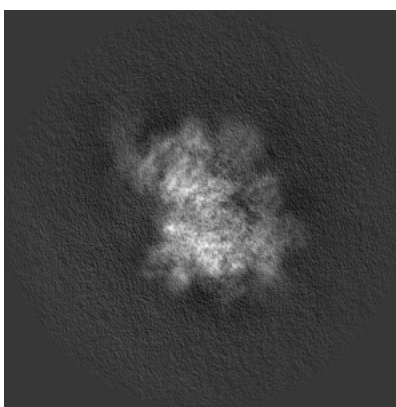


Z

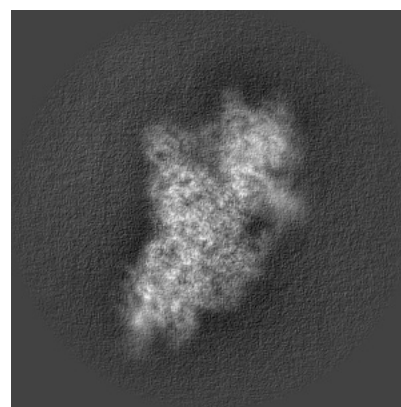
6.1.2 Raw map



X



Y

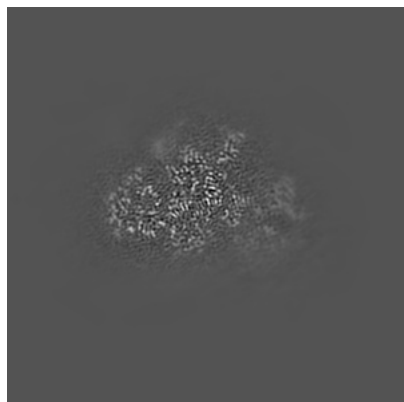


Z

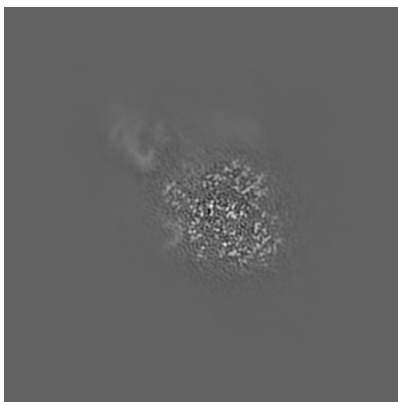
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

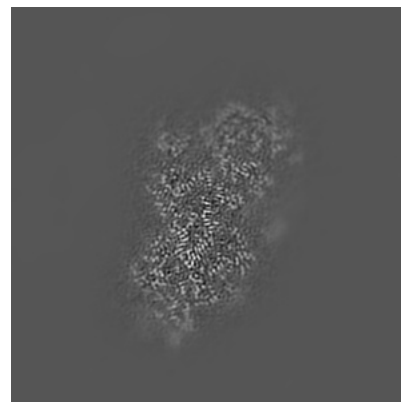
6.2.1 Primary map



X Index: 180

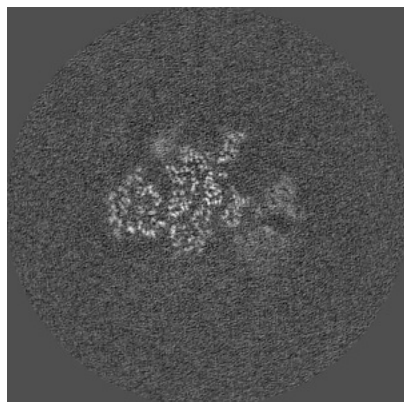


Y Index: 180

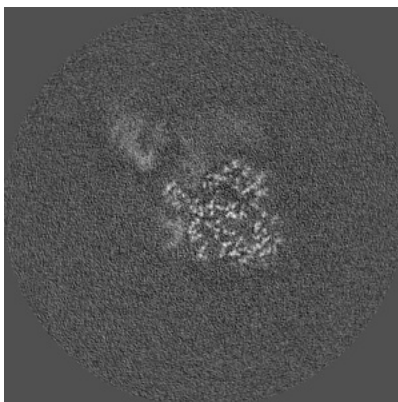


Z Index: 180

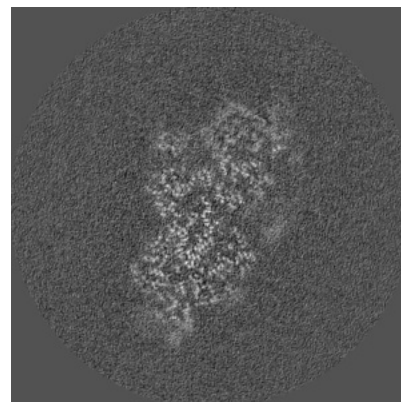
6.2.2 Raw map



X Index: 180



Y Index: 180

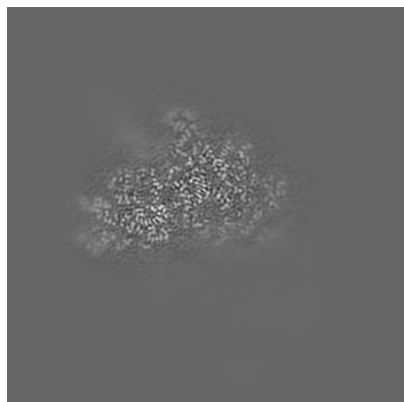


Z Index: 180

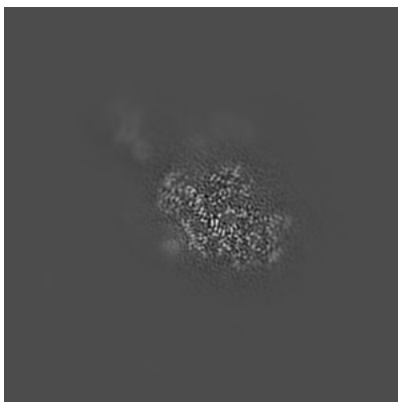
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

