



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 05:55 AM UTC

PDB ID : 9N5T / pdb_00009n5t
EMDB ID : EMD-49038
Title : Mycobacterium smegmatis 70S ribosome with small molecule drug MK-7762
Authors : Zhu, J.
Deposited on : 2025-02-04
Resolution : 2.01 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

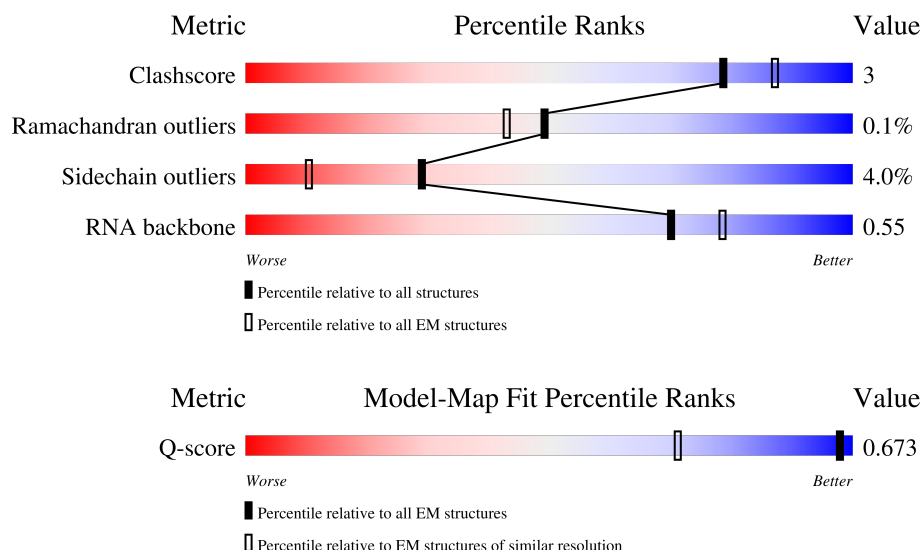
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.01 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	1691 (1.52 - 2.51)

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	3	24	
2	A	3120	
3	B	118	

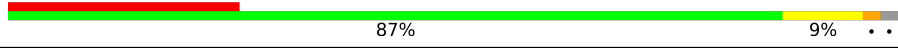
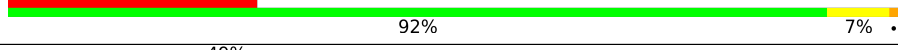
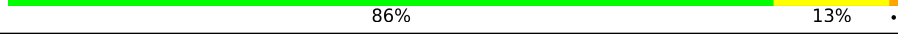
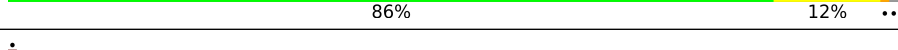
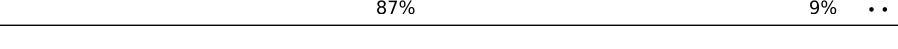
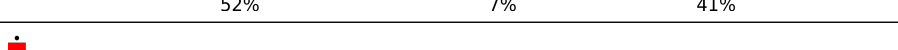
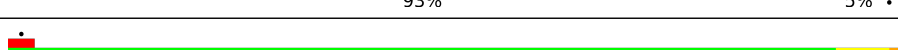
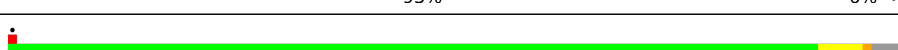
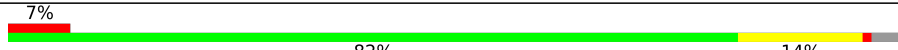
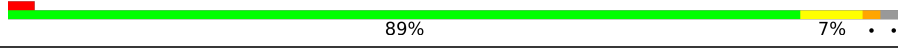
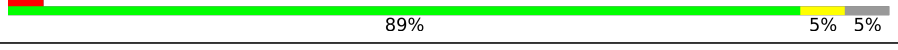
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Mol	Chain	Length	Quality of chain
4	BA	1528	
5	BB	33	
6	BC	275	
7	BD	201	
8	BE	214	
9	BF	96	
10	BG	156	
11	BH	132	
12	BI	150	
13	BJ	101	
14	BK	138	
15	BL	124	
16	BM	124	
17	BN	61	
18	BO	89	
19	BP	156	
20	BQ	98	
21	BR	84	
22	BS	93	
23	BT	86	
24	BV	277	
25	BW	76	
26	I	15	
27	C	278	
28	D	217	

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Mol	Chain	Length	Quality of chain
29	E	215	
30	F	187	
31	G	179	
32	H	151	
33	J	142	
34	K	147	
35	L	122	
36	M	147	
37	N	138	
38	O	199	
39	P	127	
40	Q	113	
41	R	129	
42	S	103	
43	T	153	
44	U	100	
45	V	105	
46	W	215	
47	X	88	
48	Y	64	
49	Z	77	
50	a	61	
51	b	57	
52	c	55	
53	d	47	

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Mol	Chain	Length	Quality of chain
54	e	64	 77% 19%
55	f	37	 86% 14%
56	g	75	 9% 68% 11% 21%
57	s	5	 40% 20% 20% 60%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 156393 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	3	23	Total	C	N	O	0	0
			190	111	50	29		

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	3085	Total	C	N	O	P	0	0
			66255	29532	12188	21450	3085		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	118	Total	C	N	O	P	0	0
			2522	1126	468	810	118		

- Molecule 4 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BA	1512	Total	C	N	O	P	0	0
			32462	14458	5935	10557	1512		

- Molecule 5 is a protein called Conserved domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BB	32	Total	C	N	O	S	0	0
			281	172	71	37	1		

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BC	208	Total	C	N	O	S	0	0
			1660	1036	322	298	4		

- Molecule 7 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BD	200	Total	C	N	O	S	0	0
			1642	1028	316	296	2		

- Molecule 8 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BE	180	Total	C	N	O	S	0	0
			1297	812	245	236	4		

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BF	96	Total	C	N	O	S	0	0
			772	486	138	146	2		

- Molecule 10 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BG	155	Total	C	N	O	S	0	0
			1233	768	241	222	2		

- Molecule 11 is a protein called 30S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BH	131	Total	C	N	O	S	0	0
			1011	633	189	188	1		

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	BI	126	Total	C	N	O	0	0
			995	630	194	171		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BJ	99	Total	C	N	O	S	0	0
			789	495	146	145	3		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BK	115	Total	C	N	O	S	0	0
			855	528	170	156	1		

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BL	122	Total	C	N	O	S	0	0
			958	594	197	165	2		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BM	116	Total	C	N	O	S	0	0
			935	572	191	169	3		

- Molecule 17 is a protein called 30S Ribosomal Protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BN	60	Total	C	N	O	S	0	0
			478	302	97	74	5		

- Molecule 18 is a protein called 30S Ribosomal Protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	BO	88	Total	C	N	O	0	0
			721	449	147	125		

- Molecule 19 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	BP	113	Total	C	N	O	0	0
			891	570	162	159		

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BQ	94	Total	C	N	O	S	0	0
			748	469	142	135	2		

- Molecule 21 is a protein called 30S Ribosomal Protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BR	65	Total	C	N	O	S	0	0
			513	318	102	90	3		

- Molecule 22 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BS	82	Total	C	N	O	S	0	0
			662	425	124	112	1		

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BT	85	Total	C	N	O		0	0
			661	402	139	120			

- Molecule 24 is a protein called 30S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BV	228	Total	C	N	O	S	0	0
			1793	1132	322	330	9		

- Molecule 25 is a RNA chain called P/P-site Phe-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BW	76	Total	C	N	O	P	0	0
			1622	723	290	533	76		

- Molecule 26 is a RNA chain called mRNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	I	6	Total	C	N	O	P	0	0
			125	56	20	43	6		

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	C	275	Total	C	N	O	S	0	0
			2110	1298	438	370	4		

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	D	214	Total	C	N	O	S	0	0
			1587	982	310	290	5		

- Molecule 29 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	E	209	Total	C	N	O	S	0	0
			1569	969	295	303	2		

- Molecule 30 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	182	Total	C	N	O	S	0	0
			1446	907	271	262	6		

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	G	176	Total	C	N	O	S	0	0
			1348	845	249	253	1		

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	H	151	Total	C	N	O	S	0	0
			1120	695	209	215	1		

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	J	69	Total	C	N	O	S	0	0
			505	315	91	98	1		

- Molecule 34 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	K	146	Total	C	N	O	S	0	0
			1131	722	207	201	1		

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L	122	Total	C	N	O	S	0	0
			939	586	179	171	3		

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	M	145	Total	C	N	O	S	0	0
			1079	676	205	195	3		

- Molecule 37 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	N	136	Total	C	N	O	S	0	0
			1092	690	213	187	2		

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	O	118	Total	C	N	O	S	0	0
			928	583	180	163	2		

- Molecule 39 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	P	126	Total	C	N	O	S	0	0
			956	586	199	171			

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Q	113	Total	C	N	O	S	0	0
			908	570	171	166	1		

- Molecule 41 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	R	124	Total	C	N	O	S	0	0
			988	613	203	172			

- Molecule 42 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	S	100	Total	C	N	O	0	0
			754	478	137	139		

- Molecule 43 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	T	114	Total	C	N	O	0	0
			873	543	171	159		

- Molecule 44 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	U	97	Total	C	N	O	0	0
			756	479	138	139		

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	V	97	Total	C	N	O	S	0	0
			732	456	137	137	2		

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	W	192	Total	C	N	O	0	0
			1428	881	255	292		

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	X	79	Total	C	N	O	0	0
			586	361	123	102		

- Molecule 48 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Y	63	Total	C	N	O	S	0	0
			471	283	103	81	4		

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Z	66	Total	C	N	O	S	0	0
			544	333	105	105	1		

- Molecule 50 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	a	59	Total	C	N	O	0	0
			474	292	95	87		

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	b	54	Total	C	N	O	S	0	0
			423	260	93	69	1		

- Molecule 52 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	c	49	Total	C	N	O	S	0	0
			405	248	82	71	4		

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	d	46	Total	C	N	O	S	0	0
			378	225	97	55	1		

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	e	63	Total	C	N	O	0	0
			503	302	115	86		

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	f	37	Total	C	N	O	S	0	0
			299	181	66	47	5		

- Molecule 56 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	g	59	Total	C	N	O	S	0	0
			458	284	84	85	5		

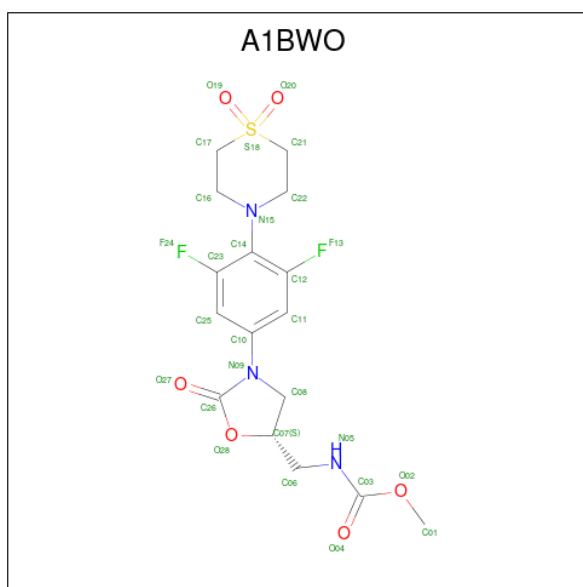
- Molecule 57 is a protein called Nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	s	2	Total	C	N	O	0	0
			16	12	2	2		

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	A	250	Total	Mg	0
			250	250	
58	B	5	Total	Mg	0
			5	5	
58	BA	85	Total	Mg	0
			85	85	
58	BM	1	Total	Mg	0
			1	1	
58	BR	1	Total	Mg	0
			1	1	
58	BW	1	Total	Mg	0
			1	1	
58	C	2	Total	Mg	0
			2	2	
58	D	1	Total	Mg	0
			1	1	
58	M	1	Total	Mg	0
			1	1	

- Molecule 59 is methyl ({(5S)-3-[4-(1,1-dioxo-1λ⁶-thiomorpholin-4-yl)-3,5-difluorophenyl]-2-oxo-1,3-oxazolidin-5-yl}methyl)carbamate (CCD ID: A1BWO) (formula: C₁₆H₁₉F₂N₃O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
59	A	1	Total	C	F	N	O	S	0
			28	16	2	3	6	1	

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
60	BN	1	Total	Zn	0
			1	1	
60	BR	1	Total	Zn	0
			1	1	
60	Y	1	Total	Zn	0
			1	1	
60	c	1	Total	Zn	0
			1	1	
60	f	1	Total	Zn	0
			1	1	
60	g	1	Total	Zn	0
			1	1	

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	3	3	Total	O	0
			3	3	
61	A	5185	Total	O	0
			5185	5185	

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Mol	Chain	Residues	Atoms		AltConf
61	B	55	Total 55	O 55	0
61	BA	1204	Total 1204	O 1204	0
61	BB	2	Total 2	O 2	0
61	BC	1	Total 1	O 1	0
61	BD	1	Total 1	O 1	0
61	BE	2	Total 2	O 2	0
61	BG	1	Total 1	O 1	0
61	BH	5	Total 5	O 5	0
61	BI	10	Total 10	O 10	0
61	BJ	4	Total 4	O 4	0
61	BK	10	Total 10	O 10	0
61	BL	7	Total 7	O 7	0
61	BN	4	Total 4	O 4	0
61	BO	4	Total 4	O 4	0
61	BP	4	Total 4	O 4	0
61	BR	5	Total 5	O 5	0
61	BT	4	Total 4	O 4	0
61	BW	9	Total 9	O 9	0
61	I	7	Total 7	O 7	0
61	C	100	Total 100	O 100	0
61	D	53	Total 53	O 53	0

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Mol	Chain	Residues	Atoms		AltConf
61	E	43	Total 43	O 43	0
61	F	2	Total 2	O 2	0
61	G	1	Total 1	O 1	0
61	H	3	Total 3	O 3	0
61	K	14	Total 14	O 14	0
61	L	9	Total 9	O 9	0
61	M	39	Total 39	O 39	0
61	N	33	Total 33	O 33	0
61	O	26	Total 26	O 26	0
61	P	11	Total 11	O 11	0
61	Q	15	Total 15	O 15	0
61	R	46	Total 46	O 46	0
61	S	19	Total 19	O 19	0
61	T	29	Total 29	O 29	0
61	U	20	Total 20	O 20	0
61	V	5	Total 5	O 5	0
61	W	3	Total 3	O 3	0
61	X	25	Total 25	O 25	0
61	Y	23	Total 23	O 23	0
61	Z	2	Total 2	O 2	0
61	a	10	Total 10	O 10	0

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Mol	Chain	Residues	Atoms		AltConf
61	b	12	Total 12	O 12	0
61	c	8	Total 8	O 8	0
61	d	22	Total 22	O 22	0
61	e	32	Total 32	O 32	0
61	f	3	Total 3	O 3	0

3 Residue-property plots [i](#)

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.

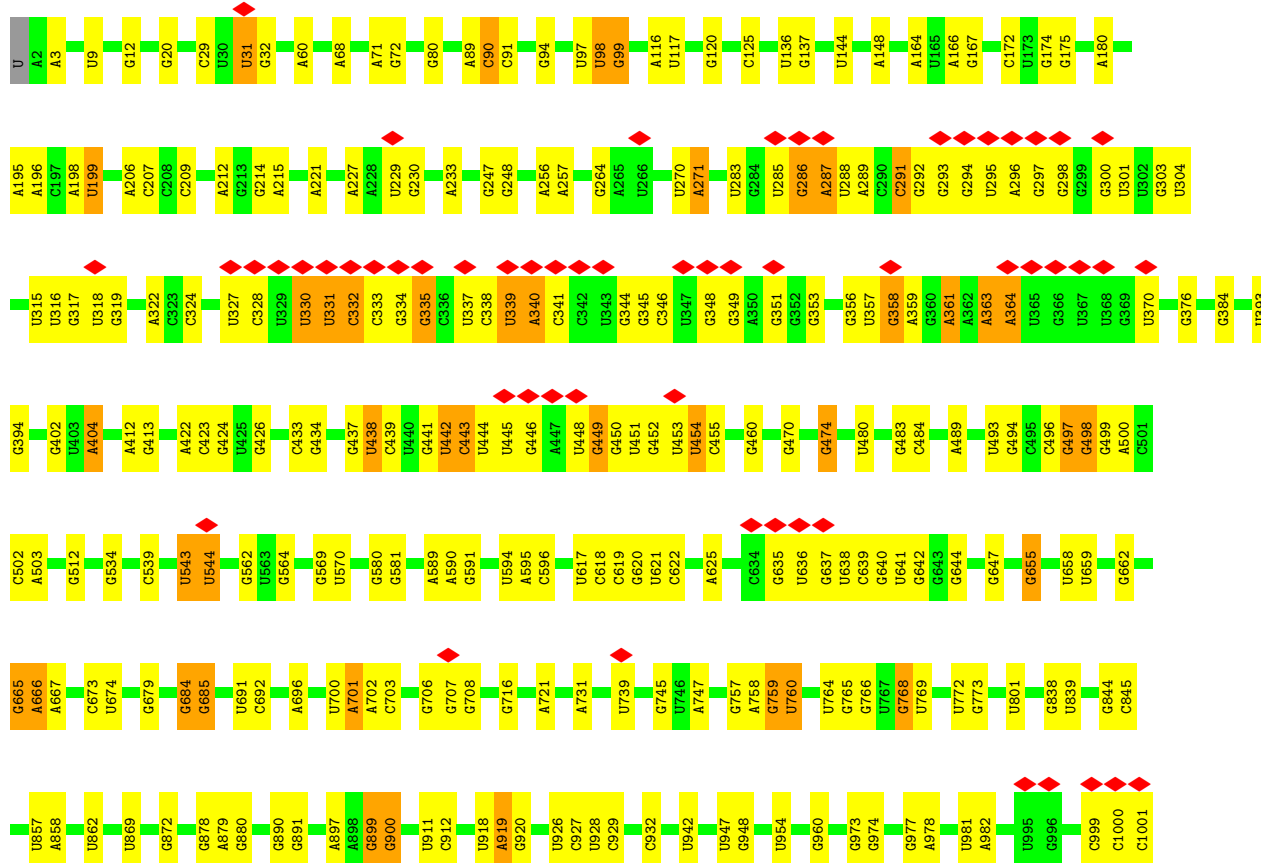
• Molecule 1: 50S Ribosomal Protein L27

Chain 3:  79% 12%

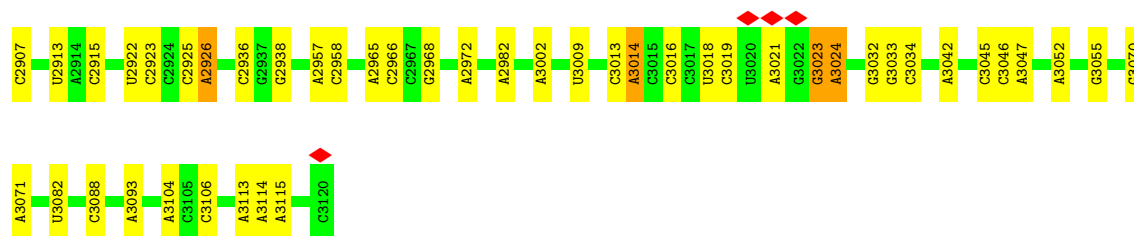


• Molecule 2: 23S rRNA

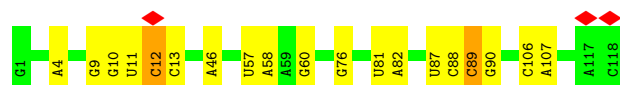
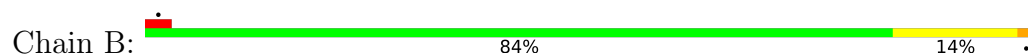
Chain A:  10% 75% 20%



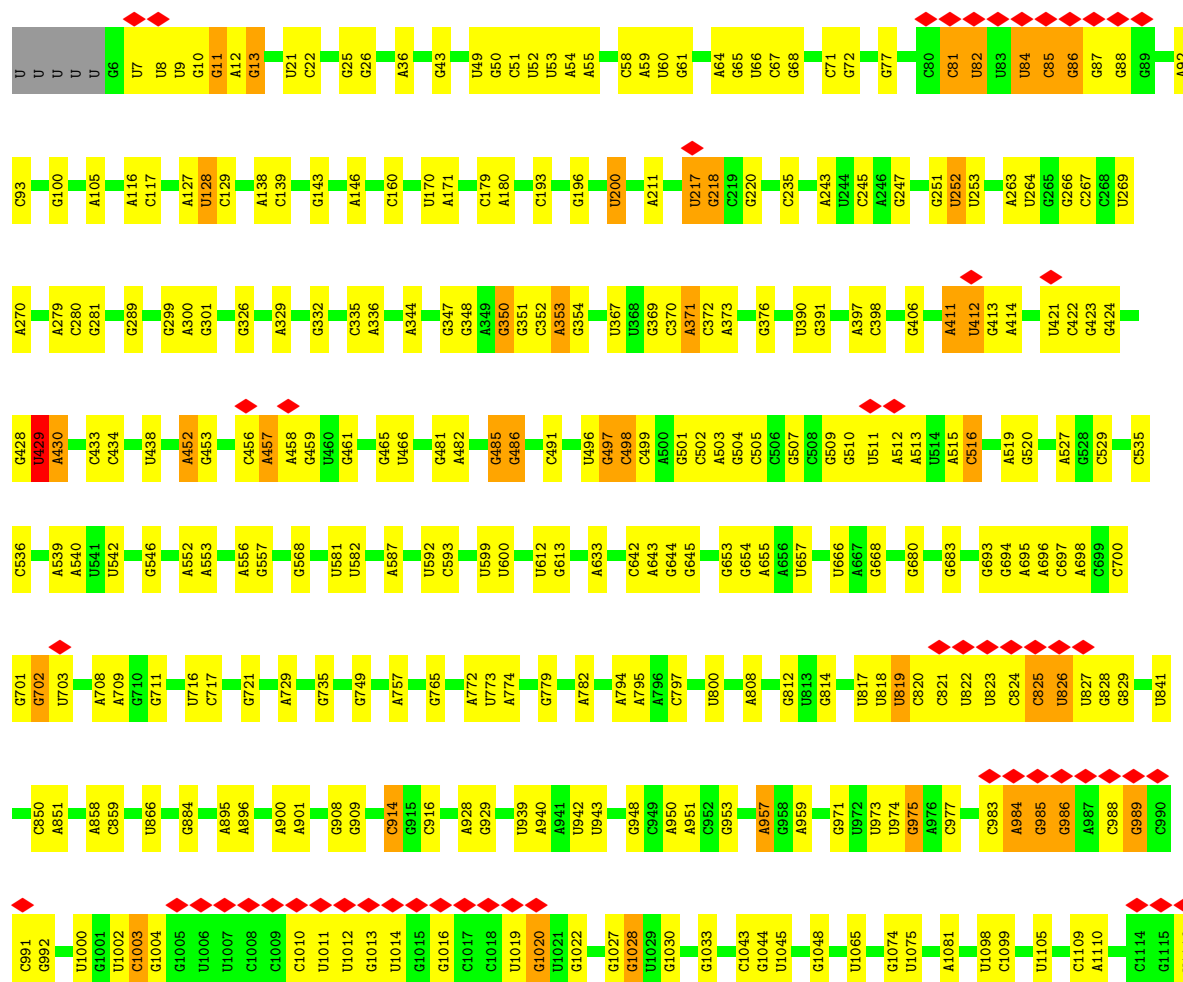
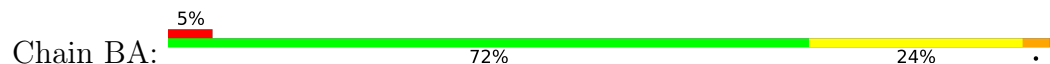


