



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 01:22 PM UTC

PDB ID : 6N8N / pdb_00006n8n
EMDB ID : EMD-0373
Title : Cryo-EM structure of Lsg1-engaged (LE) pre-60S ribosomal subunit
Authors : Zhou, Y.; Musalgaonkar, S.; Johnson, A.W.; Taylor, D.W.
Deposited on : 2018-11-29
Resolution : 3.80 Å(reported)
Based on initial model : 5T62

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

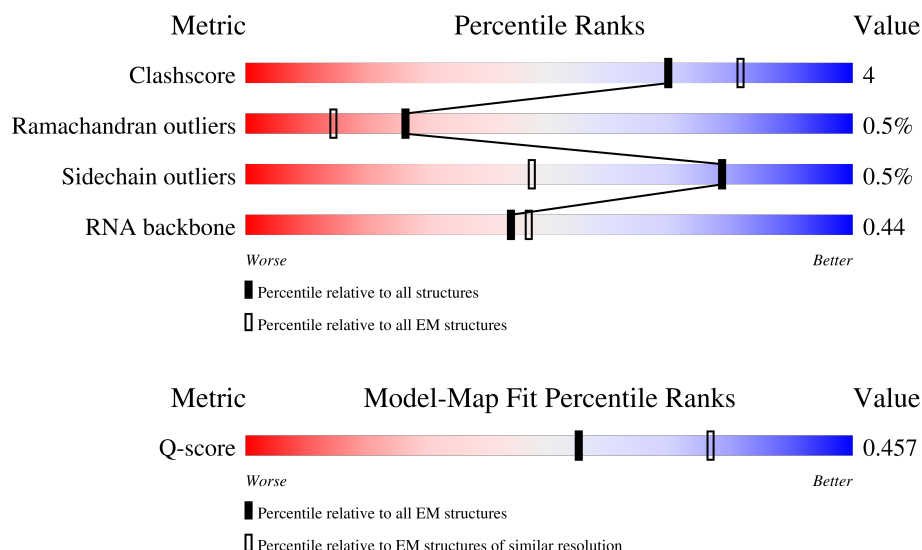
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

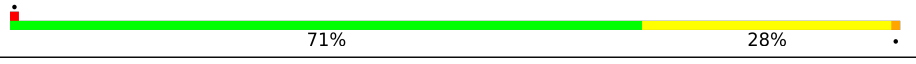
The reported resolution of this entry is 3.80 Å.

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



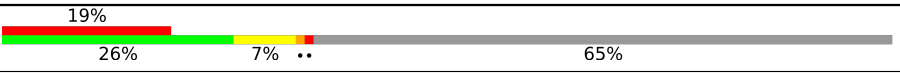
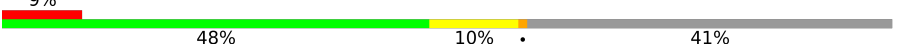
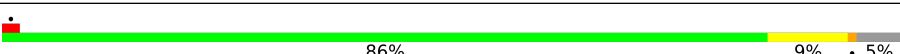
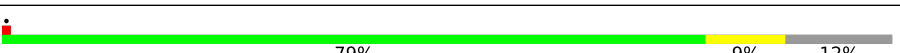
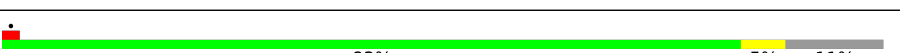
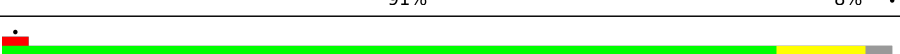
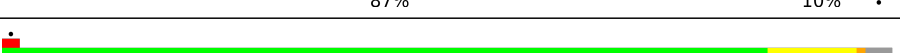
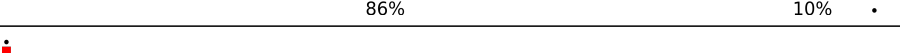
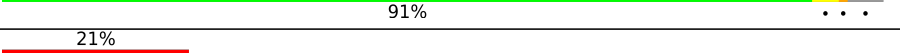
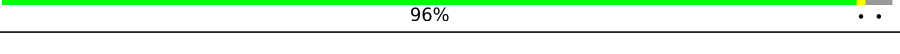
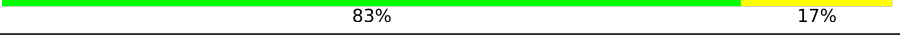
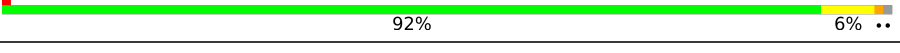
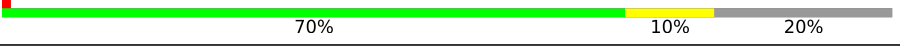
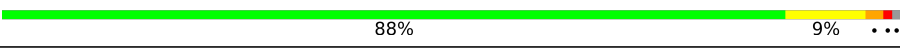
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	A	3396	
2	B	121	
3	C	158	

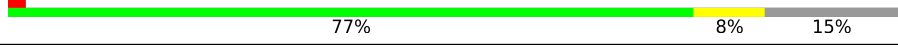
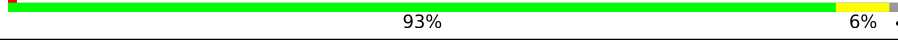
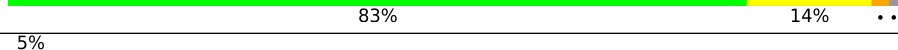
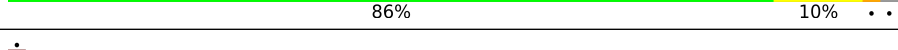
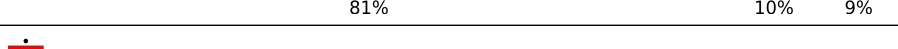
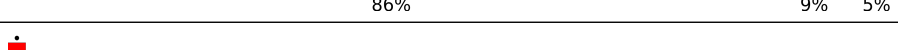
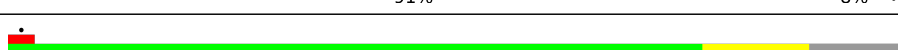
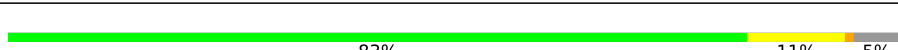
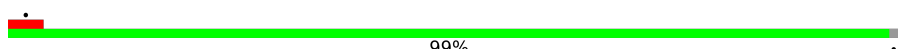
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Mol	Chain	Length	Quality of chain
4	Y	364	
5	X	245	
6	W	640	
7	V	518	
8	D	254	
9	E	387	
10	F	362	
11	G	297	
12	H	176	
13	I	244	
14	J	256	
15	K	191	
16	M	174	
17	N	199	
18	O	138	
19	Q	106	
20	R	92	
21	S	217	
22	a	204	
23	b	199	
24	c	184	
25	d	186	
26	e	189	
27	f	172	
28	g	160	

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Mol	Chain	Length	Quality of chain
29	h	121	
30	i	137	
31	j	155	
32	k	142	
33	l	127	
34	m	136	
35	n	149	
36	o	59	
37	p	105	
38	q	113	
39	r	130	
40	s	107	
41	t	121	
42	u	120	
43	v	100	
44	w	88	
45	x	78	
46	y	51	
47	z	128	
48	L	165	

2 Entry composition [i](#)

There are 48 unique types of molecules in this entry. The entry contains 131813 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 *Saccharomyces cerevisiae* S288C 35S pre-ribosomal RNA (RDN37-1), miscRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3203	Total	C	N	O	P	0	0
			68513	30603	12353	22354	3203		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 4 is a protein called Tyrosine-protein phosphatase YVH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Y	128	Total	C	N	O	S	0	0
			991	625	179	179	8		

- Molecule 5 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	X	234	Total	C	N	O	S	0	0
			1710	1063	294	346	7		

- Molecule 6 is a protein called Large subunit GTPase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	W	377	Total	C	N	O	S	0	0
			2972	1903	516	546	7		

- Molecule 7 is a protein called 60S ribosomal export protein NMD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	V	392	Total	C	N	O	S	0	0
			3034	1930	523	561	20		

- Molecule 8 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	246	Total	C	N	O	S	0	0
			1874	1168	380	325	1		

- Molecule 9 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	384	Total	C	N	O	S	0	0
			3059	1940	582	529	8		

- Molecule 10 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 11 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	283	Total	C	N	O	S	0	0
			2280	1441	397	440	2		

- Molecule 12 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	155	Total	C	N	O	S	0	0
			1217	785	220	211	1		

- Molecule 13 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	220	Total	C	N	O	S	0	0
			1770	1143	322	304	1		

- Molecule 14 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	227	Total	C	N	O	S	0	0
			1762	1128	315	316	3		

- Molecule 15 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	188	Total	C	N	O	S	0	0
			1493	948	271	270	4		

- Molecule 16 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	168	Total	C	N	O	S	0	0
			1344	841	251	248	4		

- Molecule 17 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	193	Total	C	N	O		0	0
			1539	959	314	266			

- Molecule 18 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 19 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	102	Total	C	N	O	S	0	0
			819	514	166	134	5		

- Molecule 20 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	88	Total	C	N	O	S	0	0
			673	416	135	116	6		

- Molecule 21 is a protein called Ribosomal Protein uL1.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	S	210	Total	C	N	O	0	0
			1050	630	210	210		

- Molecule 22 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 23 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 24 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	c	183	Total	C	N	O	0	0
			1420	882	281	257		

- Molecule 25 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	d	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 26 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	e	151	Total	C	N	O	0	0
			1219	757	258	204		

- Molecule 27 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	f	170	Total	C	N	O	S	0	0
			1432	922	265	242	3		

- Molecule 28 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	g	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 29 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	h	97	Total	C	N	O		0	0
			766	496	126	144			

- Molecule 30 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	i	132	Total	C	N	O	S	0	0
			981	617	184	173	7		

- Molecule 31 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	61	Total	C	N	O	S	0	0
			509	328	100	80	1		

- Molecule 32 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	k	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 33 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	l	125	Total	C	N	O		0	0
			984	620	191	173			

- Molecule 34 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	m	135	Total	C	N	O		0	0
			1092	710	202	180			

- Molecule 35 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	n	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 36 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	o	58	Total	C	N	O		0	0
			462	289	100	73			

- Molecule 37 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	p	96	Total	C	N	O	S	0	0
			737	476	123	137	1		

- Molecule 38 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	q	107	Total	C	N	O	S	0	0
			866	550	165	150	1		

- Molecule 39 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	r	126	Total	C	N	O	S	0	0
			1012	641	204	166	1		

- Molecule 40 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	s	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 41 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	t	109	Total	C	N	O	S	0	0
			861	533	175	149	4		

- Molecule 42 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 43 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	98	Total	C	N	O	S	0	0
			753	471	150	130	2		

- Molecule 44 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	84	Total	C	N	O	S	0	0
			665	405	145	110	5		

- Molecule 45 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	77	Total	C	N	O		0	0
			608	388	114	106			

- Molecule 46 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	y	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 47 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z	51	Total	C	N	O	S	0	0
			408	253	84	66	5		

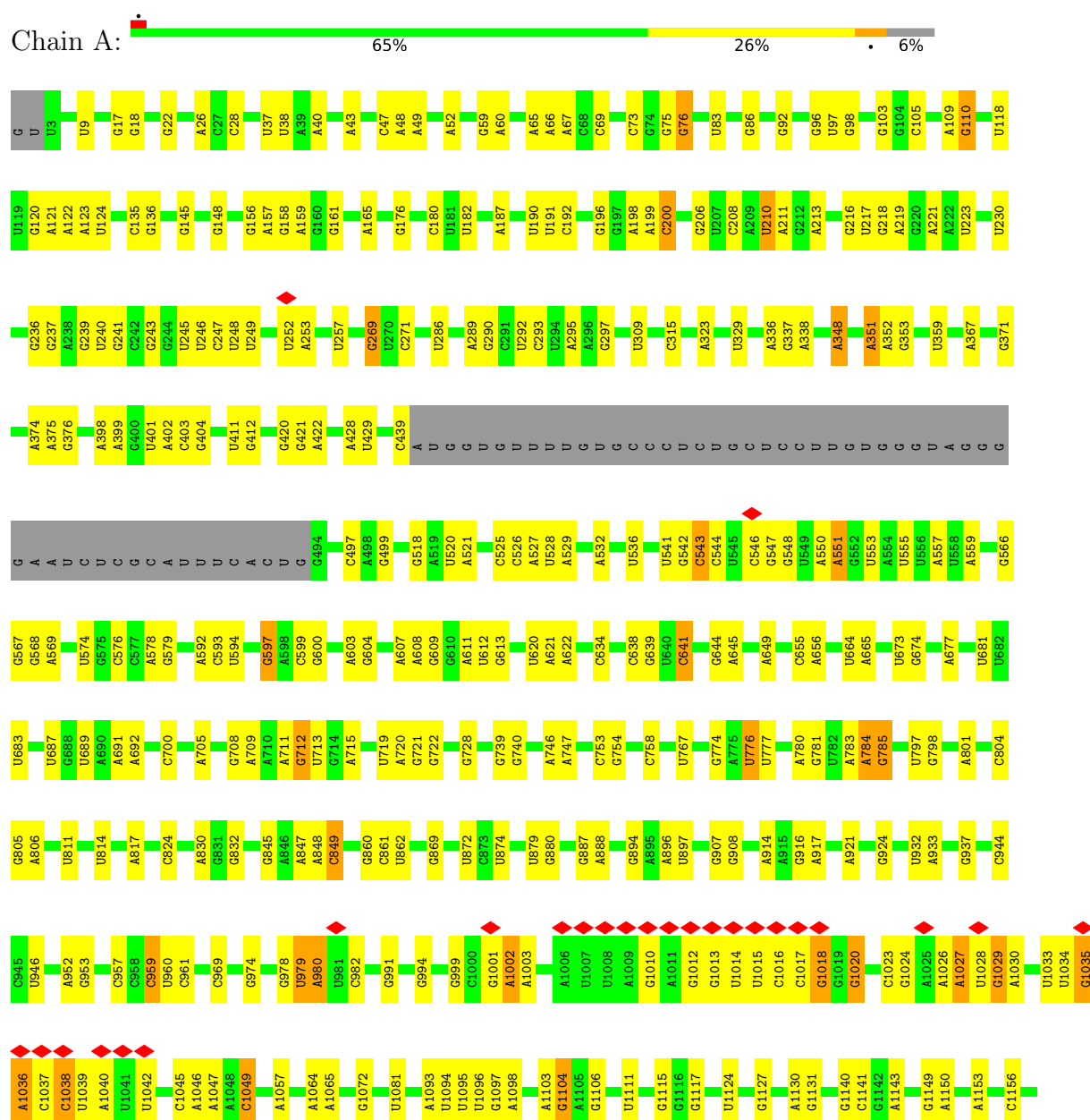
- Molecule 48 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	L	147	Total	C	N	O		0	0
			821	502	160	159			

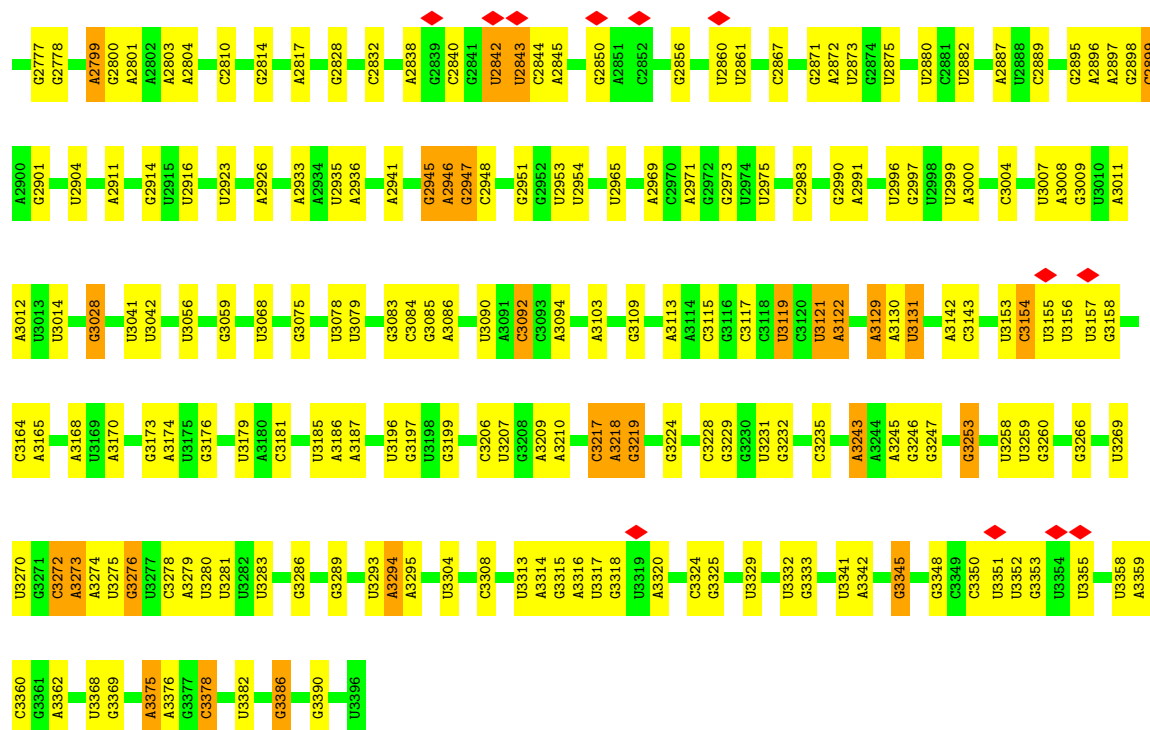
3 Residue-property plots

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: *Saccharomyces cerevisiae* S288C 35S pre-ribosomal RNA (RDN37-1), miscRNA

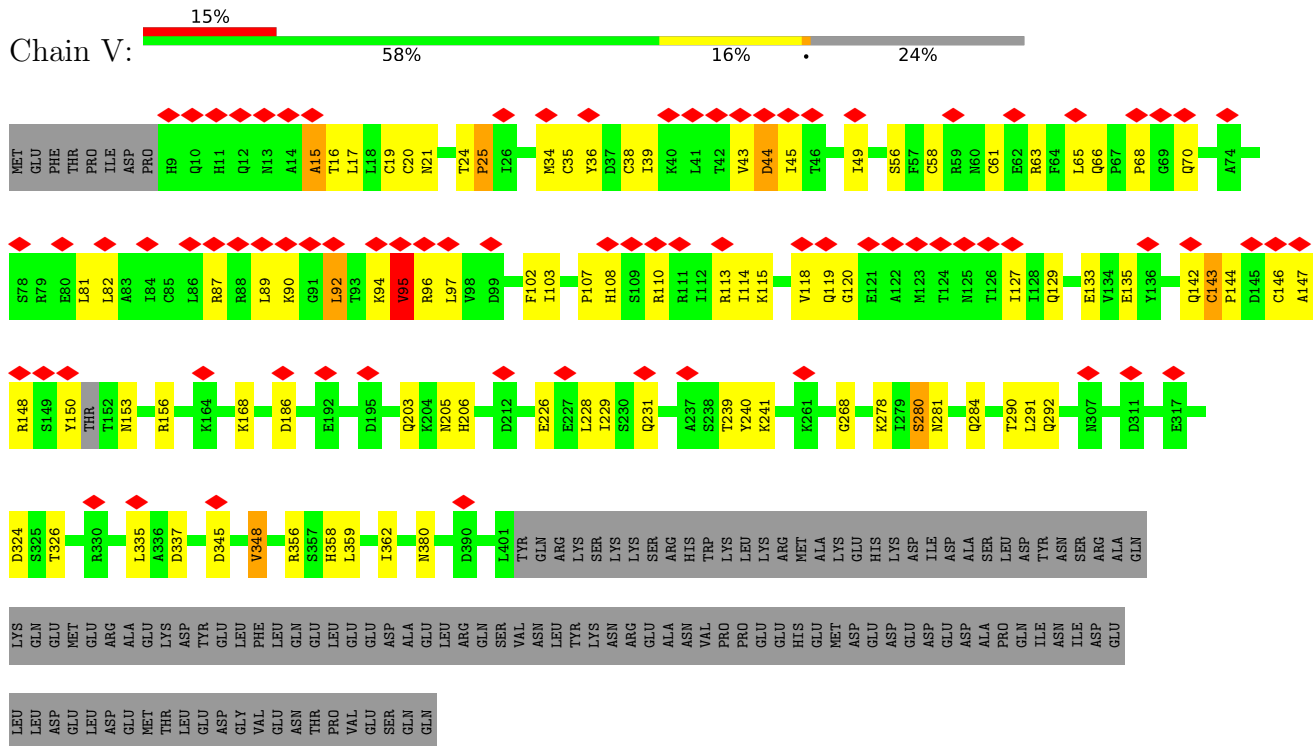




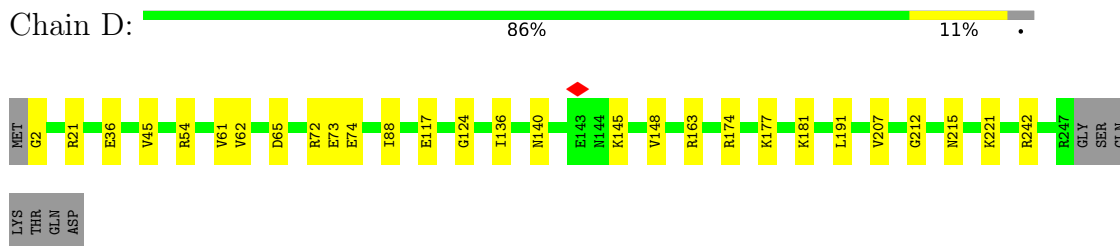




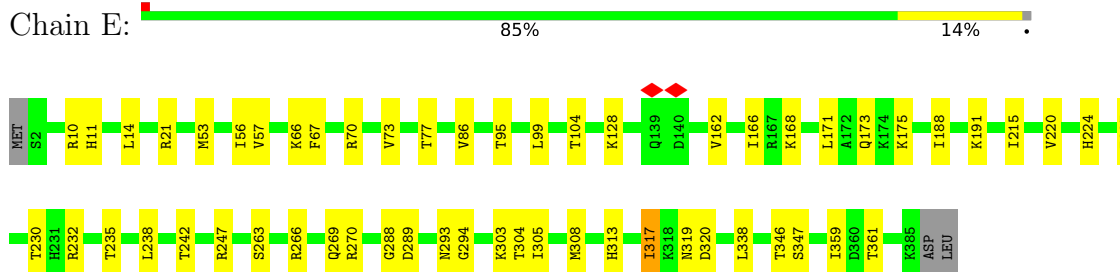
- Molecule 7: 60S ribosomal export protein NMD3



