



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 06:25 AM UTC

PDB ID : 8P2F / pdb_00008p2f
EMDB ID : EMD-17363
Title : Staphylococcus aureus 70S ribosome with elongation factor G locked with fusidic acid cyclopentane in post-translocational state
Authors : Gonzalez-Lopez, A.; Selmer, M.
Deposited on : 2023-05-16
Resolution : 2.44 Å (reported)
Based on initial models : 2XEX, 7SSD, 7K00, 7NHM

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:

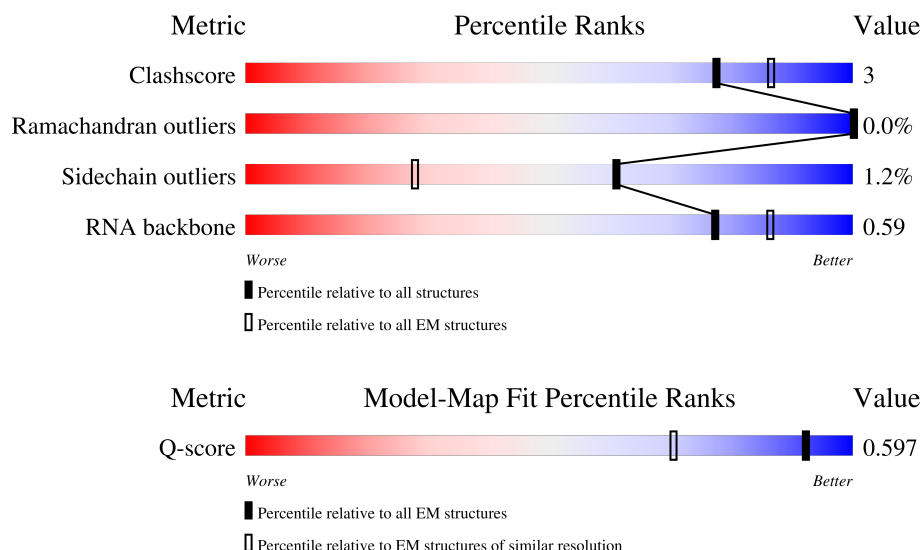
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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

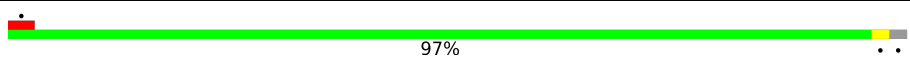
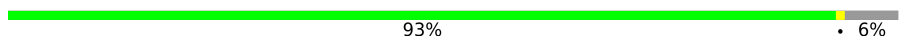
The reported resolution of this entry is 2.44 Å.

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	5856 (1.94 - 2.94)

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	1	62	 97%
2	2	69	 93% 6%
3	3	59	 90% 5% 5%

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Mol	Chain	Length	Quality of chain
4	4	84	
5	5	57	
6	6	49	
7	7	45	
8	8	66	
9	9	37	
10	A	2923	
11	B	115	
12	D	77	
12	F	77	
13	E	693	
14	G	277	
15	H	220	
16	I	207	
17	J	179	
18	K	178	
19	M	145	
20	N	122	
21	O	146	
22	P	144	
23	Q	122	
24	R	119	
25	S	116	
26	T	118	
27	U	102	

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Mol	Chain	Length	Quality of chain
28	V	117	
29	W	91	
30	X	105	
31	Y	217	
32	Z	94	
33	a	1555	
34	b	24	
35	c	255	
36	d	217	
37	e	200	
38	f	166	
39	g	98	
40	h	156	
41	i	132	
42	j	132	
43	k	102	
44	l	129	
45	m	137	
46	n	121	
47	o	61	
48	p	89	
49	q	91	
50	r	87	
51	s	80	
52	t	92	

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Mol	Chain	Length	Quality of chain
53	u	83	7% 88% 7% . .

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 149413 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 L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	61	Total	C	N	O	S	0	0
			481	298	104	78	1		

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	65	Total	C	N	O	S	0	0
			535	329	100	105	1		

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	56	Total	C	N	O	0	0
			436	271	82	83		

- Molecule 4 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	80	Total	C	N	O	S	0	0
			654	417	111	123	3		

- Molecule 5 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	53	Total	C	N	O	S	0	0
			422	256	86	75	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	?	-	ARG	deletion	UNP Q2FZF1

- Molecule 6 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	48	Total	C	N	O	S	0	0
			402	245	79	73	5		

- Molecule 7 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 8 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 9 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

- Molecule 10 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	2844	Total	C	N	O	P	0	0
			60978	27229	11150	19755	2844		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	G	A	conflict	GB CP000253
A	1584	U	A	conflict	GB CP000253
A	2261	G	A	conflict	GB CP000253

- Molecule 11 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	113	Total	C	N	O	P	0	0
			2408	1076	431	788	113		

- Molecule 12 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		
12	F	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 13 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	670	Total	C	N	O	S	0	0
			5181	3250	869	1033	29		

- Molecule 14 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	273	Total	C	N	O	S	0	0
			2085	1297	413	370	5		

- Molecule 15 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	216	Total	C	N	O	S	0	0
			1637	1024	301	307	5		

- Molecule 16 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	204	Total	C	N	O	S	0	0
			1564	981	286	295	2		

- Molecule 17 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	176	Total	C	N	O	S	0	0
			1392	885	238	262	7		

- Molecule 18 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	176	Total	C	N	O	S	0	0
			1372	852	251	266	3		

- Molecule 19 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	144	Total	C	N	O	S	0	0
			1146	715	210	218	3		

- Molecule 20 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	122	Total	C	N	O	S	0	0
			920	572	174	170	4		

- Molecule 21 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	145	Total	C	N	O	S	0	0
			1090	674	214	201	1		

- Molecule 22 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	136	Total	C	N	O	S	0	0
			1089	698	206	181	4		

- Molecule 23 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	120	Total	C	N	O	S	0	0
			952	584	182	185	1		

- Molecule 24 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	119	Total	C	N	O	S	0	0
			922	574	174	173	1		

- Molecule 25 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	114	Total	C	N	O	S	0	0
			922	580	185	157			

- Molecule 26 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	116	Total	C	N	O	S	0	0
			943	593	189	157	4		

- Molecule 27 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	101	Total	C	N	O	S	0	0
			793	503	141	148	1		

- Molecule 28 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	111	Total	C	N	O	S	0	0
			853	532	163	155	3		

- Molecule 29 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	89	Total	C	N	O	S	0	0
			725	457	130	134	4		

- Molecule 30 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	102	Total	C	N	O	S	0	0
			787	497	144	144	2		

- Molecule 31 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	94	Total	C	N	O	S	0	0
			738	471	131	134	2		

- Molecule 32 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Z	84	Total	C	N	O	0	0
			637	392	124	121		

- Molecule 33 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	1526	Total	C	N	O	P	0	0
			32707	14608	5975	10598	1526		

- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	8	Total	C	N	O	P	0	0
			176	79	37	52	8		

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	221	Total	C	N	O	S	0	0
			1781	1136	310	328	7		

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	204	Total	C	N	O	S	0	0
			1612	1015	302	293	2		

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	199	Total	C	N	O	S	0	0
			1617	1020	302	293	2		

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	156	Total	C	N	O	S	0	0
			1160	730	213	215	2		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	93	Total	C	N	O	S	0	0
			773	489	136	146	2		

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	148	Total	C	N	O	S	0	0
			1180	734	226	216	4		

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	131	Total	C	N	O	S	0	0
			1032	652	183	193	4		

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	128	Total	C	N	O	S	0	0
			1016	629	203	183	1		

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	99	Total	C	N	O	S	0	0
			792	499	145	147	1		