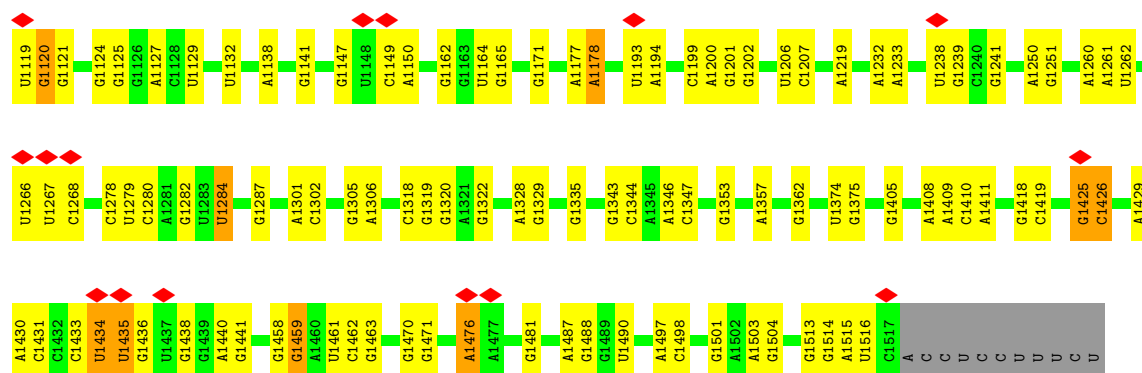


• Molecule 3: 5S rRNA

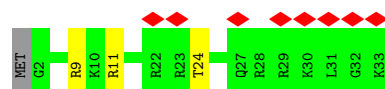


• Molecule 4: 16S rRNA

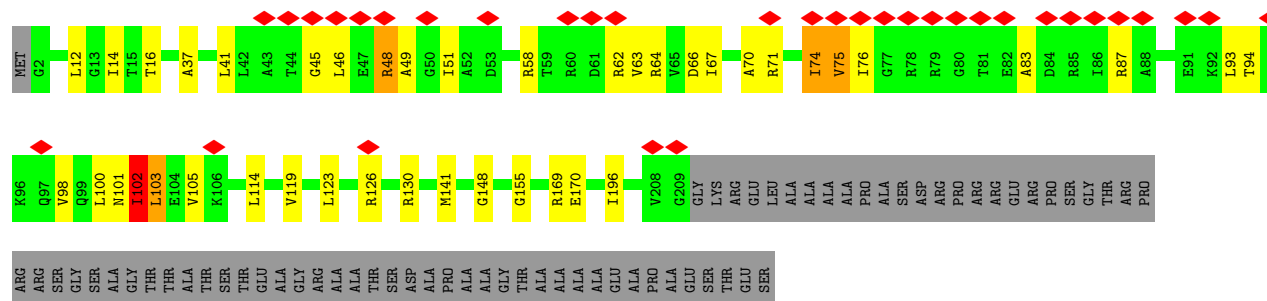




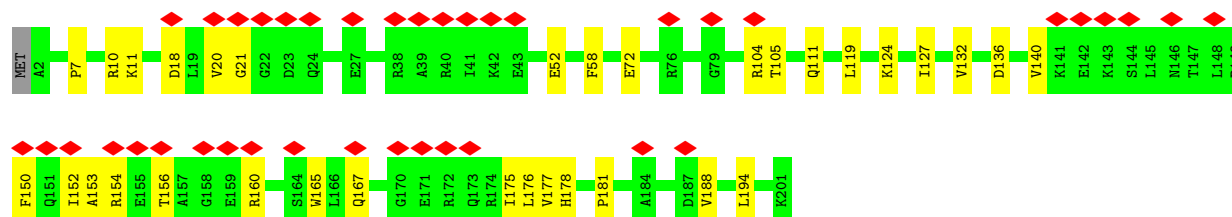
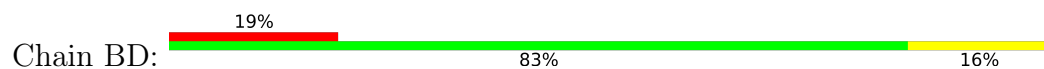
• Molecule 5: Conserved domain protein



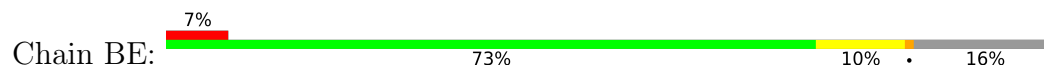
• Molecule 6: 30S ribosomal protein S3

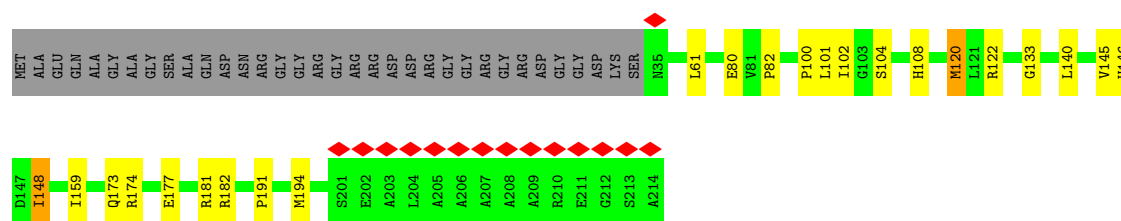


• Molecule 7: 30S ribosomal protein S4

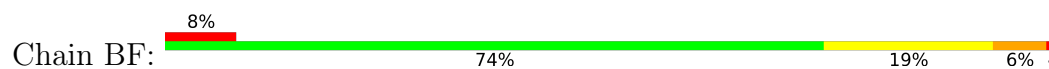


• Molecule 8: 30S Ribosomal Protein S5

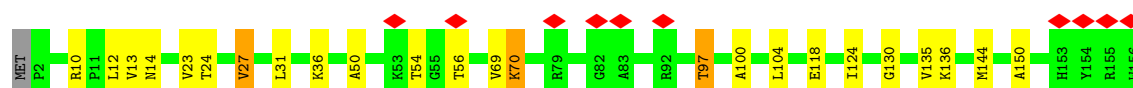
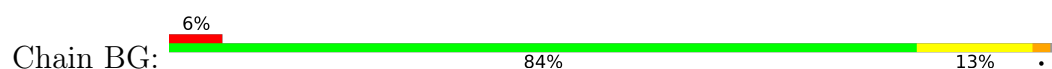




• Molecule 9: 30S ribosomal protein S6



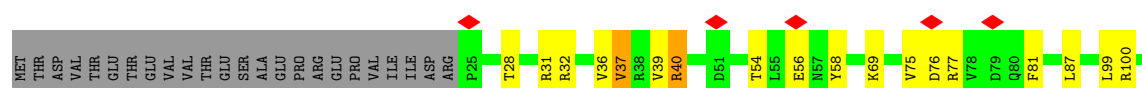
• Molecule 10: 30S ribosomal protein S7



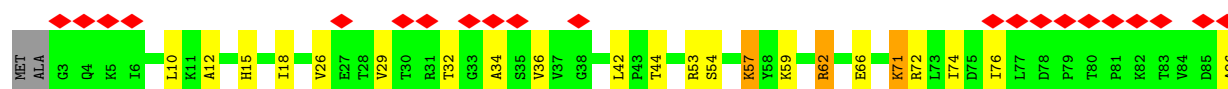
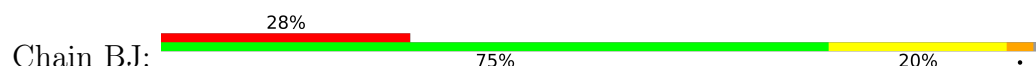
• Molecule 11: 30S Ribosomal Protein S8

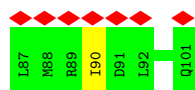


• Molecule 12: 30S ribosomal protein S9

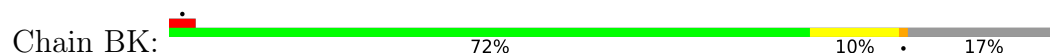


• Molecule 13: 30S ribosomal protein S10

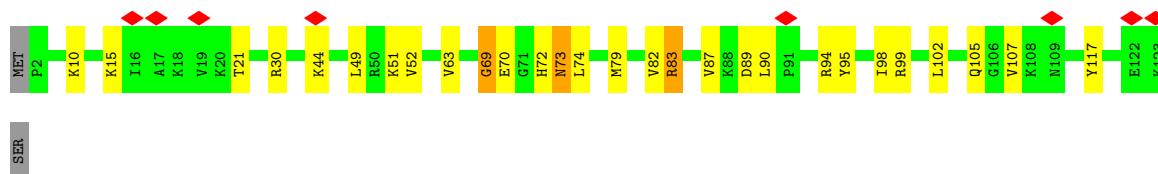
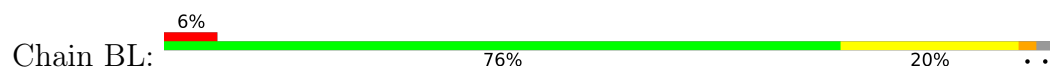




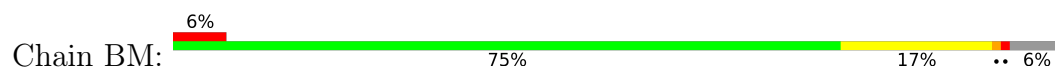
- Molecule 14: 30S ribosomal protein S11



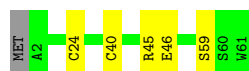
- Molecule 15: 30S ribosomal protein S12



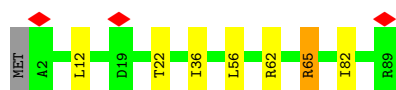
- Molecule 16: 30S ribosomal protein S13



- Molecule 17: 30S Ribosomal Protein S14



- Molecule 18: 30S Ribosomal Protein S15



- Molecule 19: 30S ribosomal protein S16



- Molecule 20: 30S ribosomal protein S17

NET	ALA	ASP	Q4	K5	K8	A13	E14	K15	R19	S29	M32	Q33	K34	T35	I36	V37	E41	R54	K57	K58	V59	K60	A61	H62	D63	E64	M65	G66	E67	A68	L82	T85	K86	R87	I93	L94	E95	K96	A97		
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- Molecule 21: 30S Ribosomal Protein S18

Category	Count
NET	1
ALA	1
LYS	1
SER	1
ASN	1
LYS	1
ARG	1
ARG	1
PRO	1
ALA	1
PRO	1
GLU	1
PRO	1
VAL	1
LYS	1
T17	1
R18	1
K25	1
K26	1
G27	1
Q28	1
K33	1
E44	1
R45	1
A50	1
V58	1
R62	1
S81	1
SER	1
THR	1
ARG	1

- Molecule 22: 30S ribosomal protein S19

NET	P2	P9	D12	D13	H14	L15	L16	K17	K18	V19	D20	E24	K25	N26	T27	K28	Q29	T39	F49	A50	V51	H52	H57	T77	F78	T79	H83	I85	L86	L87	L88	L89	L90	L91	L92	L93	L94	L95	L96	L97	L98	L99	L100	L101	L102	L103	L104	L105	L106	L107	L108	L109	L110	L111	L112	L113	L114	L115	L116	L117	L118	L119	L120	L121	L122	L123	L124	L125	L126	L127	L128	L129	L130	L131	L132	L133	L134	L135	L136	L137	L138	L139	L140	L141	L142	L143	L144	L145	L146	L147	L148	L149	L150	L151	L152	L153	L154	L155	L156	L157	L158	L159	L160	L161	L162	L163	L164	L165	L166	L167	L168	L169	L170	L171	L172	L173	L174	L175	L176	L177	L178	L179	L180	L181	L182	L183	L184	L185	L186	L187	L188	L189	L190	L191	L192	L193	L194	L195	L196	L197	L198	L199	L200	L201	L202	L203	L204	L205	L206	L207	L208	L209	L210	L211	L212	L213	L214	L215	L216	L217	L218	L219	L220	L221	L222	L223	L224	L225	L226	L227	L228	L229	L230	L231	L232	L233	L234	L235	L236	L237	L238	L239	L240	L241	L242	L243	L244	L245	L246	L247	L248	L249	L250	L251	L252	L253	L254	L255	L256	L257	L258	L259	L260	L261	L262	L263	L264	L265	L266	L267	L268	L269	L270	L271	L272	L273	L274	L275	L276	L277	L278	L279	L280	L281	L282	L283	L284	L285	L286	L287	L288	L289	L290	L291	L292	L293	L294	L295	L296	L297	L298	L299	L300	L301	L302	L303	L304	L305	L306	L307	L308	L309	L310	L311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L57
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- Molecule 23: 30S ribosomal protein S20

Diagram illustrating the schematic representation of the protein structure of the 12S ribosomal protein L24. The protein is shown as a linear sequence of residues: MET, A2, N3, I4, E15, R16, R20, L28, F35, A41, G42, D43, L51, H68, P69, N70, K85, and L86. Residues A41, G42, and D43 are highlighted in green, while the others are yellow. Red diamonds are placed above residues A41, G42, D43, and K85, indicating sites of phosphorylation.

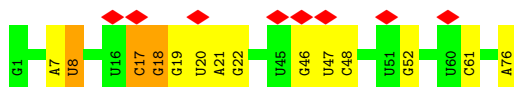
● Molecule 24: 30S Ribosomal Protein S2

[illegible]

ALA
PRO
GLU
SER
SER
THR
ASP
ALA
SER

- Molecule 25: P/P-site Phe-tRNA

Chain BW:  11% 82% 14%



- Molecule 26: mRNA fragment

Chain I:  40% 60%



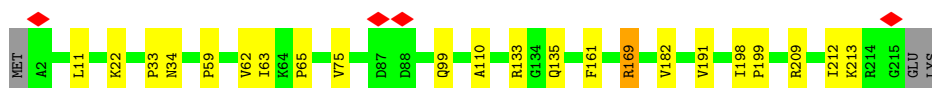
- Molecule 27: 50S ribosomal protein L2

Chain C:  90% 7%



- Molecule 28: 50S ribosomal protein L3

Chain D:  88% 10%



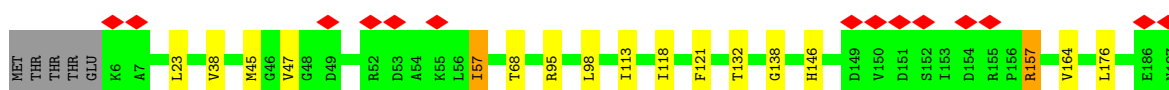
- Molecule 29: Large ribosomal subunit protein uL4

Chain E:  89% 7%



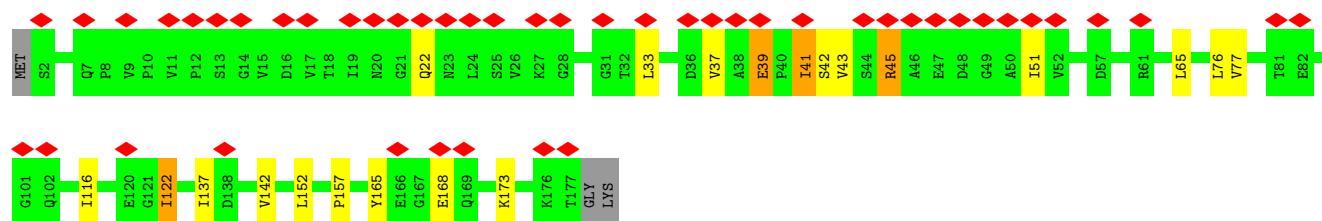
- Molecule 30: 50S Ribosomal Protein L5

Chain F:  7% 88% 8%

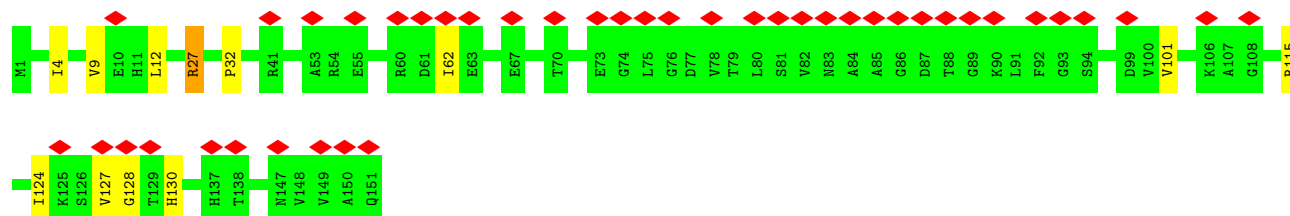


- Molecule 31: 50S ribosomal protein L6

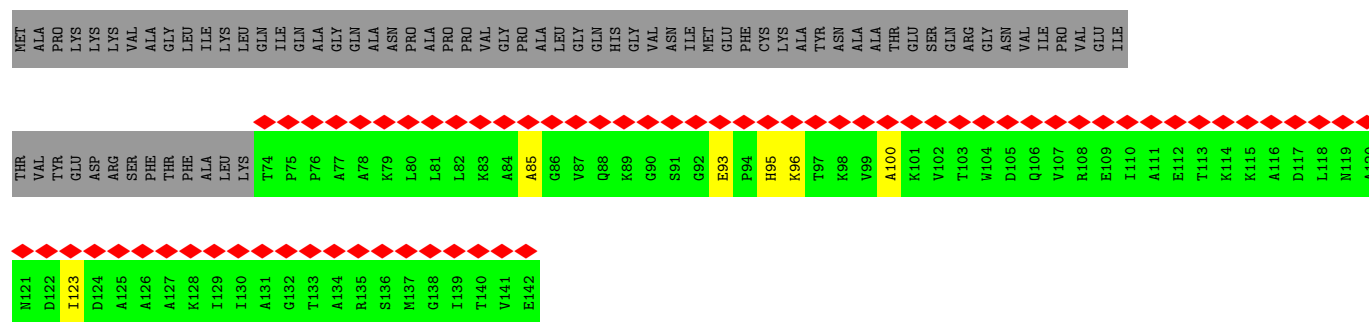
Chain G:  26% 87% 9%



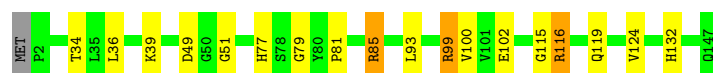
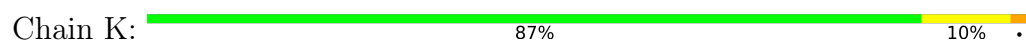
• Molecule 32: 50S ribosomal protein L9



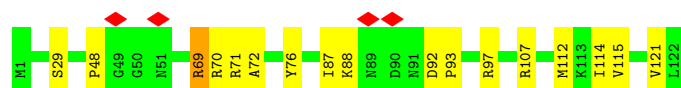
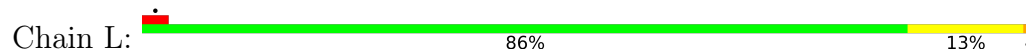
• Molecule 33: 50S ribosomal protein L11



• Molecule 34: Large ribosomal subunit protein uL13

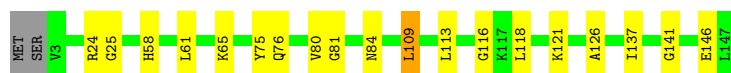


• Molecule 35: 50S ribosomal protein L14

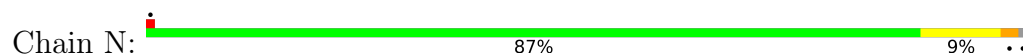


• Molecule 36: 50S ribosomal protein L15





- Molecule 37: Large ribosomal subunit protein uL16



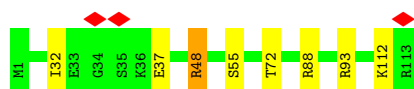
- Molecule 38: 50S ribosomal protein L17



- Molecule 39: Large ribosomal subunit protein uL18



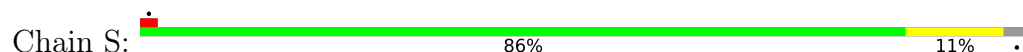
- Molecule 40: 50S ribosomal protein L19



- Molecule 41: Large ribosomal subunit protein bL20

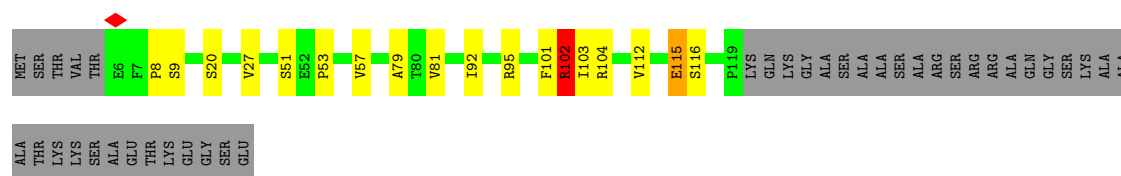


- Molecule 42: Large ribosomal subunit protein bL21



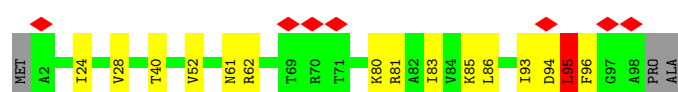
- Molecule 43: Large ribosomal subunit protein uL22

Chain T: 



- Molecule 44: Large ribosomal subunit protein uL23

Chain U: 



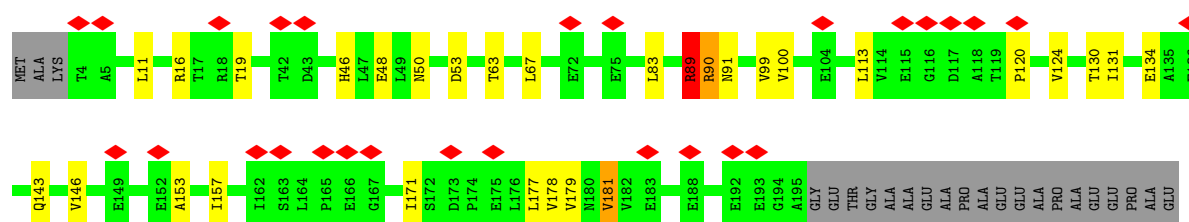
- Molecule 45: 50S ribosomal protein L24

Chain V: 



- Molecule 46: 50S ribosomal protein L25

Chain W: 



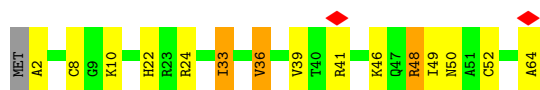
- Molecule 47: 50S ribosomal protein L27

Chain X: 

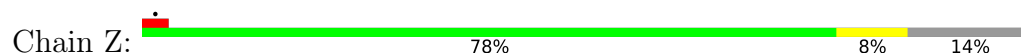


- Molecule 48: Large ribosomal subunit protein bL28

Chain Y: 



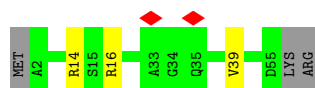
- Molecule 49: 50S ribosomal protein L29



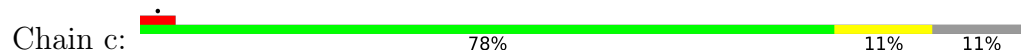
- Molecule 50: 50S ribosomal protein L30



- Molecule 51: 50S ribosomal protein L32



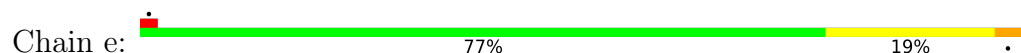
- Molecule 52: 50S Ribosomal Protein L33



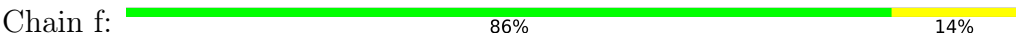
- Molecule 53: 50S ribosomal protein L34



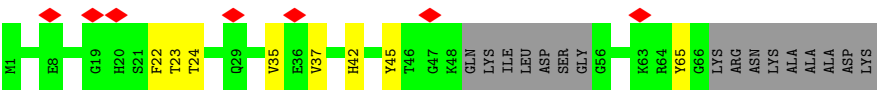
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



● Molecule 56: 50S Ribosomal Protein L31



● Molecule 57: Nascent peptide



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	638803	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.131	Depositor
Minimum map value	-0.407	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	528.768, 528.768, 528.768	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8262, 0.8262, 0.8262	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, A1BWO

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	3	0.47	0/192	0.60	0/247
2	A	0.17	0/74190	0.40	0/115759
3	B	0.15	0/2821	0.35	0/4396
4	BA	0.17	0/36335	0.39	3/56698 (0.0%)
5	BB	0.11	0/281	0.37	0/359
6	BC	0.31	0/1684	0.47	0/2261
7	BD	0.19	0/1673	0.42	0/2251
8	BE	0.25	0/1313	0.45	0/1772
9	BF	0.27	0/783	0.45	0/1059
10	BG	0.10	0/1253	0.32	0/1690
11	BH	0.10	0/1026	0.35	0/1385
12	BI	0.30	0/1013	0.47	0/1362
13	BJ	0.28	0/803	0.52	1/1086 (0.1%)
14	BK	0.32	0/873	0.46	0/1180
15	BL	0.32	0/969	0.53	1/1294 (0.1%)
16	BM	0.43	0/942	0.64	0/1260
17	BN	0.12	0/489	0.33	0/650
18	BO	0.11	0/730	0.32	0/977
19	BP	0.39	0/908	0.58	0/1226
20	BQ	0.40	0/759	0.57	1/1016 (0.1%)
21	BR	0.09	0/518	0.33	0/693
22	BS	0.28	0/680	0.49	0/915
23	BT	0.10	0/664	0.30	0/882
24	BV	0.32	0/1822	0.47	1/2457 (0.0%)
25	BW	0.18	0/1812	0.37	0/2823
26	I	0.13	0/138	0.34	0/212
27	C	0.28	0/2153	0.48	0/2895
28	D	0.37	0/1609	0.56	0/2165
29	E	0.12	0/1592	0.35	0/2153
30	F	0.23	0/1468	0.39	0/1973
31	G	0.31	0/1369	0.45	0/1848
32	H	0.38	0/1130	0.50	1/1524 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	J	0.10	0/510	0.30	0/687
34	K	0.22	0/1158	0.39	0/1567
35	L	0.12	0/947	0.36	0/1268
36	M	0.35	0/1092	0.56	1/1457 (0.1%)
37	N	0.34	0/1118	0.47	0/1506
38	O	0.12	0/945	0.36	0/1267
39	P	0.11	0/966	0.35	0/1298
40	Q	0.23	0/922	0.39	0/1236
41	R	0.21	0/1000	0.39	0/1341
42	S	0.23	0/764	0.41	0/1030
43	T	0.12	0/887	0.37	0/1204
44	U	0.23	0/766	0.39	0/1030
45	V	0.11	0/738	0.35	0/987
46	W	0.10	0/1443	0.32	0/1970
47	X	0.44	0/595	0.65	1/798 (0.1%)
48	Y	0.15	0/479	0.45	0/641
49	Z	0.10	0/547	0.27	0/731
50	a	0.10	0/477	0.34	0/640
51	b	0.14	0/427	0.42	0/572
52	c	0.10	0/413	0.34	0/553
53	d	0.12	0/381	0.40	0/500
54	e	0.38	0/508	0.53	0/672
55	f	0.13	0/303	0.41	0/401
56	g	0.08	0/467	0.30	0/626
57	s	0.07	0/16	0.15	0/20
All	All	0.20	0/161861	0.41	10/242470 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	3	0	1
5	BB	0	2
6	BC	0	7
7	BD	0	3
8	BE	0	2
9	BF	0	7
11	BH	0	3
12	BI	0	7
13	BJ	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
15	BL	0	3
16	BM	0	5
17	BN	0	1
18	BO	0	2
19	BP	0	3
20	BQ	0	1
21	BR	0	1
23	BT	0	1
24	BV	0	5
27	C	0	7
28	D	0	3
29	E	0	2
30	F	0	1
31	G	0	1
32	H	0	2
34	K	0	3
35	L	0	3
37	N	0	2
38	O	0	2
39	P	0	2
40	Q	0	2
41	R	0	1
43	T	0	1
44	U	0	2
45	V	0	1
46	W	0	2
47	X	0	3
48	Y	0	3
50	a	0	2
51	b	0	2
52	c	0	1
53	d	0	2
54	e	0	4
All	All	0	111

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BA	457	A	C2'-C3'-O3'	6.17	118.75	109.50
36	M	25	GLY	CA-C-O	-5.64	118.56	122.22
4	BA	429	U	C2'-C3'-O3'	5.61	117.92	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BV	155	GLN	N-CA-C	-5.60	107.45	114.56
47	X	44	HIS	N-CA-C	-5.33	104.88	111.33
20	BQ	82	LEU	N-CA-C	-5.29	106.87	113.38
4	BA	429	U	O3'-P-O5'	5.28	111.92	104.00
15	BL	69	GLY	CA-C-O	-5.27	118.35	122.52
13	BJ	57	LYS	N-CA-CB	-5.03	108.44	114.17
32	H	128	GLY	CA-C-O	-5.03	118.04	122.16

There are no chirality outliers.