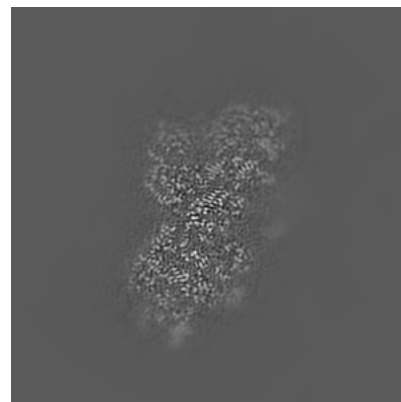
6.3.1 Primary map



X Index: 159

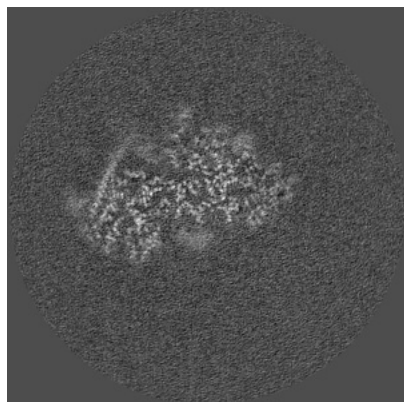


Y Index: 172

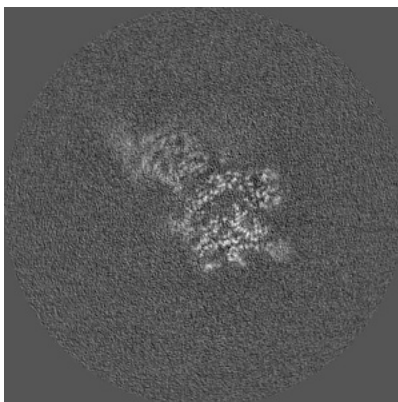


Z Index: 184

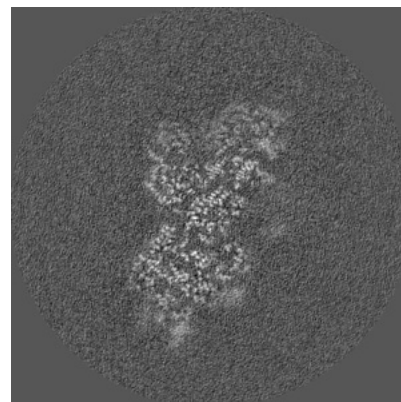
6.3.2 Raw map



X Index: 147



Y Index: 196

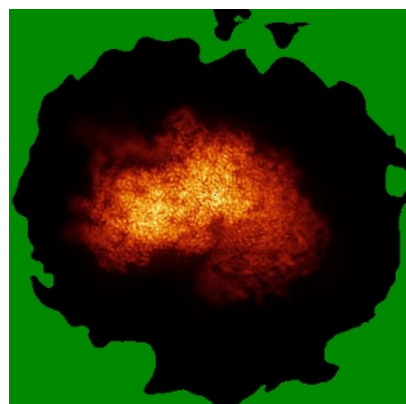


Z Index: 184

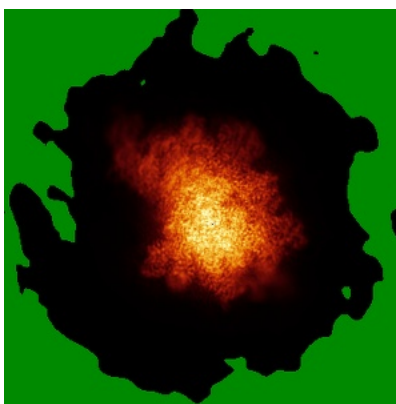
The images above show the largest variance slices of the map in three orthogonal directions.