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	118	Total	C	N	O	S	0	0
			876	542	166	165	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	113	Total	C	N	O	S	0	0
			902	554	179	168	1		

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	60	Total	C	N	O	S	0	0
			501	317	100	79	5		

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	86	Total	C	N	O	S	0	0
			721	445	148	127	1		

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	90	Total	C	N	O	S	0	0
			712	448	132	131	1		

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	80	Total	C	N	O	S	0	0
			662	419	120	122	1		

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	63	Total	C	N	O	S	0	0
			516	330	96	87	3		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	80	Total	C	N	O	S	0	0
			651	419	117	113	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	80	Total	C	N	O	S	0	0
			606	367	119	118	2		

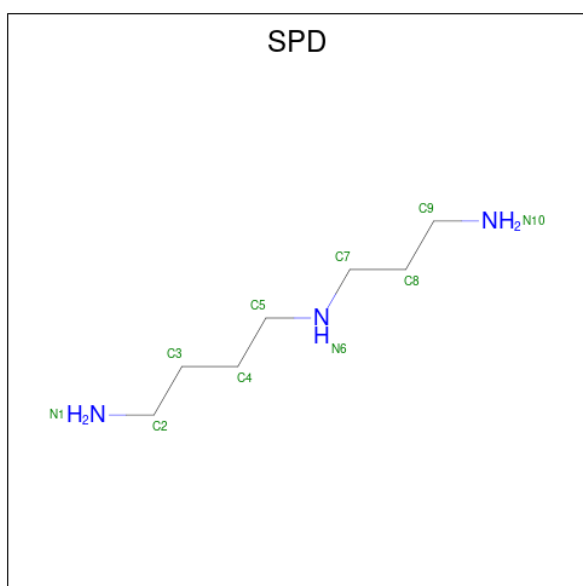
- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	5	1	Total	Zn	0
			1	1	
54	9	1	Total	Zn	0
			1	1	
54	o	1	Total	Zn	0
			1	1	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

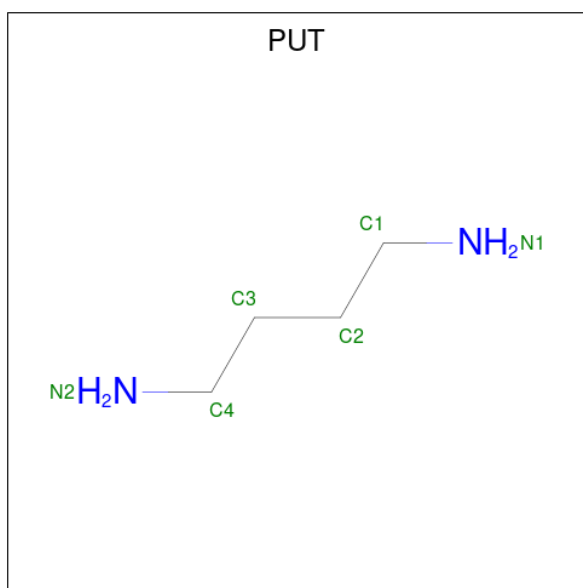
Mol	Chain	Residues	Atoms		AltConf
55	8	1	Total	Mg	0
			1	1	
55	A	131	Total	Mg	0
			131	131	
55	E	1	Total	Mg	0
			1	1	
55	F	2	Total	Mg	0
			2	2	
55	a	10	Total	Mg	0
			10	10	

- Molecule 56 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



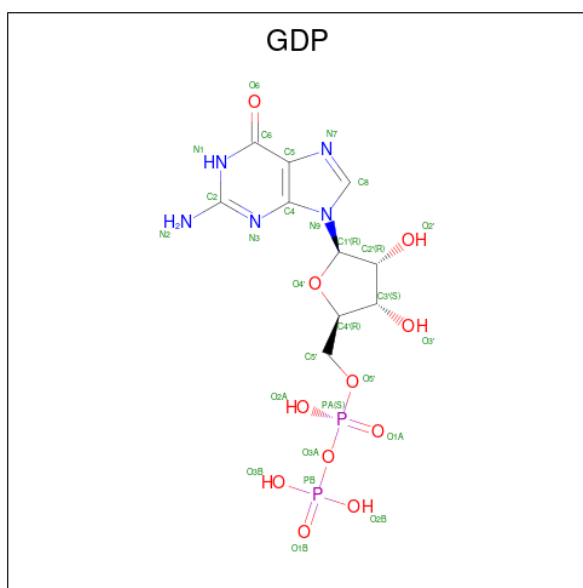
Mol	Chain	Residues	Atoms			AltConf
56	A	1	Total	C	N	0
			10	7	3	

- Molecule 57 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).

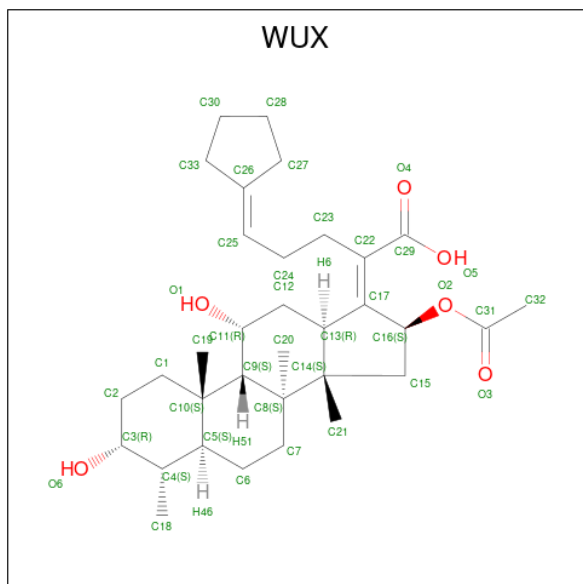


Mol	Chain	Residues	Atoms			AltConf
57	A	1	Total	C	N	0
			6	4	2	

- Molecule 58 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



acetyloxy-4,8,10,14-tetramethyl-3,11-bis(oxidanyl)-1,2,3,4,5,6,7,9,11,12,13,15,16,17-tetra decahydrocyclopenta[a]phenanthren-17-yl]-5-cyclopentyl-pentanoic acid (CCD ID: WUX) (formula: C₃₃H₅₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
59	E	1	Total	C	O	0
			39	33	6	

- Molecule 60 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
60	P	1	Total	K	0
			1	1	

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	1	1	Total	O	0
			1	1	
61	5	7	Total	O	0
			7	7	
61	7	12	Total	O	0
			12	12	
61	8	12	Total	O	0
			12	12	
61	9	1	Total	O	0
			1	1	
61	A	1409	Total	O	0
			1409	1409	

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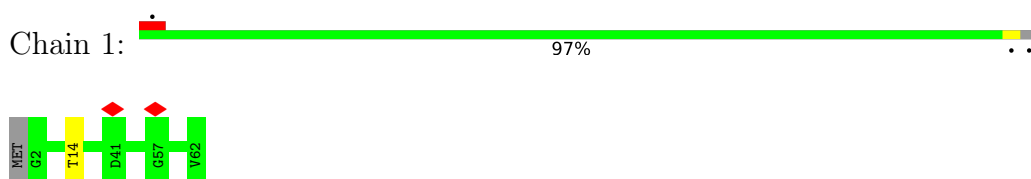
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Mol	Chain	Residues	Atoms		AltConf
61	B	3	Total 3	O 3	0
61	E	6	Total 6	O 6	0
61	G	43	Total 43	O 43	0
61	H	18	Total 18	O 18	0
61	I	24	Total 24	O 24	0
61	M	5	Total 5	O 5	0
61	N	4	Total 4	O 4	0
61	O	19	Total 19	O 19	0
61	P	8	Total 8	O 8	0
61	Q	3	Total 3	O 3	0
61	S	2	Total 2	O 2	0
61	T	9	Total 9	O 9	0
61	U	5	Total 5	O 5	0
61	V	13	Total 13	O 13	0
61	W	2	Total 2	O 2	0
61	X	1	Total 1	O 1	0
61	Z	6	Total 6	O 6	0
61	a	6	Total 6	O 6	0

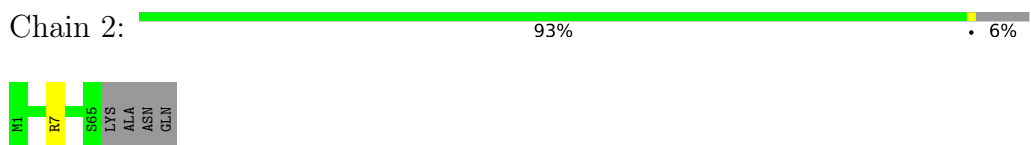
3 Residue-property plots [i](#)

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.