All (111) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	3	11	ARG	Sidechain
5	BB	11	ARG	Sidechain
5	BB	9	ARG	Sidechain
6	BC	126	ARG	Sidechain
6	BC	130	ARG	Sidechain
6	BC	169	ARG	Sidechain
6	BC	48	ARG	Sidechain
6	BC	58	ARG	Sidechain
6	BC	62	ARG	Sidechain
6	BC	64	ARG	Sidechain
7	BD	104	ARG	Sidechain
7	BD	154	ARG	Sidechain
7	BD	160	ARG	Sidechain
8	BE	181	ARG	Sidechain
8	BE	182	ARG	Sidechain
9	BF	2	ARG	Sidechain
9	BF	31	ARG	Sidechain
9	BF	46	ARG	Sidechain
9	BF	47	ARG	Sidechain
9	BF	77	ARG	Sidechain
9	BF	87	ARG	Sidechain
9	BF	92	ARG	Sidechain
11	BH	116	ARG	Sidechain
11	BH	70	ARG	Sidechain
11	BH	72	ARG	Sidechain
12	BI	100	ARG	Sidechain
12	BI	129	ARG	Sidechain
12	BI	133	ARG	Sidechain
12	BI	142	ARG	Sidechain
12	BI	32	ARG	Sidechain

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Mol	Chain	Res	Type	Group
12	BI	40	ARG	Sidechain
12	BI	77	ARG	Sidechain
13	BJ	53	ARG	Sidechain
13	BJ	62	ARG	Sidechain
13	BJ	72	ARG	Sidechain
15	BL	30	ARG	Sidechain
15	BL	83	ARG	Sidechain
15	BL	99	ARG	Sidechain
16	BM	108	ARG	Sidechain
16	BM	11	ARG	Sidechain
16	BM	14	ARG	Sidechain
16	BM	79	ARG	Sidechain
16	BM	80	ARG	Sidechain
17	BN	45	ARG	Sidechain
18	BO	62	ARG	Sidechain
18	BO	65	ARG	Sidechain
19	BP	14	ARG	Sidechain
19	BP	19	ARG	Sidechain
19	BP	29	ARG	Sidechain
20	BQ	87	ARG	Sidechain
21	BR	62	ARG	Sidechain
23	BT	20	ARG	Sidechain
24	BV	129	ARG	Sidechain
24	BV	139	ARG	Sidechain
24	BV	146	ARG	Sidechain
24	BV	152	ARG	Sidechain
24	BV	21	ARG	Sidechain
27	C	13	ARG	Sidechain
27	C	183	ARG	Sidechain
27	C	184	ARG	Sidechain
27	C	218	ARG	Sidechain
27	C	26	ARG	Sidechain
27	C	52	ARG	Sidechain
27	C	68	ARG	Sidechain
28	D	133	ARG	Sidechain
28	D	169	ARG	Sidechain
28	D	209	ARG	Sidechain
29	E	67	ARG	Sidechain
29	E	73	ARG	Sidechain
30	F	157	ARG	Sidechain
31	G	45	ARG	Sidechain
32	H	115	ARG	Sidechain

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Mol	Chain	Res	Type	Group
32	H	27	ARG	Sidechain
34	K	116	ARG	Sidechain
34	K	85	ARG	Sidechain
34	K	99	ARG	Sidechain
35	L	69	ARG	Sidechain
35	L	70	ARG	Sidechain
35	L	97	ARG	Sidechain
37	N	60	ARG	Sidechain
37	N	82	ARG	Sidechain
38	O	33	ARG	Sidechain
38	O	64	ARG	Sidechain
39	P	104	ARG	Sidechain
39	P	26	ARG	Sidechain
40	Q	48	ARG	Sidechain
40	Q	93	ARG	Sidechain
41	R	25	ARG	Sidechain
43	T	102	ARG	Sidechain
44	U	62	ARG	Sidechain
44	U	81	ARG	Sidechain
45	V	40	ARG	Sidechain
46	W	89	ARG	Sidechain
46	W	90	ARG	Sidechain
47	X	11	ARG	Sidechain
47	X	73	ARG	Sidechain
47	X	75	ARG	Sidechain
48	Y	24	ARG	Sidechain
48	Y	41	ARG	Sidechain
48	Y	48	ARG	Sidechain
50	a	20	ARG	Sidechain
50	a	37	ARG	Sidechain
51	b	14	ARG	Sidechain
51	b	16	ARG	Sidechain
52	c	8	ARG	Sidechain
53	d	26	ARG	Sidechain
53	d	28	ARG	Sidechain
54	e	15	ARG	Sidechain
54	e	29	ARG	Sidechain
54	e	30	ARG	Sidechain
54	e	43	ARG	Sidechain

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	3	190	0	205	3	0
2	A	66255	0	33335	215	0
3	B	2522	0	1285	5	0
4	BA	32462	0	16331	141	0
5	BB	281	0	342	0	0
6	BC	1660	0	1707	18	0
7	BD	1642	0	1668	15	0
8	BE	1297	0	1360	15	0
9	BF	772	0	797	8	0
10	BG	1233	0	1282	13	0
11	BH	1011	0	1046	3	0
12	BI	995	0	1050	10	0
13	BJ	789	0	819	10	0
14	BK	855	0	863	14	0
15	BL	958	0	1045	17	0
16	BM	935	0	986	12	0
17	BN	478	0	499	2	0
18	BO	721	0	760	2	0
19	BP	891	0	935	13	0
20	BQ	748	0	795	9	0
21	BR	513	0	537	3	0
22	BS	662	0	677	11	0
23	BT	661	0	712	3	0
24	BV	1793	0	1839	34	0
25	BW	1622	0	820	2	0
26	I	125	0	65	0	0
27	C	2110	0	2165	11	0
28	D	1587	0	1630	13	0
29	E	1569	0	1607	8	0
30	F	1446	0	1476	9	0
31	G	1348	0	1399	9	0
32	H	1120	0	1170	3	0
33	J	505	0	533	5	0
34	K	1131	0	1167	9	0
35	L	939	0	1000	8	0
36	M	1079	0	1151	14	0
37	N	1092	0	1128	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	O	928	0	972	7	0
39	P	956	0	991	3	0
40	Q	908	0	938	4	0
41	R	988	0	1038	6	0
42	S	754	0	802	6	0
43	T	873	0	909	9	0
44	U	756	0	802	6	0
45	V	732	0	782	9	0
46	W	1428	0	1443	14	0
47	X	586	0	601	6	0
48	Y	471	0	480	8	0
49	Z	544	0	557	3	0
50	a	474	0	500	2	0
51	b	423	0	463	0	0
52	c	405	0	407	2	0
53	d	378	0	411	5	0
54	e	503	0	541	7	0
55	f	299	0	321	2	0
56	g	458	0	443	4	0
57	s	16	0	13	0	0
58	A	250	0	0	0	0
58	B	5	0	0	0	0
58	BA	85	0	0	0	0
58	BM	1	0	0	0	0
58	BR	1	0	0	0	0
58	BW	1	0	0	0	0
58	C	2	0	0	0	0
58	D	1	0	0	0	0
58	M	1	0	0	0	0
59	A	28	0	0	0	0
60	BN	1	0	0	0	0
60	BR	1	0	0	0	0
60	Y	1	0	0	0	0
60	c	1	0	0	0	0
60	f	1	0	0	0	0
60	g	1	0	0	0	0
61	3	3	0	0	0	0
61	A	5185	0	0	3	0
61	B	55	0	0	0	0
61	BA	1204	0	0	1	0
61	BB	2	0	0	0	0
61	BC	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	BD	1	0	0	0	0
61	BE	2	0	0	0	0
61	BG	1	0	0	0	0
61	BH	5	0	0	0	0
61	BI	10	0	0	0	0
61	BJ	4	0	0	0	0
61	BK	10	0	0	0	0
61	BL	7	0	0	0	0
61	BN	4	0	0	0	0
61	BO	4	0	0	0	0
61	BP	4	0	0	0	0
61	BR	5	0	0	0	0
61	BT	4	0	0	0	0
61	BW	9	0	0	0	0
61	C	100	0	0	0	0
61	D	53	0	0	0	0
61	E	43	0	0	0	0
61	F	2	0	0	0	0
61	G	1	0	0	0	0
61	H	3	0	0	0	0
61	I	7	0	0	0	0
61	K	14	0	0	1	0
61	L	9	0	0	0	0
61	M	39	0	0	0	0
61	N	33	0	0	0	0
61	O	26	0	0	0	0
61	P	11	0	0	0	0
61	Q	15	0	0	0	0
61	R	46	0	0	0	0
61	S	19	0	0	0	0
61	T	29	0	0	0	0
61	U	20	0	0	0	0
61	V	5	0	0	0	0
61	W	3	0	0	0	0
61	X	25	0	0	0	0
61	Y	23	0	0	0	0
61	Z	2	0	0	0	0
61	a	10	0	0	0	0
61	b	12	0	0	0	0
61	c	8	0	0	0	0
61	d	22	0	0	0	0
61	e	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	f	3	0	0	0	0
All	All	156393	0	99600	691	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 3.