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

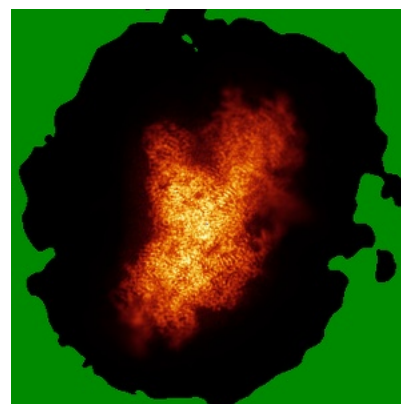
6.4.1 Primary map



X

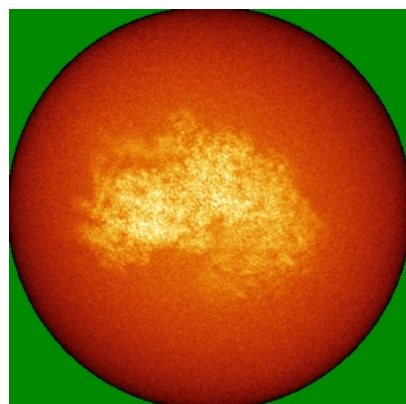


Y

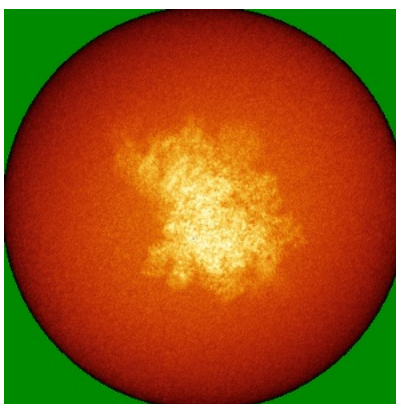


Z

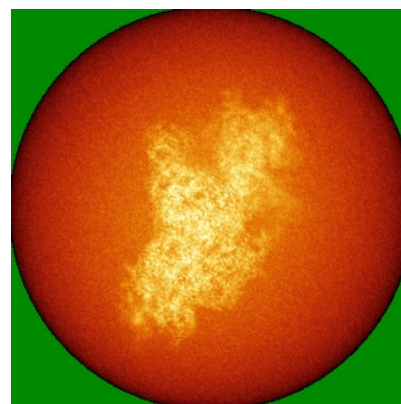
6.4.2 Raw map



X



Y

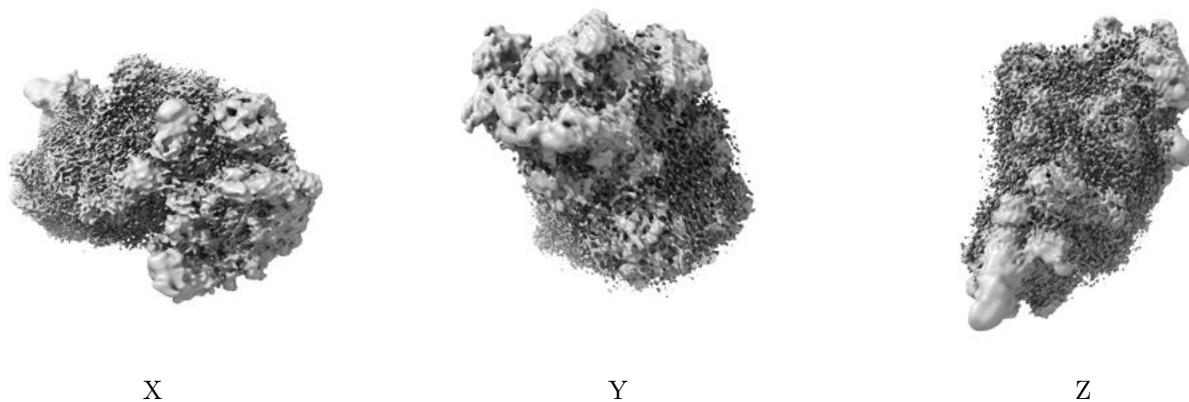


Z

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.

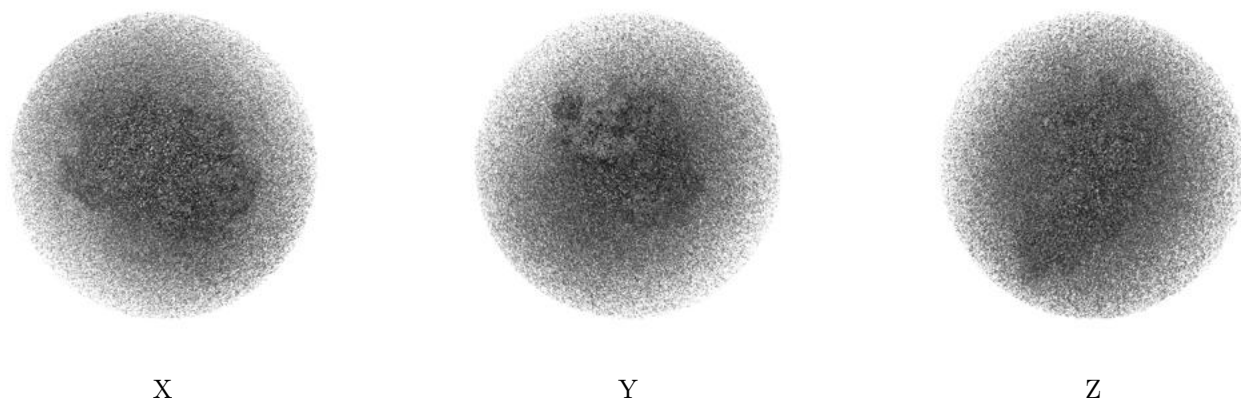
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