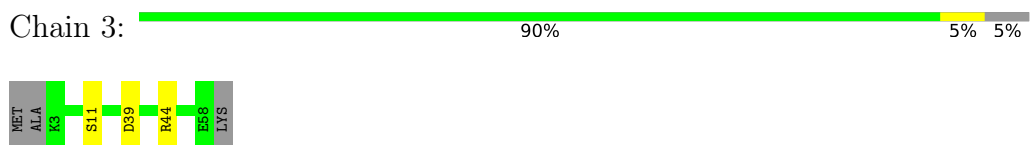
- Molecule 1: 50S ribosomal protein L28



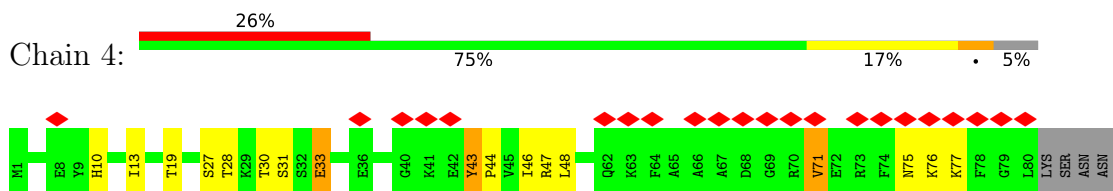
- Molecule 2: 50S ribosomal protein L29



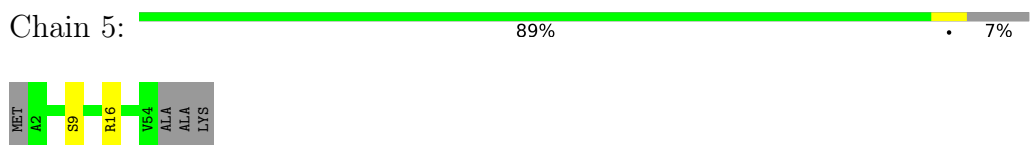
- Molecule 3: 50S ribosomal protein L30



- Molecule 4: 50S ribosomal protein L31 type B

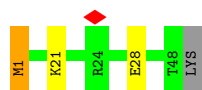


- Molecule 5: 50S ribosomal protein L32



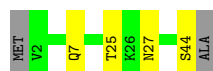
- Molecule 6: 50S ribosomal protein L33 1

Chain 6:  92%

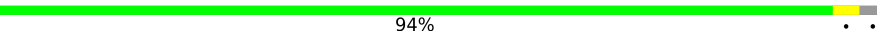


- Molecule 7: 50S ribosomal protein L34

Chain 7:  87% 9%



- Molecule 8: 50S ribosomal protein L35

Chain 8:  94%



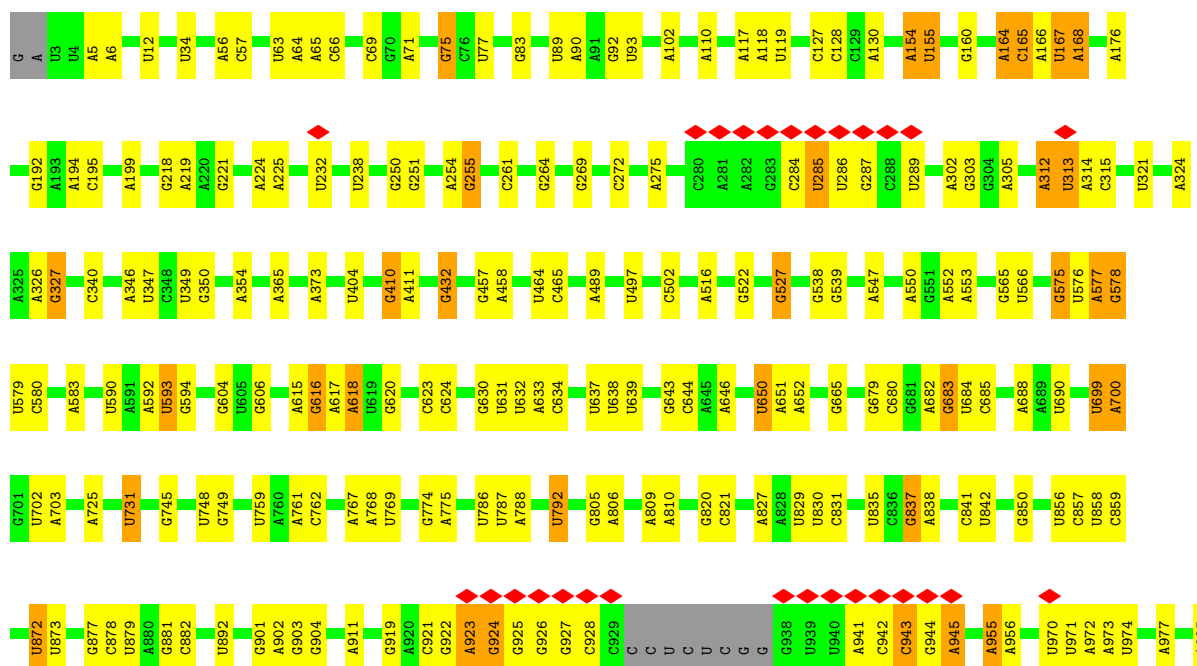
- Molecule 9: 50S ribosomal protein L36

Chain 9:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: 23S ribosomal RNA

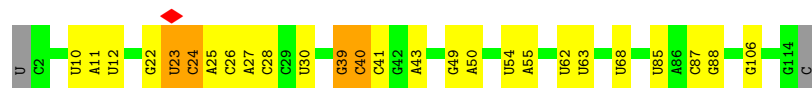
Chain A:  75% 20%





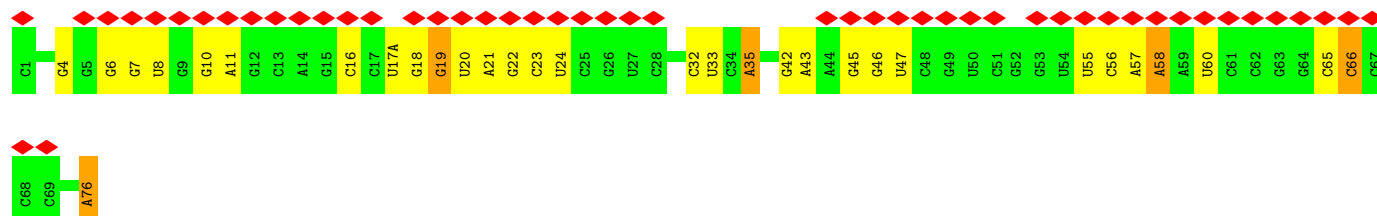
- Molecule 11: 5S ribosomal RNA

Chain B: 