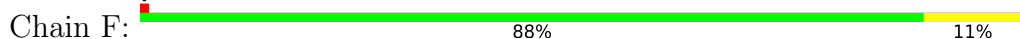
- Molecule 8: 60S ribosomal protein L2-A

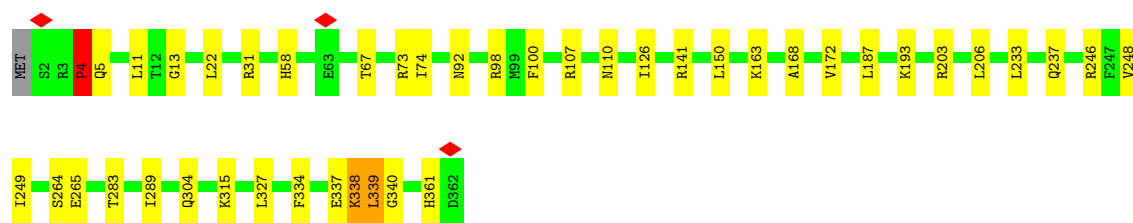


- Molecule 9: 60S ribosomal protein L3



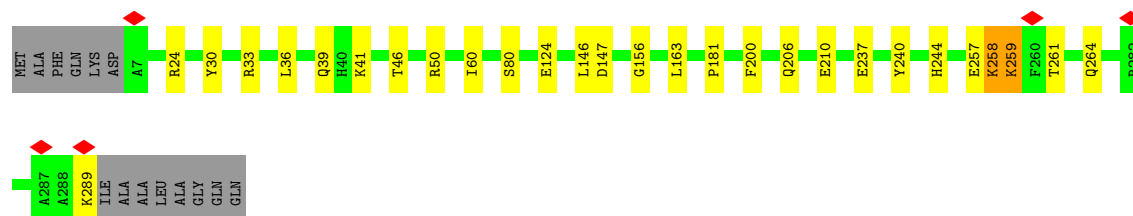
- Molecule 10: 60S ribosomal protein L4-A





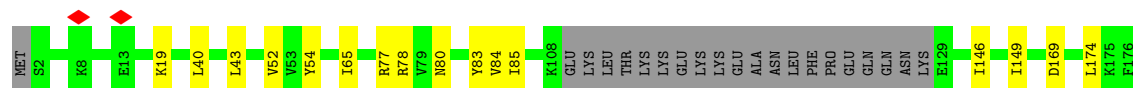
- Molecule 11: 60S ribosomal protein L5

Chain G: 86% 9% 5%



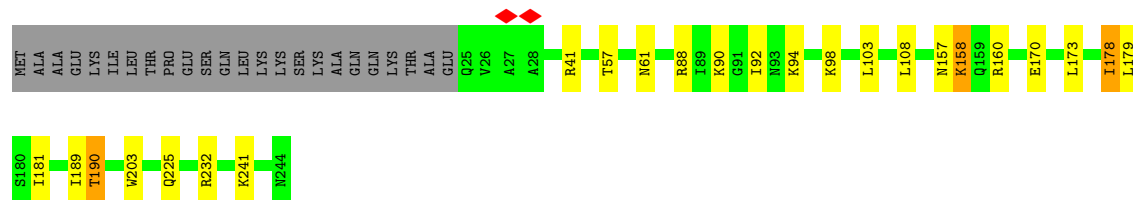
- Molecule 12: 60S ribosomal protein L6-A

Chain H: 79% 9% 12%



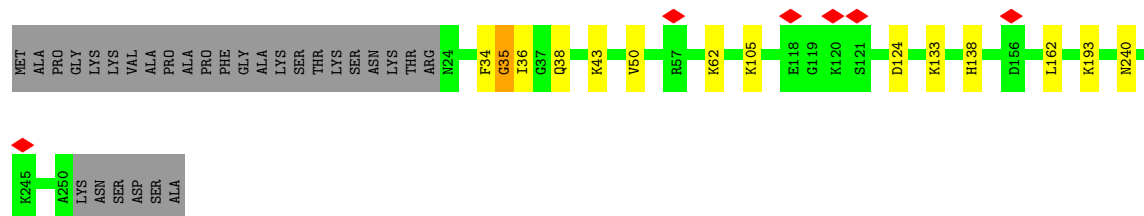
- Molecule 13: 60S ribosomal protein L7-A

Chain I: 80% 9% 10%



- Molecule 14: 60S ribosomal protein L8-A

Chain J: 83% 5% 11%



- Molecule 15: 60S ribosomal protein L9-A

Chain K:  91% 8%



- Molecule 16: 60S ribosomal protein L11-A

Chain M:  87% 10%



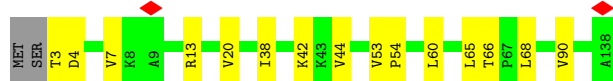
- Molecule 17: 60S ribosomal protein L13-A

Chain N:  86% 10%



- Molecule 18: 60S ribosomal protein L14-A

Chain O:  88% 11%



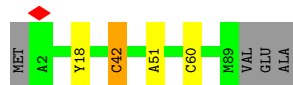
- Molecule 19: 60S ribosomal protein L42-A

Chain Q:  7% 86% 10%

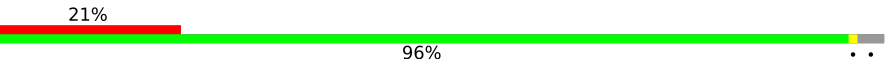


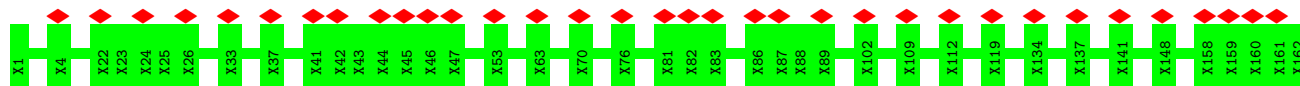
- Molecule 20: 60S ribosomal protein L43-A

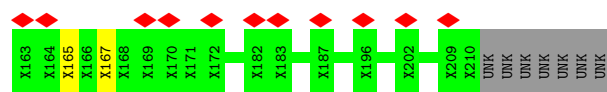
Chain R:  91% 10%



- Molecule 21: Ribosomal Protein uL1

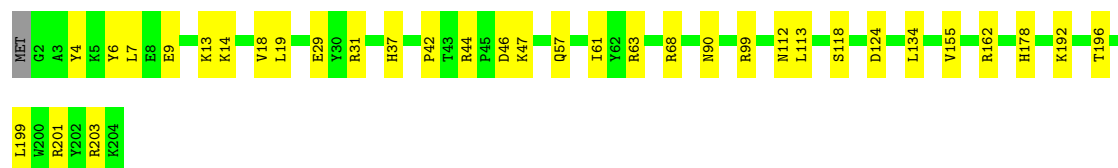
Chain S:  21% 96%





- Molecule 22: 60S ribosomal protein L15-A

Chain a: 83% 17%



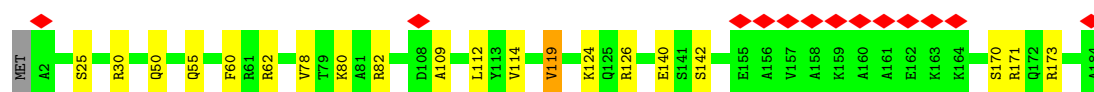
- Molecule 23: 60S ribosomal protein L16-A

Chain b: 89% 10%



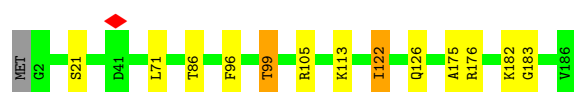
- Molecule 24: 60S ribosomal protein L17-A

Chain c: 7% 89% 10%



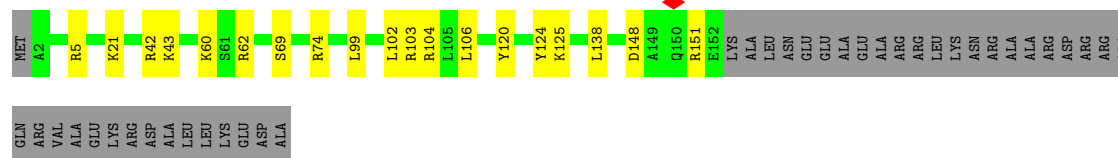
- Molecule 25: 60S ribosomal protein L18-A

Chain d: 92% 6%



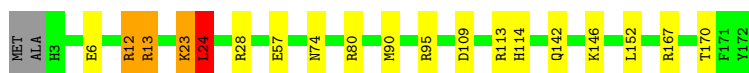
- Molecule 26: 60S ribosomal protein L19-A

Chain e: 70% 10% 20%



- Molecule 27: 60S ribosomal protein L20-A

Chain f: 88% 9%



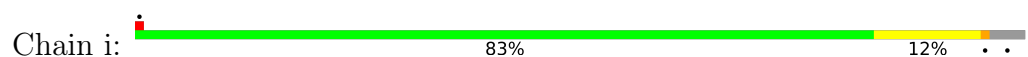
- Molecule 28: 60S ribosomal protein L21-A



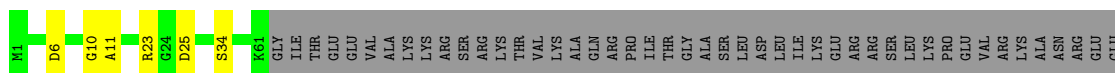
- Molecule 29: 60S ribosomal protein L22-A



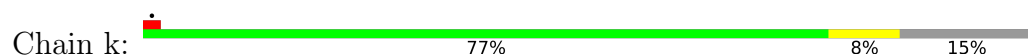
- Molecule 30: 60S ribosomal protein L23-A



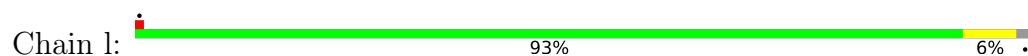
- Molecule 31: 60S ribosomal protein L24-A



- Molecule 32: 60S ribosomal protein L25

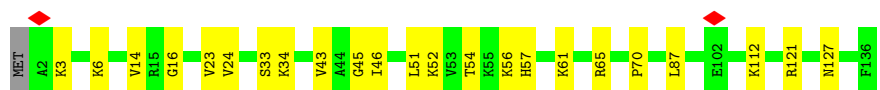


- Molecule 33: 60S ribosomal protein L26-A



- Molecule 34: 60S ribosomal protein L27-A

Chain m:  82% 17%



- Molecule 35: 60S ribosomal protein L28

Chain n:  83% 14%



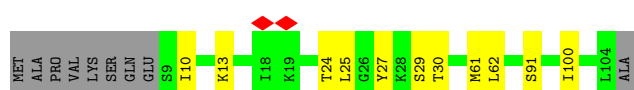
- Molecule 36: 60S ribosomal protein L29

Chain o:  5% 86% 10%



- Molecule 37: 60S ribosomal protein L30

Chain p:  81% 10% 9%



- Molecule 38: 60S ribosomal protein L31-A

Chain q:  86% 9% 5%



- Molecule 39: 60S ribosomal protein L32

Chain r:  91% 6%

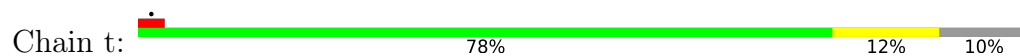


- Molecule 40: 60S ribosomal protein L33-A

Chain s:  91% 8%



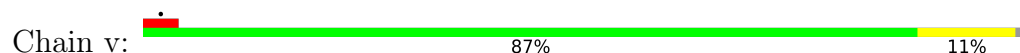
- Molecule 41: 60S ribosomal protein L34-A



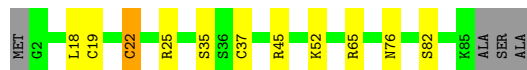
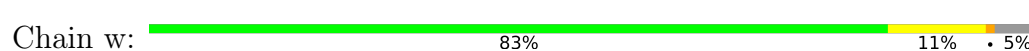
- Molecule 42: 60S ribosomal protein L35-A



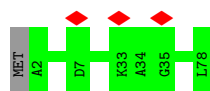
- Molecule 43: 60S ribosomal protein L36-A



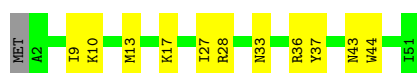
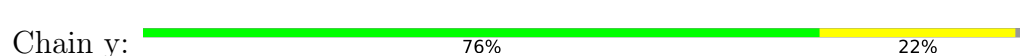
- Molecule 44: 60S ribosomal protein L37-A



- Molecule 45: 60S ribosomal protein L38



- Molecule 46: 60S ribosomal protein L39



- Molecule 47: Ubiquitin-60S ribosomal protein L40



MET	ILE	GLN	ILE	PHE	GLU	SER	VAL	THR	LEU	THR	THR	GLY	LEU	THR	THR	ILE	THR	GLY	LEU	THR	THR	GLY	VAL	GLU	SER	SER	ASP	THR	ILE	ILE	ASN	ASP	VAL	SER	LYS	SER	LYS	LYS	ILE	GLN	ASP	LYS	LYS	GLY	GLY	ILE	PRO	PRO	ASP	GLN	ARG	ARG	LEU	ILE	ILE	PHE	ALA	GLY	LYS	GLN	GLN	LEU	GLU	ASP	GLY	ARG	THR	LEU	SER	ASP	TYR	ASN
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ILE	GLN	LYS	GLU	SER	THR	LEU	HIS	VAL	LEU	ARG	LEU	ARG	GLY	GLY	I77	I78	E79	P90	K83	S87	D92	R97	Y100	P104	P105	R106	R113	R122	P123	K124	L127	LYS
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• Molecule 48: Ribosomal protein L12



MET	PRO	PRO	LYS	PHE	ASP	PRO	ASN	GLU	X10	X11	X12	X17	X18	X19	X20	X21	X22	X23	X24	X25	X26	X27	X28	X29	X30	X31	X32	X33	X34	X35	X36	X37	X38	X39	X40	X41	X44	X45	X46	X47	X48	A49	T50	K51	E52	F53	K54	G55	I56	K57	V58	T59	V60	Q61	L62	K63	I64
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Q65	N66	R67	Q68	A69	A70	A71	S72	V73	V74	V75	S76	A77	S78	S79	L80	V81	I82	T83	A84	L85	K86	E87	P88	PRO	ARG	ASP	ARG	LYS	LYS	ASP	K96	N97	V98	K99	H100	S101	G102	N103	I104	Q105	L106	D107	E108	I109	I110	X111	E112	X113	X114	X115	X116	X117	X118	X119	X120	X121	X122	X123	X124
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X125	X126	X127	X128	X129	X130	X131	X132	X133	X134	X135	X138	X139	X140	X141	X142	X143	X144	X145	X146	X147	X148	X149	X150	X151	X152	X153	X154	X155	X156	X157	X158	X159	X160	X161	X162	X163	GLU	ASN
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	54188	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.137	Depositor
Minimum map value	-0.091	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.022	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	1/76692 (0.0%)	0.36	7/119572 (0.0%)
2	B	0.27	0/2883	0.31	0/4491
3	C	0.32	0/3746	0.34	0/5832
4	Y	0.38	0/1016	1.09	12/1368 (0.9%)
5	X	0.27	0/1729	0.61	2/2355 (0.1%)
6	W	0.33	0/3035	0.86	10/4119 (0.2%)
7	V	0.32	0/3093	0.79	8/4203 (0.2%)
8	D	0.35	0/1908	0.62	2/2564 (0.1%)
9	E	0.35	0/3130	0.64	4/4206 (0.1%)
10	F	0.33	0/2800	0.67	4/3790 (0.1%)
11	G	0.28	0/2329	0.64	4/3142 (0.1%)
12	H	0.28	0/1236	0.58	0/1661
13	I	0.33	0/1807	0.64	1/2432 (0.0%)
14	J	0.30	0/1794	0.61	0/2425
15	K	0.29	0/1514	0.64	0/2039
16	M	0.27	0/1365	0.66	2/1831 (0.1%)
17	N	0.33	0/1564	0.72	3/2102 (0.1%)
18	O	0.29	0/1068	0.56	0/1438
19	Q	0.30	0/831	0.59	0/1097
20	R	0.33	0/680	0.68	0/905
22	a	0.36	0/1757	0.60	0/2354
23	b	0.32	0/1585	0.54	0/2128
24	c	0.34	0/1443	0.64	0/1944
25	d	0.32	0/1465	0.63	1/1965 (0.1%)
26	e	0.31	0/1236	0.56	0/1650
27	f	0.33	0/1468	0.62	3/1973 (0.2%)
28	g	0.30	0/1300	0.63	0/1743
29	h	0.27	0/781	0.60	0/1058
30	i	0.34	0/996	0.55	0/1340
31	j	0.27	0/521	0.55	0/691
32	k	0.32	0/979	0.57	0/1321
33	l	0.29	0/995	0.57	0/1329
34	m	0.33	0/1118	0.62	0/1497
35	n	0.34	0/1204	0.79	5/1612 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
36	o	0.32	0/473	0.83	1/629 (0.2%)
37	p	0.26	0/745	0.48	0/1001
38	q	0.35	0/880	0.66	0/1182
39	r	0.30	0/1033	0.59	2/1383 (0.1%)
40	s	0.37	0/868	0.60	0/1168
41	t	0.37	0/871	0.61	1/1164 (0.1%)
42	u	0.30	0/978	0.60	0/1301
43	v	0.28	0/759	0.64	0/1009
44	w	0.36	0/680	0.70	0/901
45	x	0.28	0/614	0.56	0/822
46	y	0.33	0/443	0.65	0/588
47	z	0.23	0/414	0.54	0/551
48	L	0.33	0/363	0.94	4/493 (0.8%)
All	All	0.31	1/140189 (0.0%)	0.49	76/206369 (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
4	Y	0	3
5	X	0	2
6	W	0	17
7	V	0	4
9	E	0	1
10	F	0	2
11	G	0	2
13	I	0	3
14	J	0	2
15	K	0	1
16	M	0	2
17	N	0	1
27	f	0	1
35	n	0	3
36	o	0	2
42	u	0	1
All	All	0	47

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2259	A	C1'-N9	-6.05	1.38	1.48

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	t	81	CYS	CA-CB-SG	8.42	133.76	114.40
6	W	337	ILE	CA-C-N	7.36	135.60	121.54
6	W	337	ILE	C-N-CA	7.36	135.60	121.54
11	G	258	LYS	CA-C-N	7.24	135.37	121.54
11	G	258	LYS	C-N-CA	7.24	135.37	121.54
4	Y	331	ILE	CG1-CB-CG2	-7.11	89.38	110.70
4	Y	328	LYS	CA-C-N	6.90	134.72	121.54
4	Y	328	LYS	C-N-CA	6.90	134.72	121.54
4	Y	331	ILE	N-CA-C	-6.81	94.17	108.88
35	n	47	LYS	CA-C-N	6.76	134.45	121.54
35	n	47	LYS	C-N-CA	6.76	134.45	121.54
11	G	257	GLU	CA-C-N	6.68	134.30	121.54
11	G	257	GLU	C-N-CA	6.68	134.30	121.54
7	V	44	ASP	CA-C-N	6.54	133.74	121.97
7	V	44	ASP	C-N-CA	6.54	133.74	121.97
17	N	93	ILE	N-CA-C	-6.47	105.04	111.77
4	Y	325	SER	CA-C-N	6.28	133.53	121.54
4	Y	325	SER	C-N-CA	6.28	133.53	121.54
25	d	99	THR	N-CA-C	6.21	118.31	110.24
7	V	95	VAL	N-CA-C	6.10	122.03	109.34
35	n	116	GLY	N-CA-C	6.08	127.60	113.18
27	f	13	ARG	N-CA-CB	-6.01	100.33	110.49
7	V	43	VAL	CA-C-N	-5.99	113.71	121.79
7	V	43	VAL	C-N-CA	-5.99	113.71	121.79
4	Y	329	TRP	N-CA-C	-5.98	98.06	110.80
4	Y	330	VAL	CA-C-N	5.92	133.08	122.13
4	Y	330	VAL	C-N-CA	5.92	133.08	122.13
4	Y	326	CYS	CB-CA-C	-5.79	98.91	110.42
1	A	1576	G	P-O3'-C3'	5.74	128.81	120.20
5	X	161	VAL	CA-C-N	5.72	128.80	120.51
5	X	161	VAL	C-N-CA	5.72	128.80	120.51
36	o	22	LYS	N-CA-C	5.67	118.29	110.35
1	A	2541	U	P-O3'-C3'	5.61	128.61	120.20
10	F	13	GLY	CA-C-N	5.57	129.01	120.82
10	F	13	GLY	C-N-CA	5.57	129.01	120.82
1	A	1029	G	P-O3'-C3'	5.55	128.52	120.20
7	V	348	VAL	CA-C-N	5.50	128.91	120.82
7	V	348	VAL	C-N-CA	5.50	128.91	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	W	306	LYS	CA-C-N	5.42	127.60	120.60
6	W	306	LYS	C-N-CA	5.42	127.60	120.60
9	E	313	HIS	CA-C-N	-5.42	115.07	121.90
9	E	313	HIS	C-N-CA	-5.42	115.07	121.90
6	W	363	SER	CA-C-N	5.39	128.65	120.13
6	W	363	SER	C-N-CA	5.39	128.65	120.13
35	n	23	GLY	CA-C-N	5.39	131.84	121.54
35	n	23	GLY	C-N-CA	5.39	131.84	121.54
27	f	23	LYS	CA-C-N	5.34	131.74	121.54
27	f	23	LYS	C-N-CA	5.34	131.74	121.54
1	A	1038	C	P-O3'-C3'	5.34	128.21	120.20
1	A	1815	U	P-O3'-C3'	5.33	128.20	120.20
48	L	105	GLN	CA-C-N	5.33	127.73	120.54
48	L	105	GLN	C-N-CA	5.33	127.73	120.54
16	M	54	VAL	CA-C-N	5.32	131.71	121.54
16	M	54	VAL	C-N-CA	5.32	131.71	121.54
10	F	337	GLU	CA-C-N	5.29	131.65	121.54
10	F	337	GLU	C-N-CA	5.29	131.65	121.54
4	Y	326	CYS	N-CA-C	5.28	122.04	110.80
8	D	212	GLY	CA-C-N	5.26	131.72	121.41
8	D	212	GLY	C-N-CA	5.26	131.72	121.41
17	N	75	PHE	CA-C-N	5.25	131.57	121.54
17	N	75	PHE	C-N-CA	5.25	131.57	121.54
4	Y	323	ARG	N-CA-CB	-5.24	101.64	110.49
1	A	979	U	P-O3'-C3'	5.23	128.04	120.20
6	W	314	GLU	CA-C-N	5.12	131.32	121.54
6	W	314	GLU	C-N-CA	5.12	131.32	121.54
6	W	241	LEU	CA-C-N	5.11	131.30	121.54
6	W	241	LEU	C-N-CA	5.11	131.30	121.54
1	A	1027	A	P-O3'-C3'	5.11	127.87	120.20
48	L	106	LEU	CA-C-N	5.09	129.29	121.19
48	L	106	LEU	C-N-CA	5.09	129.29	121.19
9	E	220	VAL	CA-C-N	5.05	128.38	120.75
9	E	220	VAL	C-N-CA	5.05	128.38	120.75
39	r	11	LYS	CA-C-N	5.04	131.16	121.54
39	r	11	LYS	C-N-CA	5.04	131.16	121.54
7	V	153	ASN	N-CA-C	-5.02	106.08	113.61
13	I	158	LYS	N-CA-CB	-5.01	102.02	110.49

There are no chirality outliers.