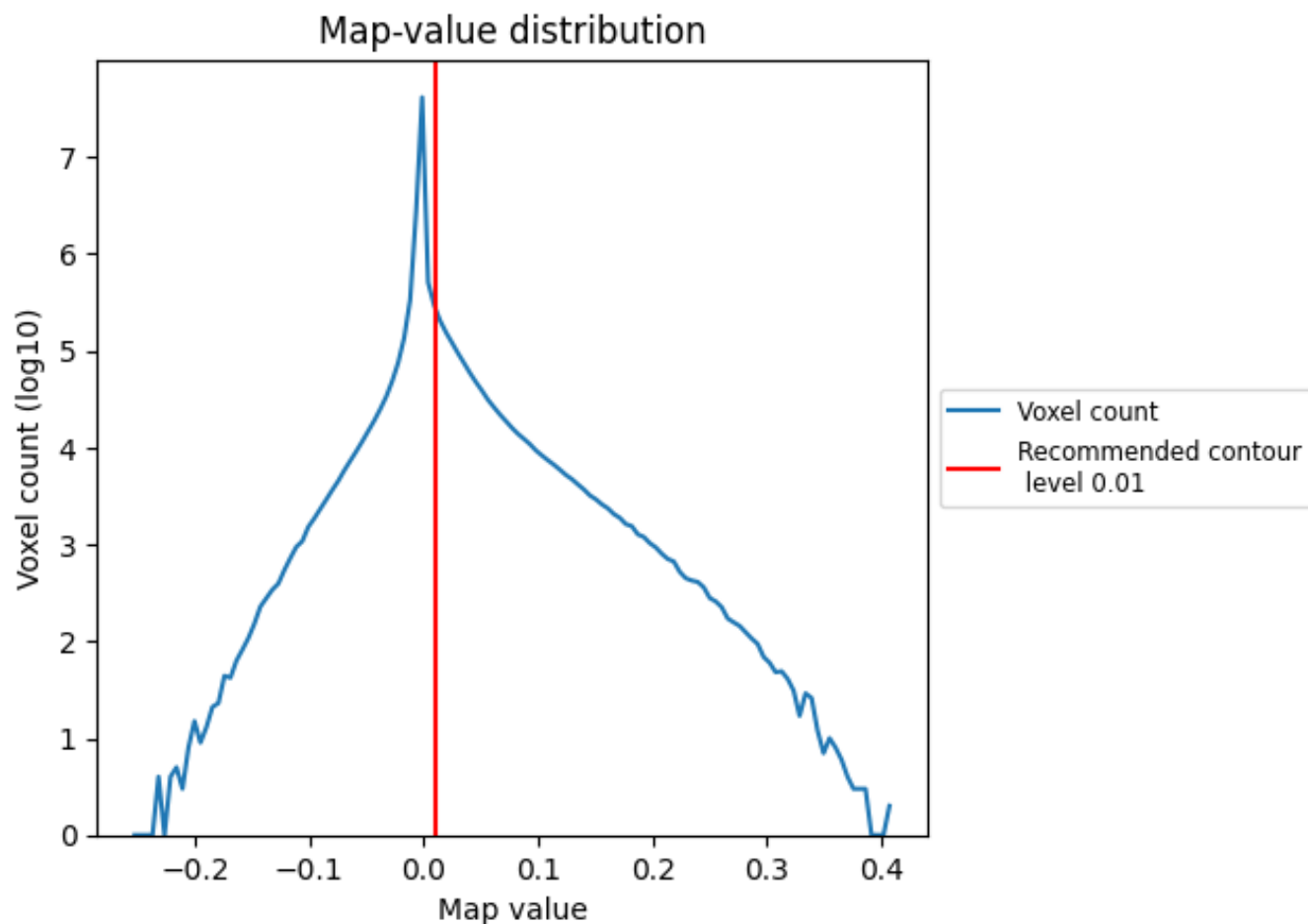
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