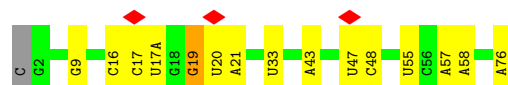
- Molecule 12: tRNA

Chain D: 



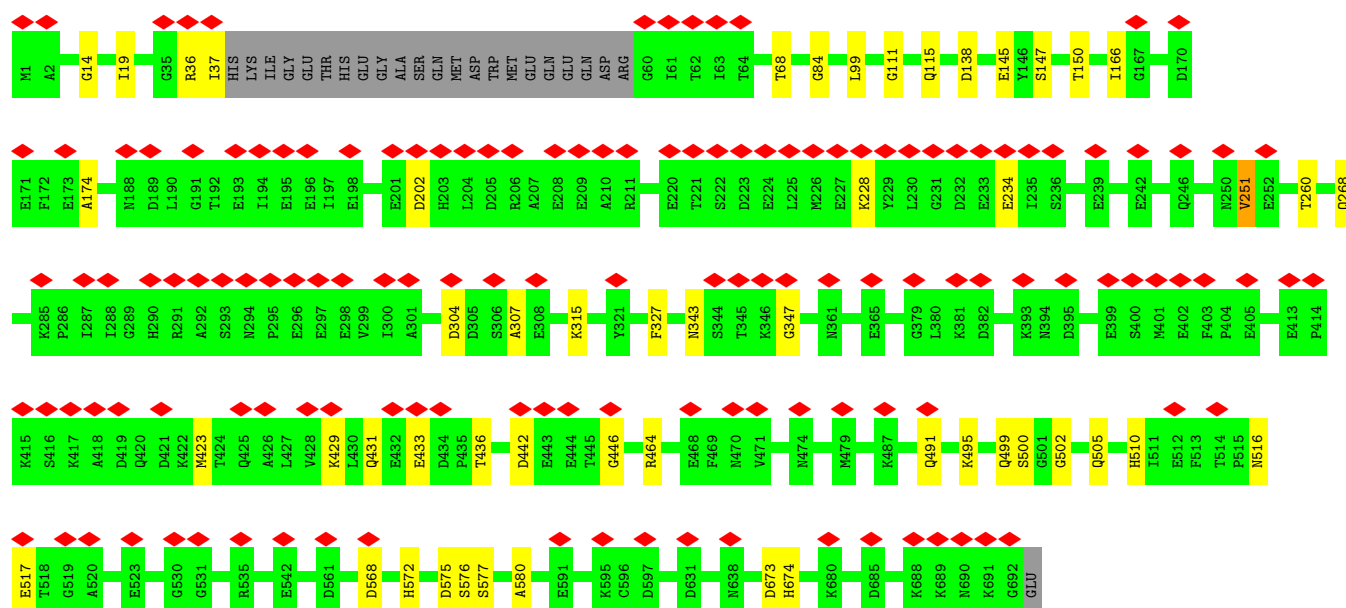
- Molecule 12: tRNA

Chain F: 

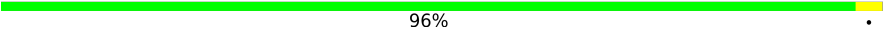


- Molecule 13: Elongation factor G

Chain E: 

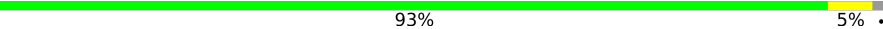


- Molecule 14: 50S ribosomal protein L2

Chain G:  96% ..

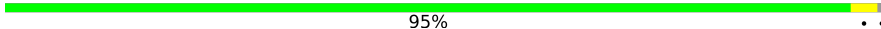


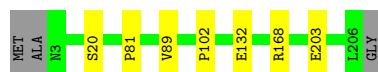
- Molecule 15: 50S ribosomal protein L3

Chain H:  93% 5% .

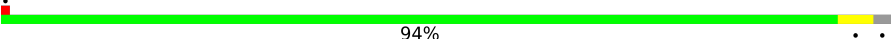


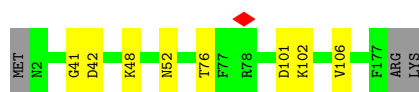
- Molecule 16: 50S ribosomal protein L4

Chain I:  95% ..



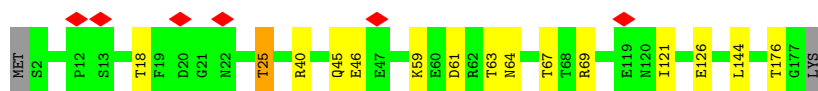
- Molecule 17: 50S ribosomal protein L5

Chain J:  94% ..

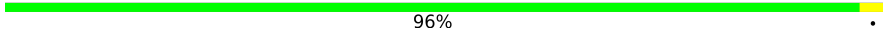


- Molecule 18: 50S ribosomal protein L6

Chain K:  90% 8% ..

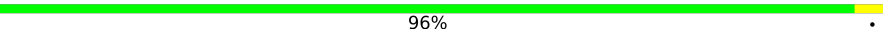


- Molecule 19: 50S ribosomal protein L13

Chain M:  96% ..

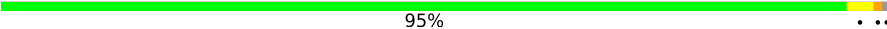


- Molecule 20: 50S ribosomal protein L14

Chain N:  96% .



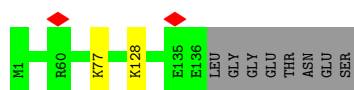
- Molecule 21: 50S ribosomal protein L15

Chain O:  95% ..



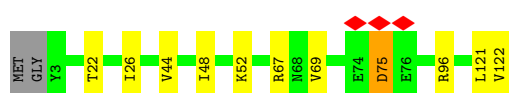
- Molecule 22: 50S ribosomal protein L16

Chain P:  93% • 6%



- Molecule 23: 50S ribosomal protein L17

Chain Q:  89% 8% ..



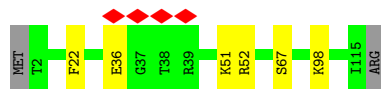
- Molecule 24: 50S ribosomal protein L18

Chain R:  93% 7%

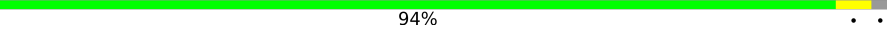


- Molecule 25: 50S ribosomal protein L19

Chain S:  93% 5% •



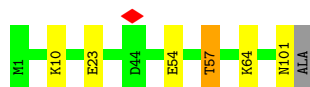
- Molecule 26: 50S ribosomal protein L20