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	E	346	THR	Peptide
10	F	338	LYS	Peptide
10	F	4	PRO	Peptide
11	G	124	GLU	Peptide
11	G	258	LYS	Peptide
13	I	157	ASN	Peptide
13	I	190	THR	Peptide
13	I	232	ARG	Peptide
14	J	34	PHE	Peptide
14	J	35	GLY	Peptide
15	K	21	LYS	Peptide
16	M	171	VAL	Peptide
16	M	7	ASN	Peptide
17	N	46	ILE	Peptide
7	V	15	ALA	Peptide
7	V	25	PRO	Peptide
7	V	280	SER	Peptide
7	V	44	ASP	Peptide
6	W	134	LEU	Peptide
6	W	136	VAL	Peptide
6	W	142	TRP	Peptide
6	W	176	LEU	Peptide
6	W	225	SER	Peptide
6	W	337	ILE	Peptide
6	W	362	VAL	Peptide
6	W	363	SER	Peptide
6	W	364	VAL	Peptide
6	W	371	THR	Peptide
6	W	373	HIS	Peptide
6	W	379	LEU	Peptide
6	W	394	PRO	Peptide
6	W	427	ARG	Peptide
6	W	441	ILE	Peptide
6	W	445	SER	Peptide
6	W	467	ALA	Peptide
5	X	142	ILE	Peptide
5	X	7	PHE	Peptide
4	Y	325	SER	Peptide
4	Y	326	CYS	Peptide
4	Y	327	GLY	Peptide
27	f	12	ARG	Peptide
35	n	116	GLY	Peptide
35	n	14	HIS	Peptide

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Mol	Chain	Res	Type	Group
35	n	23	GLY	Peptide
36	o	21	ILE	Peptide
36	o	25	LYS	Peptide
42	u	83	LYS	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	A	68513	0	34427	315	0
2	B	2579	0	1304	15	0
3	C	3353	0	1695	14	0
4	Y	991	0	980	19	0
5	X	1710	0	1667	9	0
6	W	2972	0	2973	29	0
7	V	3034	0	3004	70	0
8	D	1874	0	1943	18	0
9	E	3059	0	3127	35	0
10	F	2748	0	2859	30	0
11	G	2280	0	2230	16	0
12	H	1217	0	1308	10	0
13	I	1770	0	1851	15	0
14	J	1762	0	1839	10	0
15	K	1493	0	1566	10	0
16	M	1344	0	1370	8	0
17	N	1539	0	1597	12	0
18	O	1053	0	1149	9	0
19	Q	819	0	890	7	0
20	R	673	0	715	3	0
21	S	1050	0	235	1	0
22	a	1720	0	1779	27	0
23	b	1555	0	1659	12	0
24	c	1420	0	1437	12	0
25	d	1441	0	1543	8	0
26	e	1219	0	1301	13	0
27	f	1432	0	1470	14	0
28	g	1276	0	1323	10	0
29	h	766	0	782	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	i	981	0	1031	13	0
31	j	509	0	537	3	0
32	k	964	0	1025	7	0
33	l	984	0	1075	6	0
34	m	1092	0	1155	15	0
35	n	1173	0	1215	13	0
36	o	462	0	491	5	0
37	p	737	0	792	7	0
38	q	866	0	908	7	0
39	r	1012	0	1079	4	0
40	s	850	0	880	6	0
41	t	861	0	919	10	0
42	u	969	0	1078	4	0
43	v	753	0	826	8	0
44	w	665	0	668	10	0
45	x	608	0	671	0	0
46	y	436	0	475	7	0
47	z	408	0	446	5	0
48	L	821	0	434	19	0
All	All	131813	0	95728	730	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 4.