All (691) 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)
4:BA:697:C:C4'	14:BK:128:ASN:HD22	1.27	1.44
4:BA:697:C:H4'	14:BK:128:ASN:ND2	1.38	1.39
24:BV:73:LYS:HE2	24:BV:205:ASP:HA	1.33	1.05
16:BM:65:LYS:NZ	16:BM:73:GLU:OE1	1.94	1.01
24:BV:90:PRO:HG2	24:BV:154:MET:SD	2.01	1.01
24:BV:73:LYS:NZ	24:BV:205:ASP:OD1	1.92	1.00
4:BA:697:C:C4'	14:BK:128:ASN:ND2	2.08	0.96
24:BV:90:PRO:CG	24:BV:154:MET:SD	2.53	0.96
4:BA:697:C:H4'	14:BK:128:ASN:HD22	0.77	0.92
6:BC:46:LEU:HB2	6:BC:51:ILE:HD11	1.58	0.84
9:BF:30:ILE:HD11	9:BF:75:LEU:HD22	1.59	0.84
6:BC:46:LEU:HG	6:BC:75:VAL:HG13	1.64	0.79
24:BV:73:LYS:CE	24:BV:205:ASP:OD1	2.31	0.79
4:BA:501:G:H4'	15:BL:70:GLU:HG2	1.66	0.77
9:BF:40:VAL:HG13	9:BF:63:ILE:HG12	1.65	0.77
4:BA:819:U:H3	4:BA:829:G:H1	1.31	0.76
4:BA:644:G:H22	4:BA:721:G:H1	1.34	0.73
4:BA:986:G:H22	4:BA:1016:G:H1	1.37	0.73
31:G:22:GLN:HE21	31:G:39:GLU:HA	1.54	0.72
24:BV:73:LYS:HE2	24:BV:205:ASP:OD1	1.91	0.71
24:BV:92:VAL:HG22	24:BV:151:ILE:HD11	1.72	0.71
4:BA:13:G:H5'	8:BE:133:GLY:HA3	1.73	0.70
4:BA:452:A:H62	19:BP:94:LYS:H	1.40	0.69
2:A:498:G:H8	2:A:498:G:H5''	1.58	0.69
2:A:759:G:H1	47:X:64:PRO:HB3	1.58	0.68
4:BA:429:U:H1'	4:BA:430:A:H5''	1.75	0.68
36:M:84:ASN:HD21	36:M:118:LEU:HA	1.59	0.68
24:BV:117:LEU:HB3	24:BV:141:LYS:HZ2	1.59	0.67
2:A:1788:G:H5'	27:C:60:ARG:HA	1.75	0.67
32:H:9:VAL:HG13	32:H:12:LEU:HB3	1.75	0.67
8:BE:80:GLU:HG3	8:BE:82:PRO:HD2	1.76	0.67
7:BD:132:VAL:HG11	7:BD:177:VAL:HG21	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:K:102:GLU:HG3	34:K:124:VAL:HG11	1.77	0.66
41:R:28:ARG:HE	41:R:38:GLN:HE21	1.44	0.66
8:BE:140:LEU:HD13	8:BE:148:ILE:HG21	1.77	0.66
2:A:2808:U:H2'	2:A:2809:U:H2'	1.77	0.65
19:BP:86:LEU:HG	19:BP:87:PRO:HD2	1.79	0.65
4:BA:1425:G:H5'	4:BA:1426:C:H5	1.62	0.65
24:BV:90:PRO:HG3	24:BV:154:MET:SD	2.35	0.65
2:A:1223:U:H2'	2:A:1224:G:H8	1.61	0.65
4:BA:698:A:H5'	14:BK:128:ASN:HB2	1.78	0.64
2:A:2343:G:H22	2:A:2401:U:H3	1.46	0.64
6:BC:63:VAL:HG21	6:BC:94:THR:HG21	1.80	0.64
15:BL:79:MET:HG2	15:BL:102:LEU:HD13	1.79	0.64
7:BD:153:ALA:HA	7:BD:156:THR:HG22	1.80	0.63
8:BE:191:PRO:HG2	8:BE:194:MET:HB2	1.81	0.63
45:V:45:THR:HB	45:V:58:GLY:HA3	1.81	0.63
2:A:3023:G:H2'	2:A:3024:A:O4'	1.99	0.62
31:G:22:GLN:NE2	31:G:39:GLU:HA	2.15	0.62
13:BJ:26:VAL:HG22	13:BJ:36:VAL:HG21	1.80	0.62
16:BM:5:VAL:HG21	16:BM:60:ILE:HD11	1.81	0.62
8:BE:108:HIS:HE1	8:BE:173:GLN:H	1.46	0.62
4:BA:1219:A:H5'	4:BA:1318:C:H41	1.65	0.62
6:BC:70:ALA:HA	6:BC:105:VAL:HG22	1.82	0.61
2:A:1223:U:H2'	2:A:1224:G:C8	2.35	0.61
6:BC:66:ASP:HB3	6:BC:103:LEU:HD11	1.82	0.61
48:Y:33:ILE:HD12	48:Y:50:ASN:HB3	1.82	0.61
22:BS:9:PRO:HB2	22:BS:39:THR:HG21	1.82	0.61
24:BV:71:GLY:HA3	24:BV:80:ILE:HD12	1.81	0.61
14:BK:35:THR:HG23	14:BK:37:ASN:H	1.66	0.61
4:BA:235:C:H5'	20:BQ:87:ARG:HD3	1.83	0.61
6:BC:46:LEU:HB3	6:BC:49:ALA:HB3	1.82	0.60
19:BP:41:HIS:HB2	19:BP:48:LEU:HB3	1.83	0.60
10:BG:54:THR:HG23	10:BG:56:THR:H	1.66	0.60
10:BG:69:VAL:HG23	10:BG:100:ALA:HB1	1.82	0.60
2:A:543:U:H3'	2:A:544:U:C5'	2.32	0.60
6:BC:63:VAL:HB	6:BC:98:VAL:HG12	1.84	0.60
14:BK:59:VAL:HG11	14:BK:74:LEU:HB3	1.84	0.59
4:BA:975:G:H2'	4:BA:977:C:H41	1.66	0.59
6:BC:76:ILE:HG22	6:BC:83:ALA:HB2	1.84	0.59
4:BA:749:G:H4'	4:BA:1497:A:H4'	1.84	0.59
12:BI:31:ARG:HG2	12:BI:36:VAL:HG22	1.84	0.59
2:A:1620:U:H2'	2:A:1621:C:C6	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:R:28:ARG:HE	41:R:38:GLN:NE2	2.01	0.59
35:L:93:PRO:HG3	35:L:114:ILE:HG12	1.85	0.59
24:BV:126:PHE:HZ	24:BV:141:LYS:HE2	1.68	0.58
2:A:2356:G:H2'	2:A:2380:G:H1	1.67	0.58
4:BA:819:U:H2'	4:BA:820:C:C6	2.38	0.58
47:X:26:PHE:H	47:X:29:GLN:NE2	2.00	0.58
2:A:2454:G:H8	2:A:2454:G:H5''	1.68	0.58
20:BQ:32:MET:HB2	20:BQ:35:THR:OG1	2.03	0.58
2:A:470:G:H22	2:A:480:U:H3	1.52	0.58
2:A:543:U:H3'	2:A:544:U:H5'	1.86	0.58
4:BA:411:A:C4	4:BA:413:G:H1'	2.39	0.58
7:BD:165:TRP:HD1	7:BD:177:VAL:HG13	1.69	0.58
16:BM:40:ASP:HB3	16:BM:43:MET:HG3	1.86	0.57
2:A:1624:U:HO2'	2:A:1625:G:H8	1.53	0.57
2:A:2086:U:H3	2:A:2096:G:H1	1.53	0.57
2:A:291:C:H2'	2:A:292:G:C8	2.40	0.57
2:A:358:G:H22	2:A:361:A:H5''	1.70	0.57
7:BD:165:TRP:CE3	7:BD:181:PRO:HB3	2.40	0.56
34:K:77:HIS:CD2	34:K:79:GLY:H	2.22	0.56
2:A:3013:C:H5'	2:A:3014:A:H5'	1.86	0.56
15:BL:107:VAL:HG22	15:BL:117:TYR:HB3	1.85	0.56
2:A:2361:U:H3	2:A:2376:G:H22	1.51	0.56
19:BP:24:ASP:HB3	19:BP:27:THR:HG23	1.87	0.56
4:BA:1434:U:O2'	4:BA:1435:U:H5''	2.05	0.56
24:BV:111:LEU:HD11	24:BV:152:ARG:HA	1.88	0.56
2:A:1561:C:H42	2:A:1610:C:H42	1.54	0.56
4:BA:81:C:H3'	4:BA:82:U:H5''	1.87	0.56
4:BA:452:A:N6	19:BP:94:LYS:H	2.04	0.56
16:BM:65:LYS:HZ1	16:BM:73:GLU:HB2	1.69	0.56
2:A:2529:A:H5''	30:F:138:GLY:HA3	1.87	0.55
2:A:928:U:H2'	2:A:929:C:C6	2.41	0.55
16:BM:65:LYS:HE2	16:BM:69:ASP:O	2.07	0.55
16:BM:24:GLY:HA3	16:BM:66:VAL:HG12	1.88	0.55
1:3:8:LYS:O	1:3:11:ARG:HG2	2.07	0.55
49:Z:14:THR:HG23	49:Z:17:GLU:H	1.72	0.55
24:BV:187:LEU:HD21	24:BV:196:VAL:HG21	1.89	0.55
48:Y:33:ILE:HA	48:Y:52:CYS:HA	1.88	0.55
8:BE:108:HIS:CE1	8:BE:173:GLN:H	2.24	0.54
2:A:1509:U:H4'	2:A:1821:A:H4'	1.89	0.54
4:BA:1178:A:H5'	4:BA:1178:A:H8	1.73	0.54
2:A:363:A:H2'	2:A:364:A:O4'	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:496:C:H2'	2:A:497:G:H5''	1.88	0.54
2:A:1185:A:H2'	2:A:1186:G:C8	2.43	0.54
4:BA:1019:U:H5''	4:BA:1020:G:OP2	2.07	0.54
13:BJ:66:GLU:HB2	17:BN:59:SER:HB2	1.90	0.54
24:BV:162:TRP:CZ3	24:BV:214:THR:HG22	2.43	0.54
31:G:116:ILE:HD11	31:G:152:LEU:HD21	1.89	0.54
4:BA:498:C:H2'	4:BA:510:G:C8	2.42	0.54
9:BF:27:LEU:HD13	9:BF:37:VAL:HG11	1.89	0.54
54:e:23:VAL:HG11	54:e:47:ARG:HD2	1.90	0.54
4:BA:11:G:N7	8:BE:120:MET:HE1	2.22	0.54
14:BK:32:ILE:HG12	14:BK:41:VAL:HG12	1.89	0.54
2:A:2922:U:H2'	2:A:2923:C:C6	2.43	0.54
4:BA:928:A:H2'	4:BA:929:G:C8	2.43	0.54
24:BV:162:TRP:HZ3	24:BV:214:THR:HG22	1.72	0.54
8:BE:101:LEU:HD21	8:BE:145:VAL:HG22	1.88	0.54
2:A:918:U:H2'	2:A:919:A:H5''	1.89	0.53
4:BA:350:G:H8	4:BA:350:G:H5''	1.73	0.53
4:BA:939:U:H4'	22:BS:79:THR:HG23	1.91	0.53
2:A:1690:A:H2'	2:A:1691:A:C8	2.43	0.53
4:BA:21:U:H2'	4:BA:22:C:C6	2.43	0.53
25:BW:17:C:H3'	25:BW:18:G:H5''	1.90	0.53
46:W:89:ARG:HB2	46:W:91:ASN:HD22	1.72	0.53
13:BJ:10:LEU:HB3	13:BJ:18:ILE:HD11	1.90	0.53
15:BL:51:LYS:HD3	15:BL:72:HIS:HD1	1.74	0.53
2:A:1627:U:H2'	2:A:1628:A:H8	1.74	0.53
2:A:2552:A:H2'	2:A:2553:G:C8	2.44	0.53
4:BA:269:U:H2'	4:BA:270:A:C8	2.43	0.53
4:BA:1418:G:H2'	4:BA:1419:C:C6	2.44	0.53
9:BF:14:LEU:HD11	9:BF:84:SER:HB2	1.90	0.53
13:BJ:59:LYS:HE2	13:BJ:62:ARG:NH2	2.24	0.53
27:C:108:PRO:HG2	27:C:111:LEU:HB2	1.90	0.53
4:BA:1374:U:H2'	4:BA:1375:G:C8	2.44	0.53
24:BV:111:LEU:CD1	24:BV:152:ARG:HA	2.39	0.53
44:U:52:VAL:HG21	44:U:86:LEU:HD13	1.89	0.53
2:A:1402:A:H5'	38:O:103:ARG:HD2	1.91	0.53
4:BA:697:C:O5'	14:BK:128:ASN:ND2	2.41	0.53
15:BL:83:ARG:HB3	15:BL:98:ILE:HD11	1.90	0.53
2:A:1621:C:H2'	2:A:1622:G:C8	2.44	0.53
4:BA:600:U:H1'	7:BD:127:ILE:HG21	1.90	0.53
4:BA:1199:C:H2'	4:BA:1200:A:C8	2.44	0.53
10:BG:130:GLY:HA2	10:BG:135:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BT:68:HIS:CD2	23:BT:70:ASN:H	2.27	0.53
46:W:134:GLU:HB2	46:W:171:ILE:HD11	1.91	0.53
7:BD:140:VAL:HG21	7:BD:150:PHE:CZ	2.44	0.52
10:BG:50:ALA:O	10:BG:54:THR:HG22	2.09	0.52
45:V:85:TYR:CG	45:V:94:LYS:HE2	2.44	0.52
4:BA:1284:U:C5	16:BM:17:ILE:HG13	2.45	0.52
35:L:76:TYR:HB2	40:Q:72:THR:HB	1.91	0.52
7:BD:7:PRO:HB2	7:BD:10:ARG:HG2	1.92	0.52
16:BM:65:LYS:NZ	16:BM:73:GLU:HB2	2.24	0.52
46:W:146:VAL:HG21	46:W:157:ILE:HG21	1.90	0.52
4:BA:697:C:C5'	14:BK:128:ASN:ND2	2.69	0.52
13:BJ:15:HIS:O	13:BJ:18:ILE:HG22	2.09	0.52
16:BM:11:ARG:O	16:BM:45:THR:HB	2.09	0.52
2:A:497:G:H5''	2:A:497:G:H8	1.75	0.52
2:A:1544:U:H2'	2:A:1545:C:C6	2.44	0.52
4:BA:1279:U:H1'	4:BA:1280:C:H5	1.75	0.52
6:BC:141:MET:HE1	6:BC:148:GLY:HA2	1.91	0.52
2:A:700:U:H2'	2:A:701:A:H5'	1.92	0.52
4:BA:85:C:H1'	4:BA:86:G:C5	2.45	0.52
6:BC:70:ALA:HB2	6:BC:114:LEU:HD13	1.91	0.52
10:BG:23:VAL:O	10:BG:27:VAL:HG13	2.10	0.52
55:f:25:VAL:HB	55:f:34:GLN:HG2	1.91	0.52
7:BD:52:GLU:HG3	7:BD:194:LEU:HD12	1.91	0.52
36:M:65:LYS:H	54:e:25:GLN:HE22	1.56	0.52
47:X:49:VAL:HG12	47:X:50:ASN:ND2	2.25	0.52
4:BA:412:U:H4'	4:BA:413:G:H8	1.75	0.52
4:BA:1440:A:H3'	4:BA:1441:G:H8	1.74	0.52
4:BA:1278:C:H4'	4:BA:1284:U:O4	2.10	0.52
23:BT:68:HIS:HD2	23:BT:70:ASN:H	1.58	0.52
12:BI:81:PHE:HZ	12:BI:110:VAL:HG11	1.75	0.51
24:BV:6:MET:HG2	24:BV:47:LEU:HD11	1.91	0.51
4:BA:1232:A:H2'	4:BA:1233:A:C8	2.45	0.51
2:A:745:G:H5''	54:e:19:THR:HG23	1.91	0.51
52:c:13:LEU:HD21	52:c:36:LEU:HD23	1.91	0.51
4:BA:519:A:H2'	4:BA:520:G:C8	2.44	0.51
28:D:110:ALA:O	28:D:182:VAL:HG12	2.10	0.51
3:B:60:G:H4'	39:P:12:GLU:HB2	1.93	0.51
4:BA:985:G:H2'	4:BA:986:G:C8	2.46	0.51
4:BA:1458:G:H2'	4:BA:1459:G:O4'	2.10	0.51
45:V:81:THR:HG22	45:V:82:ARG:O	2.11	0.51
4:BA:252:U:H2'	4:BA:253:U:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:J:93:GLU:HB3	33:J:96:LYS:HB2	1.93	0.51
2:A:759:G:H3'	2:A:760:U:H4'	1.91	0.51
2:A:1552:A:H1'	2:A:1618:C:H42	1.75	0.51
4:BA:983:C:H2'	4:BA:984:A:C8	2.46	0.51
19:BP:16:PRO:HD2	19:BP:43:LYS:HD3	1.93	0.51
45:V:81:THR:HG23	45:V:100:THR:HG23	1.91	0.51
4:BA:825:C:H4'	4:BA:826:U:OP2	2.10	0.51
33:J:85:ALA:HB1	33:J:100:ALA:HB3	1.93	0.51
2:A:1827:A:H1'	2:A:1834:A:O4'	2.11	0.50
43:T:8:PRO:HG2	43:T:116:SER:HB3	1.92	0.50
13:BJ:29:VAL:HG13	13:BJ:34:ALA:HB3	1.93	0.50
28:D:33:PRO:C	28:D:34:ASN:HD22	2.19	0.50
29:E:119:ALA:HB2	29:E:124:ILE:HD12	1.94	0.50
2:A:2925:C:H3'	2:A:2926:A:H5'	1.94	0.50
3:B:12:C:H1'	47:X:71:ALA:HB3	1.94	0.50
4:BA:988:C:H3'	4:BA:989:G:H8	1.77	0.50
4:BA:1003:C:H2'	4:BA:1004:G:H8	1.77	0.50
4:BA:1202:G:O3'	22:BS:77:THR:HG21	2.11	0.50
30:F:45:MET:HE1	30:F:157:ARG:HB3	1.93	0.50
2:A:247:G:H4'	2:A:474:G:C5	2.46	0.50
13:BJ:42:LEU:HB2	13:BJ:71:LYS:HB3	1.94	0.50
14:BK:68:THR:HG23	14:BK:71:ALA:H	1.76	0.50
2:A:438:U:H3'	2:A:439:C:H6	1.77	0.50
4:BA:503:A:H61	15:BL:89:ASP:HB2	1.76	0.50
6:BC:155:GLY:HA3	6:BC:196:ILE:HG22	1.93	0.50
24:BV:126:PHE:CZ	24:BV:141:LYS:HE2	2.46	0.50
46:W:153:ALA:HA	46:W:181:VAL:HG12	1.92	0.50
2:A:286:G:H2'	2:A:287:A:C8	2.46	0.50
2:A:2515:U:H2'	2:A:2516:U:C6	2.47	0.50
2:A:3032:G:H5''	28:D:63:ILE:HG23	1.94	0.50
4:BA:1497:A:H2'	4:BA:1498:C:C6	2.47	0.50
44:U:61:ASN:HD21	44:U:80:LYS:HE3	1.76	0.50
46:W:113:LEU:HD13	46:W:143:GLN:HB2	1.93	0.50
4:BA:1120:G:H4'	4:BA:1121:G:H5'	1.93	0.50
24:BV:186:ILE:HD12	24:BV:213:LEU:HD12	1.94	0.50
2:A:662:G:H2'	2:A:2254:A:N7	2.26	0.50
2:A:2454:G:H5''	2:A:2454:G:C8	2.47	0.50
11:BH:76:GLY:HA3	11:BH:132:TRP:CE2	2.47	0.50
19:BP:83:PHE:CE2	19:BP:84:LYS:HD3	2.47	0.50
28:D:22:LYS:HG2	35:L:72:ALA:HB1	1.93	0.50
4:BA:85:C:H1'	4:BA:86:G:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BA:1503:A:H5''	4:BA:1504:G:OP2	2.12	0.49
2:A:2639:G:C8	2:A:2639:G:H5''	2.47	0.49
4:BA:1003:C:H2'	4:BA:1004:G:C8	2.46	0.49
7:BD:20:VAL:HG13	7:BD:105:THR:HG23	1.94	0.49
2:A:1704:U:H2'	2:A:1705:C:C6	2.47	0.49
2:A:2539:G:O2'	30:F:132:THR:HG21	2.13	0.49
4:BA:497:G:H1'	4:BA:510:G:H4'	1.93	0.49
4:BA:1284:U:C4	16:BM:17:ILE:HG13	2.47	0.49
36:M:81:GLY:HA3	36:M:116:GLY:HA3	1.93	0.49
47:X:41:ARG:NE	47:X:41:ARG:HA	2.27	0.49
2:A:2467:U:H2'	2:A:2468:U:C6	2.47	0.49
2:A:2639:G:H5''	2:A:2639:G:H8	1.76	0.49
2:A:3070:G:H4'	2:A:3071:A:H5'	1.95	0.49
4:BA:1002:U:H2'	4:BA:1003:C:C6	2.48	0.49
27:C:146:GLU:HB2	27:C:189:CYS:HB3	1.94	0.49
33:J:123:ILE:HD12	33:J:123:ILE:H	1.77	0.49
2:A:655:G:O2'	41:R:41:HIS:HE1	1.95	0.49
4:BA:376:G:H5''	19:BP:6:LYS:HB3	1.95	0.49
11:BH:94:LEU:HD22	11:BH:106:ILE:HD13	1.95	0.49
4:BA:502:C:H1'	4:BA:516:C:H5''	1.93	0.49
4:BA:1132:U:H5''	13:BJ:44:THR:HG23	1.95	0.49
2:A:1564:A:H2'	2:A:1565:A:C8	2.48	0.49
37:N:77:LYS:HE2	37:N:81:THR:HG21	1.94	0.49
2:A:1717:U:H5''	2:A:1718:C:H5	1.77	0.48
4:BA:11:G:H1	8:BE:122:ARG:HH11	1.59	0.48
6:BC:12:LEU:HA	6:BC:16:THR:HG23	1.94	0.48
12:BI:58:TYR:CE1	12:BI:87:LEU:HD12	2.48	0.48
34:K:93:LEU:HG	34:K:100:VAL:HG21	1.95	0.48
42:S:23:LYS:HG2	42:S:96:VAL:HG22	1.94	0.48
46:W:16:ARG:HG2	46:W:48:GLU:HG3	1.95	0.48
30:F:23:LEU:HD11	30:F:176:LEU:HD13	1.95	0.48
30:F:118:ILE:HB	30:F:121:PHE:HB2	1.95	0.48
45:V:81:THR:HG21	45:V:98:ALA:HB1	1.95	0.48
2:A:2094:G:HO2'	2:A:2095:G:H8	1.57	0.48
2:A:2761:U:H2'	2:A:2762:C:C6	2.49	0.48
43:T:95:ARG:HG3	43:T:101:PHE:CD2	2.48	0.48
2:A:1163:A:N6	2:A:1229:A:H2'	2.28	0.48
2:A:1194:C:H2'	2:A:1195:A:C8	2.47	0.48
37:N:45:ARG:H	37:N:45:ARG:HG2	1.39	0.48
15:BL:87:VAL:HG11	15:BL:90:LEU:HD12	1.95	0.48
29:E:127:VAL:HG21	29:E:144:PHE:HE2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:T:79:ALA:HB2	43:T:115:GLU:HG3	1.95	0.48
45:V:40:ARG:HD2	45:V:63:GLU:HG3	1.94	0.48
2:A:2826:A:H4'	2:A:2827:G:O5'	2.12	0.48
4:BA:217:U:H3'	4:BA:218:G:H4'	1.94	0.48
2:A:772:U:H2'	2:A:773:G:C8	2.49	0.48
2:A:1787:A:H2'	27:C:86:PRO:HG3	1.95	0.48
4:BA:412:U:H5'	4:BA:413:G:H5'	1.94	0.48
42:S:76:HIS:HE1	42:S:85:HIS:ND1	2.11	0.48
2:A:1046:C:H4'	2:A:1047:A:OP2	2.14	0.48
4:BA:858:A:H2'	4:BA:859:C:C6	2.49	0.48
24:BV:154:MET:HE3	24:BV:156:LYS:O	2.14	0.48
36:M:61:LEU:HD13	54:e:24:ARG:HD2	1.94	0.48
38:O:51:LEU:HD13	38:O:70:ILE:HD11	1.96	0.48
14:BK:35:THR:HA	14:BK:98:PRO:HD2	1.96	0.48
2:A:1551:U:H3'	2:A:1552:A:C8	2.49	0.48
4:BA:11:G:H1	8:BE:122:ARG:NH1	2.12	0.48
8:BE:61:LEU:HD22	8:BE:159:ILE:HD13	1.96	0.48
28:D:34:ASN:HD22	28:D:34:ASN:N	2.11	0.48
4:BA:10:G:O2'	4:BA:11:G:H5''	2.13	0.47
14:BK:56:SER:OG	14:BK:71:ALA:HB1	2.14	0.47
53:d:21:PHE:HB2	53:d:46:THR:HG21	1.96	0.47
2:A:999:C:H2'	2:A:1000:C:C6	2.49	0.47
2:A:1953:C:H2'	2:A:1954:C:O4'	2.14	0.47
2:A:580:G:H2'	2:A:581:G:O4'	2.14	0.47
2:A:1002:C:H2'	2:A:1003:A:H5''	1.95	0.47
2:A:1343:G:H2'	2:A:1345:G:C8	2.49	0.47
2:A:2070:A:H2'	2:A:2071:A:C8	2.49	0.47
12:BI:37:VAL:HG21	12:BI:99:LEU:HA	1.97	0.47
2:A:1314:C:H1'	41:R:4:VAL:HG22	1.95	0.47
4:BA:866:U:O2'	15:BL:15:LYS:HE2	2.14	0.47
29:E:112:ARG:HG2	29:E:112:ARG:HH11	1.80	0.47
2:A:1675:U:O4	38:O:67:MET:HE1	2.14	0.47
2:A:404:A:OP2	29:E:171:ASN:HB2	2.14	0.47
12:BI:75:VAL:O	12:BI:76:ASP:HB2	2.15	0.47
48:Y:36:VAL:HG22	48:Y:49:ILE:HG12	1.97	0.47
2:A:911:U:H2'	2:A:912:C:C6	2.50	0.47
2:A:1679:A:H4'	2:A:1679:A:OP1	2.14	0.47
4:BA:535:C:H2'	4:BA:536:C:C6	2.50	0.47
4:BA:1405:G:H5'	35:L:48:PRO:HB3	1.96	0.47
15:BL:73:ASN:HD21	15:BL:105:GLN:HB2	1.80	0.47
31:G:157:PRO:HB2	31:G:173:LYS:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:N:43:THR:HG22	37:N:94:VAL:HG12	1.96	0.47
46:W:131:ILE:HD11	46:W:178:VAL:HG21	1.97	0.47
4:BA:1117:U:H4'	4:BA:1118:A:OP1	2.15	0.47
7:BD:176:LEU:HB3	19:BP:106:PHE:CE1	2.50	0.47
15:BL:79:MET:HE3	15:BL:102:LEU:HD22	1.97	0.47
27:C:108:PRO:HD2	27:C:111:LEU:HD22	1.95	0.47
7:BD:18:ASP:HB3	7:BD:21:GLY:HA2	1.97	0.47
28:D:212:ILE:HG13	28:D:213:LYS:N	2.30	0.47
2:A:1122:C:H2'	2:A:1129:G:H2'	1.96	0.46
2:A:2686:U:H2'	2:A:2687:U:C6	2.49	0.46
6:BC:37:ALA:HB1	6:BC:93:LEU:HD21	1.97	0.46
7:BD:132:VAL:HG13	7:BD:136:ASP:HB2	1.97	0.46
15:BL:72:HIS:HD2	15:BL:74:LEU:H	1.61	0.46
2:A:2374:U:H2'	2:A:2375:G:C8	2.51	0.46
4:BA:413:G:O2'	4:BA:428:G:N2	2.48	0.46
4:BA:1178:A:H5'	4:BA:1178:A:C8	2.50	0.46
9:BF:7:MET:HE3	21:BR:33:LYS:NZ	2.31	0.46
43:T:102:ARG:HG2	43:T:104:ARG:CZ	2.46	0.46
2:A:404:A:OP1	29:E:170:ARG:HD2	2.15	0.46
2:A:1293:G:H1'	2:A:1294:U:C6	2.50	0.46
4:BA:501:G:H4'	15:BL:70:GLU:CG	2.41	0.46
43:T:9:SER:HB3	43:T:115:GLU:OE2	2.15	0.46
36:M:126:ALA:O	36:M:146:GLU:HA	2.15	0.46
2:A:498:G:H5''	2:A:498:G:C8	2.45	0.46
2:A:2113:A:H2'	2:A:2114:A:C8	2.51	0.46
4:BA:335:C:H2'	4:BA:336:A:C8	2.51	0.46
6:BC:71:ARG:HE	6:BC:74:ILE:HD11	1.80	0.46
2:A:1706:A:H2'	2:A:1707:G:C8	2.51	0.46
4:BA:371:A:H5''	4:BA:371:A:H8	1.81	0.46
4:BA:481:G:H2'	4:BA:482:A:C8	2.51	0.46
24:BV:141:LYS:O	24:BV:145:GLU:HG3	2.16	0.46
38:O:45:ARG:HB3	38:O:46:PRO:HD3	1.97	0.46
55:f:19:ARG:HG2	55:f:20:HIS:CD2	2.50	0.46
2:A:1759:A:O5'	2:A:1759:A:H8	1.99	0.46
24:BV:114:LEU:HD13	24:BV:144:LEU:HB3	1.98	0.46
4:BA:540:A:H5'	4:BA:546:G:N2	2.30	0.45
31:G:37:VAL:HG11	31:G:43:VAL:HG21	1.98	0.45
46:W:124:VAL:HG12	46:W:181:VAL:HG22	1.98	0.45
2:A:1392:G:H4'	38:O:20:LEU:HD11	1.99	0.45
25:BW:8:U:H2'	25:BW:46:G:H21	1.81	0.45
2:A:2548:U:H5''	2:A:2548:U:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Y:8:CYS:SG	48:Y:10:LYS:HB2	2.55	0.45
2:A:166:A:H2'	2:A:167:G:O4'	2.17	0.45
2:A:402:G:H4'	2:A:404:A:N7	2.32	0.45
2:A:483:G:H2'	2:A:484:C:C6	2.52	0.45
2:A:2381:A:H4'	2:A:2382:G:O5'	2.16	0.45
8:BE:104:SER:HB2	8:BE:146:HIS:HD2	1.80	0.45
36:M:80:VAL:HG12	36:M:118:LEU:HD13	1.96	0.45
44:U:28:VAL:HG22	44:U:85:LYS:HG3	1.98	0.45
2:A:1678:U:H5'	2:A:1679:A:OP2	2.15	0.45
2:A:2343:G:H2'	2:A:2344:G:C8	2.52	0.45
2:A:2907:C:H5'	40:Q:55:SER:HB2	1.98	0.45
4:BA:657:U:H3	4:BA:693:G:H22	1.63	0.45
4:BA:1043:C:H2'	4:BA:1044:G:C8	2.51	0.45
9:BF:2:ARG:HD3	9:BF:92:ARG:NE	2.31	0.45
30:F:57:ILE:H	30:F:57:ILE:HG13	1.61	0.45
2:A:1640:A:H2'	2:A:1642:G:N7	2.32	0.45
2:A:2569:G:N3	2:A:2605:C:H2'	2.31	0.45
4:BA:263:A:H2'	4:BA:264:U:C6	2.52	0.45
2:A:899:G:H5'	2:A:900:G:OP1	2.15	0.45
2:A:1628:A:H4'	2:A:1629:G:H4'	1.99	0.45
2:A:2262:C:H2'	2:A:2263:G:O4'	2.17	0.45
45:V:40:ARG:HG2	45:V:61:THR:HG22	1.98	0.45
2:A:684:G:H3'	2:A:685:G:C5'	2.47	0.45
54:e:27:ALA:O	54:e:28:ASN:HB2	2.16	0.45
2:A:869:U:P	53:d:2:ALA:HB2	2.57	0.45
3:B:89:C:H2'	3:B:90:G:O4'	2.17	0.45
4:BA:1125:G:N2	4:BA:1127:A:H62	2.14	0.45
37:N:68:ILE:HD13	37:N:103:LEU:HD22	1.99	0.45
2:A:2245:C:OP1	41:R:25:ARG:HD3	2.16	0.45
4:BA:299:G:H2'	4:BA:300:A:C8	2.52	0.45
4:BA:695:A:H2'	4:BA:696:A:C8	2.51	0.45
4:BA:1098:U:H2'	4:BA:1099:C:C6	2.52	0.45
4:BA:1410:C:H2'	4:BA:1411:A:C8	2.51	0.45
31:G:33:LEU:HB3	31:G:76:LEU:HD11	1.98	0.45
31:G:122:ILE:HD11	31:G:142:VAL:HA	1.98	0.45
2:A:270:U:H2'	2:A:271:A:H5'	1.99	0.44
4:BA:49:U:H2'	4:BA:50:G:C8	2.52	0.44
4:BA:353:A:H5'	4:BA:353:A:H8	1.82	0.44
4:BA:485:G:H2'	4:BA:486:G:C8	2.52	0.44
4:BA:914:C:H5''	4:BA:914:C:H6	1.82	0.44
28:D:59:PRO:HA	28:D:62:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Z:22:LEU:HD11	49:Z:54:ILE:HG23	1.99	0.44
1:3:7:LYS:HE2	1:3:7:LYS:HB3	1.76	0.44
2:A:691:U:H2'	2:A:692:C:C6	2.52	0.44
2:A:1621:C:H2'	2:A:1622:G:H8	1.81	0.44
4:BA:25:G:H2'	4:BA:26:G:C8	2.52	0.44
4:BA:128:U:H2'	4:BA:129:C:C6	2.52	0.44
4:BA:694:G:H2'	4:BA:695:A:C8	2.52	0.44
24:BV:76:ALA:HB2	24:BV:164:VAL:HG11	1.98	0.44
46:W:50:ASN:HD22	46:W:53:ASP:CG	2.25	0.44
48:Y:39:VAL:HG22	48:Y:46:LYS:HG2	1.99	0.44
2:A:621:U:H2'	2:A:622:C:C6	2.53	0.44
2:A:1990:A:H5''	61:A:4992:HOH:O	2.17	0.44
4:BA:81:C:H42	4:BA:88:G:H1	1.65	0.44
4:BA:100:G:H4'	4:BA:171:A:O4'	2.17	0.44
4:BA:1476:A:H5''	15:BL:44:LYS:HE3	1.99	0.44
8:BE:104:SER:HB2	8:BE:146:HIS:CD2	2.52	0.44
18:BO:36:ILE:HG23	18:BO:56:LEU:HD11	2.00	0.44
22:BS:50:ALA:HB1	22:BS:57:HIS:HB3	1.99	0.44
36:M:118:LEU:HD22	36:M:137:ILE:HD13	1.98	0.44
44:U:24:ILE:HD11	44:U:96:PHE:CD1	2.52	0.44
2:A:1476:G:H2'	2:A:1477:C:C6	2.53	0.44
2:A:1704:U:H3	2:A:1725:G:H1	1.64	0.44
4:BA:1408:A:H2'	4:BA:1409:A:O4'	2.17	0.44
12:BI:150:ARG:H	12:BI:150:ARG:HG2	1.62	0.44
2:A:2070:A:N1	2:A:2310:G:H1'	2.33	0.44
2:A:2448:G:H4'	2:A:2450:C:C2	2.53	0.44
4:BA:581:U:H2'	4:BA:582:U:C6	2.53	0.44
6:BC:101:ASN:O	6:BC:103:LEU:HG	2.17	0.44
10:BG:13:VAL:O	10:BG:24:THR:HG21	2.18	0.44
36:M:121:LYS:HE3	36:M:141:GLY:O	2.16	0.44
4:BA:66:U:H2'	4:BA:67:C:C6	2.52	0.44
4:BA:814:G:H5''	21:BR:58:VAL:HG21	2.00	0.44
35:L:107:ARG:HE	35:L:112:MET:HE1	1.81	0.44
2:A:332:C:H2'	2:A:333:C:C6	2.52	0.44
2:A:334:G:H3'	2:A:335:G:H8	1.82	0.44
2:A:422:A:H2'	2:A:423:C:O4'	2.17	0.44
2:A:454:U:H2'	2:A:455:C:C6	2.53	0.44
10:BG:12:LEU:HD23	10:BG:12:LEU:HA	1.81	0.44
13:BJ:86:ALA:O	13:BJ:90:ILE:HG13	2.18	0.44
4:BA:452:A:O2'	19:BP:76:ILE:HD11	2.16	0.44
4:BA:850:C:H2'	4:BA:851:A:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BA:1019:U:H6	4:BA:1019:U:O5'	2.01	0.44
27:C:16:ALA:HB2	27:C:207:GLY:HA3	1.99	0.44
2:A:331:U:H2'	2:A:332:C:H6	1.82	0.44
2:A:443:C:H2'	2:A:444:U:C6	2.53	0.44
2:A:932:C:O2'	2:A:954:U:H5''	2.18	0.44
2:A:1546:A:H2'	2:A:1547:G:C8	2.53	0.44
12:BI:54:THR:HG23	12:BI:56:GLU:H	1.82	0.44
22:BS:12:ASP:HB3	22:BS:14:HIS:CE1	2.53	0.44
24:BV:148:LEU:HA	24:BV:151:ILE:HD13	1.99	0.44
28:D:212:ILE:HG13	28:D:213:LYS:HG3	2.00	0.44
2:A:716:G:H8	2:A:716:G:H5''	1.82	0.43
2:A:857:U:H2'	2:A:858:A:C8	2.52	0.43
2:A:947:U:H2'	2:A:948:G:C8	2.53	0.43
2:A:1146:A:N6	2:A:1243:G:H2'	2.33	0.43
2:A:1838:G:H4'	53:d:3:LYS:O	2.17	0.43
17:BN:24:CYS:HB2	17:BN:40:CYS:HB3	1.99	0.43
36:M:84:ASN:ND2	36:M:118:LEU:HA	2.31	0.43
2:A:80:G:N2	2:A:99:G:H1'	2.33	0.43
2:A:1302:G:H5''	42:S:84:TYR:CE1	2.53	0.43
4:BA:138:A:H2'	4:BA:139:C:O4'	2.17	0.43
10:BG:104:LEU:HD21	10:BG:124:ILE:HG12	2.00	0.43
15:BL:21:THR:HG22	15:BL:21:THR:O	2.18	0.43
20:BQ:41:GLU:CD	20:BQ:54:ARG:HD2	2.43	0.43
31:G:41:ILE:HG12	31:G:65:LEU:HB3	2.00	0.43
35:L:115:VAL:HG13	35:L:121:VAL:HG21	2.00	0.43
36:M:65:LYS:H	54:e:25:GLN:NE2	2.16	0.43
39:P:18:ARG:HD2	39:P:107:TYR:CZ	2.53	0.43
43:T:27:VAL:HG11	43:T:51:SER:HA	2.00	0.43
2:A:1791:A:H2'	2:A:1792:A:C8	2.53	0.43
2:A:2457:U:H2'	2:A:2458:G:C8	2.53	0.43
4:BA:519:A:H2'	4:BA:520:G:H8	1.84	0.43
4:BA:642:C:H2'	4:BA:643:A:C8	2.53	0.43
20:BQ:29:SER:HB3	20:BQ:37:VAL:HB	2.00	0.43
34:K:115:GLY:O	34:K:119:GLN:HG3	2.18	0.43
46:W:157:ILE:HB	46:W:179:VAL:HB	2.00	0.43
2:A:256:A:H2'	2:A:257:A:C8	2.53	0.43
2:A:658:U:H2'	2:A:659:U:O4'	2.19	0.43
2:A:1195:A:H5'	33:J:95:HIS:ND1	2.33	0.43
2:A:1822:C:H5'	61:A:4384:HOH:O	2.19	0.43
4:BA:1278:C:H4'	4:BA:1284:U:C4	2.54	0.43
7:BD:11:LYS:HE3	7:BD:58:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BL:69:GLY:HA3	15:BL:107:VAL:HG11	2.01	0.43
2:A:673:C:H2'	2:A:674:U:C6	2.53	0.43
2:A:929:C:H1'	2:A:1339:G:N2	2.34	0.43
2:A:2003:A:H1'	2:A:2162:A:N6	2.33	0.43
2:A:2406:U:H2'	2:A:2407:C:C6	2.54	0.43
18:BO:12:LEU:HD13	18:BO:22:THR:HG22	2.00	0.43
27:C:217:LYS:HB3	27:C:217:LYS:HE2	1.31	0.43
34:K:36:LEU:O	34:K:51:GLY:HA3	2.18	0.43
40:Q:32:ILE:HG13	40:Q:37:GLU:HG2	1.99	0.43
54:e:23:VAL:CG1	54:e:47:ARG:HD2	2.48	0.43
2:A:438:U:H3'	2:A:439:C:C6	2.52	0.43
2:A:1541:G:H1	2:A:1631:A:H61	1.66	0.43
2:A:1636:A:H2'	2:A:1637:G:O4'	2.19	0.43
10:BG:13:VAL:HG22	10:BG:14:ASN:H	1.83	0.43
20:BQ:60:LYS:HD2	20:BQ:85:THR:OG1	2.19	0.43
4:BA:1027:G:H2'	4:BA:1028:G:H5''	2.01	0.43
20:BQ:35:THR:HG22	20:BQ:86:LYS:HZ2	1.83	0.43
2:A:1303:U:H4'	42:S:82:THR:HG23	2.00	0.43
2:A:1650:G:H2'	2:A:1651:C:C6	2.54	0.43
2:A:3033:G:H2'	2:A:3034:C:C6	2.53	0.43
4:BA:1019:U:H3'	4:BA:1020:G:C5'	2.49	0.43
6:BC:119:VAL:O	6:BC:123:LEU:HG	2.18	0.43
22:BS:15:LEU:O	22:BS:19:VAL:HG12	2.19	0.43
34:K:49:ASP:HA	61:K:201:HOH:O	2.19	0.43
2:A:768:G:H2'	2:A:769:U:C6	2.53	0.43
4:BA:1461:U:H2'	4:BA:1462:C:C6	2.53	0.43
10:BG:150:ALA:HB1	14:BK:68:THR:HG21	2.01	0.43
15:BL:94:ARG:HB2	15:BL:95:TYR:CE1	2.54	0.43
22:BS:9:PRO:HD3	56:g:65:TYR:CD1	2.54	0.43
2:A:1294:U:H2'	2:A:1295:U:C6	2.53	0.43
2:A:2088:C:H2'	2:A:2089:C:C6	2.53	0.43
2:A:2386:U:H2'	2:A:2388:G:OP2	2.18	0.43
4:BA:200:U:O4	20:BQ:8:LYS:HE3	2.19	0.43
9:BF:38:ASP:O	9:BF:39:LYS:HB2	2.19	0.43
19:BP:84:LYS:HA	19:BP:84:LYS:HD2	1.80	0.43
2:A:1338:U:H4'	42:S:89:GLY:O	2.19	0.42
2:A:2029:A:H2'	2:A:2030:C:C6	2.54	0.42
2:A:2046:A:H2'	2:A:2047:C:H5'	2.01	0.42
1:3:4:ARG:HH21	2:A:2680:C:H5'	1.84	0.42
2:A:448:U:H5''	2:A:449:G:OP2	2.19	0.42
2:A:502:C:H2'	2:A:503:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BA:1201:G:H1'	22:BS:52:HIS:HD2	1.84	0.42
24:BV:4:VAL:HG13	24:BV:8:GLN:HB3	2.00	0.42
28:D:161:PHE:CG	34:K:81:PRO:HG3	2.53	0.42
2:A:331:U:H2'	2:A:332:C:C6	2.55	0.42
2:A:402:G:H4'	2:A:404:A:C8	2.55	0.42
2:A:1249:G:O2'	2:A:2250:A:H5'	2.20	0.42
2:A:2546:A:H2'	2:A:2547:G:O4'	2.19	0.42
6:BC:67:ILE:HG23	6:BC:102:ILE:HA	2.00	0.42
24:BV:24:ASN:ND2	24:BV:192:ASP:HA	2.34	0.42
24:BV:144:LEU:HD12	24:BV:144:LEU:HA	1.86	0.42
27:C:201:GLN:HE21	27:C:201:GLN:HB2	1.63	0.42
30:F:68:THR:HB	30:F:98:LEU:HD21	2.01	0.42
2:A:2846:C:H5'	28:D:169:ARG:HG3	2.02	0.42
9:BF:43:TRP:CD1	9:BF:43:TRP:N	2.88	0.42
32:H:124:ILE:HG23	32:H:130:HIS:CD2	2.54	0.42
2:A:288:U:H3'	2:A:289:A:C2	2.54	0.42
2:A:327:U:H2'	2:A:328:C:C6	2.55	0.42
2:A:1010:U:H3'	2:A:1011:A:H5''	2.01	0.42
2:A:1862:C:H5''	2:A:1862:C:H6	1.85	0.42
34:K:34:THR:HG23	34:K:39:LYS:HB2	2.00	0.42
48:Y:2:ALA:HA	48:Y:33:ILE:HD11	2.01	0.42
2:A:291:C:H2'	2:A:292:G:H8	1.81	0.42
2:A:702:A:H2'	2:A:703:C:O4'	2.19	0.42
2:A:1296:G:H2'	2:A:1297:G:C8	2.55	0.42
2:A:2286:A:N3	2:A:2286:A:H2'	2.35	0.42
2:A:2495:G:OP1	47:X:18:ALA:HB1	2.20	0.42
2:A:2904:C:H5'	28:D:199:PRO:HA	2.01	0.42
4:BA:84:U:H3'	4:BA:85:C:C2	2.54	0.42
8:BE:100:PRO:HB3	8:BE:174:ARG:HG2	2.01	0.42
24:BV:186:ILE:HA	24:BV:200:ILE:O	2.18	0.42
24:BV:197:ASP:O	24:BV:199:PRO:HD3	2.19	0.42
29:E:27:VAL:HG21	29:E:112:ARG:HB3	2.01	0.42
33:J:95:HIS:CD2	46:W:120:PRO:HG2	2.54	0.42
2:A:2096:G:H2'	2:A:2097:G:C8	2.55	0.42
2:A:3018:U:H2'	2:A:3019:C:C6	2.54	0.42
4:BA:700:C:H5''	21:BR:50:ALA:HA	2.01	0.42
19:BP:22:VAL:HG21	19:BP:59:TRP:CD1	2.55	0.42
4:BA:1470:G:H2'	4:BA:1471:G:O4'	2.20	0.42
20:BQ:85:THR:OG1	20:BQ:86:LYS:N	2.52	0.42
30:F:113:ILE:HD11	56:g:22:PHE:HZ	1.84	0.42
45:V:85:TYR:CD1	45:V:94:LYS:HE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:199:U:H4'	48:Y:22:HIS:HB3	2.00	0.42
3:B:81:U:H2'	3:B:82:A:C8	2.55	0.42
4:BA:653:G:H2'	4:BA:654:G:C8	2.55	0.42
10:BG:31:LEU:HD13	10:BG:36:LYS:HA	2.01	0.42
22:BS:15:LEU:HD11	22:BS:49:PHE:CE1	2.55	0.42
36:M:80:VAL:HG23	36:M:113:LEU:O	2.20	0.42
56:g:42:HIS:HB3	56:g:45:TYR:CD1	2.55	0.42
2:A:926:U:H2'	36:M:24:ARG:HA	2.02	0.42
2:A:2383:U:C4	2:A:2384:C:H1'	2.55	0.42
12:BI:28:THR:HG21	12:BI:106:ALA:HB2	2.02	0.42
29:E:20:LEU:HB3	29:E:25:PHE:CD1	2.55	0.42
30:F:146:HIS:CE1	56:g:35:VAL:HG23	2.55	0.42
32:H:32:PRO:HB3	48:Y:64:ALA:HA	2.02	0.42
37:N:42:ILE:HD12	37:N:97:VAL:HG21	2.02	0.42
2:A:90:C:H2'	2:A:91:C:O4'	2.20	0.41
4:BA:592:U:H2'	4:BA:593:C:C6	2.55	0.41
4:BA:716:U:H2'	4:BA:717:C:C6	2.55	0.41
6:BC:87:ARG:HG3	6:BC:100:LEU:HD12	2.02	0.41
16:BM:49:THR:OG1	16:BM:52:GLN:HG3	2.19	0.41
29:E:196:PHE:HB3	29:E:201:LEU:HB2	2.02	0.41
36:M:75:TYR:CE1	36:M:109:LEU:HD23	2.55	0.41
2:A:442:U:H2'	2:A:443:C:C6	2.55	0.41
2:A:564:G:H4'	2:A:589:A:N1	2.35	0.41
2:A:973:G:N3	2:A:2492:A:H2'	2.36	0.41
4:BA:390:U:H2'	4:BA:391:G:C8	2.56	0.41
19:BP:21:ILE:HG22	19:BP:36:VAL:HG12	2.02	0.41
24:BV:20:THR:HG23	24:BV:39:TYR:CZ	2.55	0.41
27:C:158:SER:O	27:C:161:VAL:HG22	2.19	0.41
42:S:72:LYS:HA	42:S:91:ARG:HG2	2.02	0.41
2:A:1187:A:H4'	2:A:1188:A:H5''	2.02	0.41
2:A:2156:A:H2'	2:A:2157:G:O4'	2.19	0.41
2:A:2802:G:H21	28:D:135:GLN:NE2	2.18	0.41
2:A:3046:C:H2'	2:A:3047:A:O4'	2.20	0.41
4:BA:654:G:H2'	4:BA:655:A:C8	2.55	0.41
4:BA:708:A:H2'	4:BA:709:A:C8	2.55	0.41
10:BG:12:LEU:HD13	10:BG:24:THR:HG23	2.02	0.41
24:BV:114:LEU:HD11	24:BV:145:GLU:HG2	2.01	0.41
53:d:18:VAL:O	53:d:23:LEU:HD22	2.20	0.41
4:BA:1206:U:H2'	4:BA:1207:C:C5	2.56	0.41
7:BD:119:LEU:HG	7:BD:124:LYS:HA	2.02	0.41
10:BG:70:LYS:HD3	10:BG:97:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:O:10:LEU:HD13	38:O:40:LYS:HG2	2.02	0.41
39:P:77:LYS:CB	39:P:112:ARG:HD3	2.51	0.41
40:Q:88:ARG:HB2	40:Q:112:LYS:HB2	2.02	0.41
43:T:102:ARG:HG3	43:T:103:ILE:N	2.31	0.41
44:U:95:LEU:HD23	44:U:95:LEU:HA	1.77	0.41
2:A:977:G:H2'	2:A:978:A:O4'	2.19	0.41
4:BA:60:U:H2'	4:BA:61:G:C8	2.56	0.41
4:BA:127:A:H1'	4:BA:263:A:O2'	2.20	0.41
31:G:165:TYR:HB2	31:G:168:GLU:HB2	2.03	0.41
49:Z:32:LEU:HD21	49:Z:46:ARG:HD2	2.03	0.41
2:A:3:A:O2'	34:K:132:HIS:HD2	2.03	0.41
12:BI:133:ARG:HG2	12:BI:134:LYS:N	2.35	0.41
22:BS:14:HIS:CD2	22:BS:14:HIS:H	2.38	0.41
22:BS:25:LYS:O	22:BS:26:ASN:C	2.62	0.41
2:A:1561:C:H2'	2:A:1562:C:C6	2.56	0.41
2:A:1825:C:H4'	2:A:1826:A:O5'	2.20	0.41
15:BL:72:HIS:CD2	15:BL:74:LEU:H	2.39	0.41
20:BQ:34:LYS:O	20:BQ:62:HIS:HD2	2.04	0.41
2:A:356:G:H4'	2:A:358:G:C6	2.56	0.41
2:A:1191:A:H2'	2:A:1192:G:H5'	2.01	0.41
2:A:2412:U:H2'	2:A:2413:G:C8	2.55	0.41
4:BA:64:A:H4'	4:BA:65:G:O5'	2.21	0.41
4:BA:957:A:H5'	4:BA:957:A:N3	2.36	0.41
2:A:206:A:H2'	2:A:207:C:O4'	2.21	0.41
2:A:209:C:OP1	53:d:28:ARG:HD3	2.21	0.41
2:A:1640:A:O2'	2:A:1641:U:H5''	2.21	0.41
3:B:76:G:H5'	46:W:46:HIS:CE1	2.56	0.41
4:BA:693:G:H2'	4:BA:694:G:C8	2.56	0.41
4:BA:900:A:H2'	4:BA:901:A:C8	2.56	0.41
4:BA:988:C:H3'	4:BA:989:G:C8	2.56	0.41
11:BH:10:PHE:HD1	11:BH:27:LEU:HD22	1.85	0.41
24:BV:126:PHE:HZ	24:BV:141:LYS:CE	2.32	0.41
35:L:88:LYS:HE3	35:L:92:ASP:HB2	2.03	0.41
43:T:81:VAL:HG23	43:T:112:VAL:HG22	2.03	0.41
45:V:2:LYS:HB3	45:V:83:VAL:HG21	2.03	0.41
46:W:63:THR:HG23	46:W:83:LEU:HD12	2.03	0.41
50:a:6:ILE:HD11	50:a:47:ILE:HD11	2.02	0.41
2:A:31:U:H6	2:A:31:U:H2'	1.74	0.41
2:A:332:C:H2'	2:A:333:C:H6	1.85	0.41
2:A:625:A:H61	2:A:647:G:H1'	1.86	0.41
2:A:1786:G:OP1	27:C:211:ARG:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1815:G:OP1	44:U:40:THR:HG22	2.21	0.41
2:A:3045:C:H2'	2:A:3046:C:O4'	2.20	0.41
4:BA:481:G:H1'	4:BA:529:C:H1'	2.02	0.41
4:BA:504:G:H2'	4:BA:505:C:C6	2.56	0.41
13:BJ:12:ALA:HB3	13:BJ:18:ILE:HB	2.03	0.41
24:BV:165:ASP:O	24:BV:169:GLU:HB2	2.21	0.41
37:N:40:ALA:HB2	37:N:127:ILE:HG23	2.03	0.41
50:a:37:ARG:HE	50:a:37:ARG:HB3	1.72	0.41
52:c:16:GLU:HG3	52:c:50:PRO:HB2	2.03	0.41
2:A:120:G:H5''	2:A:1490:U:O2'	2.20	0.40
2:A:2261:U:H2'	2:A:2262:C:C6	2.56	0.40
2:A:2899:A:H4'	35:L:29:SER:HB2	2.03	0.40
4:BA:71:C:H2'	4:BA:72:G:C8	2.56	0.40
4:BA:105:A:C6	4:BA:326:G:C6	3.08	0.40
4:BA:800:U:H5'	61:BA:1761:HOH:O	2.21	0.40
38:O:56:LYS:HE3	38:O:56:LYS:HB3	1.86	0.40
43:T:53:PRO:O	43:T:57:VAL:HG23	2.20	0.40
2:A:339:U:H2'	2:A:340:A:C8	2.56	0.40
2:A:844:G:H4'	2:A:878:G:H5''	2.04	0.40
2:A:1615:G:H8	2:A:1615:G:O5'	2.04	0.40
2:A:98:U:H3'	2:A:99:G:C5'	2.52	0.40
2:A:1947:U:H6	2:A:1947:U:H2'	1.76	0.40
2:A:2965:A:H2'	2:A:2966:C:O4'	2.21	0.40
2:A:3052:A:OP1	2:A:3055:G:H4'	2.22	0.40
61:A:4970:HOH:O	36:M:58:HIS:HD2	2.03	0.40
4:BA:1305:G:H2'	4:BA:1306:A:C8	2.56	0.40
8:BE:174:ARG:HB2	8:BE:177:GLU:HG3	2.04	0.40
2:A:665:G:O2'	2:A:666:A:H3'	2.21	0.40
2:A:1787:A:C2'	27:C:86:PRO:HG3	2.52	0.40
2:A:1937:U:H2'	2:A:1938:G:O4'	2.20	0.40
2:A:2147:U:H2'	2:A:2148:C:C6	2.55	0.40
2:A:3033:G:H2'	2:A:3034:C:H6	1.87	0.40
4:BA:702:G:N3	4:BA:702:G:H2'	2.36	0.40
12:BI:69:LYS:HB2	12:BI:69:LYS:HE3	1.81	0.40
24:BV:54:TYR:HE1	24:BV:58:LYS:HE3	1.85	0.40
28:D:63:ILE:HG22	28:D:65:PRO:HD2	2.04	0.40
46:W:11:LEU:HD12	46:W:67:LEU:HD13	2.02	0.40
2:A:330:U:H6	2:A:330:U:H2'	1.69	0.40
2:A:1553:C:N4	2:A:1618:C:H1'	2.37	0.40
4:BA:510:G:N3	4:BA:510:G:H2'	2.37	0.40
7:BD:167:GLN:HB2	7:BD:178:HIS:HE1	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BM:51:ASP:O	16:BM:55:VAL:HG23	2.21	0.40
23:BT:35:PHE:CE1	23:BT:51:LEU:HB2	2.57	0.40
41:R:109:LEU:HD23	41:R:109:LEU:HA	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	21/24 (88%)	21 (100%)	0	0	100	100
5	BB	30/33 (91%)	30 (100%)	0	0	100	100
6	BC	206/275 (75%)	190 (92%)	14 (7%)	2 (1%)	12	8
7	BD	198/201 (98%)	197 (100%)	1 (0%)	0	100	100
8	BE	178/214 (83%)	175 (98%)	3 (2%)	0	100	100
9	BF	94/96 (98%)	89 (95%)	4 (4%)	1 (1%)	11	7
10	BG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
11	BH	129/132 (98%)	127 (98%)	2 (2%)	0	100	100
12	BI	124/150 (83%)	117 (94%)	7 (6%)	0	100	100
13	BJ	97/101 (96%)	93 (96%)	4 (4%)	0	100	100
14	BK	113/138 (82%)	107 (95%)	5 (4%)	1 (1%)	14	9
15	BL	120/124 (97%)	118 (98%)	2 (2%)	0	100	100
16	BM	114/124 (92%)	106 (93%)	7 (6%)	1 (1%)	14	9
17	BN	58/61 (95%)	58 (100%)	0	0	100	100
18	BO	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
19	BP	111/156 (71%)	109 (98%)	2 (2%)	0	100	100
20	BQ	92/98 (94%)	88 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	BR	63/84 (75%)	61 (97%)	2 (3%)	0	100	100
22	BS	80/93 (86%)	76 (95%)	4 (5%)	0	100	100
23	BT	83/86 (96%)	83 (100%)	0	0	100	100
24	BV	226/277 (82%)	213 (94%)	12 (5%)	1 (0%)	30	27
27	C	273/278 (98%)	269 (98%)	4 (2%)	0	100	100
28	D	212/217 (98%)	205 (97%)	7 (3%)	0	100	100
29	E	207/215 (96%)	205 (99%)	2 (1%)	0	100	100
30	F	180/187 (96%)	170 (94%)	10 (6%)	0	100	100
31	G	174/179 (97%)	169 (97%)	5 (3%)	0	100	100
32	H	149/151 (99%)	141 (95%)	8 (5%)	0	100	100
33	J	67/142 (47%)	64 (96%)	3 (4%)	0	100	100
34	K	144/147 (98%)	144 (100%)	0	0	100	100
35	L	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
36	M	143/147 (97%)	139 (97%)	4 (3%)	0	100	100
37	N	134/138 (97%)	132 (98%)	2 (2%)	0	100	100
38	O	116/199 (58%)	112 (97%)	4 (3%)	0	100	100
39	P	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
40	Q	111/113 (98%)	109 (98%)	2 (2%)	0	100	100
41	R	122/129 (95%)	122 (100%)	0	0	100	100
42	S	98/103 (95%)	97 (99%)	1 (1%)	0	100	100
43	T	112/153 (73%)	111 (99%)	1 (1%)	0	100	100
44	U	95/100 (95%)	94 (99%)	0	1 (1%)	11	7
45	V	93/105 (89%)	89 (96%)	4 (4%)	0	100	100
46	W	190/215 (88%)	189 (100%)	1 (0%)	0	100	100
47	X	77/88 (88%)	75 (97%)	2 (3%)	0	100	100
48	Y	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
49	Z	64/77 (83%)	64 (100%)	0	0	100	100
50	a	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
51	b	52/57 (91%)	52 (100%)	0	0	100	100
52	c	47/55 (86%)	47 (100%)	0	0	100	100
53	d	44/47 (94%)	43 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	e	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
55	f	35/37 (95%)	35 (100%)	0	0	100	100
56	g	55/75 (73%)	54 (98%)	1 (2%)	0	100	100
All	All	5793/6504 (89%)	5640 (97%)	146 (2%)	7 (0%)	49	46