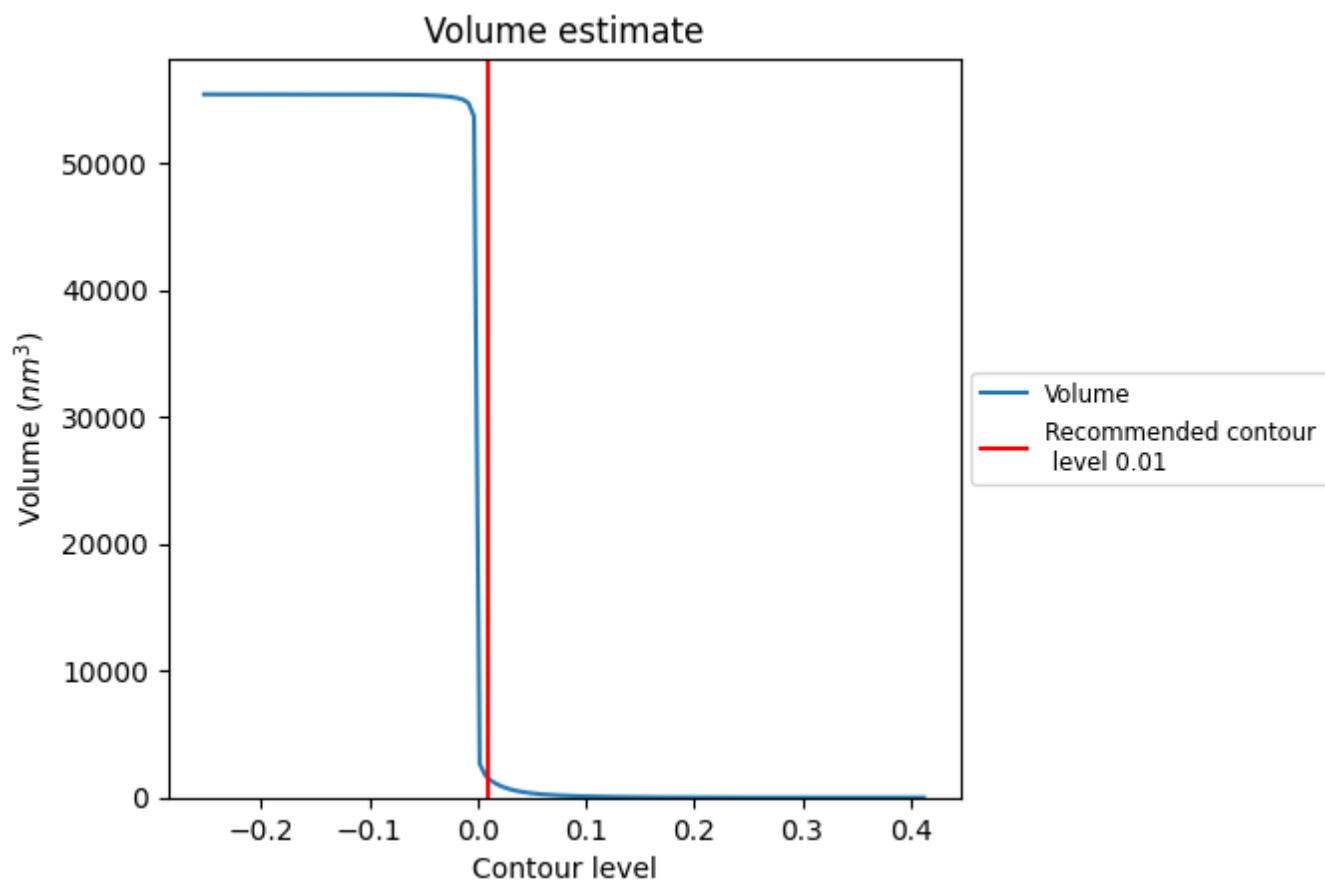
This section contains the results of statistical analysis of the map.

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.

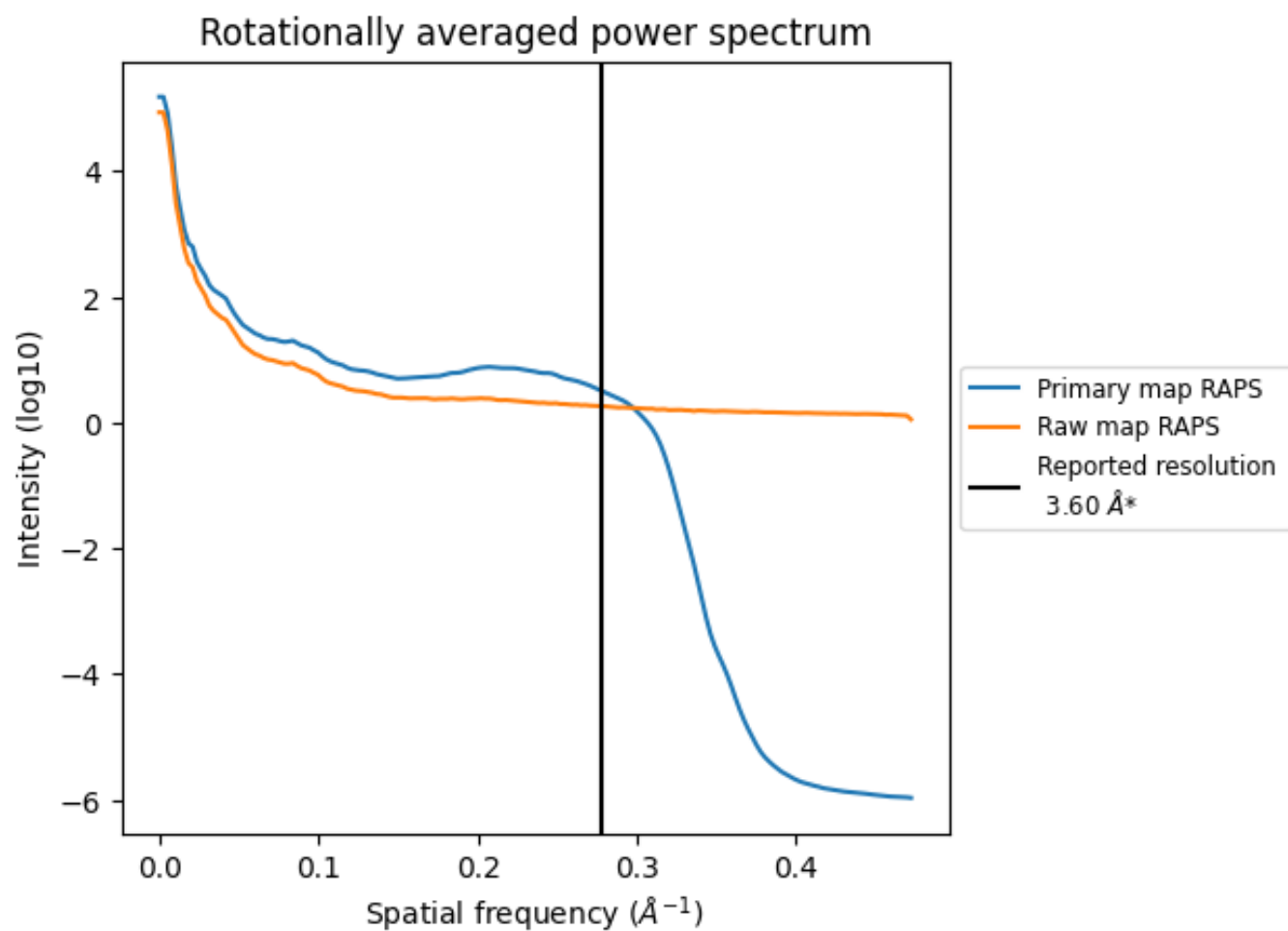
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1517 nm^3 ; this corresponds to an approximate mass of 1370 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