All (730) 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)
48:L:97:ASN:O	48:L:99:LYS:HD2	1.47	1.14
7:V:49:ILE:HG22	7:V:90:LYS:HG3	1.28	1.08
7:V:96:ARG:HD3	7:V:119:GLN:HE22	1.14	1.06
1:A:2247:G:C6	1:A:2248:C:C5	2.44	1.05
7:V:90:LYS:HE2	7:V:90:LYS:HA	1.41	1.00
7:V:49:ILE:CG2	7:V:90:LYS:HG3	1.90	1.00
7:V:95:VAL:CB	7:V:120:GLY:H	1.73	1.00
1:A:2247:G:C5	1:A:2248:C:C5	2.56	0.93
7:V:96:ARG:HD3	7:V:119:GLN:NE2	1.83	0.92
1:A:2249:G:N7	1:A:2272:G:C5	2.40	0.90
1:A:2249:G:O6	1:A:2272:G:N1	2.06	0.89
48:L:97:ASN:O	48:L:99:LYS:CD	2.20	0.89
48:L:28:UNK:O	48:L:32:UNK:N	2.05	0.88
7:V:95:VAL:CB	7:V:120:GLY:N	2.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:49:ILE:HG22	7:V:90:LYS:CG	2.05	0.86
7:V:94:LYS:HE3	7:V:97:LEU:HD11	1.57	0.86
7:V:92:LEU:H	7:V:92:LEU:HD23	1.42	0.83
7:V:95:VAL:CB	7:V:120:GLY:CA	2.58	0.81
1:A:2247:G:C5	1:A:2248:C:H5	1.98	0.81
7:V:89:LEU:HD13	7:V:89:LEU:O	1.82	0.79
7:V:90:LYS:HE2	7:V:90:LYS:CA	2.13	0.77
7:V:95:VAL:CB	7:V:120:GLY:HA3	2.14	0.77
4:Y:307:CYS:SG	4:Y:310:CYS:N	2.60	0.75
7:V:92:LEU:H	7:V:92:LEU:CD2	2.00	0.73
1:A:3274:A:H2'	24:c:171:ARG:HH12	1.57	0.70
1:A:2254:U:H5''	1:A:2259:A:H61	1.57	0.68
23:b:37:ARG:HH21	23:b:160:ARG:HH22	1.39	0.68
1:A:2254:U:C5'	1:A:2259:A:H61	2.06	0.68
9:E:53:MET:HG2	9:E:77:THR:HG22	1.74	0.68
7:V:58:CYS:SG	7:V:61:CYS:N	2.66	0.67
48:L:28:UNK:O	48:L:32:UNK:CB	2.43	0.67
4:Y:276:SER:HB3	4:Y:326:CYS:HA	1.76	0.67
7:V:92:LEU:HD23	7:V:92:LEU:N	2.10	0.66
27:f:80:ARG:HE	28:g:156:TYR:HB2	1.58	0.66
1:A:664:U:H5'	10:F:107:ARG:HA	1.78	0.66
1:A:1383:G:OP1	10:F:203:ARG:NH2	2.29	0.66
1:A:2249:G:C6	1:A:2272:G:C6	2.83	0.65
9:E:10:ARG:NH2	9:E:263:SER:O	2.29	0.65
1:A:2249:G:O2'	1:A:2250:G:P	2.54	0.65
30:i:87:ARG:HH22	30:i:137:VAL:HG21	1.61	0.65
44:w:19:CYS:SG	44:w:22:CYS:N	2.70	0.64
27:f:109:ASP:OD1	27:f:113:ARG:NH1	2.30	0.63
30:i:17:LEU:HB2	30:i:52:ALA:HB3	1.81	0.62
28:g:75:ILE:HG22	28:g:88:ARG:HG2	1.81	0.62
1:A:2290:C:O2'	6:W:413:GLN:NE2	2.32	0.62
10:F:327:LEU:HD23	13:I:181:ILE:HG21	1.82	0.62
1:A:1020:G:H1	1:A:1033:U:H1'	1.65	0.62
1:A:2249:G:H8	1:A:2249:G:H5''	1.65	0.62
16:M:15:GLU:OE1	16:M:132:ASN:ND2	2.32	0.62
1:A:1057:A:OP1	13:I:98:LYS:NZ	2.33	0.62
48:L:60:VAL:HB	48:L:80:LEU:HD11	1.80	0.62
1:A:2254:U:H3'	1:A:2259:A:H61	1.65	0.61
1:A:499:G:H5''	40:s:48:ARG:HH22	1.65	0.61
11:G:50:ARG:NH1	11:G:147:ASP:OD2	2.33	0.61
48:L:99:LYS:HD2	48:L:99:LYS:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2137:U:OP2	1:A:2142:A:N6	2.32	0.61
1:A:2249:G:O6	1:A:2272:G:C6	2.53	0.61
14:J:162:LEU:HA	22:a:7:LEU:HD11	1.81	0.61
22:a:42:PRO:HG3	22:a:61:ILE:HG13	1.82	0.61
1:A:2727:A:OP2	1:A:2728:G:N2	2.33	0.61
35:n:104:THR:HG21	35:n:112:ILE:HD11	1.83	0.61
11:G:261:THR:OG1	11:G:264:GLN:NE2	2.33	0.61
38:q:44:MET:O	38:q:77:ARG:NH1	2.34	0.61
3:C:141:C:O2	22:a:112:ASN:ND2	2.34	0.61
7:V:89:LEU:HD13	7:V:89:LEU:C	2.25	0.61
24:c:126:ARG:NH2	24:c:140:GLU:OE2	2.34	0.60
34:m:121:ARG:NH2	34:m:127:ASN:OD1	2.35	0.60
1:A:2247:G:C4	1:A:2248:C:C6	2.89	0.60
1:A:3231:U:H2'	1:A:3232:G:H8	1.66	0.60
7:V:56:SER:HB2	7:V:65:LEU:HB3	1.83	0.60
26:e:102:LEU:HD22	26:e:138:LEU:HD13	1.84	0.60
1:A:804:C:OP1	10:F:98:ARG:NH2	2.35	0.60
1:A:2440:G:N2	1:A:2508:U:O2	2.33	0.60
1:A:1578:C:OP1	14:J:43:LYS:NZ	2.34	0.60
41:t:29:ILE:HD11	41:t:31:ARG:HH21	1.67	0.60
1:A:2262:A:N6	1:A:2263:C:N3	2.50	0.60
26:e:148:ASP:OD1	26:e:151:ARG:NH2	2.34	0.59
1:A:526:C:N3	1:A:527:A:N6	2.50	0.59
6:W:217:ASP:OD1	6:W:220:ARG:NH2	2.35	0.59
7:V:278:LYS:HB2	7:V:284:GLN:HB3	1.85	0.59
7:V:16:THR:HG22	7:V:17:LEU:HD12	1.84	0.59
18:O:13:ARG:NH1	18:O:65:LEU:O	2.35	0.59
38:q:55:LEU:HB2	38:q:95:PRO:HD3	1.85	0.58
39:r:42:VAL:HG12	39:r:52:GLN:HE21	1.66	0.58
1:A:1635:G:N2	1:A:1638:A:OP2	2.35	0.58
24:c:50:GLN:HB3	24:c:55:GLN:HB2	1.85	0.58
1:A:1192:C:N4	1:A:1302:A:OP2	2.36	0.58
30:i:69:LEU:HD12	30:i:74:MET:HE1	1.84	0.58
3:C:94:C:H5''	44:w:76:ASN:HD21	1.67	0.58
1:A:3041:U:OP1	30:i:12:ARG:NH1	2.35	0.58
1:A:1724:U:O4	26:e:125:LYS:NZ	2.36	0.58
6:W:139:ARG:HH22	6:W:196:GLU:HB2	1.67	0.58
1:A:2249:G:N7	1:A:2272:G:N7	2.52	0.58
1:A:1210:U:H5''	15:K:62:ARG:HD3	1.85	0.58
2:B:7:G:OP1	11:G:33:ARG:NH1	2.36	0.58
34:m:46:ILE:HA	34:m:70:PRO:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3042:U:OP2	1:A:3092:C:N4	2.37	0.57
1:A:2843:U:H3	4:Y:269:ARG:HA	1.68	0.57
41:t:44:CYS:SG	41:t:45:GLY:N	2.77	0.57
7:V:19:CYS:SG	7:V:20:CYS:N	2.78	0.57
5:X:4:ARG:NH1	5:X:210:THR:O	2.38	0.57
1:A:2180:G:OP1	8:D:174:ARG:NH2	2.38	0.57
7:V:268:GLY:O	7:V:292:GLN:NE2	2.38	0.57
1:A:428:A:O2'	40:s:88:ASN:ND2	2.37	0.57
1:A:1834:U:OP2	46:y:10:LYS:NZ	2.38	0.57
1:A:2284:C:O2	7:V:205:ASN:ND2	2.37	0.57
11:G:41:LYS:HE3	28:g:93:VAL:HG11	1.87	0.57
1:A:2254:U:H3'	1:A:2259:A:N1	2.19	0.57
1:A:217:U:O2	33:l:103:LYS:NZ	2.35	0.57
1:A:1223:A:OP2	1:A:1285:G:N2	2.36	0.56
26:e:103:ARG:NH1	26:e:124:TYR:OH	2.37	0.56
1:A:269:G:OP2	22:a:44:ARG:NH1	2.38	0.56
5:X:106:ASN:ND2	5:X:150:SER:OG	2.38	0.56
7:V:21:ASN:HD22	7:V:38:CYS:HB3	1.69	0.56
7:V:81:LEU:HD22	7:V:114:ILE:HD11	1.86	0.56
23:b:61:ALA:HA	23:b:70:PRO:HD2	1.88	0.56
1:A:1156:C:OP2	13:I:94:LYS:NZ	2.38	0.56
1:A:2249:G:O6	1:A:2272:G:C2	2.59	0.56
4:Y:331:ILE:HG22	4:Y:332:PRO:HD2	1.85	0.56
19:Q:65:THR:O	19:Q:87:ARG:NH1	2.38	0.56
28:g:17:ARG:NH1	28:g:45:ASN:OD1	2.38	0.56
46:y:28:ARG:NH1	46:y:36:ARG:O	2.39	0.56
1:A:2799:A:O2'	35:n:42:ARG:NH1	2.38	0.56
1:A:3185:U:HO2'	27:f:170:THR:HG1	1.54	0.56
11:G:41:LYS:NZ	28:g:30:TYR:O	2.36	0.56
12:H:54:TYR:HA	12:H:65:ILE:HG22	1.87	0.56
19:Q:38:GLN:OE1	19:Q:41:ARG:NH2	2.39	0.56
7:V:103:ILE:HD11	7:V:113:ARG:HD2	1.86	0.56
13:I:88:ARG:NH1	13:I:90:LYS:O	2.38	0.56
24:c:78:VAL:HG12	24:c:80:LYS:H	1.70	0.56
28:g:18:ASP:HB2	28:g:21:LYS:HB2	1.88	0.56
1:A:1941:C:H42	1:A:2107:A:H61	1.54	0.56
1:A:776:U:OP1	36:o:41:ARG:NH2	2.39	0.56
4:Y:260:PHE:HB2	4:Y:274:GLN:HB2	1.86	0.56
9:E:238:LEU:HB3	9:E:242:THR:HG21	1.88	0.56
11:G:240:TYR:O	11:G:244:HIS:ND1	2.38	0.56
34:m:3:LYS:O	34:m:6:LYS:NZ	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2608:G:OP1	8:D:2:GLY:N	2.39	0.56
6:W:202:VAL:HB	6:W:341:LEU:HD23	1.87	0.56
7:V:115:LYS:HB3	7:V:133:GLU:HG2	1.88	0.56
1:A:597:G:OP1	13:I:41:ARG:NH2	2.38	0.56
1:A:1219:C:O2'	1:A:1286:A:N1	2.35	0.56
48:L:105:GLN:HA	48:L:143:UNK:HA	1.87	0.56
1:A:959:C:O2	1:A:2614:G:O2'	2.24	0.56
3:C:131:A:H2'	3:C:132:G:H8	1.70	0.56
1:A:566:G:H2'	1:A:567:G:H8	1.71	0.55
1:A:814:U:H5'	44:w:45:ARG:HH22	1.71	0.55
1:A:1513:G:OP1	26:e:5:ARG:NH2	2.39	0.55
1:A:1863:G:N1	1:A:1866:C:OP2	2.39	0.55
1:A:3186:A:N3	15:K:44:THR:OG1	2.39	0.55
11:G:60:ILE:HB	11:G:80:SER:HB3	1.88	0.55
25:d:86:THR:HG22	25:d:105:ARG:HB2	1.87	0.55
1:A:712:G:OP1	17:N:174:ARG:NH1	2.39	0.55
4:Y:227:VAL:HG23	4:Y:346:LEU:HB3	1.87	0.55
1:A:687:U:OP2	17:N:36:ARG:NH2	2.37	0.55
29:h:25:ASN:HD22	29:h:107:PHE:HE2	1.53	0.55
1:A:180:C:H42	1:A:236:G:H1	1.55	0.55
3:C:43:A:H62	44:w:65:ARG:HH12	1.55	0.55
1:A:1203:A:OP2	1:A:1301:A:N6	2.37	0.55
7:V:96:ARG:CD	7:V:119:GLN:HE22	2.04	0.55
24:c:109:ALA:HA	24:c:112:LEU:HD13	1.87	0.55
48:L:97:ASN:O	48:L:99:LYS:CE	2.54	0.55
1:A:3386:G:H4'	38:q:10:ARG:HH12	1.70	0.55
47:z:78:ILE:HG21	47:z:83:LYS:HE3	1.87	0.55
1:A:1035:G:N2	1:A:1036:A:N3	2.55	0.55
23:b:119:VAL:HG11	27:f:167:ARG:HE	1.72	0.55
1:A:351:A:N6	46:y:37:TYR:O	2.37	0.55
32:k:50:ALA:HB1	42:u:66:VAL:HG11	1.89	0.55
34:m:24:VAL:HG11	34:m:87:LEU:HD23	1.88	0.55
1:A:1106:G:O2'	36:o:25:LYS:NZ	2.40	0.54
1:A:1447:G:N7	24:c:25:SER:OG	2.35	0.54
1:A:2247:G:C2'	1:A:2248:C:H5'	2.37	0.54
1:A:69:C:OP1	22:a:178:HIS:ND1	2.36	0.54
1:A:1671:C:OP1	26:e:60:LYS:NZ	2.40	0.54
6:W:403:LEU:HB3	6:W:409:LEU:HD23	1.87	0.54
25:d:182:LYS:NZ	35:n:55:LYS:O	2.35	0.54
7:V:229:ILE:HD11	7:V:241:LYS:HB2	1.89	0.54
22:a:37:HIS:HE1	22:a:63:ARG:HH11	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:t:44:CYS:SG	41:t:46:ASP:N	2.79	0.54
1:A:641:C:OP2	35:n:21:ARG:NH1	2.37	0.54
1:A:2254:U:H5''	1:A:2259:A:N6	2.22	0.54
1:A:3129:A:N6	1:A:3131:U:O2	2.41	0.54
2:B:96:U:H2'	2:B:97:A:H8	1.72	0.54
7:V:90:LYS:CA	7:V:90:LYS:CE	2.85	0.54
1:A:980:A:H2	1:A:1104:G:H21	1.56	0.54
6:W:237:LYS:HB2	6:W:240:LEU:HD13	1.89	0.54
35:n:112:ILE:HB	35:n:130:VAL:HG12	1.89	0.54
7:V:49:ILE:CB	7:V:90:LYS:HG3	2.38	0.54
22:a:68:ARG:NH1	22:a:124:ASP:O	2.39	0.54
1:A:2946:A:H5''	1:A:2947:G:H5'	1.89	0.54
17:N:43:ALA:HB1	17:N:137:GLN:HE22	1.71	0.54
1:A:2249:G:O2'	1:A:2250:G:OP1	2.26	0.54
7:V:148:ARG:NH2	7:V:150:TYR:OH	2.41	0.54
1:A:3235:C:O2	1:A:3253:G:N1	2.40	0.54
6:W:203:GLN:HB2	6:W:233:LEU:HD23	1.90	0.54
8:D:65:ASP:OD2	8:D:72:ARG:NH2	2.41	0.54
11:G:36:LEU:HB3	11:G:50:ARG:HD3	1.89	0.54
1:A:2275:A:H5''	6:W:360:LYS:HD3	1.90	0.53
1:A:3272:C:OP1	12:H:78:ARG:NH2	2.41	0.53
1:A:3294:A:OP1	9:E:128:LYS:NZ	2.40	0.53
7:V:326:THR:HG21	7:V:356:ARG:HH22	1.73	0.53
1:A:2197:C:O2	1:A:2198:A:N6	2.41	0.53
9:E:303:LYS:HD2	9:E:361:THR:HG21	1.91	0.53
1:A:845:G:O2'	1:A:847:A:N7	2.41	0.53
1:A:1666:G:HO2'	1:A:1742:U:HO2'	1.54	0.53
3:C:144:G:OP1	22:a:57:GLN:NE2	2.41	0.53
6:W:208:ARG:O	6:W:500:ASN:ND2	2.42	0.53
7:V:107:PRO:O	7:V:110:ARG:NH1	2.36	0.53
11:G:39:GLN:NE2	11:G:46:THR:O	2.42	0.53
1:A:371:G:N1	1:A:374:A:OP2	2.41	0.53
6:W:186:GLU:HG2	6:W:371:THR:HB	1.90	0.53
7:V:280:SER:OG	7:V:281:ASN:N	2.41	0.53
16:M:47:GLN:HG2	16:M:67:VAL:HG12	1.91	0.53
1:A:337:G:N2	3:C:27:U:O2	2.41	0.53
1:A:953:G:N2	1:A:1115:G:OP1	2.42	0.53
7:V:96:ARG:N	7:V:118:VAL:O	2.33	0.53
35:n:100:PRO:HG2	35:n:123:VAL:HG12	1.89	0.53
43:v:5:THR:HG23	43:v:12:ASN:HB2	1.89	0.53
48:L:99:LYS:CD	48:L:99:LYS:H	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:110:ASN:HD22	22:a:201:ARG:HB3	1.73	0.53
33:l:51:ARG:NH1	33:l:112:ASP:OD2	2.42	0.53
1:A:412:G:OP1	24:c:62:ARG:NH1	2.42	0.53
1:A:1468:A:N6	1:A:1508:C:O2	2.42	0.53
1:A:2880:U:OP1	30:i:47:ASN:ND2	2.42	0.53
10:F:92:ASN:HD22	10:F:100:PHE:HB2	1.73	0.53
43:v:57:LEU:HD12	43:v:90:MET:HG3	1.91	0.53
1:A:518:G:N2	1:A:518:G:OP2	2.42	0.52
1:A:1821:U:H3	41:t:67:LYS:HD3	1.73	0.52
30:i:81:GLN:HE21	30:i:83:LYS:HB3	1.74	0.52
44:w:35:SER:O	44:w:45:ARG:NH1	2.41	0.52
1:A:3345:G:O6	1:A:3359:A:N6	2.42	0.52
6:W:137:PRO:HB2	6:W:192:TRP:HZ2	1.74	0.52
1:A:674:G:OP1	10:F:31:ARG:NH1	2.42	0.52
1:A:2899:C:O2'	1:A:2901:G:OP2	2.27	0.52
3:C:97:A:OP1	42:u:63:ARG:NH2	2.38	0.52
8:D:36:GLU:OE1	8:D:163:ARG:NH1	2.42	0.52
10:F:338:LYS:O	10:F:340:GLY:N	2.42	0.52
1:A:352:A:N7	1:A:367:A:N6	2.58	0.52
1:A:1521:G:O6	46:y:17:LYS:NZ	2.42	0.52
1:A:2896:A:O2'	47:z:122:ARG:NH2	2.42	0.52
1:A:3090:U:OP2	9:E:224:HIS:NE2	2.43	0.52
11:G:146:LEU:HG	11:G:163:LEU:HD12	1.92	0.52
13:I:57:THR:O	13:I:61:ASN:ND2	2.43	0.52
46:y:27:ILE:O	46:y:33:ASN:ND2	2.43	0.52
48:L:99:LYS:CD	48:L:99:LYS:N	2.73	0.52
7:V:49:ILE:HG22	7:V:90:LYS:CD	2.40	0.52
23:b:10:ASP:HB2	23:b:117:ARG:HB3	1.91	0.52
1:A:708:G:N2	1:A:711:A:OP2	2.43	0.52
1:A:2176:U:OP1	8:D:54:ARG:NH2	2.39	0.52
1:A:2631:U:OP2	28:g:4:SER:OG	2.28	0.52
10:F:4:PRO:HD2	10:F:22:LEU:HD13	1.92	0.52
1:A:9:U:O2	3:C:150:G:N2	2.43	0.51
1:A:2457:G:H22	1:A:2487:U:H3	1.58	0.51
1:A:2568:C:O2'	1:A:2569:A:O4'	2.25	0.51
7:V:102:PHE:HA	7:V:114:ILE:HA	1.92	0.51
9:E:305:ILE:HD11	9:E:317:ILE:HG21	1.92	0.51
43:v:34:SER:HG	43:v:37:THR:H	1.54	0.51
1:A:860:G:OP2	8:D:181:LYS:NZ	2.39	0.51
9:E:173:GLN:HG2	9:E:175:LYS:H	1.76	0.51
1:A:2249:G:H2'	1:A:2250:G:O4'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1486:G:H21	41:t:6:THR:HG22	1.76	0.51
1:A:2241:U:H4'	8:D:242:ARG:HG3	1.92	0.51
12:H:146:ILE:HD13	12:H:149:ILE:HD12	1.93	0.51
1:A:673:U:H2'	1:A:674:G:H8	1.74	0.51
1:A:2247:G:C5	1:A:2248:C:C6	2.99	0.51
1:A:2832:C:O2	1:A:2856:G:N2	2.40	0.51
1:A:3243:A:H4'	9:E:95:THR:HG22	1.92	0.51
8:D:140:ASN:HD22	8:D:145:LYS:HB2	1.76	0.51
10:F:187:LEU:HD11	10:F:193:LYS:HD3	1.92	0.51
42:u:104:GLN:OE1	42:u:108:GLN:NE2	2.44	0.51
46:y:9:ILE:HG22	46:y:13:MET:HE3	1.92	0.51
1:A:2249:G:C5	1:A:2272:G:C6	2.99	0.51
1:A:2768:U:O2'	19:Q:82:GLN:NE2	2.42	0.51
1:A:1496:C:H42	1:A:1520:G:H1	1.59	0.51
1:A:2483:G:N2	1:A:2486:A:OP2	2.43	0.51
9:E:67:PHE:HD1	9:E:70:ARG:HG2	1.76	0.51
10:F:237:GLN:O	10:F:246:ARG:NH1	2.44	0.51
1:A:2247:G:C2	1:A:2248:C:C6	2.99	0.51
7:V:65:LEU:O	7:V:87:ARG:NH1	2.44	0.51
1:A:576:C:OP1	13:I:241:LYS:NZ	2.32	0.50
1:A:1489:A:OP2	1:A:1838:G:N1	2.37	0.50
16:M:32:ARG:NH1	16:M:120:ILE:O	2.44	0.50
40:s:6:ARG:NH1	40:s:8:TYR:O	2.44	0.50
1:A:2584:G:O2'	14:J:240:ASN:ND2	2.44	0.50
7:V:142:GLN:HB3	7:V:147:ALA:HB2	1.91	0.50
27:f:23:LYS:O	28:g:146:ASN:ND2	2.43	0.50
1:A:824:C:H5''	8:D:21:ARG:HD3	1.93	0.50
1:A:2185:G:O2'	1:A:2314:U:OP2	2.28	0.50
9:E:10:ARG:NH1	9:E:11:HIS:O	2.44	0.50
1:A:3329:U:H5''	9:E:308:MET:HE2	1.94	0.50
34:m:51:LEU:HB2	34:m:65:ARG:HD2	1.94	0.50
7:V:108:HIS:O	7:V:110:ARG:NH2	2.45	0.50
7:V:144:PRO:HA	7:V:147:ALA:HB3	1.92	0.50
13:I:189:ILE:HG23	13:I:190:THR:HG23	1.94	0.50
1:A:609:G:OP2	10:F:315:LYS:NZ	2.36	0.50
4:Y:264:ALA:HB3	4:Y:269:ARG:HB3	1.93	0.50
3:C:21:C:OP1	10:F:193:LYS:NZ	2.37	0.50
6:W:462:VAL:O	6:W:466:ARG:N	2.43	0.50
1:A:1629:U:H5'	34:m:112:LYS:HE2	1.92	0.50
1:A:2969:A:N7	8:D:215:ASN:ND2	2.59	0.50
2:B:44:C:OP2	16:M:137:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:k:103:TYR:HB3	32:k:135:ILE:HD11	1.94	0.50
1:A:1675:G:H2'	1:A:1676:A:H8	1.77	0.50
6:W:207:ALA:HA	6:W:210:PRO:HG3	1.93	0.50
9:E:294:GLY:HA2	9:E:359:ILE:HD12	1.93	0.50
12:H:43:LEU:HD11	12:H:85:ILE:HG13	1.93	0.50
16:M:133:ARG:NH2	16:M:158:ASP:OD2	2.45	0.50
1:A:123:A:OP1	14:J:105:LYS:NZ	2.38	0.49
1:A:700:C:OP1	17:N:65:TYR:OH	2.28	0.49
1:A:758:C:OP1	19:Q:15:LYS:NZ	2.45	0.49
1:A:1150:A:N6	1:A:2369:G:O2'	2.45	0.49
7:V:49:ILE:HA	7:V:90:LYS:HD2	1.92	0.49
7:V:56:SER:H	7:V:87:ARG:HH12	1.60	0.49
1:A:2745:G:N2	1:A:2748:A:OP2	2.39	0.49
1:A:2149:A:N6	1:A:2187:G:O2'	2.43	0.49
1:A:3258:U:O2'	1:A:3260:G:OP1	2.25	0.49
6:W:425:ALA:HB1	6:W:455:PRO:HG2	1.92	0.49
25:d:96:PHE:HE2	25:d:113:LYS:HE3	1.76	0.49
1:A:86:G:O2'	1:A:98:G:O6	2.29	0.49
1:A:1220:U:O2	1:A:1222:G:N1	2.46	0.49
25:d:122:ILE:HG23	25:d:126:GLN:HB2	1.94	0.49
48:L:110:ILE:O	48:L:114:UNK:N	2.45	0.49
12:H:40:LEU:HD13	12:H:84:VAL:HG11	1.95	0.49
18:O:38:ILE:HG22	18:O:44:VAL:HG12	1.95	0.49
1:A:348:A:N3	1:A:352:A:O2'	2.45	0.49
1:A:1193:A:OP2	23:b:49:ARG:NH1	2.38	0.49
1:A:1949:G:OP1	26:e:104:ARG:NH2	2.41	0.49
5:X:146:ILE:HG13	5:X:147:LEU:HD12	1.94	0.49
6:W:380:SER:HB2	6:W:383:VAL:H	1.78	0.49
7:V:290:THR:HA	7:V:335:LEU:HD11	1.94	0.49
29:h:29:ASP:OD1	29:h:29:ASP:N	2.46	0.49
1:A:2131:A:H61	20:R:18:TYR:HD1	1.61	0.49
1:A:2150:G:O2'	1:A:2189:U:OP1	2.31	0.49
30:i:74:MET:HE3	30:i:102:ILE:HG21	1.94	0.49
1:A:1637:A:H5''	34:m:16:GLY:HA3	1.94	0.49
1:A:2365:C:H1'	23:b:68:ARG:HH22	1.78	0.49
1:A:2402:A:H2'	10:F:67:THR:HG21	1.93	0.49
10:F:334:PHE:HA	10:F:339:LEU:HD12	1.95	0.49
1:A:1431:G:OP2	35:n:12:ARG:NH1	2.39	0.49
1:A:2953:U:H2'	1:A:2954:U:H2'	1.94	0.49
1:A:3348:G:N2	1:A:3358:U:O2	2.46	0.49
7:V:94:LYS:HD2	7:V:97:LEU:HD21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:170:GLU:HG3	13:I:179:LEU:HB2	1.95	0.49
1:A:3008:A:OP2	23:b:74:ARG:NH1	2.46	0.48
6:W:242:THR:HG23	6:W:245:GLN:H	1.77	0.48
25:d:175:ALA:HB2	35:n:56:VAL:HG13	1.94	0.48
32:k:115:ARG:NH1	32:k:119:THR:OG1	2.46	0.48
1:A:2712:U:O2'	1:A:2743:A:O2'	2.31	0.48
1:A:1220:U:OP1	1:A:1221:A:O2'	2.26	0.48
23:b:157:GLU:OE1	23:b:160:ARG:NH2	2.47	0.48
24:c:170:SER:HA	24:c:173:ARG:HD2	1.96	0.48
1:A:1302:A:N1	1:A:2832:C:O2'	2.45	0.48
7:V:228:LEU:HD21	7:V:231:GLN:HB2	1.96	0.48
1:A:3085:G:OP1	31:j:34:SER:OG	2.30	0.48
4:Y:232:CYS:HA	4:Y:341:VAL:HG23	1.94	0.48
4:Y:304:LYS:HA	4:Y:316:GLY:HA2	1.95	0.48
10:F:283:THR:HB	10:F:289:ILE:HD11	1.96	0.48
6:W:314:GLU:HG2	6:W:315:GLU:H	1.76	0.48
30:i:10:LYS:HD3	30:i:125:LEU:HD22	1.94	0.48
31:j:6:ASP:N	31:j:11:ALA:O	2.46	0.48
1:A:2094:C:H2'	1:A:2095:G:H8	1.78	0.48
1:A:3375:A:O2'	1:A:3378:C:OP2	2.24	0.48
17:N:24:VAL:HG12	22:a:199:LEU:HB2	1.96	0.48
1:A:38:U:H4'	35:n:32:ARG:HD2	1.96	0.48
1:A:1385:C:OP1	10:F:141:ARG:NH1	2.43	0.48
1:A:2254:U:C6	1:A:2259:A:C6	3.02	0.48
1:A:3276:G:O6	24:c:171:ARG:NH2	2.46	0.48
9:E:230:THR:HA	9:E:235:THR:HG22	1.95	0.48
9:E:293:ASN:HB2	9:E:304:THR:HA	1.96	0.48
48:L:64:ILE:H	48:L:71:ALA:HB3	1.79	0.48
9:E:188:ILE:HG22	9:E:191:LYS:HD2	1.96	0.47
9:E:232:ARG:NH1	9:E:269:GLN:O	2.47	0.47
15:K:20:ILE:HG12	15:K:25:VAL:HG22	1.95	0.47
1:A:309:U:OP1	43:v:84:LYS:NZ	2.47	0.47
1:A:2895:G:O2'	47:z:100:TYR:O	2.27	0.47
7:V:113:ARG:HG3	7:V:135:GLU:HG2	1.95	0.47
1:A:216:G:OP1	33:l:16:ARG:NH1	2.47	0.47
1:A:1765:U:H3'	26:e:43:LYS:HZ3	1.80	0.47
1:A:1793:C:OP1	8:D:177:LYS:NZ	2.37	0.47
34:m:52:LYS:O	34:m:65:ARG:NH1	2.47	0.47
1:A:797:U:H2'	1:A:798:G:H8	1.80	0.47
1:A:2218:G:H2'	1:A:2219:A:H8	1.78	0.47
6:W:202:VAL:HG13	6:W:232:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:3:TYR:HA	27:f:142:GLN:HE22	1.79	0.47
34:m:23:VAL:HG12	34:m:45:GLY:HA3	1.95	0.47
1:A:593:C:OP2	12:H:19:LYS:NZ	2.45	0.47
1:A:1756:C:N4	1:A:1769:G:O6	2.48	0.47
1:A:2249:G:N7	1:A:2272:G:C4	2.81	0.47
1:A:3084:C:O2'	1:A:3332:U:OP1	2.28	0.47
6:W:205:VAL:HG13	6:W:213:PHE:HB2	1.97	0.47