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	BC	102	ILE
16	BM	11	ARG
24	BV	124	GLY
44	U	95	LEU
9	BF	39	LYS
14	BK	128	ASN
6	BC	45	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	18/19 (95%)	18 (100%)	0	100	100
5	BB	30/31 (97%)	29 (97%)	1 (3%)	33	34
6	BC	170/212 (80%)	162 (95%)	8 (5%)	23	22
7	BD	175/176 (99%)	170 (97%)	5 (3%)	37	40
8	BE	127/147 (86%)	124 (98%)	3 (2%)	43	47
9	BF	85/85 (100%)	74 (87%)	11 (13%)	4	2
10	BG	131/132 (99%)	124 (95%)	7 (5%)	20	18
11	BH	107/108 (99%)	105 (98%)	2 (2%)	50	56
12	BI	102/125 (82%)	93 (91%)	9 (9%)	9	6
13	BJ	89/90 (99%)	83 (93%)	6 (7%)	15	11
14	BK	89/105 (85%)	85 (96%)	4 (4%)	24	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	BL	103/105 (98%)	97 (94%)	6 (6%)	18	15
16	BM	99/104 (95%)	95 (96%)	4 (4%)	28	27
17	BN	49/50 (98%)	48 (98%)	1 (2%)	48	54
18	BO	76/77 (99%)	74 (97%)	2 (3%)	40	44
19	BP	92/118 (78%)	90 (98%)	2 (2%)	45	50
20	BQ	80/83 (96%)	75 (94%)	5 (6%)	16	13
21	BR	55/72 (76%)	55 (100%)	0	100	100
22	BS	73/84 (87%)	71 (97%)	2 (3%)	39	42
23	BT	69/70 (99%)	65 (94%)	4 (6%)	18	15
24	BV	191/218 (88%)	184 (96%)	7 (4%)	30	30
27	C	215/218 (99%)	207 (96%)	8 (4%)	30	30
28	D	160/163 (98%)	155 (97%)	5 (3%)	35	37
29	E	169/173 (98%)	164 (97%)	5 (3%)	36	38
30	F	151/156 (97%)	146 (97%)	5 (3%)	33	34
31	G	148/150 (99%)	140 (95%)	8 (5%)	20	17
32	H	116/116 (100%)	111 (96%)	5 (4%)	26	25
33	J	51/108 (47%)	51 (100%)	0	100	100
34	K	119/120 (99%)	116 (98%)	3 (2%)	42	45
35	L	100/100 (100%)	97 (97%)	3 (3%)	36	38
36	M	112/114 (98%)	110 (98%)	2 (2%)	51	58
37	N	114/116 (98%)	108 (95%)	6 (5%)	20	18
38	O	97/158 (61%)	95 (98%)	2 (2%)	47	52
39	P	93/94 (99%)	90 (97%)	3 (3%)	34	35
40	Q	100/100 (100%)	99 (99%)	1 (1%)	68	75
41	R	97/99 (98%)	96 (99%)	1 (1%)	68	75
42	S	81/83 (98%)	79 (98%)	2 (2%)	42	45
43	T	90/117 (77%)	86 (96%)	4 (4%)	25	24
44	U	83/85 (98%)	79 (95%)	4 (5%)	23	21
45	V	81/86 (94%)	74 (91%)	7 (9%)	10	6
46	W	155/168 (92%)	147 (95%)	8 (5%)	21	18
47	X	58/63 (92%)	56 (97%)	2 (3%)	32	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	Y	50/51 (98%)	47 (94%)	3 (6%)	17	14
49	Z	59/66 (89%)	59 (100%)	0	100	100
50	a	52/54 (96%)	51 (98%)	1 (2%)	50	56
51	b	43/46 (94%)	42 (98%)	1 (2%)	44	49
52	c	47/52 (90%)	46 (98%)	1 (2%)	47	52
53	d	35/36 (97%)	33 (94%)	2 (6%)	18	15
54	e	53/54 (98%)	48 (91%)	5 (9%)	8	5
55	f	35/35 (100%)	34 (97%)	1 (3%)	37	40
56	g	51/63 (81%)	48 (94%)	3 (6%)	18	14
57	s	1/4 (25%)	0	1 (100%)	0	0
All	All	4826/5259 (92%)	4635 (96%)	191 (4%)	29	27

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	BB	24	THR
6	BC	14	ILE
6	BC	41	LEU
6	BC	48	ARG
6	BC	74	ILE
6	BC	75	VAL
6	BC	102	ILE
6	BC	103	LEU
6	BC	170	GLU
7	BD	72	GLU
7	BD	111	GLN
7	BD	152	ILE
7	BD	175	ILE
7	BD	188	VAL
8	BE	102	ILE
8	BE	120	MET
8	BE	148	ILE
9	BF	1	MET
9	BF	26	PHE
9	BF	31	ARG
9	BF	38	ASP
9	BF	45	ARG
9	BF	57	GLU