Chain T:  94% • •

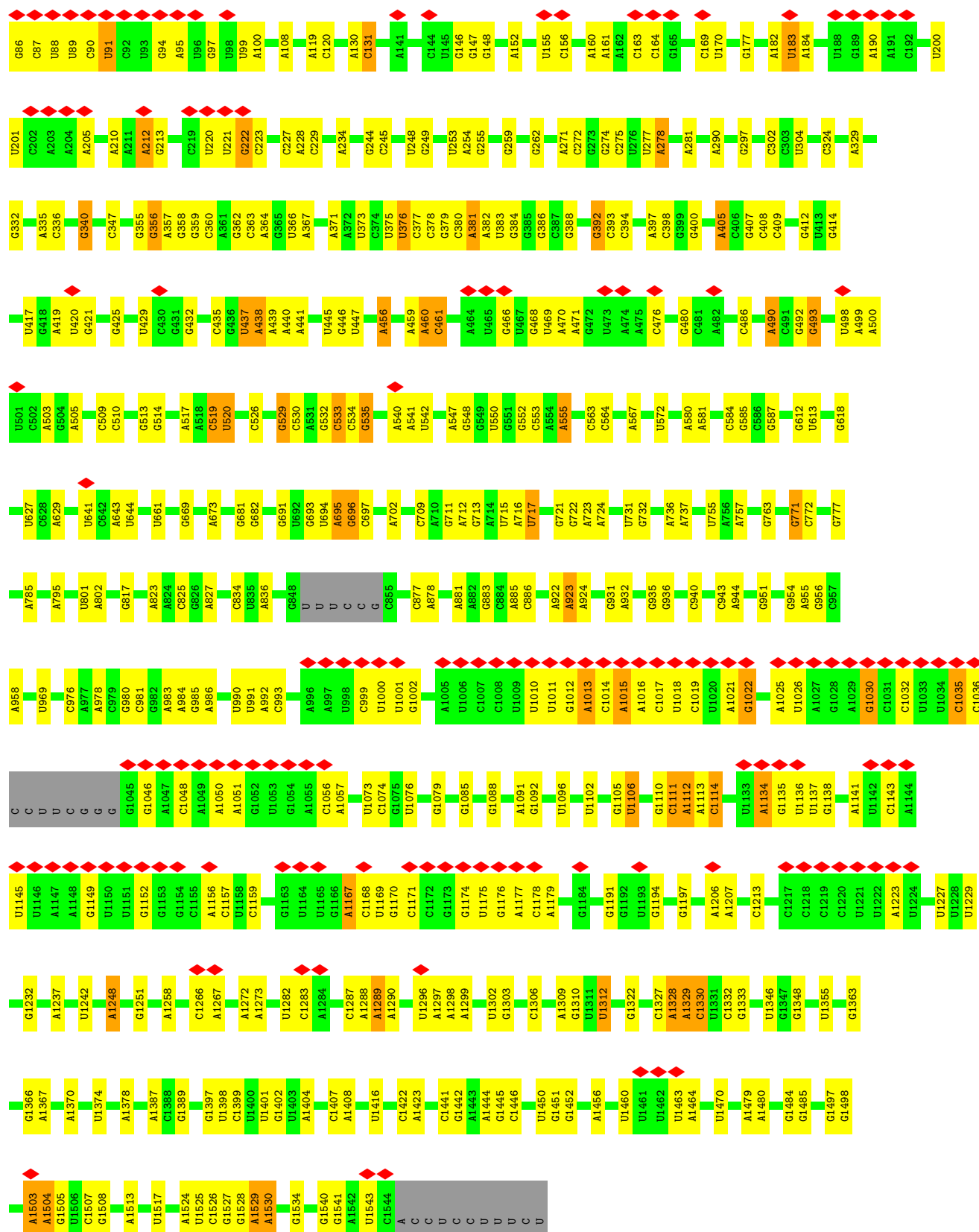


- Molecule 27: 50S ribosomal protein L21

Chain U:  93% 5% ..

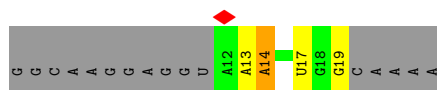


- [illegible]



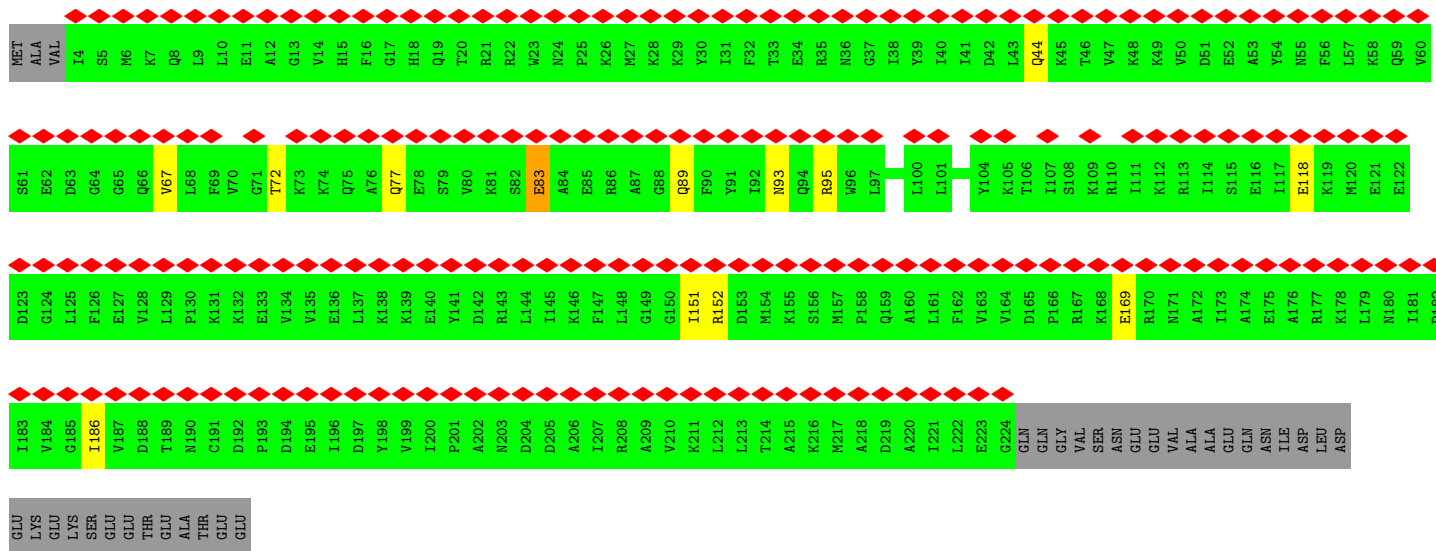
• Molecule 34: mRNA

Chain b: 

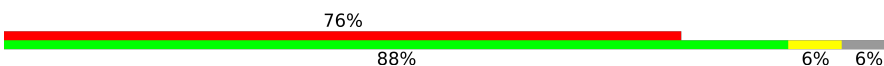


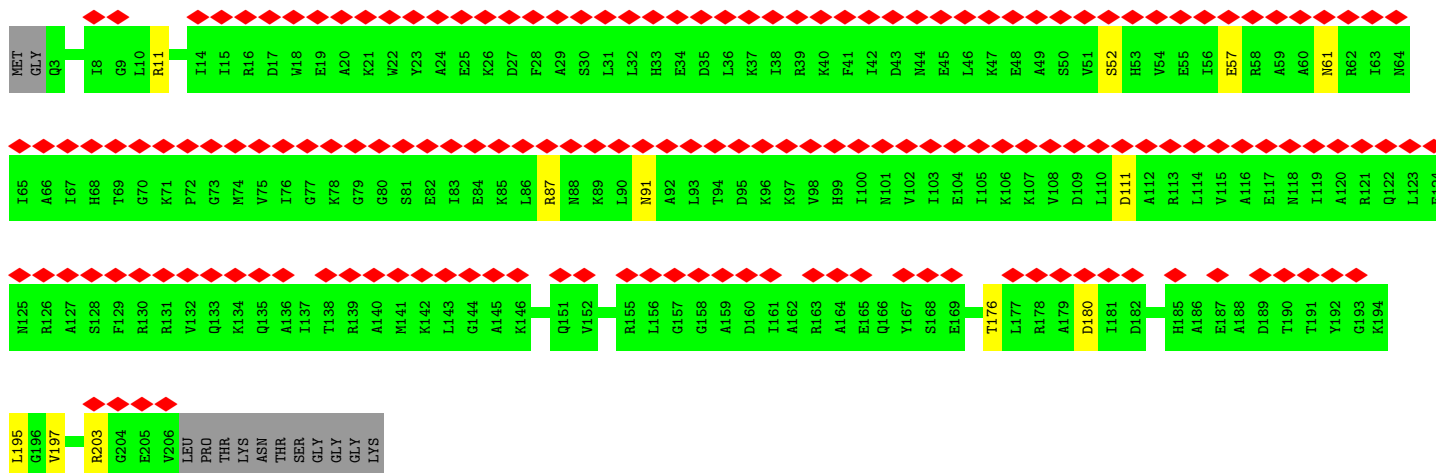
• Molecule 35: 30S ribosomal protein S2

Chain c: 