7:V:380:ASN:O	19:Q:61:LYS:NZ	2.39	0.47
1:A:28:C:OP1	22:a:192:LYS:NZ	2.41	0.47
1:A:52:A:N3	1:A:811:U:O2'	2.48	0.47
1:A:805:G:O2'	10:F:73:ARG:NH2	2.45	0.47
1:A:1523:U:OP1	1:A:1607:U:N3	2.40	0.47
2:B:40:C:O2	16:M:72:ARG:NE	2.41	0.47
4:Y:324:CYS:SG	4:Y:327:GLY:N	2.88	0.47
7:V:186:ASP:OD2	7:V:206:HIS:ND1	2.48	0.47
9:E:57:VAL:HG22	9:E:73:VAL:HG12	1.96	0.47
25:d:71:LEU:HD13	25:d:99:THR:HG21	1.97	0.47
1:A:353:G:O6	44:w:52:LYS:NZ	2.47	0.47
15:K:20:ILE:HB	18:O:7:VAL:HG13	1.97	0.47
23:b:25:LYS:HE3	23:b:29:ASN:HD21	1.79	0.47
27:f:12:ARG:NE	27:f:57:GLU:OE2	2.39	0.47
42:u:85:THR:O	42:u:89:ARG:NE	2.37	0.47
1:A:158:G:H2'	1:A:159:A:H8	1.80	0.47
39:r:83:GLU:O	39:r:86:THR:OG1	2.31	0.47
1:A:1794:G:H4'	8:D:191:LEU:HD12	1.96	0.47
1:A:2168:A:N6	1:A:2170:U:O2	2.48	0.47
1:A:2254:U:C5'	1:A:2259:A:N6	2.77	0.47
1:A:2290:C:H5''	7:V:82:LEU:HD23	1.97	0.47
1:A:2375:G:O2'	1:A:2377:G:OP2	2.28	0.47
7:V:34:MET:HE2	7:V:39:ILE:HG22	1.97	0.47
1:A:110:G:OP2	17:N:73:ARG:NH1	2.49	0.46
1:A:2157:G:N2	1:A:2177:G:O2'	2.48	0.46
1:A:3092:C:O2'	1:A:3094:A:OP2	2.28	0.46
2:B:64:A:OP2	11:G:289:LYS:NZ	2.41	0.46
9:E:227:GLU:HG3	9:E:270:ARG:HE	1.80	0.46
12:H:52:VAL:HG11	12:H:65:ILE:HD13	1.97	0.46
12:H:169:ASP:HB3	12:H:174:LEU:HD11	1.97	0.46
1:A:2677:G:H1	1:A:2680:A:H62	1.63	0.46
22:a:113:LEU:HD23	22:a:134:LEU:HB3	1.97	0.46
48:L:99:LYS:HD2	48:L:99:LYS:H	1.78	0.46
1:A:1601:U:OP2	26:e:42:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:G:OP2	11:G:30:TYR:OH	2.29	0.46
2:B:97:A:O4'	13:I:225:GLN:NE2	2.47	0.46
7:V:58:CYS:HB3	7:V:63:ARG:H	1.80	0.46
7:V:89:LEU:C	7:V:89:LEU:CD1	2.88	0.46
10:F:361:HIS:O	27:f:28:ARG:NH2	2.49	0.46
1:A:2208:A:H2	1:A:2236:G:H1	1.63	0.46
1:A:608:A:OP1	10:F:315:LYS:NZ	2.42	0.46
1:A:655:C:H2'	1:A:656:A:C8	2.51	0.46
1:A:2451:G:O2'	1:A:2497:U:O2	2.33	0.46
2:B:12:U:OP2	2:B:68:C:O2'	2.33	0.46
7:V:203:GLN:HB2	7:V:206:HIS:HD2	1.80	0.46
1:A:665:A:OP1	22:a:203:ARG:NH1	2.47	0.46
1:A:832:G:H1	1:A:862:U:H3	1.64	0.46
1:A:1524:A:O2'	1:A:1526:U:OP2	2.32	0.46
1:A:2254:U:H3'	1:A:2259:A:N6	2.30	0.46
1:A:2945:G:O2'	1:A:2948:C:OP2	2.25	0.46
6:W:344:TYR:HE1	6:W:393:PHE:HD2	1.63	0.46
13:I:88:ARG:HD2	13:I:108:LEU:HB3	1.97	0.46
15:K:92:TYR:HB2	15:K:142:ASP:HB3	1.98	0.46
17:N:46:ILE:HG22	17:N:49:ARG:HB2	1.97	0.46
23:b:36:VAL:HB	23:b:108:ILE:HG12	1.98	0.46
1:A:1477:A:OP1	1:A:3075:G:O2'	2.33	0.46
2:B:107:C:H2'	2:B:108:A:H8	1.81	0.46
34:m:54:THR:HG22	34:m:57:HIS:CD2	2.51	0.46
38:q:20:LEU:HD11	38:q:32:ALA:HB2	1.97	0.46
1:A:2469:G:N2	1:A:2488:A:N3	2.62	0.46
7:V:345:ASP:HA	7:V:348:VAL:HG12	1.98	0.46
34:m:14:VAL:HG22	41:t:86:LYS:HG2	1.98	0.46
1:A:2514:U:OP2	1:A:2586:G:N2	2.49	0.45
37:p:10:ILE:HD12	37:p:13:LYS:HD2	1.98	0.45
1:A:2991:A:O3'	9:E:21:ARG:NH2	2.49	0.45
7:V:24:THR:OG1	7:V:35:CYS:SG	2.63	0.45
10:F:150:LEU:HD21	10:F:172:VAL:HG11	1.99	0.45
14:J:50:VAL:HG12	32:k:30:ALA:HA	1.98	0.45
7:V:119:GLN:HG2	7:V:129:GLN:HB3	1.97	0.45
1:A:1196:C:OP1	1:A:1309:U:O2'	2.34	0.45
1:A:2312:A:O2'	1:A:2315:G:N3	2.40	0.45
1:A:2516:U:H5'	22:a:31:ARG:HH21	1.81	0.45
9:E:317:ILE:O	9:E:319:ASN:N	2.48	0.45
10:F:11:LEU:HD22	10:F:168:ALA:HB1	1.98	0.45
1:A:2196:C:H2'	1:A:2242:A:H61	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2247:G:C6	1:A:2248:C:H5	2.15	0.45
1:A:2341:A:OP2	9:E:247:ARG:NH1	2.43	0.45
1:A:2882:U:O2'	9:E:263:SER:OG	2.26	0.45
5:X:101:LEU:HA	30:i:135:VAL:HG22	1.98	0.45
11:G:206:GLN:NE2	11:G:210:GLU:OE2	2.49	0.45
15:K:41:ILE:HD11	15:K:67:ALA:HB1	1.98	0.45
41:t:41:ARG:HG2	41:t:56:THR:HG21	1.98	0.45
1:A:103:G:OP1	17:N:70:ARG:NH2	2.49	0.45
1:A:293:C:O2'	43:v:76:ARG:O	2.33	0.45
1:A:612:U:H2'	1:A:613:G:H8	1.81	0.45
1:A:3068:U:OP2	26:e:62:ARG:NH1	2.39	0.45
6:W:239:ASP:OD1	6:W:239:ASP:N	2.46	0.45
8:D:61:VAL:O	8:D:74:GLU:N	2.45	0.45
1:A:2897:A:OP2	47:z:124:LYS:NZ	2.43	0.45
18:O:3:THR:OG1	18:O:4:ASP:N	2.49	0.45
27:f:6:GLU:OE2	27:f:28:ARG:NH1	2.50	0.45
22:a:18:VAL:HG13	22:a:19:LEU:HD12	1.98	0.45
26:e:69:SER:HB2	26:e:74:ARG:HG3	1.99	0.45
34:m:57:HIS:HB3	34:m:61:LYS:HB2	1.98	0.45
2:B:19:C:H2'	2:B:20:A:H8	1.82	0.45
14:J:133:LYS:HD3	14:J:138:HIS:HE1	1.82	0.45
32:k:105:VAL:HG11	32:k:126:LEU:HD22	1.99	0.45
1:A:3154:C:OP1	1:A:3293:U:O2'	2.34	0.44
5:X:38:PHE:HE1	5:X:205:VAL:HG21	1.83	0.44
7:V:324:ASP:O	7:V:337:ASP:N	2.48	0.44
11:G:200:PHE:HB3	11:G:237:GLU:HG3	1.98	0.44
37:p:61:MET:HE3	37:p:62:LEU:HG	1.99	0.44
40:s:14:LEU:HD11	40:s:31:LYS:HB2	1.99	0.44
1:A:76:G:OP1	17:N:70:ARG:NH1	2.49	0.44
1:A:721:G:H2'	1:A:722:G:H8	1.82	0.44
1:A:2094:C:H2'	1:A:2095:G:C8	2.52	0.44
10:F:126:ILE:HD11	10:F:233:LEU:HD13	2.00	0.44
1:A:196:G:N1	1:A:199:A:OP2	2.51	0.44
1:A:1597:C:OP1	41:t:8:ARG:NH2	2.50	0.44
9:E:86:VAL:HG22	9:E:162:VAL:HG12	2.00	0.44
1:A:746:A:H2'	1:A:747:A:H8	1.83	0.44
18:O:60:LEU:HD13	27:f:152:LEU:HD11	2.00	0.44
22:a:9:GLU:OE2	22:a:13:LYS:NZ	2.50	0.44
22:a:112:ASN:OD1	22:a:112:ASN:N	2.49	0.44
1:A:497:C:O3'	40:s:86:ARG:NH2	2.51	0.44
37:p:27:TYR:O	37:p:30:THR:OG1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:99:ARG:NH2	22:a:118:SER:O	2.45	0.44
1:A:848:A:C5	1:A:849:C:H1'	2.53	0.44
1:A:957:C:H1'	35:n:43:ILE:HD11	2.00	0.44
4:Y:262:LYS:HB3	4:Y:272:ASP:HB2	2.00	0.44
7:V:226:GLU:HG3	7:V:240:TYR:CD2	2.53	0.44
8:D:136:ILE:HG12	8:D:148:VAL:HG12	1.99	0.44
25:d:176:ARG:HA	25:d:183:GLY:HA3	1.99	0.44
1:A:145:G:OP2	14:J:193:LYS:NZ	2.37	0.44
1:A:208:C:OP2	10:F:163:LYS:NZ	2.32	0.44
1:A:1705:U:O2	1:A:1786:G:O2'	2.36	0.44
1:A:2660:G:N3	1:A:2744:U:O2'	2.50	0.44
15:K:23:ARG:NH1	15:K:42:ASP:OD1	2.47	0.44
28:g:79:MET:HB3	28:g:84:TYR:CE1	2.52	0.44
1:A:1235:U:H4'	1:A:1236:G:H5'	1.99	0.44
7:V:359:LEU:HD22	7:V:362:ILE:HD11	1.99	0.44
34:m:33:SER:OG	34:m:34:LYS:N	2.51	0.44
1:A:200:C:OP1	33:l:60:ARG:NH1	2.50	0.43
7:V:291:LEU:HD11	7:V:358:HIS:HB3	1.99	0.43
1:A:120:G:N2	14:J:124:ASP:OD1	2.49	0.43
1:A:221:A:O2'	1:A:223:U:OP2	2.34	0.43
1:A:297:G:H2'	43:v:41:ARG:HH12	1.82	0.43
1:A:536:U:OP1	27:f:146:LYS:NZ	2.43	0.43
1:A:1906:G:N2	1:A:1909:A:N1	2.65	0.43
1:A:2965:U:O2	8:D:221:LYS:NZ	2.45	0.43
4:Y:330:VAL:HG13	4:Y:331:ILE:H	1.82	0.43
10:F:206:LEU:HB3	10:F:248:VAL:HG22	2.01	0.43
13:I:160:ARG:HD2	13:I:203:TRP:CE2	2.53	0.43
29:h:15:PHE:HB2	29:h:65:VAL:HB	2.00	0.43
38:q:10:ARG:HE	38:q:44:MET:HE1	1.84	0.43
39:r:100:ILE:O	39:r:105:ARG:NH1	2.49	0.43
1:A:634:C:H4'	39:r:47:ARG:HH12	1.82	0.43
1:A:1363:A:OP1	13:I:160:ARG:NH1	2.42	0.43
1:A:1761:C:O2	1:A:1765:U:N3	2.51	0.43
1:A:2221:G:N2	1:A:2224:A:OP2	2.44	0.43
1:A:2415:C:H5'	8:D:207:VAL:HG12	1.99	0.43
3:C:95:G:OP1	44:w:76:ASN:ND2	2.37	0.43
23:b:113:ASP:O	23:b:117:ARG:NH1	2.51	0.43
1:A:1127:G:N2	1:A:1130:A:OP2	2.39	0.43
1:A:1821:U:N3	41:t:67:LYS:HD3	2.34	0.43
7:V:119:GLN:HA	7:V:129:GLN:HA	2.01	0.43
20:R:42:CYS:HB3	20:R:60:CYS:HB3	1.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:L:19:UNK:HA	48:L:59:THR:H	1.84	0.43
1:A:542:G:C5	1:A:543:C:H1'	2.53	0.43
1:A:1228:C:O2	1:A:1282:G:N1	2.45	0.43
1:A:1506:A:H5''	1:A:1507:G:H5''	2.01	0.43
9:E:288:GLY:N	9:E:320:ASP:OD1	2.50	0.43
1:A:1003:A:N1	1:A:1049:C:O2'	2.45	0.43
1:A:3314:A:H2'	1:A:3315:G:H8	1.84	0.43
2:B:4:U:H2'	2:B:5:G:C8	2.54	0.43
7:V:229:ILE:HD12	7:V:239:THR:HG22	2.00	0.43
14:J:35:GLY:HA3	14:J:38:GLN:HE21	1.84	0.43
16:M:12:LEU:HD12	16:M:131:MET:HE3	1.99	0.43
17:N:23:LYS:HE2	17:N:25:HIS:CE1	2.54	0.43
22:a:192:LYS:O	22:a:196:THR:OG1	2.30	0.43
30:i:80:ARG:HD3	30:i:117:PRO:HG2	2.01	0.43
32:k:67:ILE:HD12	32:k:83:VAL:HG12	2.00	0.43
35:n:94:ALA:HB1	35:n:122:PRO:HD2	2.00	0.43
1:A:3083:G:N2	1:A:3333:G:OP1	2.50	0.43
9:E:168:LYS:O	9:E:319:ASN:ND2	2.52	0.43
9:E:215:ILE:HD12	9:E:338:LEU:HD12	2.01	0.43
1:A:3119:U:H4'	47:z:104:PRO:HG2	2.01	0.43
1:A:269:G:H5''	22:a:14:LYS:HE2	2.00	0.43
1:A:1624:G:O2'	1:A:1643:A:N1	2.46	0.43
1:A:3004:C:O2'	9:E:99:LEU:O	2.35	0.43
8:D:62:VAL:HA	8:D:73:GLU:HA	2.01	0.43
14:J:62:LYS:HD3	22:a:29:GLU:HG3	2.01	0.43
18:O:42:LYS:HA	18:O:60:LEU:HD12	2.01	0.43
23:b:77:SER:HB2	23:b:104:VAL:HG12	2.01	0.43
1:A:289:A:H2'	1:A:290:G:H8	1.84	0.43
1:A:673:U:H2'	1:A:674:G:C8	2.53	0.43
1:A:2219:A:H2'	1:A:2220:A:H8	1.84	0.43
4:Y:238:LYS:HD3	5:X:230:GLU:HG2	2.01	0.43
6:W:465:ALA:HB2	6:W:483:ALA:HB2	2.01	0.43
18:O:53:VAL:HA	18:O:54:PRO:HD3	1.91	0.43
37:p:25:LEU:O	37:p:29:SER:OG	2.36	0.43
48:L:17:UNK:N	48:L:61:GLN:O	2.52	0.43
1:A:3121:U:H1'	1:A:3122:A:H5''	2.01	0.42
9:E:56:ILE:HD12	9:E:56:ILE:HA	1.93	0.42
35:n:64:GLN:HB2	35:n:67:HIS:HD2	1.84	0.42
1:A:952:A:OP1	36:o:14:ARG:NH2	2.51	0.42
19:Q:99:GLN:OE1	19:Q:102:GLN:NE2	2.48	0.42
1:A:1411:C:H2'	1:A:1412:G:H8	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:C:H42	2:B:49:G:H1	1.65	0.42
4:Y:352:PRO:HB2	7:V:15:ALA:HB3	2.00	0.42
22:a:6:TYR:HE1	43:v:40:VAL:HG22	1.84	0.42
24:c:30:ARG:HA	24:c:119:VAL:HG11	2.01	0.42
44:w:18:LEU:HD23	44:w:25:ARG:HB2	2.00	0.42
1:A:783:A:H5''	1:A:784:A:H5''	2.01	0.42
1:A:785:G:O6	35:n:77:LYS:NZ	2.51	0.42
3:C:71:A:OP2	33:l:51:ARG:NH1	2.52	0.42
12:H:80:ASN:HB3	12:H:83:TYR:HD2	1.85	0.42
18:O:20:VAL:O	18:O:66:THR:OG1	2.36	0.42
48:L:86:LYS:NZ	48:L:100:HIS:O	2.53	0.42
1:A:3273:A:OP2	12:H:77:ARG:NH2	2.44	0.42
6:W:226:ASP:HA	6:W:229:LYS:HB3	2.02	0.42
28:g:68:THR:OG1	28:g:69:LYS:N	2.44	0.42
1:A:411:U:H2'	1:A:412:G:H8	1.83	0.42
1:A:594:U:OP2	1:A:609:G:N1	2.48	0.42
4:Y:235:CYS:SG	4:Y:310:CYS:N	2.93	0.42
4:Y:330:VAL:HG22	4:Y:331:ILE:HD12	2.01	0.42
10:F:150:LEU:HD22	10:F:249:ILE:HG12	2.00	0.42
33:l:56:VAL:HG11	33:l:104:LEU:HD13	2.02	0.42
36:o:28:LYS:HE2	36:o:28:LYS:HB3	1.90	0.42
37:p:13:LYS:HB3	37:p:100:ILE:HG22	2.00	0.42
6:W:430:LYS:HE2	6:W:455:PRO:HB3	2.01	0.42
18:O:68:LEU:HD22	18:O:90:VAL:HG23	2.01	0.42
30:i:102:ILE:H	30:i:102:ILE:HG13	1.59	0.42
1:A:2661:G:O6	1:A:2709:C:N4	2.53	0.42
1:A:3009:G:O2'	9:E:14:LEU:O	2.30	0.42
1:A:3218:A:H5''	1:A:3219:G:C4	2.54	0.42
2:B:89:G:N2	2:B:92:A:OP2	2.53	0.42
3:C:148:G:H2'	3:C:149:A:H8	1.84	0.42
17:N:53:LEU:HB2	17:N:55:ARG:HH12	1.85	0.42
1:A:1018:G:N2	1:A:1035:G:N3	2.65	0.42
2:B:3:U:O2'	2:B:25:G:N3	2.53	0.42
15:K:134:ILE:HG13	15:K:146:LEU:HG	2.01	0.42
34:m:23:VAL:HB	34:m:43:VAL:HB	2.02	0.42
1:A:1390:A:N6	1:A:1418:A:O2'	2.52	0.41
1:A:1474:A:O2'	38:q:57:GLN:NE2	2.48	0.41
1:A:1874:A:OP2	26:e:21:LYS:NZ	2.51	0.41
1:A:2247:G:C4	1:A:2248:C:H6	2.34	0.41
1:A:3217:C:H6	1:A:3266:G:H21	1.67	0.41
7:V:168:LYS:H	7:V:168:LYS:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:124:LYS:NZ	24:c:142:SER:OG	2.53	0.41
1:A:753:C:H2'	1:A:754:G:H8	1.84	0.41
1:A:2768:U:H2'	1:A:2769:A:H8	1.84	0.41
1:A:3314:A:H2'	1:A:3315:G:C8	2.55	0.41
38:q:74:ARG:N	38:q:94:GLU:O	2.46	0.41
48:L:76:SER:HA	48:L:80:LEU:HD12	2.02	0.41
1:A:210:U:C2	1:A:230:U:H4'	2.55	0.41
1:A:1020:G:N1	1:A:1033:U:O2	2.53	0.41
1:A:2254:U:C3'	1:A:2259:A:H61	2.32	0.41
1:A:2406:C:HO2'	1:A:2619:G:H21	1.65	0.41
5:X:185:THR:HB	5:X:189:GLY:HA2	2.02	0.41
8:D:117:GLU:HG2	8:D:124:GLY:H	1.85	0.41
30:i:80:ARG:NH1	30:i:117:PRO:O	2.45	0.41
30:i:104:ASN:HD21	30:i:108:GLU:HB2	1.85	0.41
46:y:43:ASN:HD22	46:y:44:TRP:H	1.68	0.41
1:A:999:G:N3	1:A:1002:A:N6	2.68	0.41
1:A:1404:G:N2	1:A:1407:A:OP2	2.53	0.41
4:Y:225:SER:OG	4:Y:226:LYS:N	2.52	0.41
7:V:143:CYS:O	7:V:146:CYS:N	2.43	0.41
7:V:156:ARG:HA	7:V:241:LYS:HG3	2.03	0.41
26:e:106:LEU:HB3	26:e:120:TYR:HE1	1.85	0.41
37:p:30:THR:HG22	37:p:91:SER:HB2	2.01	0.41
1:A:1350:A:H2'	1:A:1351:U:H3'	2.02	0.41
1:A:2103:U:H2'	1:A:2104:A:H8	1.85	0.41
9:E:166:ILE:HD11	9:E:171:LEU:HD12	2.01	0.41
13:I:173:LEU:HD23	13:I:178:ILE:HD12	2.01	0.41
24:c:60:PHE:CE2	24:c:82:ARG:HB3	2.56	0.41
40:s:49:ILE:HD11	40:s:71:VAL:HG23	2.03	0.41
1:A:37:U:N3	1:A:47:C:O2	2.54	0.41
16:M:20:ASN:HB3	16:M:126:ASP:HB2	2.02	0.41
27:f:90:MET:HE1	27:f:114:HIS:CE1	2.55	0.41
1:A:2249:G:C8	1:A:2272:G:N7	2.88	0.41
1:A:2254:U:C5	1:A:2259:A:C6	3.09	0.41
1:A:2307:G:O2'	1:A:2310:U:OP2	2.39	0.41
4:Y:323:ARG:HG3	4:Y:324:CYS:H	1.85	0.41
11:G:156:GLY:HA2	11:G:181:PRO:HD3	2.02	0.41
13:I:88:ARG:HE	13:I:103:LEU:HD13	1.85	0.41
29:h:89:LEU:HB3	29:h:93:ILE:HD12	2.03	0.41
1:A:528:U:H2'	1:A:529:A:C8	2.55	0.41
1:A:638:C:N4	1:A:639:G:O6	2.54	0.41
1:A:2249:G:O2'	1:A:2250:G:O5'	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2535:A:H3'	1:A:2536:A:C8	2.56	0.41
1:A:2585:G:O5'	3:C:151:C:N4	2.54	0.41
5:X:224:LEU:H	5:X:224:LEU:HG	1.72	0.41
10:F:58:HIS:NE2	10:F:98:ARG:HD3	2.36	0.41
27:f:74:ASN:OD1	27:f:95:ARG:NH1	2.51	0.41
1:A:543:C:H2'	1:A:544:C:C2	2.56	0.41
1:A:594:U:O4	10:F:304:GLN:NE2	2.53	0.41
1:A:673:U:OP1	25:d:21:SER:OG	2.32	0.41
1:A:739:G:H2'	1:A:740:G:H8	1.86	0.41
1:A:1795:U:C4	20:R:51:ALA:HA	2.56	0.41
1:A:2424:A:OP1	22:a:90:ASN:ND2	2.54	0.41
1:A:2505:U:O2	1:A:2506:U:N3	2.45	0.41
1:A:2842:U:H6	1:A:2842:U:H2'	1.72	0.41
1:A:2999:U:H2'	1:A:3000:A:C8	2.56	0.41
1:A:3218:A:H5''	1:A:3219:G:C5	2.56	0.41
5:X:57:ARG:HH21	9:E:66:LYS:HG2	1.86	0.41
6:W:507:ASP:OD1	6:W:507:ASP:N	2.51	0.41
9:E:266:ARG:HD3	9:E:266:ARG:HA	1.91	0.41
1:A:1592:G:OP1	41:t:58:ARG:NH2	2.54	0.41
48:L:97:ASN:O	48:L:99:LYS:HE3	2.20	0.41
1:A:148:G:OP2	22:a:4:TYR:OH	2.27	0.40
1:A:292:U:OP2	22:a:68:ARG:NH2	2.54	0.40
1:A:550:A:H2'	1:A:551:A:C5	2.56	0.40
1:A:969:C:OP1	36:o:19:ASN:ND2	2.53	0.40
1:A:1149:G:H21	1:A:1199:C:N4	2.19	0.40
1:A:1362:G:H2'	1:A:1363:A:C8	2.56	0.40
1:A:2282:U:OP1	1:A:2973:G:O2'	2.39	0.40
6:W:236:ASN:HB3	6:W:263:TYR:CZ	2.57	0.40
10:F:339:LEU:HD23	10:F:339:LEU:HA	1.91	0.40
15:K:92:TYR:HD1	15:K:179:ILE:HG12	1.86	0.40
29:h:39:ASP:OD1	29:h:40:HIS:ND1	2.53	0.40
48:L:65:GLN:HA	48:L:69:ALA:HB3	2.04	0.40
1:A:2253:G:H1	1:A:2263:C:H42	1.68	0.40
1:A:2290:C:H1'	6:W:413:GLN:HE22	1.86	0.40
3:C:95:G:C4	44:w:82:SER:HA	2.57	0.40
9:E:232:ARG:HA	9:E:270:ARG:HD3	2.04	0.40
32:k:34:LEU:HA	32:k:35:PRO:HD3	1.96	0.40
34:m:54:THR:HG23	34:m:56:LYS:H	1.87	0.40
1:A:67:A:N6	1:A:271:C:O2'	2.54	0.40
1:A:1190:A:C8	1:A:1193:A:H1'	2.56	0.40
1:A:3028:G:H1'	4:Y:325:SER:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:C:H2'	2:B:108:A:C8	2.56	0.40
6:W:149:PHE:O	6:W:153:ARG:N	2.45	0.40
6:W:430:LYS:NZ	6:W:453:ASP:O	2.53	0.40
7:V:66:GLN:HB2	7:V:70:GLN:HB2	2.02	0.40
11:G:259:LYS:HE3	11:G:259:LYS:HB3	1.86	0.40
21:S:165:UNK:O	21:S:167:UNK:N	2.55	0.40
22:a:46:ASP:OD1	22:a:47:LYS:N	2.54	0.40
31:j:23:ARG:NH2	31:j:25:ASP:OD2	2.47	0.40
1:A:1342:C:H2'	1:A:1343:A:C8	2.56	0.40
1:A:3007:U:H2'	1:A:3008:A:H8	1.86	0.40
9:E:289:ASP:OD1	9:E:289:ASP:N	2.50	0.40
10:F:264:SER:OG	10:F:265:GLU:N	2.54	0.40
17:N:106:GLN:HB3	43:v:18:THR:HG23	2.03	0.40
19:Q:71:ARG:HH21	19:Q:80:ARG:HD3	1.87	0.40
22:a:155:VAL:O	22:a:162:ARG:NH2	2.45	0.40
27:f:12:ARG:HB3	27:f:24:LEU:HD13	2.02	0.40
29:h:22:PRO:HB2	29:h:28:PHE:HB3	2.03	0.40
37:p:24:THR:HG22	37:p:91:SER:HB3	2.04	0.40
44:w:22:CYS:HB3	44:w:37:CYS:HB3	1.28	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Y	126/364 (35%)	99 (79%)	22 (18%)	5 (4%)	2	20
5	X	230/245 (94%)	221 (96%)	9 (4%)	0	100	100
6	W	373/640 (58%)	313 (84%)	54 (14%)	6 (2%)	7	35
7	V	388/518 (75%)	323 (83%)	59 (15%)	6 (2%)	8	36
8	D	244/254 (96%)	225 (92%)	19 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	E	382/387 (99%)	354 (93%)	26 (7%)	2 (0%)	24	57
10	F	359/362 (99%)	330 (92%)	26 (7%)	3 (1%)	16	48
11	G	281/297 (95%)	268 (95%)	12 (4%)	1 (0%)	30	62
12	H	151/176 (86%)	142 (94%)	9 (6%)	0	100	100
13	I	218/244 (89%)	207 (95%)	9 (4%)	2 (1%)	14	45
14	J	225/256 (88%)	217 (96%)	7 (3%)	1 (0%)	30	62
15	K	186/191 (97%)	176 (95%)	10 (5%)	0	100	100
16	M	166/174 (95%)	152 (92%)	14 (8%)	0	100	100
17	N	191/199 (96%)	172 (90%)	17 (9%)	2 (1%)	12	43
18	O	134/138 (97%)	129 (96%)	5 (4%)	0	100	100
19	Q	100/106 (94%)	94 (94%)	6 (6%)	0	100	100
20	R	86/92 (94%)	80 (93%)	6 (7%)	0	100	100
22	a	201/204 (98%)	191 (95%)	10 (5%)	0	100	100
23	b	195/199 (98%)	191 (98%)	4 (2%)	0	100	100
24	c	181/184 (98%)	169 (93%)	12 (7%)	0	100	100
25	d	183/186 (98%)	175 (96%)	8 (4%)	0	100	100
26	e	149/189 (79%)	140 (94%)	9 (6%)	0	100	100
27	f	168/172 (98%)	155 (92%)	11 (6%)	2 (1%)	10	40
28	g	157/160 (98%)	149 (95%)	8 (5%)	0	100	100
29	h	95/121 (78%)	91 (96%)	3 (3%)	1 (1%)	11	41
30	i	130/137 (95%)	129 (99%)	1 (1%)	0	100	100
31	j	59/155 (38%)	56 (95%)	2 (3%)	1 (2%)	7	34
32	k	119/142 (84%)	111 (93%)	8 (7%)	0	100	100
33	l	123/127 (97%)	121 (98%)	2 (2%)	0	100	100
34	m	133/136 (98%)	122 (92%)	11 (8%)	0	100	100
35	n	146/149 (98%)	132 (90%)	11 (8%)	3 (2%)	5	31
36	o	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
37	p	94/105 (90%)	93 (99%)	1 (1%)	0	100	100
38	q	105/113 (93%)	98 (93%)	7 (7%)	0	100	100
39	r	124/130 (95%)	118 (95%)	6 (5%)	0	100	100
40	s	104/107 (97%)	96 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	t	107/121 (88%)	103 (96%)	4 (4%)	0	100	100
42	u	117/120 (98%)	114 (97%)	3 (3%)	0	100	100
43	v	96/100 (96%)	90 (94%)	6 (6%)	0	100	100
44	w	82/88 (93%)	75 (92%)	7 (8%)	0	100	100
45	x	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
46	y	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
47	z	49/128 (38%)	46 (94%)	3 (6%)	0	100	100
48	L	53/165 (32%)	48 (91%)	5 (9%)	0	100	100
All	All	6989/8269 (84%)	6483 (93%)	471 (7%)	35 (0%)	26	57