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Mol	Chain	Res	Type
9	BF	76	ASP
9	BF	77	ARG
9	BF	87	ARG
9	BF	91	LEU
9	BF	92	ARG
10	BG	10	ARG
10	BG	27	VAL
10	BG	70	LYS
10	BG	97	THR
10	BG	118	GLU
10	BG	136	LYS
10	BG	144	MET
11	BH	55	ARG
11	BH	120	ARG
12	BI	37	VAL
12	BI	39	VAL
12	BI	40	ARG
12	BI	129	ARG
12	BI	133	ARG
12	BI	135	LYS
12	BI	139	LYS
12	BI	140	LYS
12	BI	150	ARG
13	BJ	32	THR
13	BJ	54	SER
13	BJ	57	LYS
13	BJ	71	LYS
13	BJ	74	ILE
13	BJ	76	ILE
14	BK	25	VAL
14	BK	91	VAL
14	BK	102	ARG
14	BK	103	GLU
15	BL	10	LYS
15	BL	49	LEU
15	BL	52	VAL
15	BL	63	VAL
15	BL	73	ASN
15	BL	82	VAL
16	BM	13	LYS
16	BM	64	LEU
16	BM	80	ARG

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Mol	Chain	Res	Type
16	BM	111	LYS
17	BN	46	GLU
18	BO	65	ARG
18	BO	82	ILE
19	BP	21	ILE
19	BP	36	VAL
20	BQ	33	GLN
20	BQ	57	LYS
20	BQ	59	VAL
20	BQ	87	ARG
20	BQ	93	ILE
22	BS	14	HIS
22	BS	19	VAL
23	BT	4	ILE
23	BT	15	GLU
23	BT	16	ARG
23	BT	28	LEU
24	BV	4	VAL
24	BV	79	SER
24	BV	129	ARG
24	BV	141	LYS
24	BV	148	LEU
24	BV	156	LYS
24	BV	195	VAL
27	C	26	ARG
27	C	101	GLU
27	C	131	LEU
27	C	184	ARG
27	C	201	GLN
27	C	205	ASN
27	C	213	ARG
27	C	217	LYS
28	D	11	LEU
28	D	75	VAL
28	D	99	GLN
28	D	191	VAL
28	D	198	ILE
29	E	27	VAL
29	E	67	ARG
29	E	132	GLU
29	E	134	GLN
29	E	158	ILE

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Mol	Chain	Res	Type
30	F	38	VAL
30	F	47	VAL
30	F	57	ILE
30	F	95	ARG
30	F	164	VAL
31	G	39	GLU
31	G	41	ILE
31	G	42	SER
31	G	45	ARG
31	G	51	ILE
31	G	77	VAL
31	G	122	ILE
31	G	137	ILE
32	H	4	ILE
32	H	27	ARG
32	H	62	ILE
32	H	101	VAL
32	H	127	VAL
34	K	85	ARG
34	K	99	ARG
34	K	116	ARG
35	L	69	ARG
35	L	71	ARG
35	L	87	ILE
36	M	76	GLN
36	M	109	LEU
37	N	18	ARG
37	N	45	ARG
37	N	72	ARG
37	N	77	LYS
37	N	91	GLU
37	N	127	ILE
38	O	71	ARG
38	O	96	ARG
39	P	12	GLU
39	P	25	LEU
39	P	104	ARG
40	Q	48	ARG
41	R	8	LEU
42	S	58	VAL
42	S	86	LYS
43	T	20	SER

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Mol	Chain	Res	Type
43	T	92	ILE
43	T	102	ARG
43	T	115	GLU
44	U	83	ILE
44	U	93	ILE
44	U	94	ASP
44	U	95	LEU
45	V	38	VAL
45	V	40	ARG
45	V	41	ILE
45	V	42	LYS
45	V	59	ILE
45	V	72	MET
45	V	97	ILE
46	W	19	THR
46	W	89	ARG
46	W	90	ARG
46	W	99	VAL
46	W	100	VAL
46	W	130	THR
46	W	177	LEU
46	W	181	VAL
47	X	38	VAL
47	X	73	ARG
48	Y	33	ILE
48	Y	36	VAL
48	Y	48	ARG
50	a	43	THR
51	b	39	VAL
52	c	40	LYS
53	d	6	ARG
53	d	28	ARG
54	e	15	ARG
54	e	16	ARG
54	e	23	VAL
54	e	48	THR
54	e	56	SER
55	f	2	LYS
56	g	23	THR
56	g	24	THR
56	g	37	VAL
57	s	5	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	3	17	ASN
6	BC	8	HIS
6	BC	125	ASN
6	BC	176	HIS
7	BD	84	ASN
7	BD	115	HIS
7	BD	117	HIS
7	BD	151	GLN
8	BE	95	ASN
8	BE	108	HIS
8	BE	146	HIS
8	BE	160	ASN
9	BF	78	GLN
9	BF	80	ASN
10	BG	28	ASN
10	BG	106	ASN
10	BG	148	ASN
10	BG	153	HIS
12	BI	57	ASN
12	BI	146	GLN
13	BJ	64	HIS
14	BK	31	HIS
14	BK	37	ASN
14	BK	86	HIS
14	BK	128	ASN
15	BL	73	ASN
17	BN	8	HIS
17	BN	25	ASN
18	BO	46	HIS
19	BP	17	GLN
19	BP	41	HIS
20	BQ	62	HIS
22	BS	14	HIS
22	BS	57	HIS
22	BS	69	HIS
23	BT	68	HIS
23	BT	70	ASN
23	BT	84	ASN
27	C	76	ASN
27	C	87	ASN
27	C	143	HIS

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Mol	Chain	Res	Type
27	C	201	GLN
27	C	205	ASN
28	D	21	ASN
28	D	130	HIS
28	D	135	GLN
28	D	179	ASN
29	E	171	ASN
29	E	190	ASN
29	E	202	ASN
30	F	128	GLN
30	F	146	HIS
30	F	187	ASN
31	G	22	GLN
31	G	23	ASN
31	G	66	HIS
32	H	46	GLN
32	H	64	HIS
32	H	102	ASN
32	H	130	HIS
34	K	58	ASN
34	K	77	HIS
34	K	103	ASN
34	K	132	HIS
35	L	3	GLN
36	M	45	ASN
36	M	58	HIS
36	M	127	ASN
37	N	12	GLN
37	N	17	GLN
38	O	16	HIS
38	O	17	GLN
39	P	9	ASN
39	P	80	HIS
40	Q	50	GLN
40	Q	79	ASN
41	R	38	GLN
41	R	41	HIS
41	R	122	ASN
42	S	67	HIS
42	S	76	HIS
42	S	90	HIS
43	T	66	GLN

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Mol	Chain	Res	Type
44	U	61	ASN
45	V	67	HIS
46	W	9	ASN
46	W	46	HIS
46	W	50	ASN
46	W	61	HIS
46	W	91	ASN
46	W	94	HIS
47	X	19	GLN
47	X	29	GLN
47	X	50	ASN
50	a	8	GLN
52	c	22	ASN
52	c	48	HIS
54	e	25	GLN
54	e	63	ASN
55	f	20	HIS
56	g	20	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	3083/3120 (98%)	499 (16%)	63 (2%)
25	BW	75/76 (98%)	13 (17%)	2 (2%)
26	I	5/15 (33%)	0	0
3	B	117/118 (99%)	12 (10%)	5 (4%)
4	BA	1511/1528 (98%)	271 (17%)	27 (1%)
All	All	4791/4857 (98%)	795 (16%)	97 (2%)

All (795) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	9	U
2	A	12	G
2	A	20	G
2	A	29	C
2	A	31	U
2	A	32	G
2	A	60	A
2	A	68	A
2	A	71	A

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Mol	Chain	Res	Type
2	A	72	G
2	A	89	A
2	A	90	C
2	A	94	G
2	A	98	U
2	A	99	G
2	A	116	A
2	A	117	U
2	A	125	C
2	A	136	U
2	A	137	G
2	A	144	U
2	A	148	A
2	A	164	A
2	A	172	C
2	A	174	G
2	A	175	G
2	A	180	A
2	A	195	A
2	A	196	A
2	A	198	A
2	A	199	U
2	A	212	A
2	A	214	G
2	A	215	A
2	A	221	A
2	A	227	A
2	A	229	U
2	A	230	G
2	A	233	A
2	A	248	G
2	A	264	G
2	A	271	A
2	A	283	U
2	A	285	U
2	A	286	G
2	A	287	A
2	A	291	C
2	A	293	G
2	A	294	G
2	A	295	U
2	A	296	A

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Mol	Chain	Res	Type
2	A	297	G
2	A	298	G
2	A	300	G
2	A	301	U
2	A	303	G
2	A	304	U
2	A	315	U
2	A	317	G
2	A	318	U
2	A	319	G
2	A	322	A
2	A	324	C
2	A	330	U
2	A	331	U
2	A	332	C
2	A	335	G
2	A	337	U
2	A	338	C
2	A	339	U
2	A	340	A
2	A	341	C
2	A	344	G
2	A	345	G
2	A	346	C
2	A	348	G
2	A	349	G
2	A	351	G
2	A	353	G
2	A	357	U
2	A	358	G
2	A	359	A
2	A	361	A
2	A	364	A
2	A	370	U
2	A	376	G
2	A	384	G
2	A	393	U
2	A	394	G
2	A	404	A
2	A	412	A
2	A	413	G
2	A	424	G

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Mol	Chain	Res	Type
2	A	426	G
2	A	433	C
2	A	434	G
2	A	437	G
2	A	438	U
2	A	441	G
2	A	442	U
2	A	443	C
2	A	445	U
2	A	446	G
2	A	449	G
2	A	450	G
2	A	451	U
2	A	452	G
2	A	453	U
2	A	454	U
2	A	460	G
2	A	474	G
2	A	489	A
2	A	493	U
2	A	494	G
2	A	497	G
2	A	498	G
2	A	499	G
2	A	500	A
2	A	512	G
2	A	539	C
2	A	543	U
2	A	544	U
2	A	562	G
2	A	569	G
2	A	570	U
2	A	590	A
2	A	591	G
2	A	594	U
2	A	595	A
2	A	596	C
2	A	617	U
2	A	618	C
2	A	619	C
2	A	620	G
2	A	635	G

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Mol	Chain	Res	Type
2	A	636	U
2	A	637	G
2	A	638	U
2	A	639	C
2	A	640	G
2	A	641	U
2	A	642	G
2	A	644	G
2	A	655	G
2	A	665	G
2	A	667	A
2	A	679	G
2	A	684	G
2	A	685	G
2	A	696	A
2	A	701	A
2	A	706	G
2	A	707	G
2	A	708	G
2	A	721	A
2	A	731	A
2	A	739	U
2	A	747	A
2	A	757	G
2	A	758	A
2	A	760	U
2	A	764	U
2	A	765	G
2	A	766	G
2	A	768	G
2	A	801	U
2	A	838	G
2	A	839	U
2	A	845	C
2	A	862	U
2	A	872	G
2	A	879	A
2	A	880	G
2	A	890	G
2	A	891	G
2	A	897	A
2	A	899	G

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Mol	Chain	Res	Type
2	A	900	G
2	A	919	A
2	A	920	G
2	A	927	C
2	A	942	U
2	A	960	G
2	A	974	G
2	A	981	U
2	A	982	A
2	A	1001	C
2	A	1002	C
2	A	1003	A
2	A	1004	C
2	A	1005	A
2	A	1007	G
2	A	1012	C
2	A	1025	A
2	A	1046	C
2	A	1047	A
2	A	1048	A
2	A	1049	G
2	A	1063	G
2	A	1076	A
2	A	1078	G
2	A	1085	G
2	A	1092	G
2	A	1101	A
2	A	1114	G
2	A	1130	C
2	A	1131	G
2	A	1140	G
2	A	1144	A
2	A	1151	U
2	A	1164	A
2	A	1165	G
2	A	1184	U
2	A	1185	A
2	A	1186	G
2	A	1187	A
2	A	1188	A
2	A	1191	A
2	A	1192	G

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Mol	Chain	Res	Type
2	A	1197	C
2	A	1202	A
2	A	1203	A
2	A	1206	A
2	A	1207	G
2	A	1208	U
2	A	1209	G
2	A	1212	U
2	A	1213	A
2	A	1230	G
2	A	1232	G
2	A	1233	A
2	A	1238	G
2	A	1246	A
2	A	1247	A
2	A	1250	U
2	A	1251	A
2	A	1253	C
2	A	1260	C
2	A	1261	A
2	A	1290	C
2	A	1292	U
2	A	1293	G
2	A	1325	U
2	A	1344	A
2	A	1345	G
2	A	1353	G
2	A	1368	A
2	A	1369	A
2	A	1371	G
2	A	1386	G
2	A	1387	A
2	A	1389	U
2	A	1415	A
2	A	1416	A
2	A	1436	C
2	A	1447	G
2	A	1448	C
2	A	1465	C
2	A	1467	U
2	A	1480	A
2	A	1494	U

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Mol	Chain	Res	Type
2	A	1499	A
2	A	1522	G
2	A	1530	G
2	A	1533	U
2	A	1537	U
2	A	1538	G
2	A	1540	U
2	A	1541	G
2	A	1542	A
2	A	1550	G
2	A	1551	U
2	A	1552	A
2	A	1553	C
2	A	1564	A
2	A	1565	A
2	A	1625	G
2	A	1629	G
2	A	1630	U
2	A	1632	G
2	A	1636	A
2	A	1637	G
2	A	1640	A
2	A	1641	U
2	A	1648	A
2	A	1649	C
2	A	1676	G
2	A	1679	A
2	A	1680	A
2	A	1681	U
2	A	1688	G
2	A	1703	G
2	A	1710	A
2	A	1714	A
2	A	1716	A
2	A	1717	U
2	A	1728	U
2	A	1730	U
2	A	1731	A
2	A	1737	A
2	A	1746	G
2	A	1754	G
2	A	1758	G

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Mol	Chain	Res	Type
2	A	1767	U
2	A	1768	C
2	A	1769	G
2	A	1789	A
2	A	1798	U
2	A	1803	A
2	A	1826	A
2	A	1827	A
2	A	1834	A
2	A	1845	G
2	A	1864	U
2	A	1866	C
2	A	1871	G
2	A	1872	A
2	A	1892	G
2	A	1946	U
2	A	1947	U
2	A	1948	A
2	A	1949	C
2	A	1950	G
2	A	1973	C
2	A	1981	U
2	A	1990	A
2	A	1999	U
2	A	2008	A
2	A	2017	C
2	A	2018	G
2	A	2026	A
2	A	2033	U
2	A	2046	A
2	A	2065	A
2	A	2073	A
2	A	2074	G
2	A	2075	G
2	A	2086	U
2	A	2088	C
2	A	2089	C
2	A	2091	U
2	A	2092	U
2	A	2093	G
2	A	2094	G
2	A	2095	G

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Mol	Chain	Res	Type
2	A	2107	G
2	A	2111	U
2	A	2112	U
2	A	2130	G
2	A	2138	C
2	A	2153	G
2	A	2154	G
2	A	2161	A
2	A	2162	A
2	A	2179	U
2	A	2190	A
2	A	2191	C
2	A	2194	A
2	A	2195	U
2	A	2196	G
2	A	2215	U
2	A	2217	U
2	A	2221	A
2	A	2243	C
2	A	2244	A
2	A	2247	A
2	A	2255	A
2	A	2256	G
2	A	2257	A
2	A	2267	C
2	A	2279	C
2	A	2280	G
2	A	2284	A
2	A	2285	G
2	A	2299	C
2	A	2320	C
2	A	2325	U
2	A	2329	G
2	A	2334	U
2	A	2335	G
2	A	2336	U
2	A	2338	G
2	A	2339	G
2	A	2340	A
2	A	2341	U
2	A	2342	A
2	A	2343	G

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Mol	Chain	Res	Type
2	A	2346	G
2	A	2349	A
2	A	2351	A
2	A	2354	G
2	A	2355	U
2	A	2356	G
2	A	2357	A
2	A	2368	C
2	A	2371	G
2	A	2382	G
2	A	2383	U
2	A	2384	C
2	A	2386	U
2	A	2387	U
2	A	2388	G
2	A	2390	U
2	A	2391	G
2	A	2392	A
2	A	2393	A
2	A	2394	A
2	A	2395	U
2	A	2396	A
2	A	2400	C
2	A	2401	U
2	A	2402	C
2	A	2407	C
2	A	2408	G
2	A	2409	U
2	A	2410	A
2	A	2413	G
2	A	2421	A
2	A	2427	G
2	A	2434	A
2	A	2436	A
2	A	2437	U
2	A	2449	A
2	A	2454	G
2	A	2462	G
2	A	2463	G
2	A	2492	A
2	A	2507	C
2	A	2511	A

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Mol	Chain	Res	Type
2	A	2529	A
2	A	2532	G
2	A	2544	U
2	A	2545	G
2	A	2548	U
2	A	2549	G
2	A	2559	A
2	A	2571	C
2	A	2574	C
2	A	2581	G
2	A	2582	A
2	A	2607	G
2	A	2609	A
2	A	2613	G
2	A	2630	A
2	A	2639	G
2	A	2647	U
2	A	2649	A
2	A	2653	G
2	A	2654	A
2	A	2659	A
2	A	2665	C
2	A	2672	A
2	A	2694	G
2	A	2698	C
2	A	2700	A
2	A	2705	G
2	A	2726	G
2	A	2729	G
2	A	2730	U
2	A	2742	A
2	A	2744	C
2	A	2753	G
2	A	2778	U
2	A	2790	A
2	A	2791	G
2	A	2797	C
2	A	2809	U
2	A	2826	A
2	A	2827	G
2	A	2833	U
2	A	2835	U

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Mol	Chain	Res	Type
2	A	2837	U
2	A	2853	C
2	A	2865	G
2	A	2913	U
2	A	2915	C
2	A	2926	A
2	A	2936	C
2	A	2938	G
2	A	2957	A
2	A	2958	C
2	A	2968	G
2	A	2972	A
2	A	2982	A
2	A	3002	A
2	A	3009	U
2	A	3014	A
2	A	3016	C
2	A	3021	A
2	A	3023	G
2	A	3024	A
2	A	3042	A
2	A	3082	U
2	A	3088	C
2	A	3093	A
2	A	3104	A
2	A	3106	C
2	A	3114	A
2	A	3115	A
3	B	4	A
3	B	9	G
3	B	11	U
3	B	12	C
3	B	13	C
3	B	46	A
3	B	57	U
3	B	58	A
3	B	87	U
3	B	88	C
3	B	89	C
3	B	107	A
4	BA	7	U
4	BA	8	U

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Mol	Chain	Res	Type
4	BA	9	U
4	BA	11	G
4	BA	12	A
4	BA	13	G
4	BA	36	A
4	BA	43	G
4	BA	51	C
4	BA	52	U
4	BA	53	U
4	BA	54	A
4	BA	55	A
4	BA	58	C
4	BA	59	A
4	BA	68	G
4	BA	77	G
4	BA	81	C
4	BA	82	U
4	BA	84	U
4	BA	85	C
4	BA	86	G
4	BA	87	G
4	BA	92	A
4	BA	93	C
4	BA	116	A
4	BA	117	C
4	BA	128	U
4	BA	143	G
4	BA	146	A
4	BA	160	C
4	BA	170	U
4	BA	179	C
4	BA	180	A
4	BA	193	C
4	BA	196	G
4	BA	200	U
4	BA	211	A
4	BA	217	U
4	BA	218	G
4	BA	220	G
4	BA	243	A
4	BA	245	C
4	BA	247	G

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Mol	Chain	Res	Type
4	BA	251	G
4	BA	252	U
4	BA	266	G
4	BA	267	C
4	BA	279	A
4	BA	280	C
4	BA	281	G
4	BA	289	G
4	BA	301	G
4	BA	329	A
4	BA	332	G
4	BA	344	A
4	BA	347	G
4	BA	348	G
4	BA	350	G
4	BA	351	G
4	BA	352	C
4	BA	353	A
4	BA	354	G
4	BA	367	U
4	BA	369	G
4	BA	370	C
4	BA	371	A
4	BA	372	C
4	BA	373	A
4	BA	397	A
4	BA	398	C
4	BA	406	G
4	BA	411	A
4	BA	412	U
4	BA	414	A
4	BA	421	U
4	BA	422	C
4	BA	423	G
4	BA	424	G
4	BA	429	U
4	BA	430	A
4	BA	433	C
4	BA	434	C
4	BA	438	U
4	BA	452	A
4	BA	453	G

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Mol	Chain	Res	Type
4	BA	456	C
4	BA	457	A
4	BA	458	A
4	BA	459	G
4	BA	461	G
4	BA	465	G
4	BA	466	U
4	BA	486	G
4	BA	491	C
4	BA	496	U
4	BA	497	G
4	BA	498	C
4	BA	499	C
4	BA	507	G
4	BA	509	G
4	BA	511	U
4	BA	512	A
4	BA	513	A
4	BA	515	A
4	BA	516	C
4	BA	527	A
4	BA	539	A
4	BA	542	U
4	BA	552	A
4	BA	553	A
4	BA	556	A
4	BA	557	G
4	BA	568	G
4	BA	587	A
4	BA	599	U
4	BA	612	U
4	BA	613	G
4	BA	633	A
4	BA	645	G
4	BA	666	U
4	BA	668	G
4	BA	680	G
4	BA	683	G
4	BA	701	G
4	BA	702	G
4	BA	703	U
4	BA	711	G

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Mol	Chain	Res	Type
4	BA	729	A
4	BA	735	G
4	BA	757	A
4	BA	765	G
4	BA	772	A
4	BA	773	U
4	BA	774	A
4	BA	779	G
4	BA	782	A
4	BA	794	A
4	BA	795	A
4	BA	797	C
4	BA	808	A
4	BA	812	G
4	BA	817	U
4	BA	818	U
4	BA	819	U
4	BA	821	C
4	BA	822	U
4	BA	823	U
4	BA	824	C
4	BA	825	C
4	BA	826	U
4	BA	827	U
4	BA	828	G
4	BA	841	U
4	BA	884	G
4	BA	895	A
4	BA	896	A
4	BA	908	G
4	BA	909	G
4	BA	914	C
4	BA	916	C
4	BA	940	A
4	BA	942	U
4	BA	943	U
4	BA	948	G
4	BA	950	A
4	BA	951	A
4	BA	953	G
4	BA	957	A
4	BA	959	A

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Mol	Chain	Res	Type
4	BA	971	G
4	BA	973	U
4	BA	974	U
4	BA	975	G
4	BA	984	A
4	BA	985	G
4	BA	986	G
4	BA	989	G
4	BA	991	C
4	BA	992	G
4	BA	1000	U
4	BA	1003	C
4	BA	1010	C
4	BA	1011	U
4	BA	1012	U
4	BA	1013	G
4	BA	1014	U
4	BA	1020	G
4	BA	1022	G
4	BA	1028	G
4	BA	1030	G
4	BA	1033	G
4	BA	1045	U
4	BA	1048	G
4	BA	1065	U
4	BA	1074	G
4	BA	1075	U
4	BA	1081	A
4	BA	1105	U
4	BA	1110	A
4	BA	1116	U
4	BA	1117	U
4	BA	1118	A
4	BA	1119	U
4	BA	1120	G
4	BA	1124	G
4	BA	1129	U
4	BA	1138	A
4	BA	1141	G
4	BA	1147	G
4	BA	1149	C
4	BA	1150	A

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Mol	Chain	Res	Type
4	BA	1162	G
4	BA	1164	U
4	BA	1165	G
4	BA	1171	G
4	BA	1177	A
4	BA	1178	A
4	BA	1193	U
4	BA	1194	A
4	BA	1238	U
4	BA	1239	G
4	BA	1241	G
4	BA	1250	A
4	BA	1251	G
4	BA	1260	A
4	BA	1261	A
4	BA	1262	U
4	BA	1266	U
4	BA	1267	U
4	BA	1268	C
4	BA	1282	G
4	BA	1284	U
4	BA	1287	G
4	BA	1301	A
4	BA	1302	C
4	BA	1319	G
4	BA	1320	G
4	BA	1322	G
4	BA	1328	A
4	BA	1329	G
4	BA	1335	G
4	BA	1343	G
4	BA	1344	C
4	BA	1346	A
4	BA	1347	C
4	BA	1353	G
4	BA	1357	A
4	BA	1362	G
4	BA	1425	G
4	BA	1426	C
4	BA	1429	A
4	BA	1430	A
4	BA	1431	C

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Mol	Chain	Res	Type
4	BA	1433	C
4	BA	1434	U
4	BA	1435	U
4	BA	1436	G
4	BA	1438	G
4	BA	1459	G
4	BA	1463	G
4	BA	1476	A
4	BA	1481	G
4	BA	1487	A
4	BA	1488	G
4	BA	1490	U
4	BA	1501	G
4	BA	1513	G
4	BA	1514	G
4	BA	1515	A
4	BA	1516	U
25	BW	7	A
25	BW	8	U
25	BW	17	C
25	BW	18	G
25	BW	19	G
25	BW	20	U
25	BW	21	A
25	BW	22	G
25	BW	47	U
25	BW	48	C
25	BW	52	G
25	BW	61	C
25	BW	76	A

All (97) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	9	U
2	A	31	U
2	A	89	A
2	A	97	U
2	A	99	G
2	A	195	A
2	A	198	A
2	A	227	A