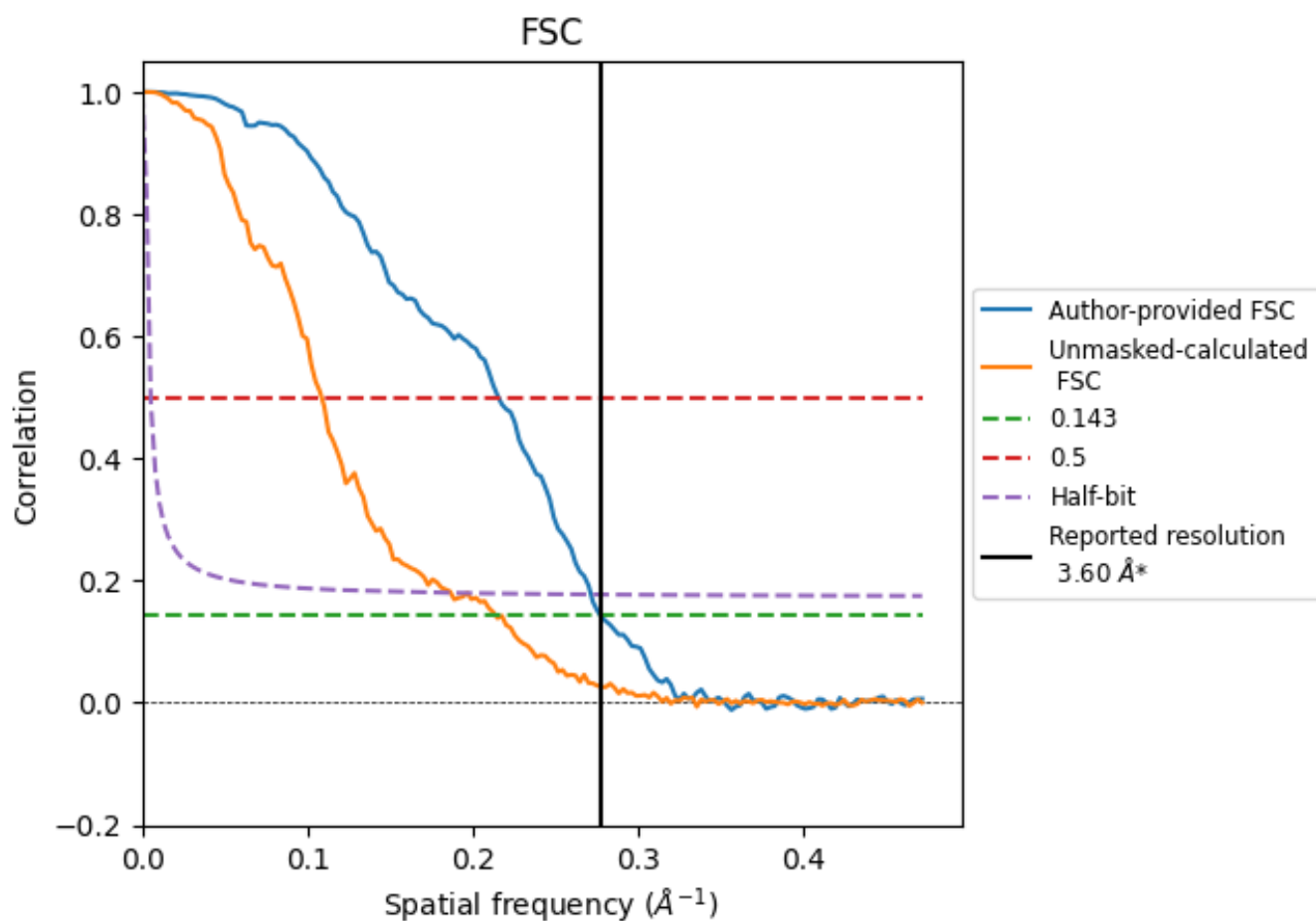


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

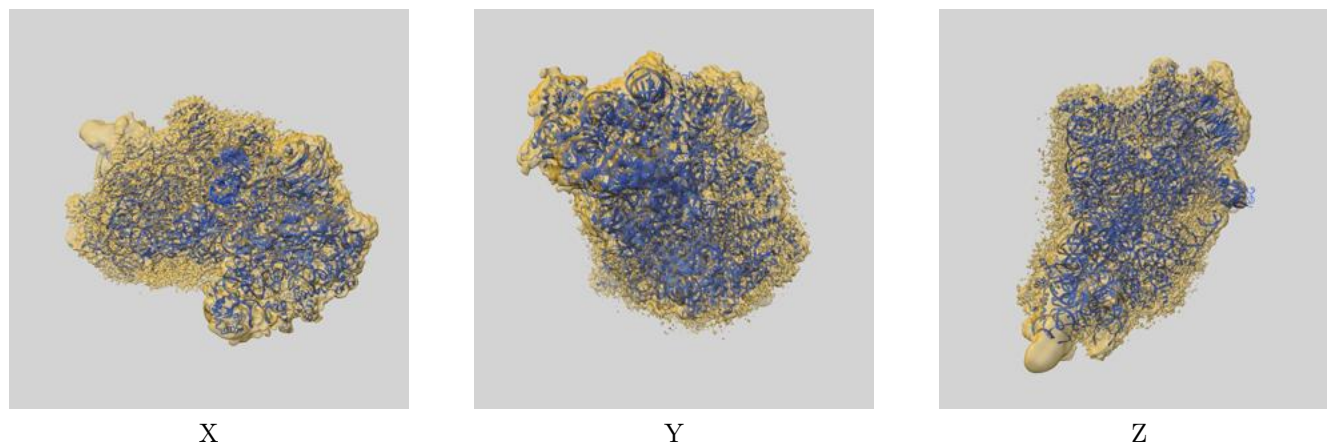
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.64	3.68
Unmasked-calculated*	4.68	9.21	5.36

*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 4.68 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