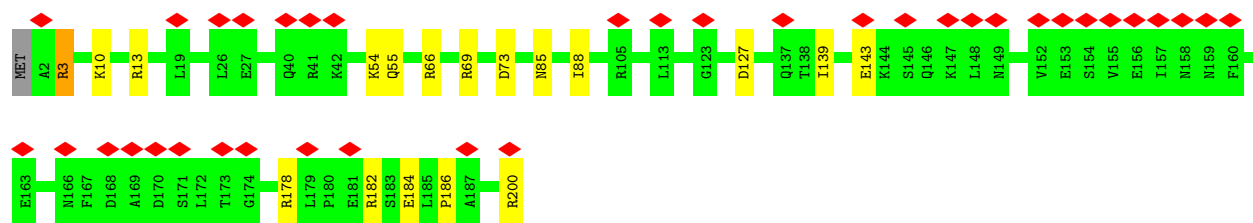
• Molecule 36: 30S ribosomal protein S3

Chain d: 

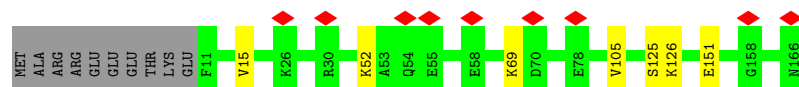
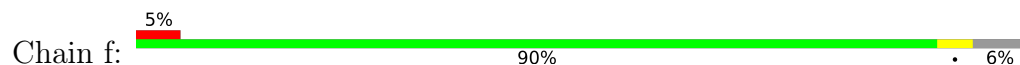


• Molecule 37: 30S ribosomal protein S4

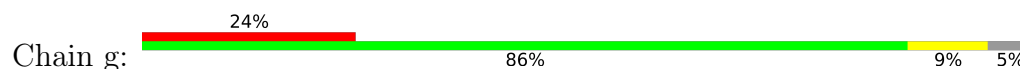
Chain e: 



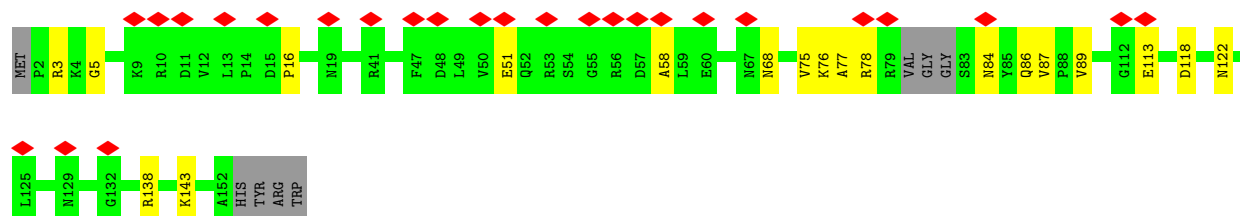
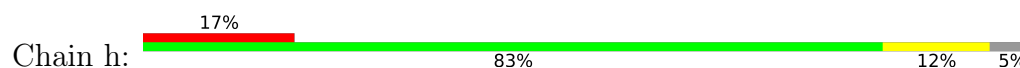
- Molecule 38: 30S ribosomal protein S5



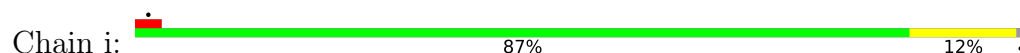
- Molecule 39: 30S ribosomal protein S6



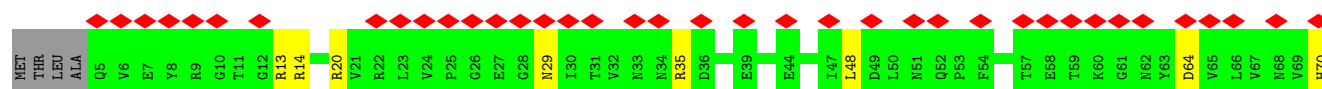
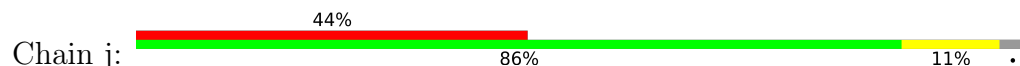
- Molecule 40: 30S ribosomal protein S7

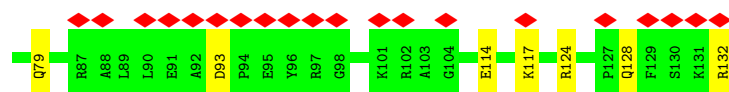


- Molecule 41: 30S ribosomal protein S8

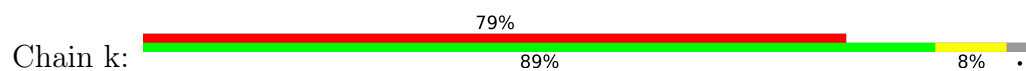


- Molecule 42: 30S ribosomal protein S9

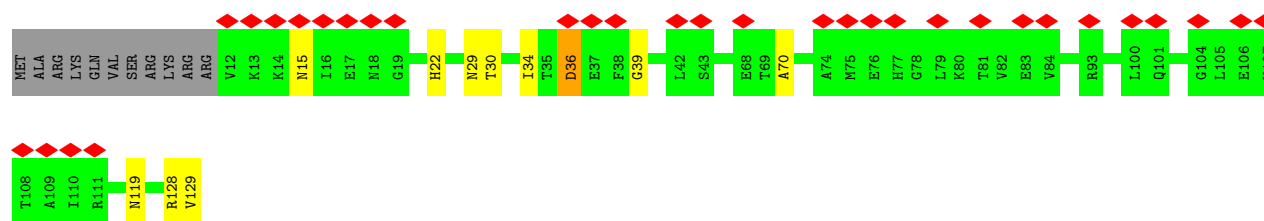
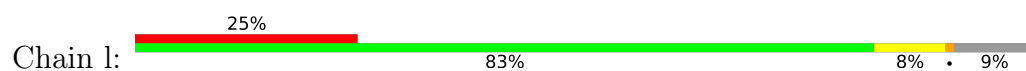




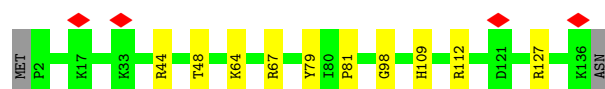
- Molecule 43: 30S ribosomal protein S10