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Mol	Chain	Res	Type
2	A	293	G
2	A	316	U
2	A	317	G
2	A	357	U
2	A	358	G
2	A	363	A
2	A	452	G
2	A	498	G
2	A	499	G
2	A	534	G
2	A	590	A
2	A	666	A
2	A	707	G
2	A	759	G
2	A	879	A
2	A	899	G
2	A	919	A
2	A	981	U
2	A	1003	A
2	A	1004	C
2	A	1046	C
2	A	1102	G
2	A	1163	A
2	A	1164	A
2	A	1186	G
2	A	1207	G
2	A	1231	U
2	A	1246	A
2	A	1368	A
2	A	1447	G
2	A	1511	U
2	A	1537	U
2	A	1541	G
2	A	1564	A
2	A	1629	G
2	A	1730	U
2	A	1757	U
2	A	1826	A
2	A	1947	U
2	A	2064	A
2	A	2073	A
2	A	2075	G

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Mol	Chain	Res	Type
2	A	2085	C
2	A	2088	C
2	A	2094	G
2	A	2153	G
2	A	2162	A
2	A	2243	C
2	A	2350	G
2	A	2381	A
2	A	2436	A
2	A	2548	U
2	A	2581	G
2	A	2826	A
2	A	3113	A
3	B	10	G
3	B	11	U
3	B	87	U
3	B	88	C
3	B	106	C
4	BA	85	C
4	BA	251	G
4	BA	280	C
4	BA	350	G
4	BA	422	C
4	BA	429	U
4	BA	457	A
4	BA	485	G
4	BA	498	C
4	BA	515	A
4	BA	542	U
4	BA	825	C
4	BA	827	U
4	BA	895	A
4	BA	975	G
4	BA	985	G
4	BA	1011	U
4	BA	1109	C
4	BA	1116	U
4	BA	1117	U
4	BA	1149	C
4	BA	1171	G
4	BA	1177	A
4	BA	1261	A

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Mol	Chain	Res	Type
4	BA	1266	U
4	BA	1301	A
4	BA	1430	A
25	BW	7	A
25	BW	21	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 354 ligands modelled in this entry, 353 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	A1BWO	A	4251	58	30,30,30	2.66	15 (50%)	40,44,44	2.99	13 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	A1BWO	A	4251	58	-	0/15/39/39	0/2/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	A	4251	A1BWO	C06-C07	5.61	1.59	1.51
59	A	4251	A1BWO	C26-N09	5.31	1.42	1.36
59	A	4251	A1BWO	C21-S18	-4.50	1.72	1.76
59	A	4251	A1BWO	C03-N05	3.73	1.42	1.34
59	A	4251	A1BWO	C17-S18	-3.55	1.73	1.76
59	A	4251	A1BWO	C16-N15	3.47	1.52	1.46
59	A	4251	A1BWO	O02-C03	3.29	1.39	1.34
59	A	4251	A1BWO	C11-C12	3.24	1.43	1.37
59	A	4251	A1BWO	O28-C26	3.17	1.40	1.35
59	A	4251	A1BWO	C22-N15	3.09	1.52	1.46
59	A	4251	A1BWO	O28-C07	-2.98	1.41	1.46
59	A	4251	A1BWO	C25-C23	2.97	1.42	1.37
59	A	4251	A1BWO	C08-C07	2.32	1.56	1.52
59	A	4251	A1BWO	C14-C12	2.29	1.44	1.39
59	A	4251	A1BWO	C14-N15	2.18	1.47	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	A	4251	A1BWO	O02-C03-N05	9.18	120.62	110.91
59	A	4251	A1BWO	C08-N09-C26	-8.64	104.78	111.17
59	A	4251	A1BWO	C07-C08-N09	7.38	108.82	101.85
59	A	4251	A1BWO	C10-N09-C26	5.04	131.26	125.98
59	A	4251	A1BWO	O02-C03-O04	-4.70	117.77	124.62
59	A	4251	A1BWO	O28-C07-C08	-3.92	100.70	104.50
59	A	4251	A1BWO	C07-O28-C26	3.15	112.62	110.10
59	A	4251	A1BWO	O28-C07-C06	2.97	112.49	109.13
59	A	4251	A1BWO	C10-C11-C12	2.84	122.02	118.86
59	A	4251	A1BWO	O04-C03-N05	-2.21	121.61	124.93
59	A	4251	A1BWO	C01-O02-C03	2.15	118.12	115.63
59	A	4251	A1BWO	C10-C25-C23	2.10	121.20	118.86
59	A	4251	A1BWO	C23-C14-C12	-2.01	112.38	116.03

There are no chirality outliers.

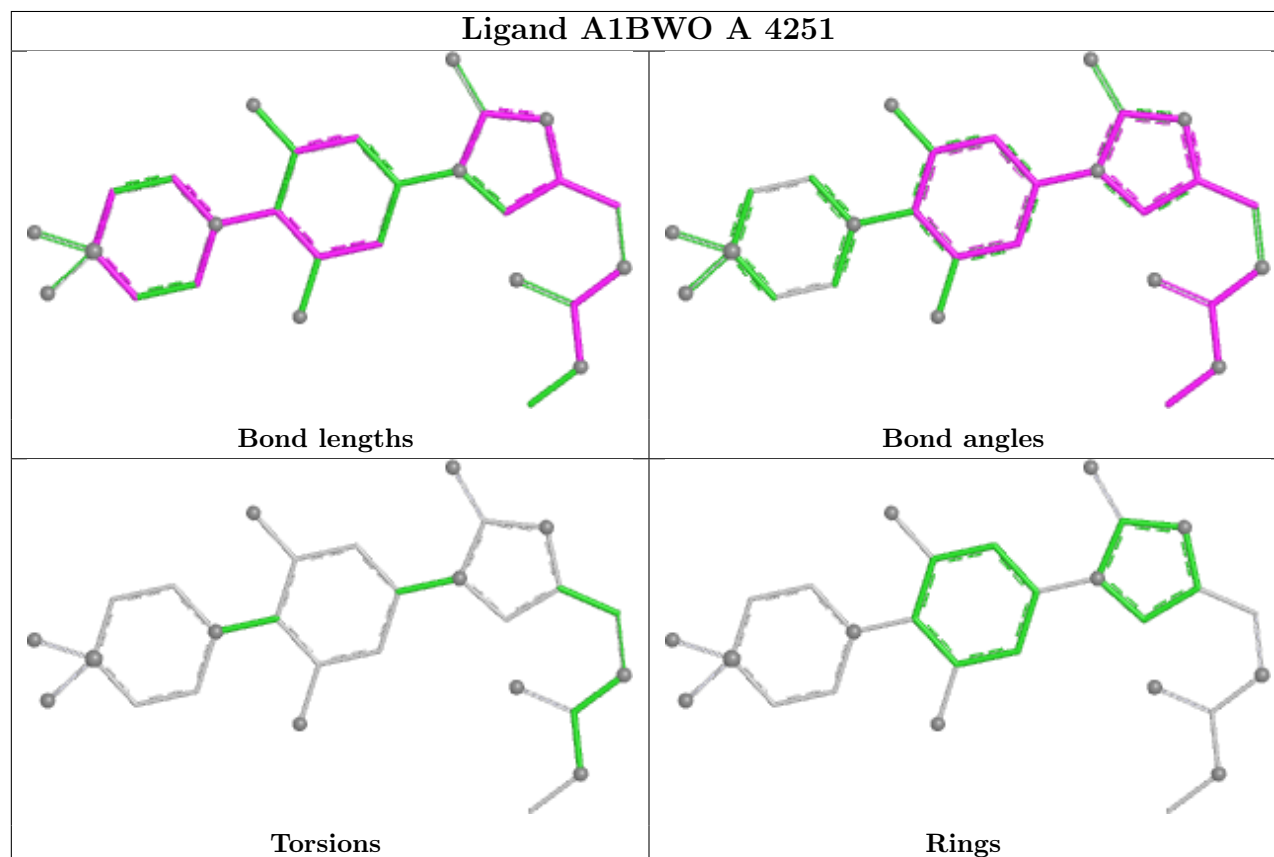
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

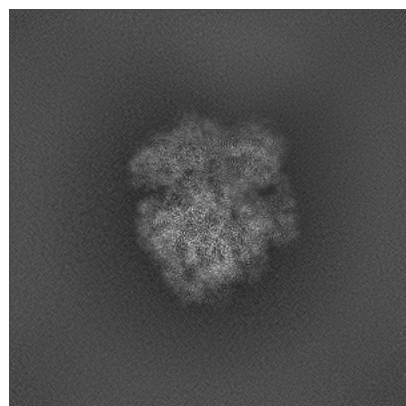
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49038. These allow visual inspection of the internal detail of the map and identification of artifacts.

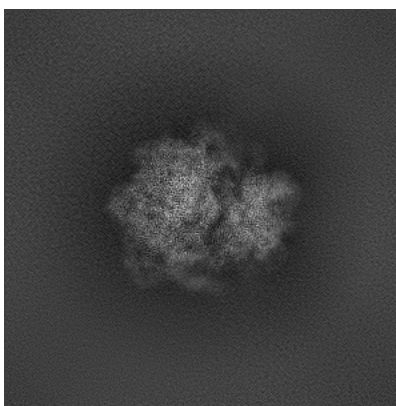
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

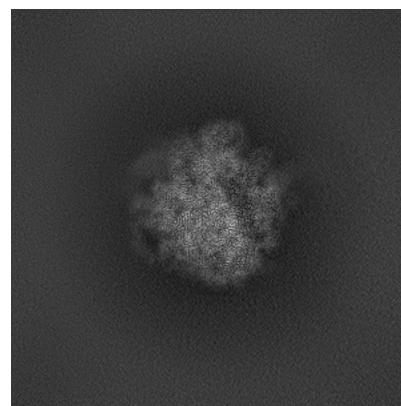
6.1.1 Primary map



X

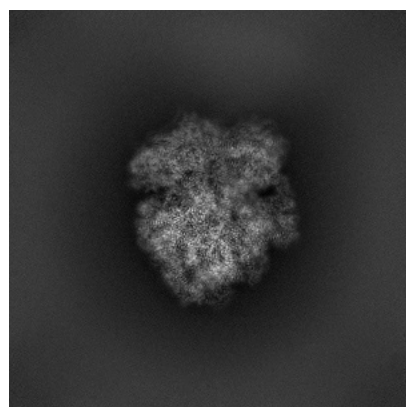


Y

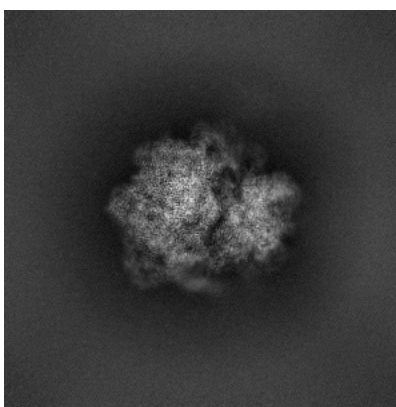


Z

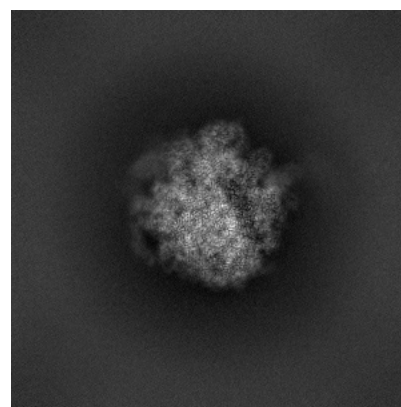
6.1.2 Raw map



X



Y

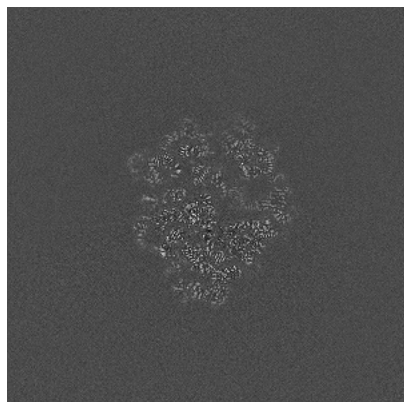


Z

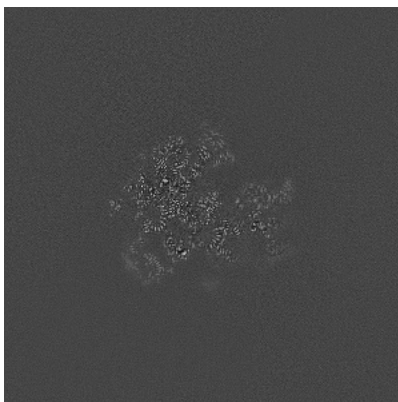
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

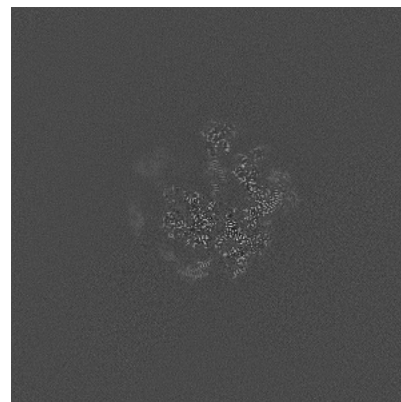
6.2.1 Primary map



X Index: 320

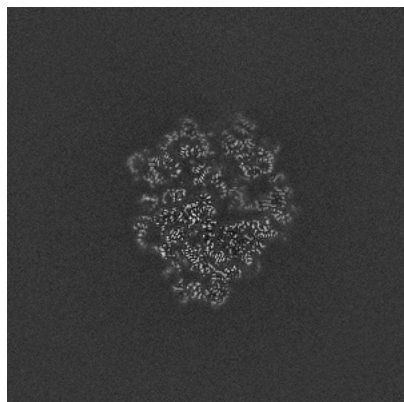


Y Index: 320

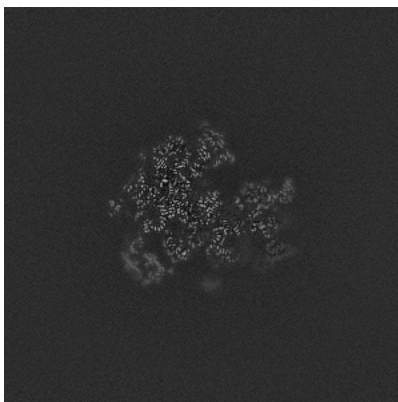


Z Index: 320

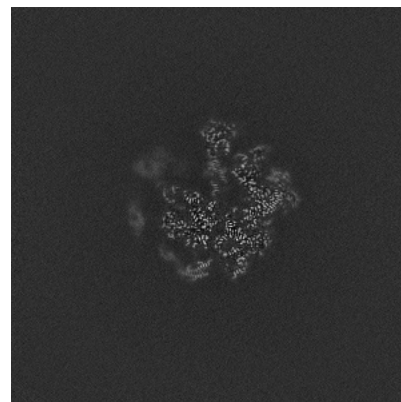
6.2.2 Raw map



X Index: 320



Y Index: 320

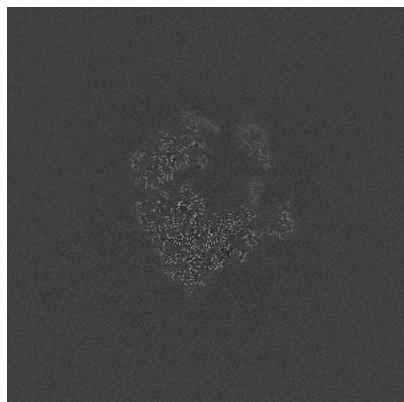


Z Index: 320

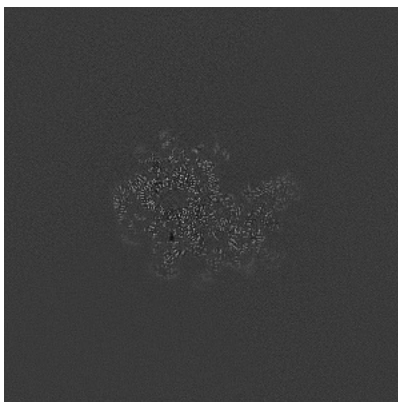
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

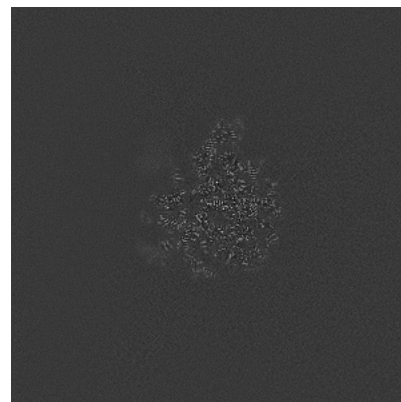
6.3.1 Primary map



X Index: 356

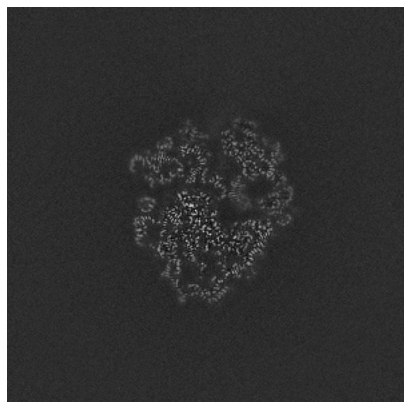


Y Index: 300

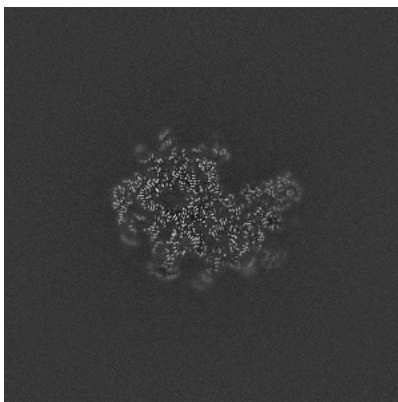


Z Index: 275

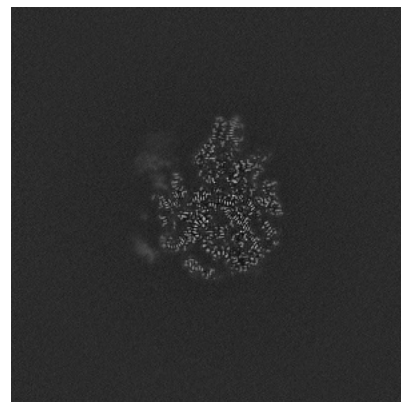
6.3.2 Raw map



X Index: 315



Y Index: 299

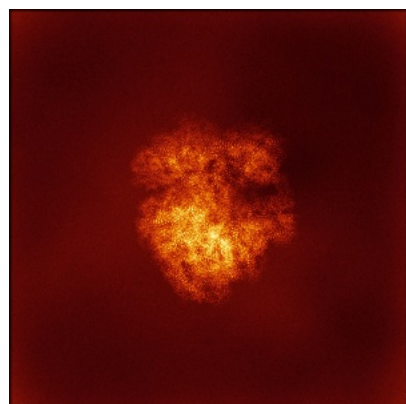


Z Index: 281

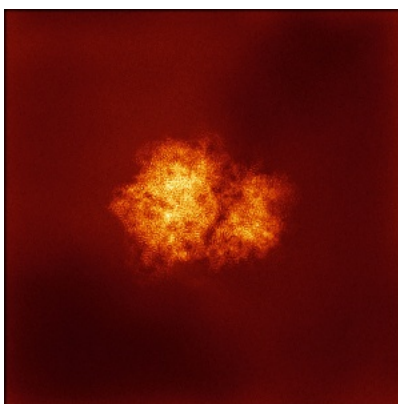
The images above show the largest variance slices of the map in three orthogonal directions.

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

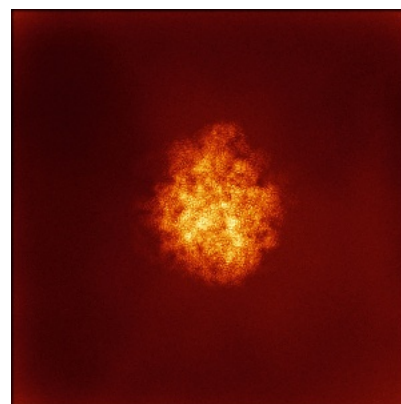
6.4.1 Primary map



X

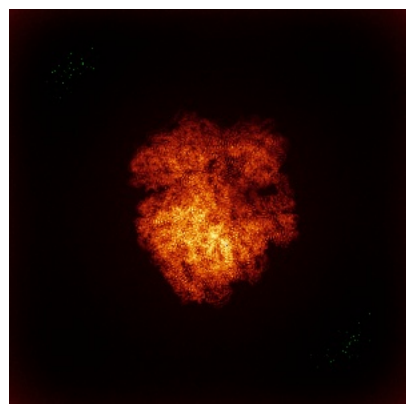


Y

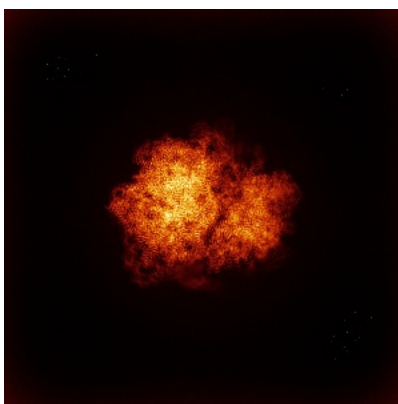


Z

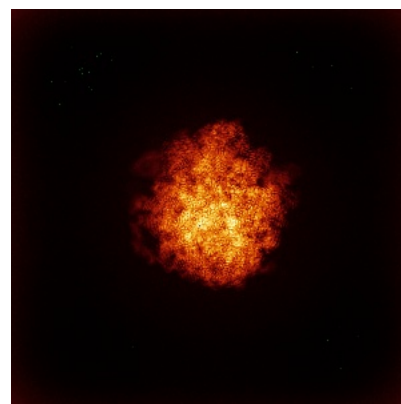
6.4.2 Raw map



X



Y

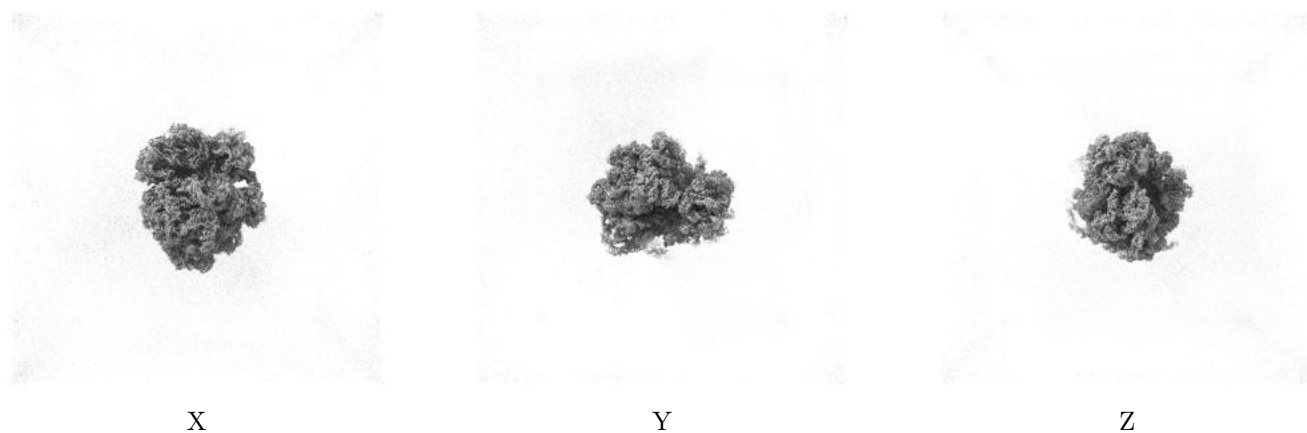


Z

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

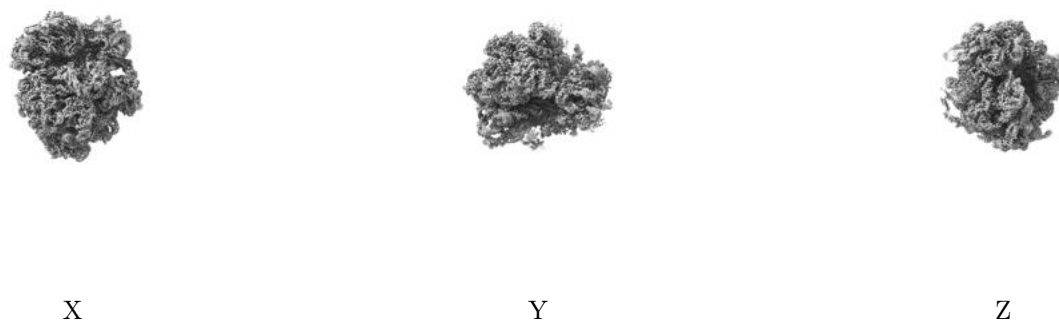
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