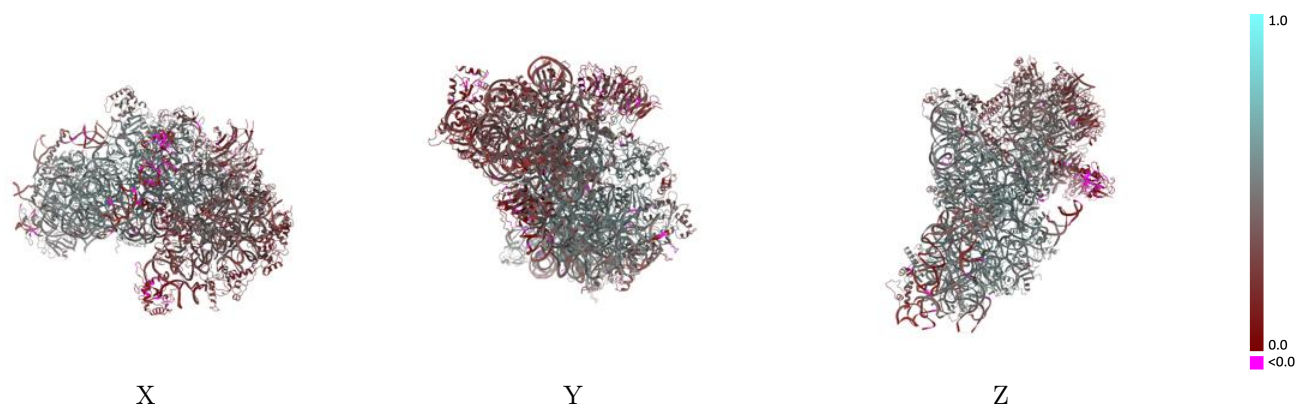
This section contains information regarding the fit between EMDB map EMD-39956 and PDB model 8ZDB. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



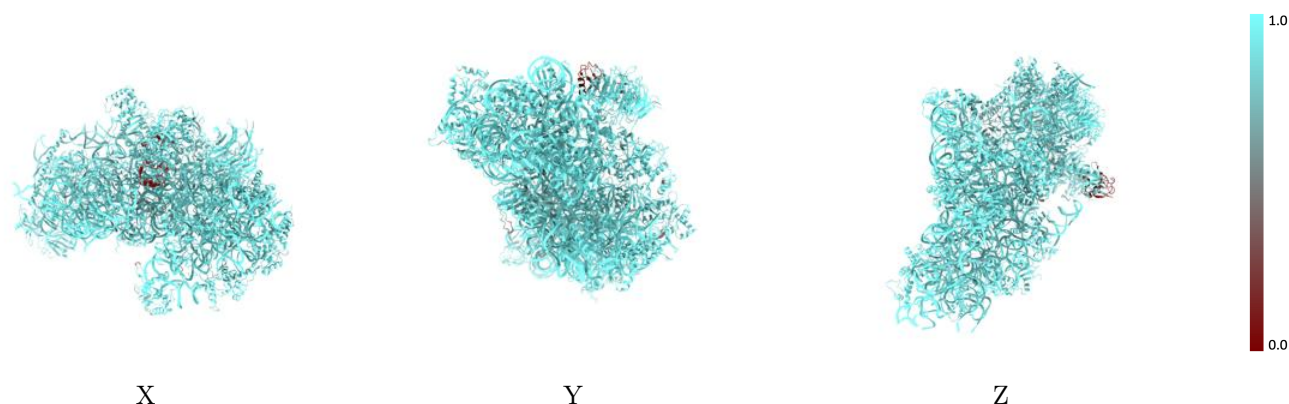
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