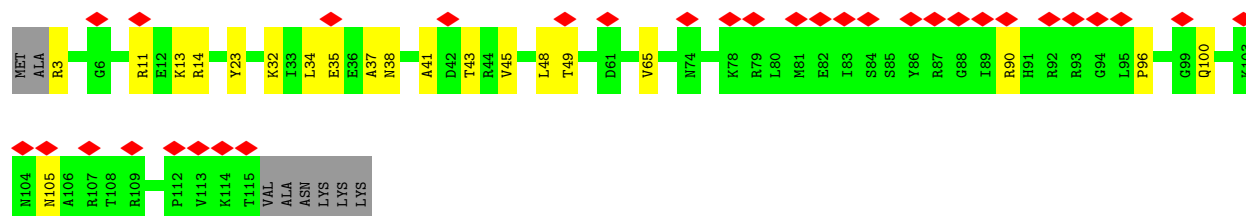
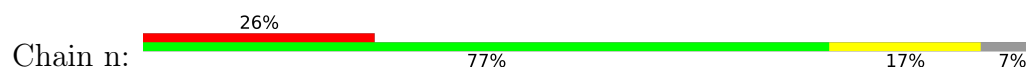
- Molecule 44: 30S ribosomal protein S11



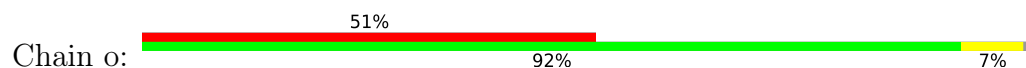
- Molecule 45: 30S ribosomal protein S12

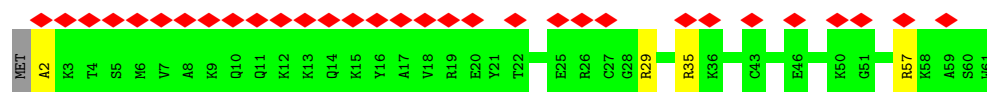


- Molecule 46: 30S ribosomal protein S13

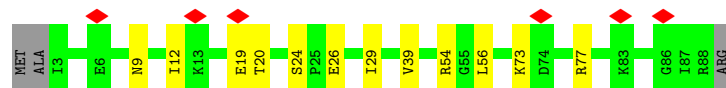
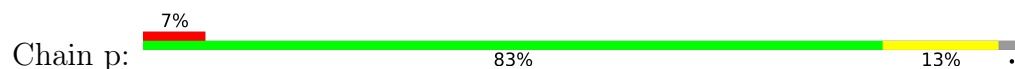


- Molecule 47: 30S ribosomal protein S14 type Z

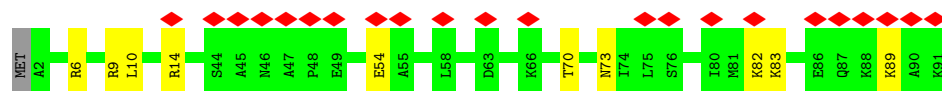
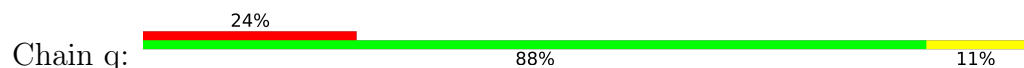




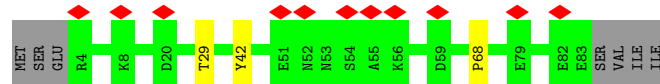
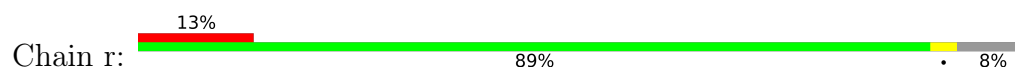
- Molecule 48: 30S ribosomal protein S15



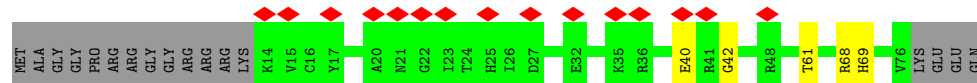
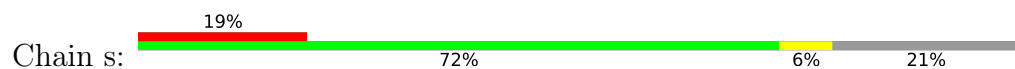
- Molecule 49: 30S ribosomal protein S16



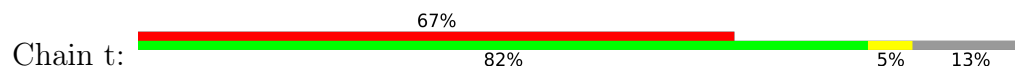
- Molecule 50: 30S ribosomal protein S17



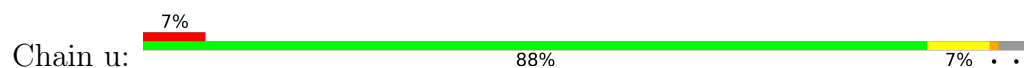
- Molecule 51: 30S ribosomal protein S18

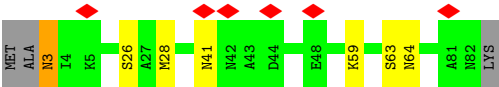


- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40800	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 ($e^-/\text{\AA}^2$)	27.77	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	3.236	Depositor
Minimum map value	-1.600	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	509.59998, 509.59998, 509.59998	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.728, 0.728, 0.728	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3TD, 4OC, MG, G7M, PUT, GDP, 2MG, H2U, SPD, 2MA, WUX, 5MC, OMG, 5MU, ZN, K, MA6, UR3

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	1	0.28	0/487	0.34	0/649
2	2	0.24	0/536	0.28	0/713
3	3	0.30	0/438	0.41	0/590
4	4	0.19	0/671	0.35	0/900
5	5	0.32	0/429	0.41	0/571
6	6	0.23	0/407	0.34	0/545
7	7	0.35	0/371	0.41	0/484
8	8	0.34	0/526	0.47	0/690
9	9	0.30	0/299	0.38	0/393
10	A	0.41	0/68117	0.40	0/106230
11	B	0.31	0/2692	0.32	0/4193
12	D	0.14	0/1832	0.27	0/2855
12	F	0.22	0/1813	0.30	0/2825
13	E	0.17	0/5271	0.28	0/7128
14	G	0.30	0/2120	0.40	0/2847
15	H	0.32	0/1661	0.44	0/2227
16	I	0.28	0/1587	0.37	0/2143
17	J	0.22	0/1410	0.31	0/1893
18	K	0.21	0/1390	0.34	0/1870
19	M	0.32	0/1168	0.40	0/1573
20	N	0.30	0/927	0.40	0/1243
21	O	0.30	0/1104	0.40	0/1471
22	P	0.32	0/1113	0.39	0/1493
23	Q	0.32	0/956	0.42	0/1277
24	R	0.24	0/931	0.32	0/1244
25	S	0.28	0/934	0.37	0/1249
26	T	0.33	0/955	0.45	0/1265
27	U	0.31	0/803	0.37	0/1073
28	V	0.33	0/861	0.45	0/1159
29	W	0.30	0/733	0.42	0/978
30	X	0.24	0/796	0.32	0/1063

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	Y	0.24	0/746	0.35	0/1000
32	Z	0.32	0/643	0.38	0/853
33	a	0.24	0/36440	0.32	0/56820
34	b	0.34	0/198	0.39	0/307
35	c	0.09	0/1808	0.23	0/2426
36	d	0.10	0/1634	0.23	0/2195
37	e	0.15	0/1647	0.26	0/2211
38	f	0.19	0/1174	0.30	0/1583
39	g	0.14	0/784	0.30	0/1052
40	h	0.15	0/1195	0.33	0/1605
41	i	0.19	0/1044	0.32	0/1401
42	j	0.12	0/1032	0.26	0/1386
43	k	0.10	0/804	0.26	0/1083
44	l	0.15	0/891	0.31	0/1203
45	m	0.18	0/1075	0.28	0/1439
46	n	0.15	0/909	0.31	0/1218
47	o	0.11	0/511	0.25	0/678
48	p	0.18	0/730	0.29	0/975
49	q	0.15	0/723	0.36	0/971
50	r	0.15	0/670	0.28	0/895
51	s	0.16	0/525	0.28	0/704
52	t	0.09	0/668	0.20	0/896
53	u	0.17	0/606	0.28	0/810
All	All	0.32	0/159795	0.37	0/238545