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	V	95	VAL
10	F	339	LEU
11	G	259	LYS
13	I	178	ILE
4	Y	326	CYS
6	W	135	ILE
6	W	442	GLN
7	V	45	ILE
14	J	36	ILE
17	N	6	ASN
17	N	63	VAL
27	f	13	ARG
4	Y	247	ALA
6	W	338	ASN
6	W	443	THR
10	F	5	GLN
13	I	158	LYS
27	f	24	LEU
4	Y	323	ARG
6	W	226	ASP
6	W	337	ILE
7	V	36	TYR
10	F	4	PRO
35	n	15	VAL
35	n	47	LYS
35	n	117	ARG

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Mol	Chain	Res	Type
7	V	68	PRO
7	V	143	CYS
9	E	347	SER
29	h	52	ASN
4	Y	246	ILE
9	E	317	ILE
31	j	10	GLY
4	Y	327	GLY
7	V	25	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	
4	Y	110/323 (34%)	109 (99%)	1 (1%)	70	74
5	X	186/211 (88%)	186 (100%)	0	100	100
6	W	316/555 (57%)	313 (99%)	3 (1%)	70	74
7	V	332/467 (71%)	330 (99%)	2 (1%)	78	79
8	D	189/196 (96%)	187 (99%)	2 (1%)	65	73
9	E	317/323 (98%)	316 (100%)	1 (0%)	86	84
10	F	288/289 (100%)	287 (100%)	1 (0%)	86	84
11	G	236/245 (96%)	235 (100%)	1 (0%)	84	83
12	H	131/153 (86%)	131 (100%)	0	100	100
13	I	185/205 (90%)	184 (100%)	1 (0%)	81	81
14	J	182/208 (88%)	182 (100%)	0	100	100
15	K	168/171 (98%)	168 (100%)	0	100	100
16	M	146/150 (97%)	146 (100%)	0	100	100
17	N	153/159 (96%)	151 (99%)	2 (1%)	61	71
18	O	107/109 (98%)	107 (100%)	0	100	100
19	Q	87/91 (96%)	87 (100%)	0	100	100
20	R	69/72 (96%)	68 (99%)	1 (1%)	59	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	a	175/176 (99%)	175 (100%)	0	100	100
23	b	160/162 (99%)	159 (99%)	1 (1%)	78	79
24	c	140/146 (96%)	138 (99%)	2 (1%)	59	70
25	d	150/151 (99%)	149 (99%)	1 (1%)	76	77
26	e	125/154 (81%)	124 (99%)	1 (1%)	73	76
27	f	155/156 (99%)	154 (99%)	1 (1%)	78	79
28	g	136/137 (99%)	134 (98%)	2 (2%)	57	69
29	h	84/107 (78%)	84 (100%)	0	100	100
30	i	102/105 (97%)	101 (99%)	1 (1%)	68	74
31	j	54/129 (42%)	54 (100%)	0	100	100
32	k	104/118 (88%)	104 (100%)	0	100	100
33	l	108/110 (98%)	108 (100%)	0	100	100
34	m	115/116 (99%)	115 (100%)	0	100	100
35	n	118/119 (99%)	117 (99%)	1 (1%)	73	76
36	o	46/47 (98%)	46 (100%)	0	100	100
37	p	81/88 (92%)	81 (100%)	0	100	100
38	q	92/97 (95%)	92 (100%)	0	100	100
39	r	108/111 (97%)	108 (100%)	0	100	100
40	s	90/91 (99%)	90 (100%)	0	100	100
41	t	94/103 (91%)	92 (98%)	2 (2%)	47	64
42	u	104/105 (99%)	104 (100%)	0	100	100
43	v	78/82 (95%)	78 (100%)	0	100	100
44	w	69/71 (97%)	68 (99%)	1 (1%)	59	70
45	x	67/69 (97%)	67 (100%)	0	100	100
46	y	45/46 (98%)	45 (100%)	0	100	100
47	z	46/116 (40%)	46 (100%)	0	100	100
48	L	31/65 (48%)	30 (97%)	1 (3%)	34	56
All	All	5879/6904 (85%)	5850 (100%)	29 (0%)	78	81

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Y	235	CYS

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Mol	Chain	Res	Type
6	W	136	VAL
6	W	392	VAL
6	W	428	ILE
7	V	92	LEU
7	V	127	ILE
8	D	45	VAL
8	D	88	ILE
9	E	104	THR
10	F	74	ILE
11	G	24	ARG
13	I	92	ILE
17	N	54	LEU
17	N	124	ILE
20	R	42	CYS
23	b	34	VAL
24	c	114	VAL
24	c	119	VAL
25	d	122	ILE
26	e	99	LEU
27	f	24	LEU
28	g	69	LYS
28	g	124	VAL
30	i	102	ILE
35	n	4	ARG
41	t	47	CYS
41	t	95	ILE
44	w	22	CYS
48	L	99	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
4	Y	274	GLN
4	Y	318	ASN
5	X	50	HIS
5	X	106	ASN
5	X	145	ASN
5	X	162	HIS
5	X	170	GLN
6	W	127	GLN
6	W	170	GLN
6	W	323	ASN

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Mol	Chain	Res	Type
6	W	413	GLN
7	V	21	ASN
7	V	119	GLN
7	V	153	ASN
7	V	231	GLN
7	V	351	GLN
8	D	132	ASN
8	D	140	ASN
8	D	187	HIS
8	D	209	HIS
8	D	218	HIS
9	E	109	HIS
10	F	43	ASN
10	F	45	ASN
10	F	110	ASN
10	F	175	HIS
10	F	221	ASN
10	F	237	GLN
10	F	279	HIS
10	F	291	ASN
10	F	322	GLN
11	G	151	GLN
11	G	264	GLN
12	H	4	GLN
12	H	28	GLN
13	I	93	ASN
13	I	112	ASN
13	I	200	ASN
14	J	24	ASN
14	J	38	GLN
14	J	61	GLN
14	J	240	ASN
16	M	68	HIS
16	M	109	HIS
17	N	19	GLN
17	N	25	HIS
17	N	103	ASN
17	N	137	GLN
18	O	41	GLN
19	Q	22	GLN
19	Q	82	GLN
19	Q	90	HIS

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Mol	Chain	Res	Type
22	a	11	GLN
22	a	37	HIS
22	a	70	ASN
22	a	95	GLN
23	b	55	HIS
24	c	55	GLN
24	c	133	HIS
25	d	15	HIS
25	d	158	HIS
27	f	88	HIS
27	f	142	GLN
28	g	22	HIS
28	g	146	ASN
29	h	25	ASN
29	h	87	ASN
30	i	81	GLN
31	j	59	HIS
35	n	14	HIS
35	n	120	ASN
37	p	36	GLN
38	q	15	ASN
38	q	21	HIS
39	r	20	HIS
39	r	26	HIS
39	r	49	ASN
39	r	52	GLN
40	s	24	ASN
40	s	88	ASN
42	u	99	GLN
42	u	104	GLN
42	u	108	GLN
44	w	57	HIS
45	x	67	GLN
46	y	43	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3200/3396 (94%)	705 (22%)	37 (1%)
2	B	120/121 (99%)	15 (12%)	0
3	C	157/158 (99%)	31 (19%)	2 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	3477/3675 (94%)	751 (21%)	39 (1%)

All (751) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	17	G
1	A	18	G
1	A	22	G
1	A	26	A
1	A	40	A
1	A	43	A
1	A	48	A
1	A	49	A
1	A	59	G
1	A	60	A
1	A	65	A
1	A	66	A
1	A	73	C
1	A	75	G
1	A	76	G
1	A	83	U
1	A	92	G
1	A	96	G
1	A	97	U
1	A	105	C
1	A	109	A
1	A	110	G
1	A	118	U
1	A	121	A
1	A	122	A
1	A	124	U
1	A	135	C
1	A	136	G
1	A	156	G
1	A	157	A
1	A	161	G
1	A	165	A
1	A	176	G
1	A	182	U
1	A	187	A
1	A	190	U
1	A	191	U

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Mol	Chain	Res	Type
1	A	192	C
1	A	198	A
1	A	200	C
1	A	206	G
1	A	210	U
1	A	211	A
1	A	213	A
1	A	218	G
1	A	219	A
1	A	237	G
1	A	240	U
1	A	241	G
1	A	243	G
1	A	245	U
1	A	246	U
1	A	247	C
1	A	248	U
1	A	249	U
1	A	252	U
1	A	253	A
1	A	257	U
1	A	269	G
1	A	286	U
1	A	295	A
1	A	315	C
1	A	323	A
1	A	329	U
1	A	336	A
1	A	338	A
1	A	348	A
1	A	351	A
1	A	359	U
1	A	375	A
1	A	376	G
1	A	398	A
1	A	399	A
1	A	401	U
1	A	402	A
1	A	403	C
1	A	404	G
1	A	420	G
1	A	421	G

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Mol	Chain	Res	Type
1	A	422	A
1	A	429	U
1	A	439	C
1	A	520	U
1	A	521	A
1	A	525	C
1	A	532	A
1	A	541	U
1	A	543	C
1	A	546	C
1	A	547	G
1	A	548	G
1	A	551	A
1	A	553	U
1	A	555	U
1	A	557	A
1	A	559	A
1	A	568	G
1	A	569	A
1	A	574	U
1	A	578	A
1	A	579	G
1	A	592	A
1	A	597	G
1	A	600	G
1	A	603	A
1	A	604	G
1	A	607	A
1	A	611	A
1	A	620	U
1	A	621	A
1	A	622	A
1	A	641	C
1	A	644	G
1	A	645	A
1	A	649	A
1	A	677	A
1	A	681	U
1	A	683	U
1	A	689	U
1	A	691	A
1	A	692	A

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Mol	Chain	Res	Type
1	A	705	A
1	A	709	A
1	A	712	G
1	A	713	U
1	A	715	A
1	A	719	U
1	A	720	A
1	A	728	G
1	A	767	U
1	A	774	G
1	A	776	U
1	A	777	U
1	A	780	A
1	A	781	G
1	A	784	A
1	A	785	G
1	A	801	A
1	A	806	A
1	A	817	A
1	A	830	A
1	A	849	C
1	A	861	C
1	A	869	G
1	A	872	U
1	A	874	U
1	A	879	U
1	A	880	G
1	A	887	G
1	A	888	A
1	A	894	G
1	A	896	A
1	A	897	U
1	A	907	G
1	A	908	G
1	A	914	A
1	A	916	G
1	A	917	A
1	A	921	A
1	A	924	G
1	A	932	U
1	A	933	A
1	A	937	G

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Mol	Chain	Res	Type
1	A	944	C
1	A	946	U
1	A	959	C
1	A	960	U
1	A	961	C
1	A	974	G
1	A	978	G
1	A	979	U
1	A	980	A
1	A	982	C
1	A	991	G
1	A	994	G
1	A	1001	G
1	A	1002	A
1	A	1010	G
1	A	1012	G
1	A	1013	G
1	A	1014	U
1	A	1015	U
1	A	1016	C
1	A	1017	C
1	A	1018	G
1	A	1020	G
1	A	1023	C
1	A	1024	G
1	A	1026	A
1	A	1027	A
1	A	1028	U
1	A	1029	G
1	A	1030	A
1	A	1034	U
1	A	1035	G
1	A	1036	A
1	A	1037	C
1	A	1038	C
1	A	1039	U
1	A	1040	A
1	A	1042	U
1	A	1045	C
1	A	1046	A
1	A	1047	A
1	A	1049	C

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Mol	Chain	Res	Type
1	A	1064	A
1	A	1065	A
1	A	1072	G
1	A	1081	U
1	A	1093	A
1	A	1094	U
1	A	1095	U
1	A	1096	U
1	A	1097	G
1	A	1098	A
1	A	1103	A
1	A	1104	G
1	A	1111	U
1	A	1117	G
1	A	1124	U
1	A	1131	G
1	A	1140	G
1	A	1141	C
1	A	1143	A
1	A	1153	A
1	A	1159	A
1	A	1177	G
1	A	1180	A
1	A	1181	U
1	A	1192	C
1	A	1193	A
1	A	1195	A
1	A	1196	C
1	A	1201	C
1	A	1209	G
1	A	1221	A
1	A	1222	G
1	A	1223	A
1	A	1235	U
1	A	1236	G
1	A	1237	G
1	A	1239	C
1	A	1240	A
1	A	1241	U
1	A	1242	G
1	A	1244	A
1	A	1245	A

Continued on next page...

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Mol	Chain	Res	Type
1	A	1246	G
1	A	1247	U
1	A	1252	A
1	A	1258	U
1	A	1262	G
1	A	1263	A
1	A	1264	G
1	A	1266	G
1	A	1273	A
1	A	1281	G
1	A	1285	G
1	A	1295	G
1	A	1307	G
1	A	1309	U
1	A	1313	G
1	A	1325	U
1	A	1330	A
1	A	1345	G
1	A	1348	U
1	A	1349	G
1	A	1351	U
1	A	1352	A
1	A	1353	U
1	A	1354	G
1	A	1356	U
1	A	1357	G
1	A	1366	A
1	A	1383	G
1	A	1386	A
1	A	1390	A
1	A	1392	G
1	A	1399	A
1	A	1400	G
1	A	1419	A
1	A	1430	U
1	A	1434	G
1	A	1437	C
1	A	1443	G
1	A	1446	A
1	A	1448	U
1	A	1450	G
1	A	1455	U

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Mol	Chain	Res	Type
1	A	1481	A
1	A	1482	A
1	A	1484	U
1	A	1487	G
1	A	1506	A
1	A	1508	C
1	A	1523	U
1	A	1526	U
1	A	1527	C
1	A	1533	U
1	A	1536	G
1	A	1547	G
1	A	1555	U
1	A	1556	C
1	A	1557	A
1	A	1559	A
1	A	1560	G
1	A	1561	G
1	A	1562	C
1	A	1563	C
1	A	1564	U
1	A	1565	G
1	A	1566	A
1	A	1567	U
1	A	1568	U
1	A	1569	U
1	A	1570	U
1	A	1571	A
1	A	1572	U
1	A	1576	G
1	A	1577	G
1	A	1579	C
1	A	1580	A
1	A	1583	A
1	A	1589	A
1	A	1593	A
1	A	1605	A
1	A	1606	U
1	A	1618	G
1	A	1619	A
1	A	1620	U
1	A	1629	U

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Mol	Chain	Res	Type
1	A	1636	U
1	A	1642	A
1	A	1643	A
1	A	1656	A
1	A	1657	C
1	A	1662	G
1	A	1666	G
1	A	1683	A
1	A	1703	U
1	A	1716	U
1	A	1717	U
1	A	1724	U
1	A	1725	C
1	A	1728	G
1	A	1736	G
1	A	1741	A
1	A	1742	U
1	A	1750	A
1	A	1751	G
1	A	1758	G
1	A	1759	C
1	A	1760	A
1	A	1762	C
1	A	1764	U
1	A	1765	U
1	A	1766	G
1	A	1770	G
1	A	1773	C
1	A	1780	G
1	A	1793	C
1	A	1797	A
1	A	1814	A
1	A	1816	A
1	A	1817	G
1	A	1820	U
1	A	1821	U
1	A	1839	A
1	A	1842	A
1	A	1849	C
1	A	1850	A
1	A	1866	C
1	A	1867	A

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Mol	Chain	Res	Type
1	A	1871	U
1	A	1880	U
1	A	1886	A
1	A	1893	A
1	A	1906	G
1	A	1907	C
1	A	1908	A
1	A	1909	A
1	A	1913	A
1	A	1926	C
1	A	1927	G
1	A	1943	C
1	A	1951	C
1	A	1952	G
1	A	1953	G
1	A	1954	G
1	A	2101	C
1	A	2102	U
1	A	2113	A
1	A	2114	C
1	A	2121	G
1	A	2122	G
1	A	2126	A
1	A	2131	A
1	A	2139	A
1	A	2142	A
1	A	2158	A
1	A	2169	G
1	A	2178	A
1	A	2184	U
1	A	2185	G
1	A	2191	U
1	A	2192	C
1	A	2205	U
1	A	2208	A
1	A	2209	U
1	A	2210	G
1	A	2244	A
1	A	2248	C
1	A	2249	G
1	A	2250	G
1	A	2253	G