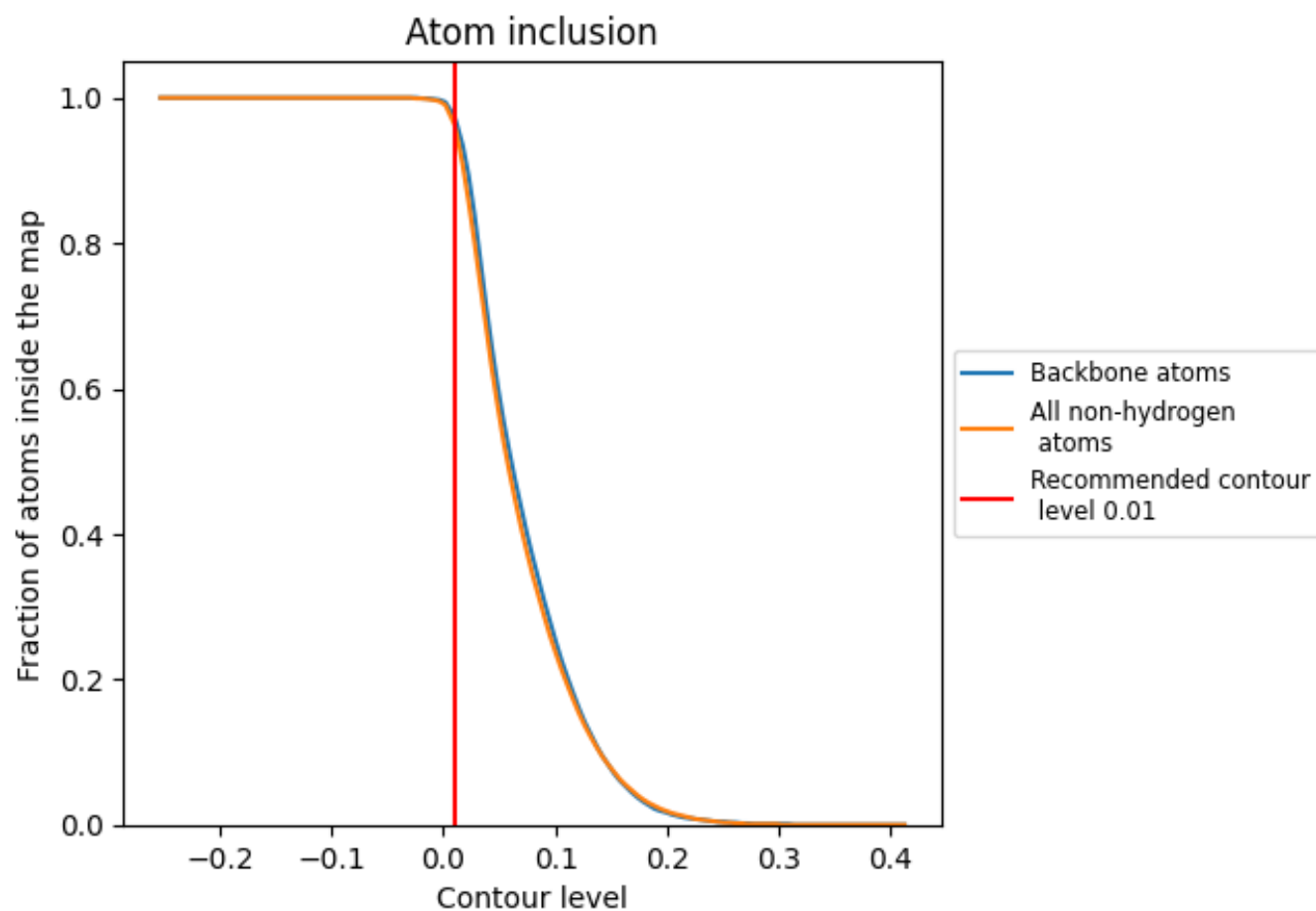
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.9630	 0.4140
2	 0.9870	 0.4410
A	 0.9790	 0.5110
B	 0.9720	 0.4570
C	 0.9780	 0.5350
D	 0.9330	 0.3480
E	 0.9860	 0.5330
F	 0.9620	 0.3740
G	 0.9820	 0.4340
H	 0.9780	 0.4270
I	 0.9820	 0.4710
J	 0.9790	 0.5230
K	 0.9530	 0.2730
L	 0.9780	 0.5210
M	 0.9160	 0.1250
N	 0.9850	 0.5050
O	 0.9730	 0.4600
P	 0.9540	 0.2570
Q	 0.9670	 0.3820
R	 0.9270	 0.3790
S	 0.9450	 0.2410
T	 0.9610	 0.3110
U	 0.9630	 0.3450
V	 0.9850	 0.5180
W	 0.9830	 0.5580
X	 0.9730	 0.5200
Y	 0.9850	 0.4920
Z	 0.9520	 0.2240
a	 0.9530	 0.4950
b	 0.9650	 0.4240
c	 0.9410	 0.3400
d	 0.9680	 0.3850
e	 0.9600	 0.4650
f	 0.8020	 0.1380
g	 0.9640	 0.2730



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Chain	Atom inclusion	Q-score
h	 0.7100	 0.2910
i	 0.2490	 0.0650
j	 0.7340	 0.0720
p	 0.8270	 0.2170