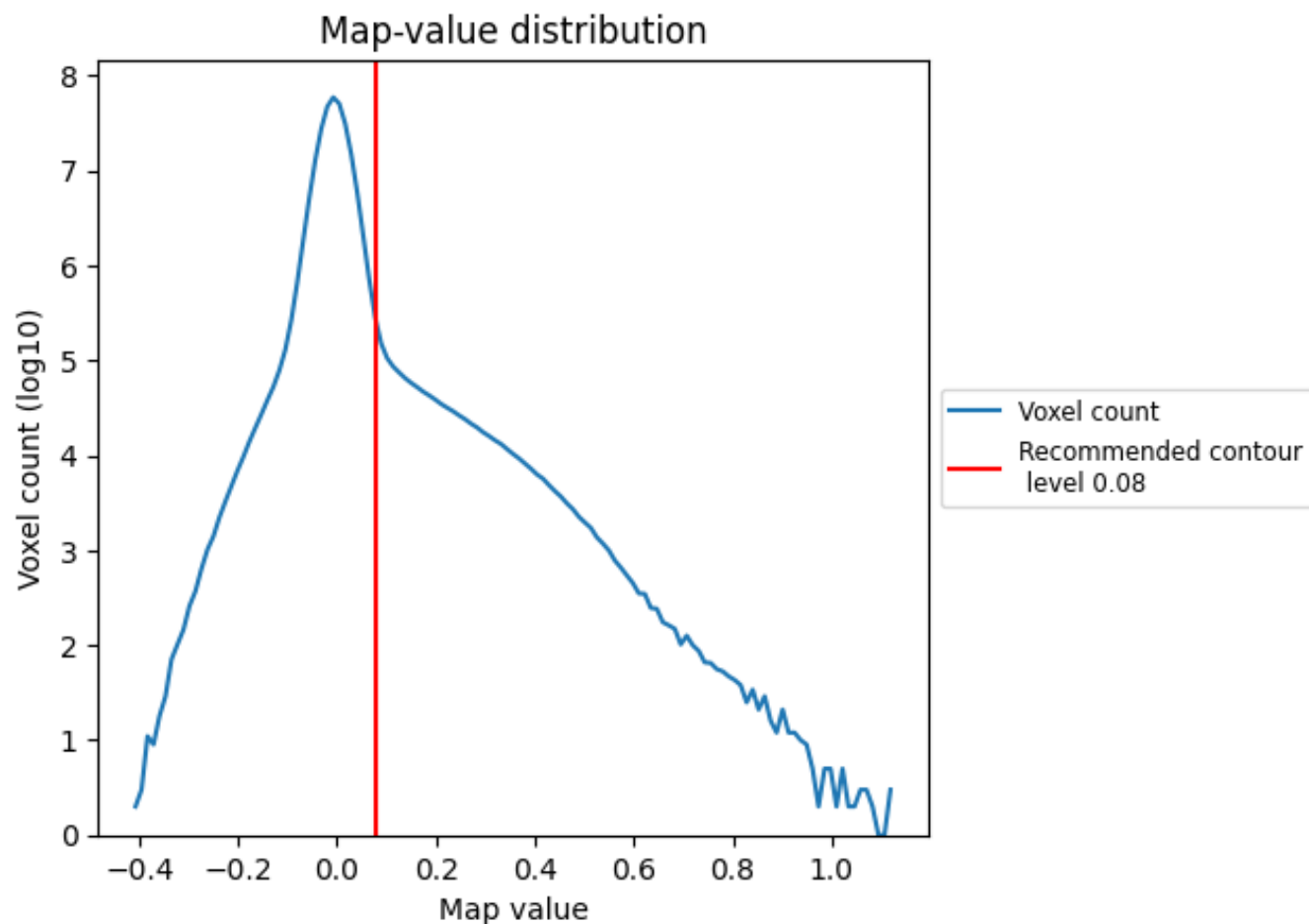
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

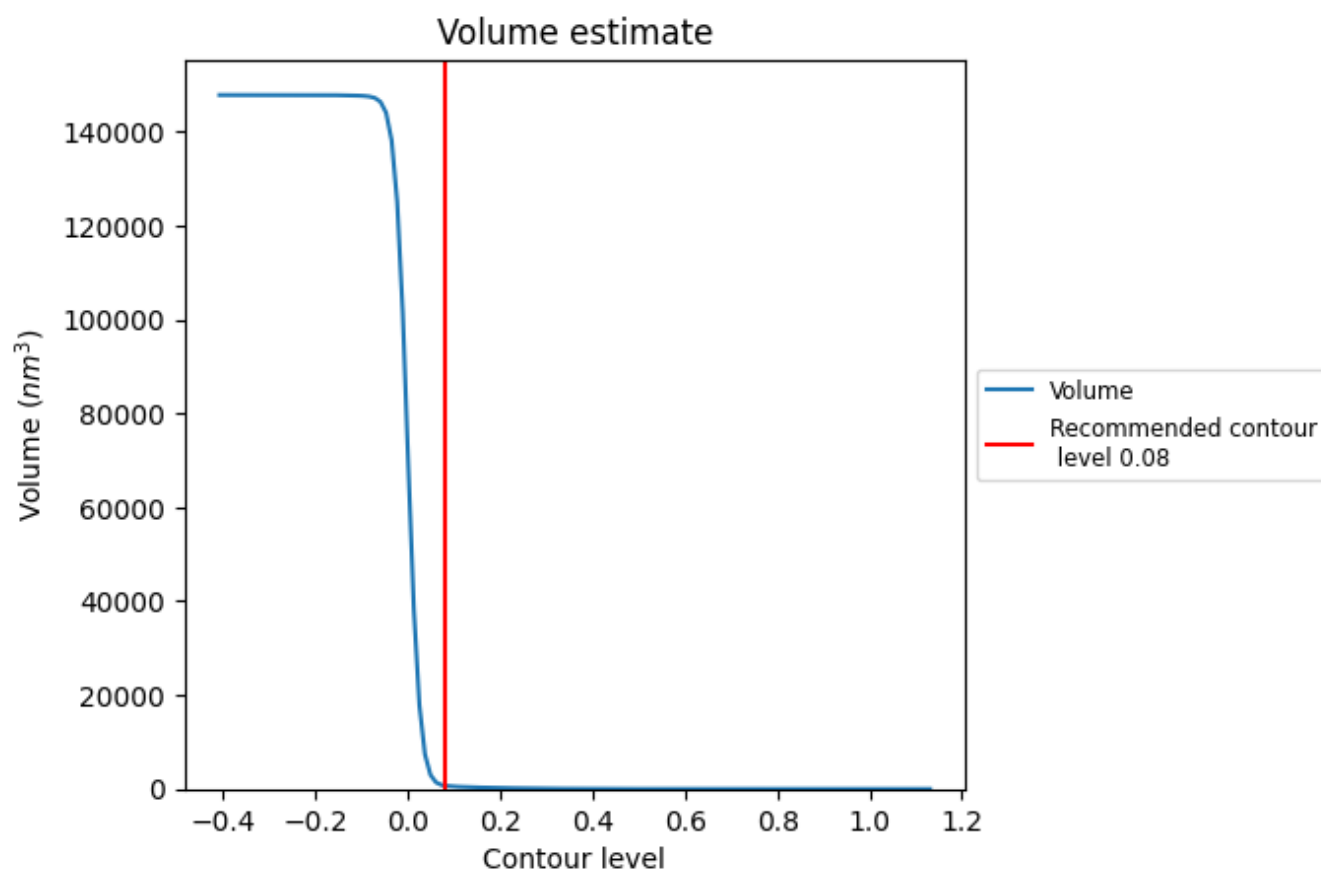
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

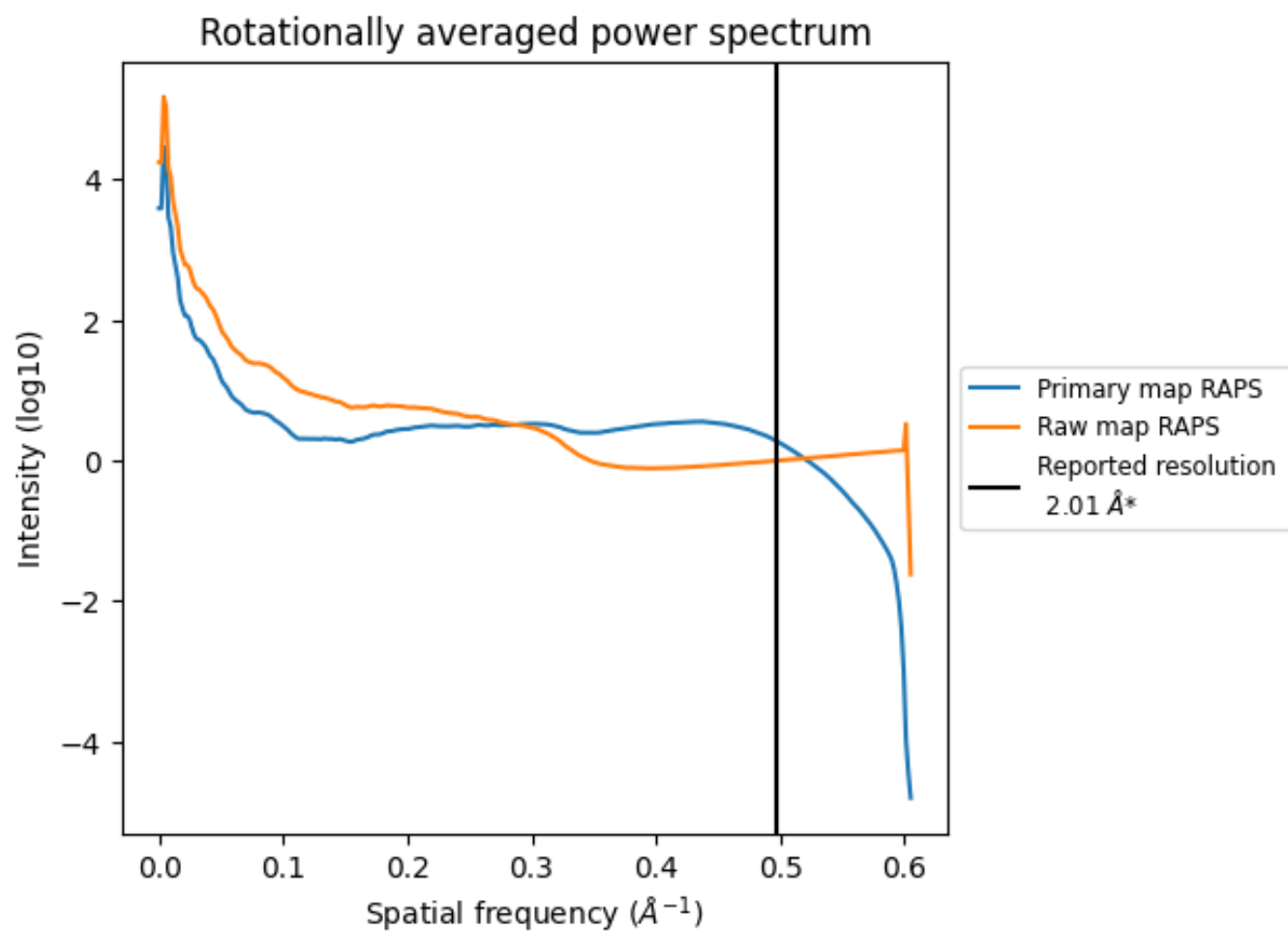
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 733 nm^3 ; this corresponds to an approximate mass of 662 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 ⓘ

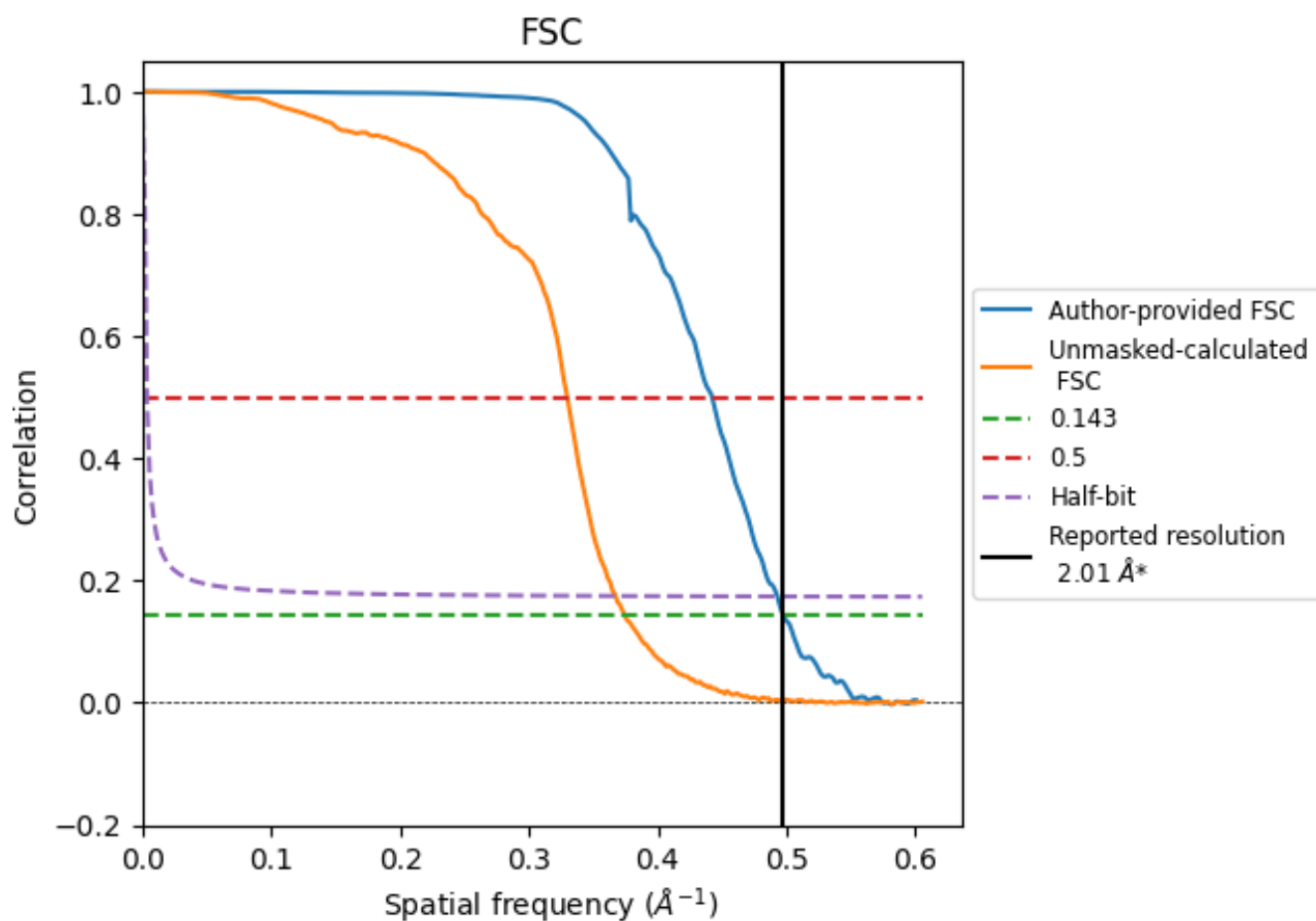


*Reported resolution corresponds to spatial frequency of 0.498 $\text{\AA}^{-1}$

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 0.498 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

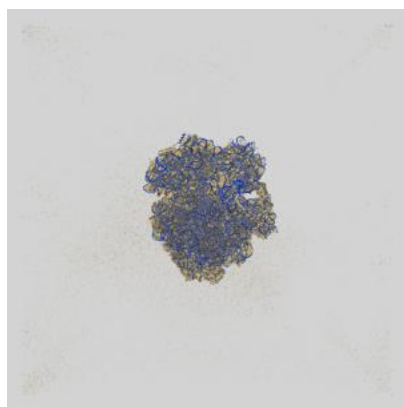
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.01	-	-
Author-provided FSC curve	2.01	2.26	2.03
Unmasked-calculated*	2.67	3.03	2.72

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.67 differs from the reported value 2.01 by more than 10 %

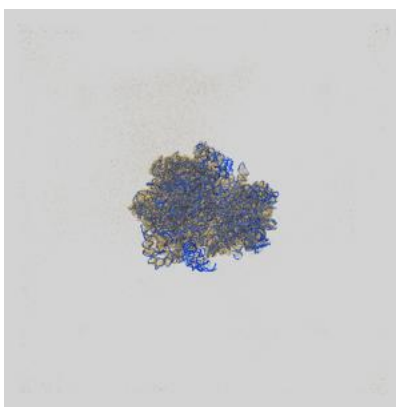
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49038 and PDB model 9N5T. Per-residue inclusion information can be found in section [3](#) on page [19](#).

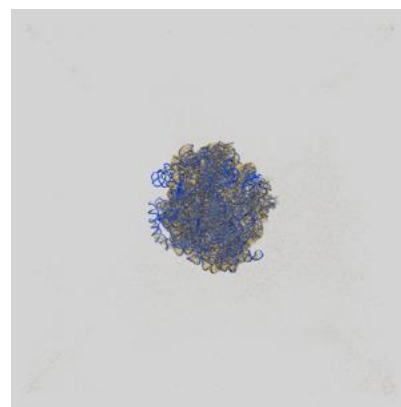
9.1 Map-model overlay [i](#)



X



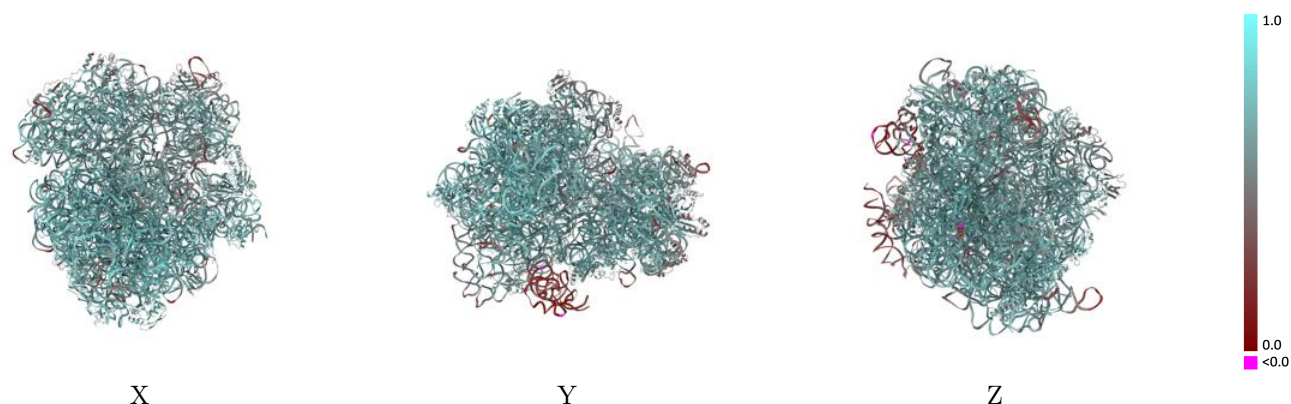
Y



Z

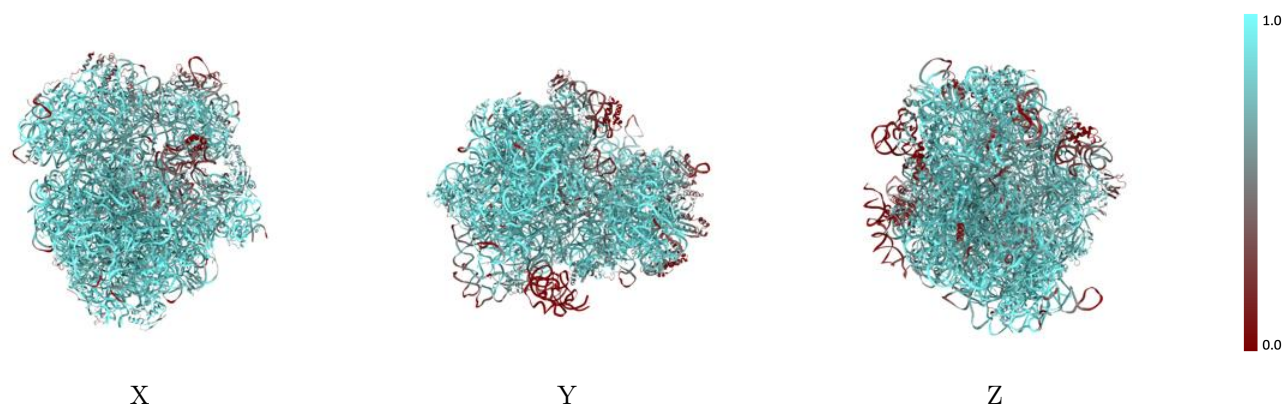
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



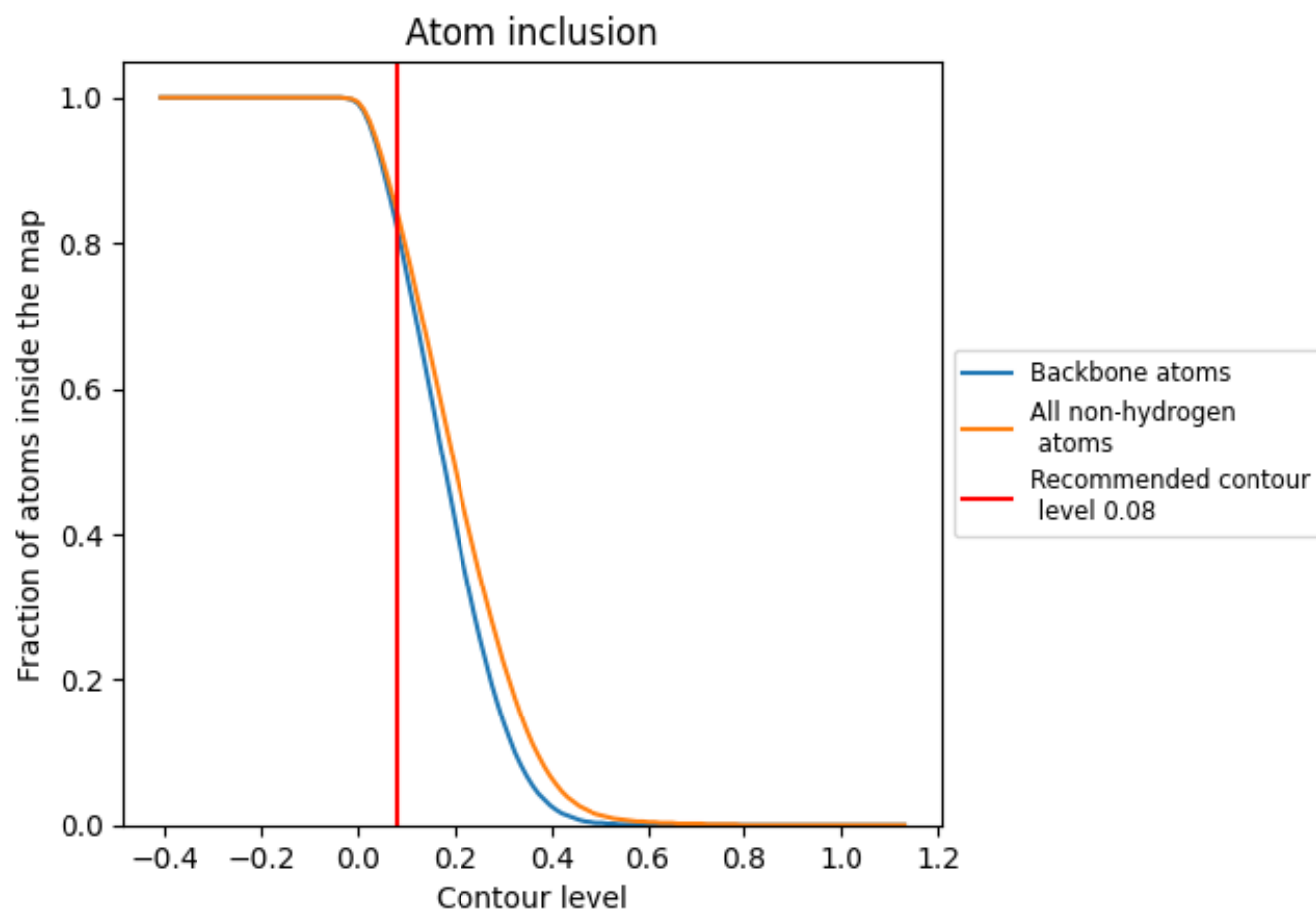
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8470	 0.6730
3	 0.9220	 0.7530
A	 0.8720	 0.6870
B	 0.9110	 0.6770
BA	 0.9000	 0.6700
BB	 0.5970	 0.6240
BC	 0.6980	 0.5980
BD	 0.6600	 0.5880
BE	 0.7940	 0.6440
BF	 0.7170	 0.6160
BG	 0.7470	 0.6250
BH	 0.8690	 0.6860
BI	 0.8010	 0.6410
BJ	 0.6380	 0.5670
BK	 0.8250	 0.6460
BL	 0.7680	 0.6390
BM	 0.7900	 0.6310
BN	 0.9090	 0.6890
BO	 0.8200	 0.6650
BP	 0.7680	 0.6410
BQ	 0.7260	 0.6140
BR	 0.7670	 0.6220
BS	 0.7470	 0.6140
BT	 0.8100	 0.6530
BV	 0.2740	 0.4890
BW	 0.6800	 0.5830
C	 0.9330	 0.7450
D	 0.9130	 0.7350
E	 0.8930	 0.7230
F	 0.7990	 0.6370
G	 0.5800	 0.5480
H	 0.5870	 0.5660
I	 0.8560	 0.6690
J	 0.0140	 0.4800
K	 0.9280	 0.7320



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Chain	Atom inclusion	Q-score
L	 0.8690	 0.7180
M	 0.8910	 0.7080
N	 0.9000	 0.7210
O	 0.9390	 0.7560
P	 0.8850	 0.6840
Q	 0.8510	 0.7000
R	 0.9480	 0.7680
S	 0.9030	 0.7160
T	 0.9170	 0.7470
U	 0.8230	 0.6790
V	 0.7080	 0.6010
W	 0.6560	 0.5990
X	 0.9240	 0.7450
Y	 0.8920	 0.7170
Z	 0.8180	 0.6610
a	 0.9130	 0.7440
b	 0.8860	 0.7200
c	 0.9040	 0.7270
d	 0.9400	 0.7580
e	 0.9610	 0.7670
f	 0.8960	 0.6970
g	 0.6720	 0.5950
s	 0.2500	 0.4800