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Mol	Chain	Res	Type
1	A	2254	U
1	A	2255	A
1	A	2256	A
1	A	2257	C
1	A	2262	A
1	A	2263	C
1	A	2265	C
1	A	2267	C
1	A	2268	U
1	A	2269	U
1	A	2270	A
1	A	2273	G
1	A	2274	U
1	A	2281	A
1	A	2282	U
1	A	2285	C
1	A	2286	U
1	A	2288	G
1	A	2291	A
1	A	2298	U
1	A	2306	C
1	A	2307	G
1	A	2308	C
1	A	2310	U
1	A	2313	A
1	A	2314	U
1	A	2315	G
1	A	2334	U
1	A	2336	U
1	A	2354	C
1	A	2364	G
1	A	2373	A
1	A	2374	C
1	A	2375	G
1	A	2376	G
1	A	2385	G
1	A	2388	U
1	A	2393	G
1	A	2394	G
1	A	2397	A
1	A	2402	A
1	A	2403	G

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Mol	Chain	Res	Type
1	A	2404	A
1	A	2411	U
1	A	2415	C
1	A	2419	A
1	A	2435	G
1	A	2437	G
1	A	2440	G
1	A	2442	G
1	A	2443	A
1	A	2444	C
1	A	2449	A
1	A	2450	G
1	A	2452	G
1	A	2453	U
1	A	2454	G
1	A	2458	A
1	A	2459	A
1	A	2460	U
1	A	2461	A
1	A	2462	A
1	A	2463	G
1	A	2464	U
1	A	2468	A
1	A	2469	G
1	A	2472	U
1	A	2474	G
1	A	2476	C
1	A	2477	G
1	A	2480	A
1	A	2484	A
1	A	2485	A
1	A	2487	U
1	A	2488	A
1	A	2490	C
1	A	2495	C
1	A	2496	C
1	A	2498	U
1	A	2499	U
1	A	2501	U
1	A	2502	A
1	A	2503	G
1	A	2505	U

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Mol	Chain	Res	Type
1	A	2506	U
1	A	2507	C
1	A	2508	U
1	A	2509	U
1	A	2514	U
1	A	2515	A
1	A	2522	G
1	A	2531	C
1	A	2533	G
1	A	2537	U
1	A	2538	U
1	A	2539	C
1	A	2540	A
1	A	2541	U
1	A	2542	U
1	A	2543	U
1	A	2544	U
1	A	2547	A
1	A	2549	G
1	A	2550	U
1	A	2552	C
1	A	2561	A
1	A	2562	A
1	A	2569	A
1	A	2570	U
1	A	2571	U
1	A	2572	C
1	A	2573	G
1	A	2577	C
1	A	2585	G
1	A	2593	A
1	A	2594	C
1	A	2599	U
1	A	2606	G
1	A	2607	G
1	A	2614	G
1	A	2620	G
1	A	2626	A
1	A	2635	A
1	A	2636	A
1	A	2648	G
1	A	2652	U

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Mol	Chain	Res	Type
1	A	2656	A
1	A	2657	A
1	A	2664	C
1	A	2674	A
1	A	2677	G
1	A	2688	U
1	A	2689	A
1	A	2691	A
1	A	2696	A
1	A	2704	A
1	A	2705	A
1	A	2713	U
1	A	2719	U
1	A	2728	G
1	A	2729	U
1	A	2753	G
1	A	2754	G
1	A	2777	G
1	A	2778	G
1	A	2799	A
1	A	2800	G
1	A	2801	A
1	A	2803	A
1	A	2804	A
1	A	2810	C
1	A	2814	G
1	A	2817	A
1	A	2828	G
1	A	2838	A
1	A	2840	C
1	A	2842	U
1	A	2843	U
1	A	2844	C
1	A	2845	A
1	A	2850	G
1	A	2860	U
1	A	2861	U
1	A	2867	C
1	A	2871	G
1	A	2872	A
1	A	2873	U
1	A	2875	U

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Mol	Chain	Res	Type
1	A	2887	A
1	A	2889	C
1	A	2898	G
1	A	2899	C
1	A	2904	U
1	A	2911	A
1	A	2914	G
1	A	2916	U
1	A	2923	U
1	A	2926	A
1	A	2933	A
1	A	2935	U
1	A	2936	A
1	A	2941	A
1	A	2945	G
1	A	2946	A
1	A	2947	G
1	A	2951	G
1	A	2971	A
1	A	2975	U
1	A	2983	C
1	A	2990	G
1	A	2996	U
1	A	2997	G
1	A	3011	A
1	A	3012	A
1	A	3014	U
1	A	3028	G
1	A	3056	U
1	A	3059	G
1	A	3078	U
1	A	3079	U
1	A	3086	A
1	A	3092	C
1	A	3103	A
1	A	3109	G
1	A	3113	A
1	A	3115	C
1	A	3117	C
1	A	3119	U
1	A	3122	A
1	A	3129	A

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Mol	Chain	Res	Type
1	A	3130	A
1	A	3131	U
1	A	3142	A
1	A	3143	C
1	A	3153	U
1	A	3154	C
1	A	3155	U
1	A	3156	U
1	A	3157	U
1	A	3158	G
1	A	3164	C
1	A	3165	A
1	A	3168	A
1	A	3170	A
1	A	3173	G
1	A	3174	A
1	A	3176	G
1	A	3179	U
1	A	3181	C
1	A	3187	A
1	A	3196	U
1	A	3197	G
1	A	3199	G
1	A	3206	C
1	A	3207	U
1	A	3209	A
1	A	3210	A
1	A	3217	C
1	A	3218	A
1	A	3219	G
1	A	3224	G
1	A	3229	G
1	A	3243	A
1	A	3245	A
1	A	3246	G
1	A	3247	G
1	A	3253	G
1	A	3259	U
1	A	3269	U
1	A	3270	U
1	A	3272	C
1	A	3273	A

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Mol	Chain	Res	Type
1	A	3275	U
1	A	3276	G
1	A	3278	C
1	A	3279	A
1	A	3280	U
1	A	3281	U
1	A	3283	U
1	A	3286	G
1	A	3289	G
1	A	3294	A
1	A	3295	A
1	A	3304	U
1	A	3308	C
1	A	3313	U
1	A	3316	A
1	A	3317	U
1	A	3318	G
1	A	3320	A
1	A	3324	C
1	A	3325	G
1	A	3341	U
1	A	3342	A
1	A	3345	G
1	A	3350	C
1	A	3351	U
1	A	3352	U
1	A	3353	G
1	A	3355	U
1	A	3360	C
1	A	3362	A
1	A	3368	U
1	A	3369	G
1	A	3375	A
1	A	3376	A
1	A	3378	C
1	A	3382	U
1	A	3386	G
1	A	3390	G
2	B	10	C
2	B	18	C
2	B	22	A
2	B	28	C

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Mol	Chain	Res	Type
2	B	38	U
2	B	49	G
2	B	52	G
2	B	65	G
2	B	71	G
2	B	73	C
2	B	99	G
2	B	102	A
2	B	112	G
2	B	114	U
2	B	121	U
3	C	34	U
3	C	35	C
3	C	39	G
3	C	45	C
3	C	51	G
3	C	58	G
3	C	59	A
3	C	62	C
3	C	63	G
3	C	67	U
3	C	80	A
3	C	82	U
3	C	83	C
3	C	84	C
3	C	85	G
3	C	86	U
3	C	90	U
3	C	95	G
3	C	102	U
3	C	104	A
3	C	106	C
3	C	111	A
3	C	113	U
3	C	125	U
3	C	126	A
3	C	127	U
3	C	129	C
3	C	138	A
3	C	144	G
3	C	155	A
3	C	158	U

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	239	G
1	A	547	G
1	A	599	C
1	A	916	G
1	A	979	U
1	A	1027	A
1	A	1029	G
1	A	1038	C
1	A	1064	A
1	A	1097	G
1	A	1103	A
1	A	1222	G
1	A	1241	U
1	A	1352	A
1	A	1355	A
1	A	1554	U
1	A	1576	G
1	A	1716	U
1	A	1815	U
1	A	2101	C
1	A	2112	U
1	A	2209	U
1	A	2249	G
1	A	2264	U
1	A	2266	U
1	A	2453	U
1	A	2495	C
1	A	2501	U
1	A	2513	U
1	A	2537	U
1	A	2541	U
1	A	2593	A
1	A	3078	U
1	A	3121	U
1	A	3218	A
1	A	3228	C
1	A	3269	U
3	C	82	U
3	C	85	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

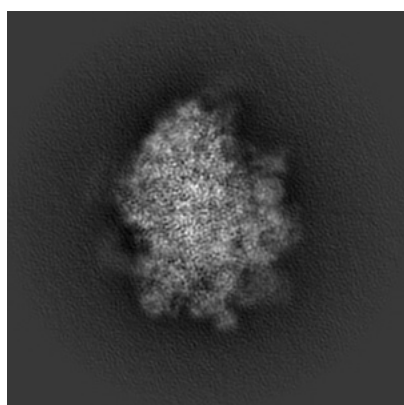
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0373. These allow visual inspection of the internal detail of the map and identification of artifacts.

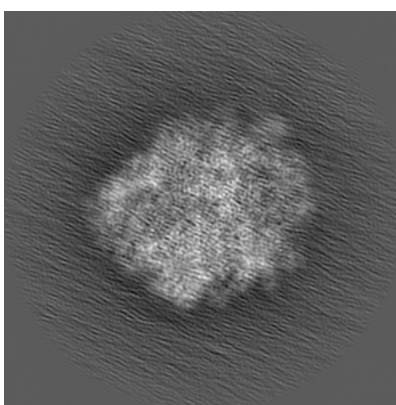
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

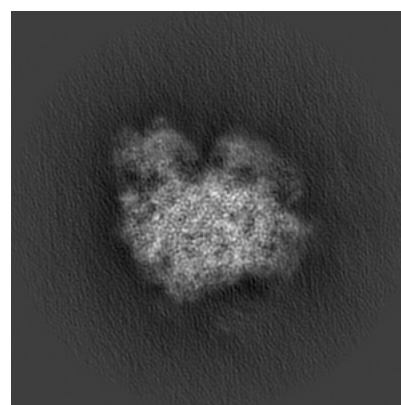
6.1.1 Primary map



X



Y

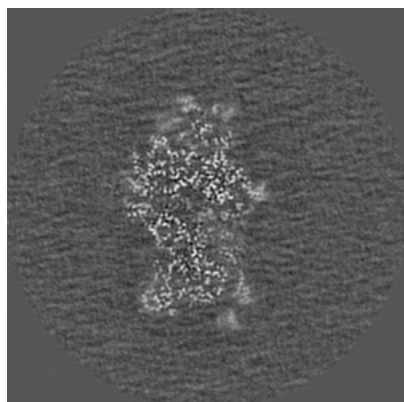


Z

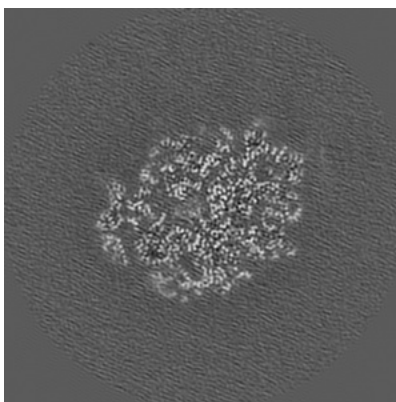
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

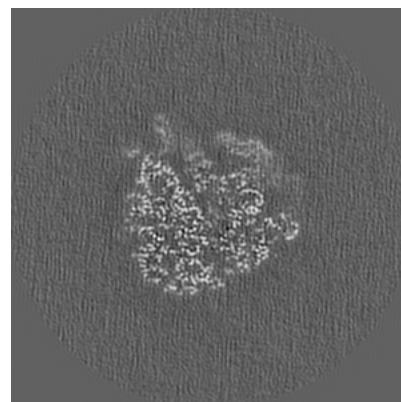
6.2.1 Primary map



X Index: 192



Y Index: 192

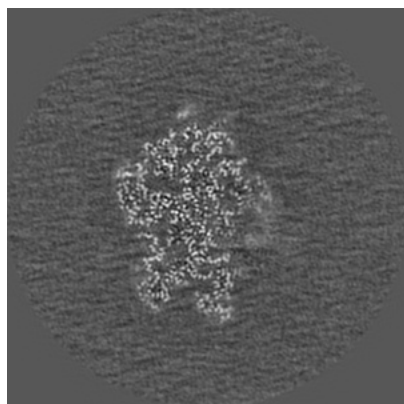


Z Index: 192

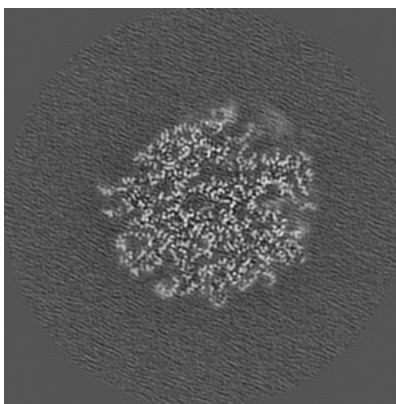
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

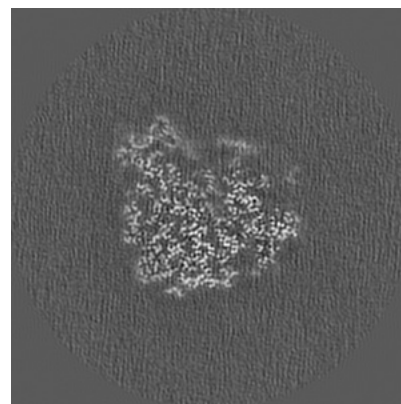
6.3.1 Primary map



X Index: 173



Y Index: 173

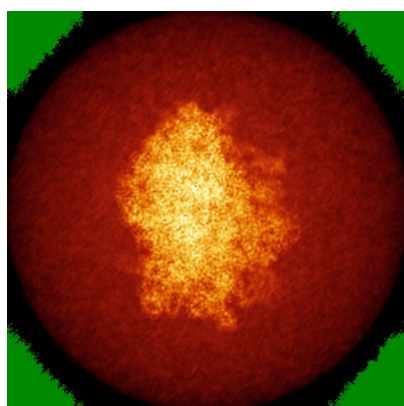


Z Index: 185

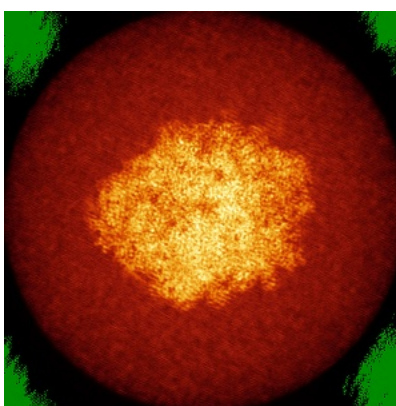
The images above show the largest variance slices of the map in three orthogonal directions.

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

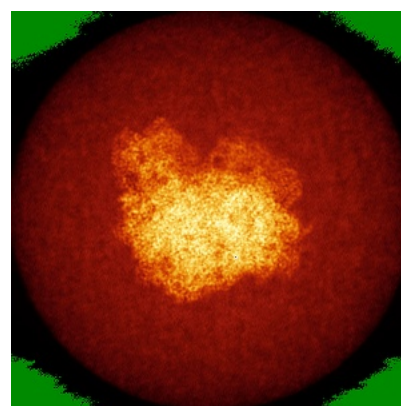
6.4.1 Primary map



X



Y

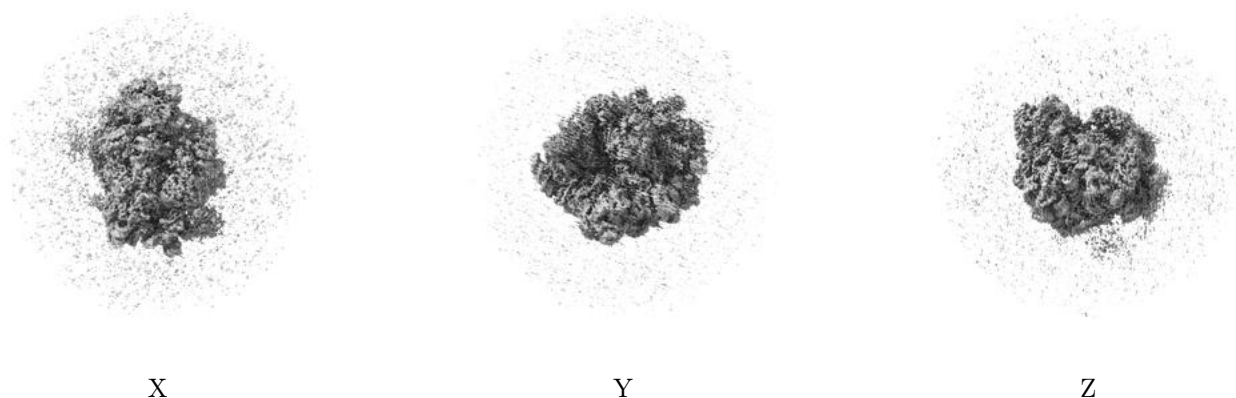


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

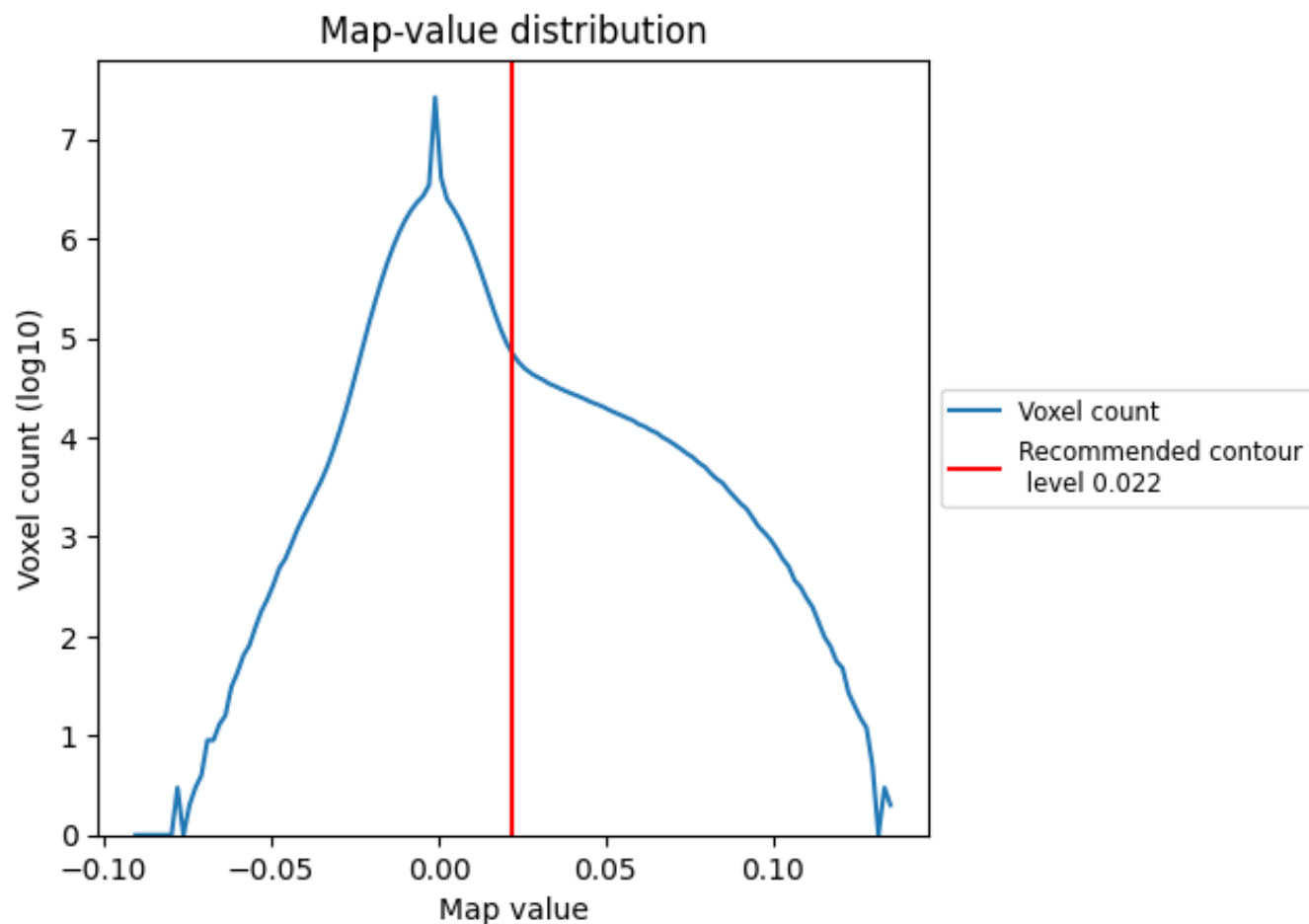
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

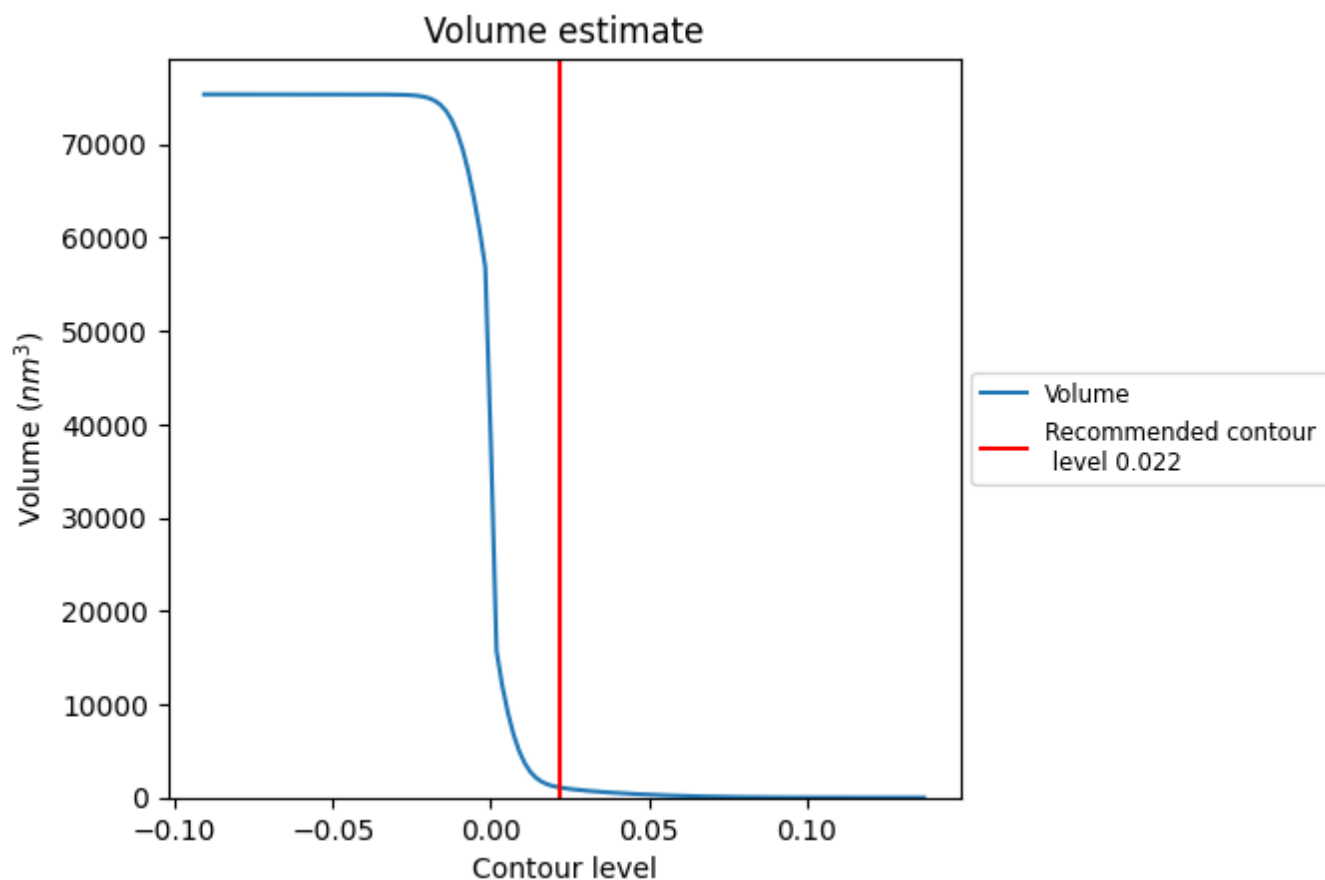
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

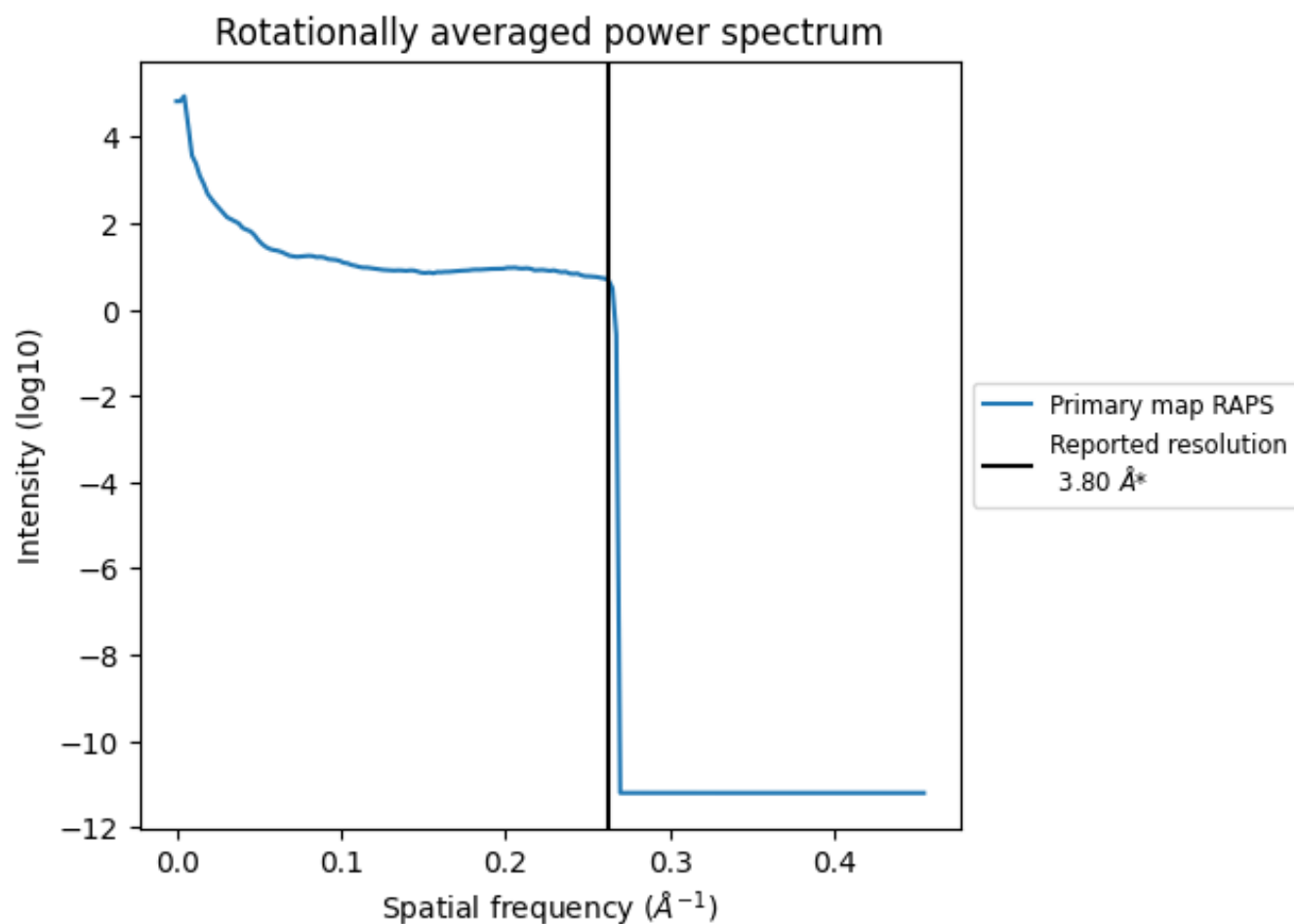
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1068 nm³; this corresponds to an approximate mass of 965 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

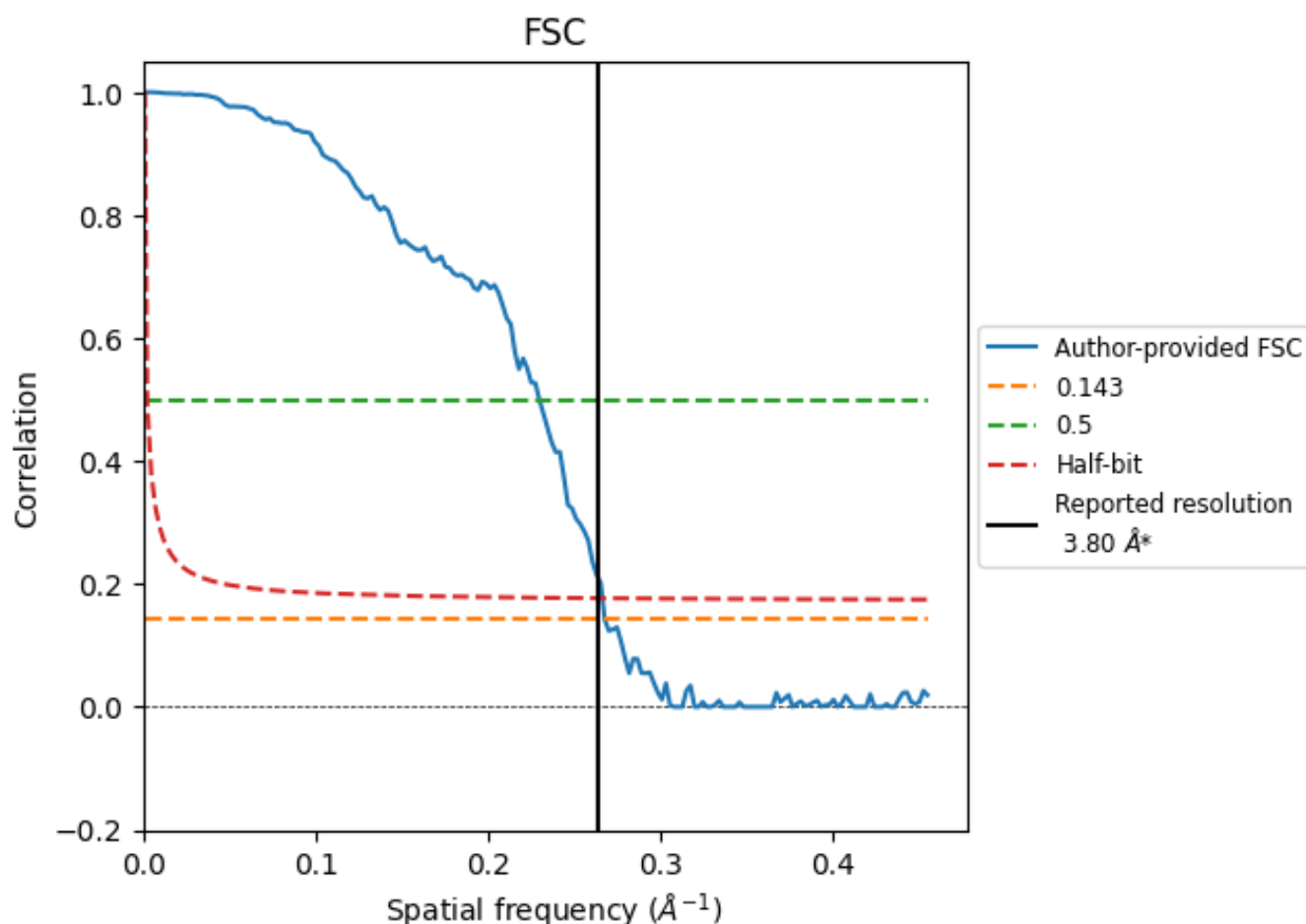


*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

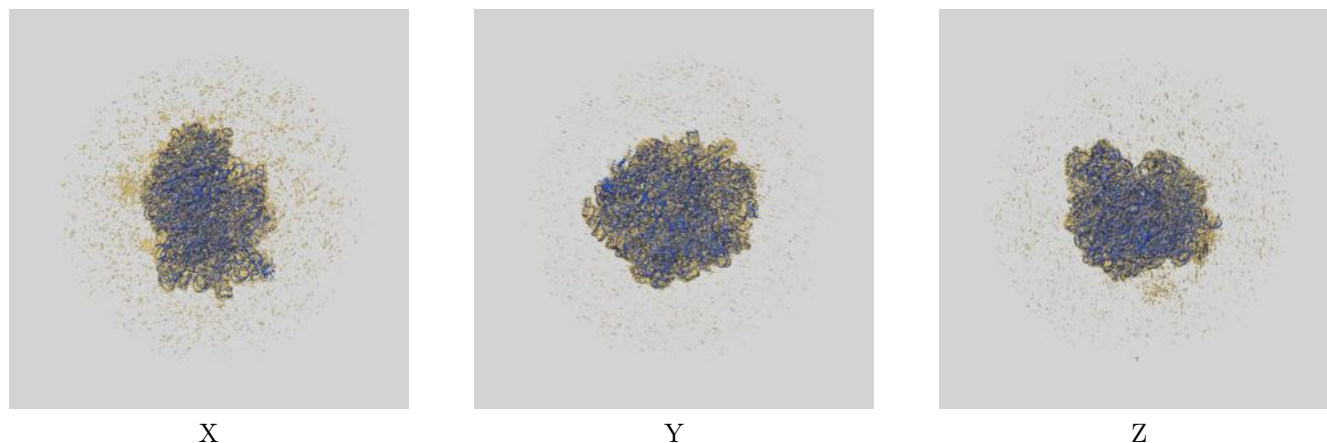
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.74	4.35	3.76
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

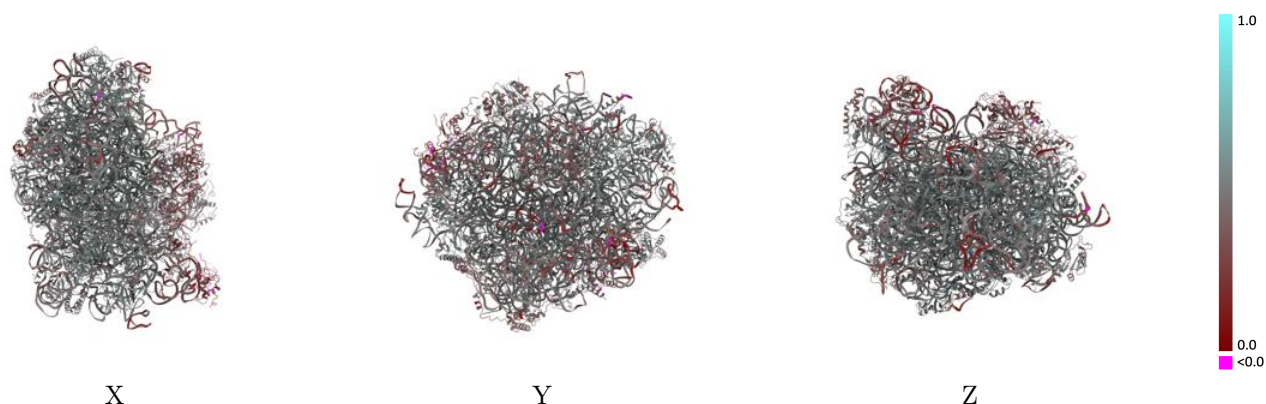
This section contains information regarding the fit between EMDB map EMD-0373 and PDB model 6N8N. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



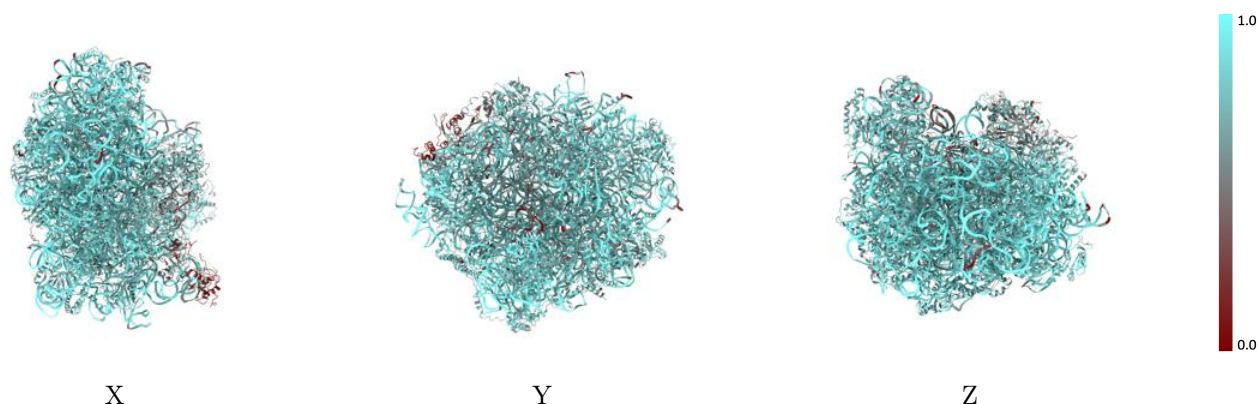
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



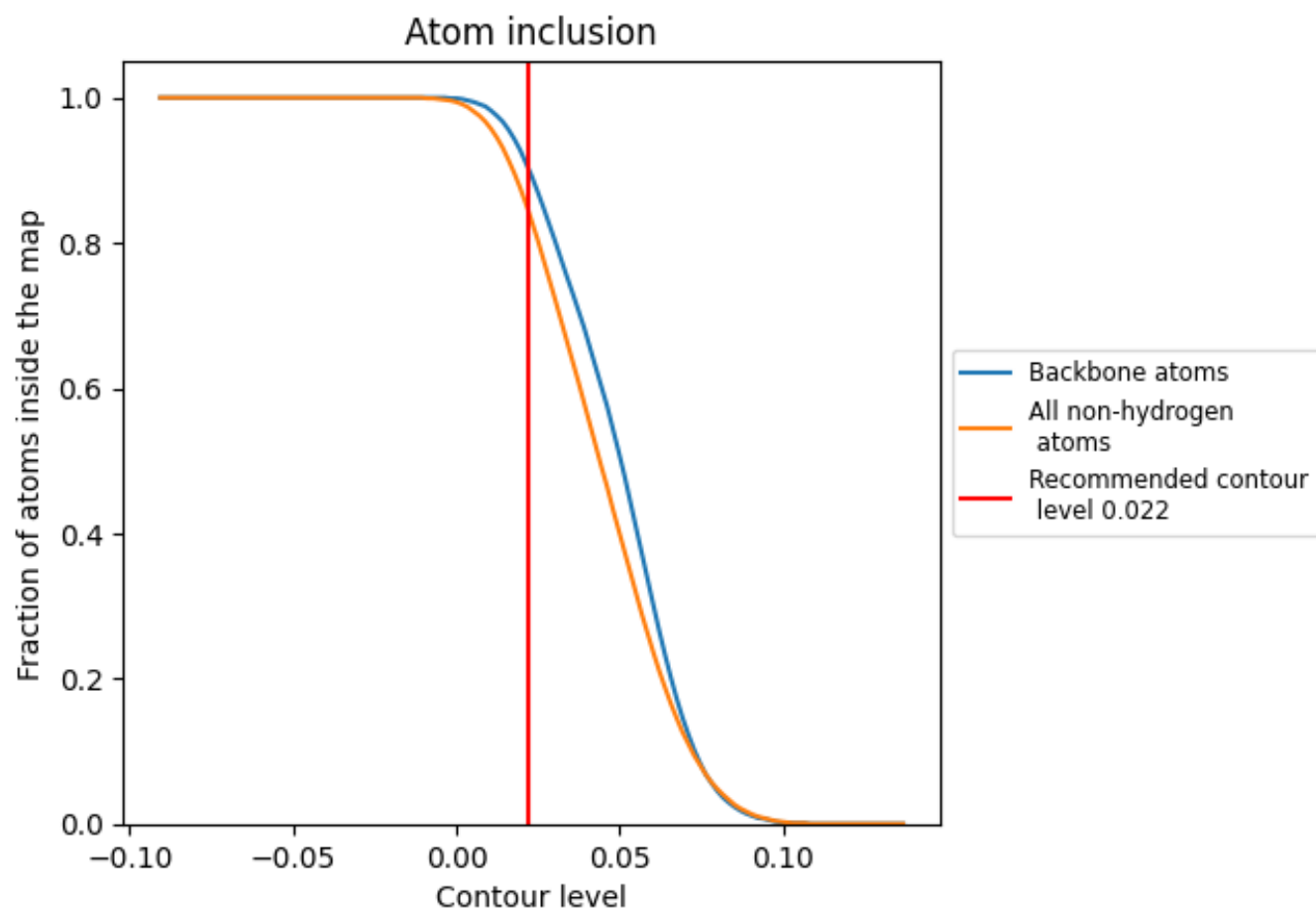
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 85% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8460	 0.4570
A	 0.9100	 0.4590
B	 0.9520	 0.4610
C	 0.9400	 0.4730
D	 0.8240	 0.5080
E	 0.8270	 0.4900
F	 0.7950	 0.4810
G	 0.7750	 0.4170
H	 0.7870	 0.4620
I	 0.8080	 0.4740
J	 0.8030	 0.4600
K	 0.7870	 0.4730
L	 0.2100	 0.2090
M	 0.7240	 0.3840
N	 0.7880	 0.4620
O	 0.8050	 0.4690
Q	 0.7450	 0.4820
R	 0.8130	 0.4930
S	 0.7010	 0.3340
V	 0.6160	 0.4010
W	 0.6460	 0.3470
X	 0.7030	 0.4330
Y	 0.3890	 0.3310
a	 0.8250	 0.5050
b	 0.8180	 0.4940
c	 0.7800	 0.4820
d	 0.7960	 0.4860
e	 0.8310	 0.4900
f	 0.8100	 0.4800
g	 0.7680	 0.4780
h	 0.7930	 0.4390
i	 0.7580	 0.4890
j	 0.7850	 0.4810
k	 0.7940	 0.4690
l	 0.7970	 0.4860



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Chain	Atom inclusion	Q-score
m	 0.8220	 0.4730
n	 0.8160	 0.4950
o	 0.7260	 0.4380
p	 0.7770	 0.4580
q	 0.7680	 0.4640
r	 0.7890	 0.4950
s	 0.8320	 0.5030
t	 0.7850	 0.4910
u	 0.8080	 0.4660
v	 0.7640	 0.4510
w	 0.8700	 0.5130
x	 0.7480	 0.4440
y	 0.7930	 0.5030
z	 0.5560	 0.4530