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	481	0	523	1	0
2	2	535	0	566	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	3	436	0	473	2	0
4	4	654	0	631	10	0
5	5	422	0	426	2	0
6	6	402	0	413	3	0
7	7	367	0	415	3	0
8	8	521	0	586	1	0
9	9	296	0	339	0	0
10	A	60978	0	30664	274	0
11	B	2408	0	1218	8	0
12	D	1640	0	837	13	0
12	F	1623	0	825	4	0
13	E	5181	0	5096	27	0
14	G	2085	0	2192	5	0
15	H	1637	0	1680	6	0
16	I	1564	0	1611	5	0
17	J	1392	0	1444	6	0
18	K	1372	0	1402	9	0
19	M	1146	0	1142	4	0
20	N	920	0	981	4	0
21	O	1090	0	1131	4	0
22	P	1089	0	1155	1	0
23	Q	952	0	999	6	0
24	R	922	0	968	5	0
25	S	922	0	994	4	0
26	T	943	0	1014	4	0
27	U	793	0	831	4	0
28	V	853	0	914	4	0
29	W	725	0	761	3	0
30	X	787	0	853	2	0
31	Y	738	0	787	2	0
32	Z	637	0	655	2	0
33	a	32707	0	16479	218	0
34	b	176	0	88	2	0
35	c	1781	0	1844	9	0
36	d	1612	0	1674	5	0
37	e	1617	0	1646	17	0
38	f	1160	0	1223	7	0
39	g	773	0	772	6	0
40	h	1180	0	1221	11	0
41	i	1032	0	1082	8	0
42	j	1016	0	1039	11	0
43	k	792	0	833	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	l	876	0	895	8	0
45	m	1058	0	1130	7	0
46	n	902	0	950	9	0
47	o	501	0	523	3	0
48	p	721	0	751	7	0
49	q	712	0	744	7	0
50	r	662	0	702	2	0
51	s	516	0	548	3	0
52	t	651	0	658	3	0
53	u	606	0	650	6	0
54	5	1	0	0	0	0
54	9	1	0	0	0	0
54	o	1	0	0	0	0
55	8	1	0	0	0	0
55	A	131	0	0	0	0
55	E	1	0	0	0	0
55	F	2	0	0	0	0
55	a	10	0	0	0	0
56	A	10	0	19	0	0
57	A	6	0	12	0	0
58	E	28	0	12	0	0
59	E	39	0	0	1	0
60	P	1	0	0	0	0
61	1	1	0	0	0	0
61	5	7	0	0	0	0
61	7	12	0	0	0	0
61	8	12	0	0	0	0
61	9	1	0	0	0	0
61	A	1409	0	0	20	0
61	B	3	0	0	0	0
61	E	6	0	0	1	0
61	G	43	0	0	1	0
61	H	18	0	0	0	0
61	I	24	0	0	0	0
61	M	5	0	0	0	0
61	N	4	0	0	0	0
61	O	19	0	0	0	0
61	P	8	0	0	0	0
61	Q	3	0	0	0	0
61	S	2	0	0	0	0
61	T	9	0	0	0	0
61	U	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	V	13	0	0	0	0
61	W	2	0	0	0	0
61	X	1	0	0	0	0
61	Z	6	0	0	0	0
61	a	6	0	0	0	0
All	All	149413	0	100021	693	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 (693) 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)
10:A:516:A:OP1	61:A:3201:HOH:O	1.83	0.94
13:E:433:GLU:OE1	13:E:464:ARG:NH2	2.01	0.94
20:N:104:ARG:NH2	25:S:36:GLU:OE1	2.04	0.90
40:h:3:ARG:NH1	40:h:5:GLY:O	2.06	0.89
39:g:88:ARG:NH1	51:s:69:HIS:O	2.08	0.86
37:e:69:ARG:NH1	37:e:73:ASP:OD1	2.10	0.84
10:A:1997:A:OP2	61:A:3202:HOH:O	1.96	0.82
20:N:120:GLU:OE1	25:S:67:SER:OG	1.96	0.82
30:X:51:ASN:ND2	30:X:53:GLU:O	2.12	0.81
33:a:371:A:OP2	45:m:44:ARG:NH1	2.14	0.81
10:A:2817:A:O2'	10:A:2818:A:O5'	1.99	0.80
10:A:1051:C:OP1	19:M:38:ARG:NH1	2.16	0.79
33:a:1327:C:O2'	33:a:1328:A:O5'	2.00	0.79
41:i:21:ARG:NH1	41:i:70:ASP:O	2.17	0.77
33:a:1013:A:O2'	33:a:1035:C:N4	2.16	0.77
32:Z:19:LYS:O	32:Z:22:ARG:NH2	2.17	0.77
33:a:435:C:OP1	37:e:13:ARG:NH2	2.19	0.76
35:c:72:THR:OG1	35:c:169:GLU:OE2	2.04	0.76
12:D:10:G:O6	12:D:45:G:N2	2.19	0.76
17:J:48:LYS:O	17:J:52:ASN:ND2	2.19	0.76
40:h:68:ASN:O	40:h:138:ARG:NE	2.18	0.75
10:A:923:A:O2'	10:A:924:G:O4'	2.03	0.75
33:a:82:G:N2	33:a:88:U:O4'	2.20	0.75
33:a:1137:U:OP1	43:k:7:ARG:NH2	2.20	0.74
12:D:42:G:OP1	40:h:143:LYS:NZ	2.17	0.74
33:a:587:G:O2'	48:p:54:ARG:NH1	2.21	0.74
10:A:1067:U:OP2	61:A:3204:HOH:O	2.05	0.74
33:a:358:G:OP1	53:u:3:ASN:ND2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:h:113:GLU:N	40:h:113:GLU:OE1	2.21	0.73
43:k:19:ASP:OD1	43:k:72:ARG:NH1	2.21	0.73
33:a:1213:C:OP1	47:o:2:ALA:N	2.22	0.73
33:a:412:G:O6	37:e:3:ARG:NH2	2.21	0.73
10:A:2276:U:OP2	61:A:3203:HOH:O	2.05	0.72
10:A:1070:A:OP1	61:A:3204:HOH:O	2.06	0.72
10:A:1795:A:N3	61:A:3216:HOH:O	2.22	0.72
10:A:2495:A:OP2	61:A:3205:HOH:O	2.08	0.72
10:A:1001:A:OP2	61:A:3206:HOH:O	2.09	0.71
48:p:26:GLU:OE2	48:p:77:ARG:NH1	2.24	0.71
33:a:691:G:N2	44:l:39:GLY:O	2.24	0.70
10:A:264:G:N7	61:A:3219:HOH:O	2.26	0.68
39:g:5:GLU:N	39:g:5:GLU:OE1	2.26	0.68
6:6:1:MET:SD	6:6:1:MET:N	2.62	0.68
21:O:83:ASN:ND2	21:O:116:SER:O	2.26	0.68
10:A:2822:C:O5'	10:A:2823:G:N2	2.27	0.67
8:8:54:ASP:OD1	8:8:57:ARG:NH2	2.26	0.66
13:E:516:ASN:OD1	13:E:517:GLU:N	2.29	0.66
10:A:1658:A:N7	61:A:3222:HOH:O	2.28	0.66
12:D:18:G:N2	12:D:58:A:OP2	2.29	0.66
33:a:400:G:OP1	49:q:9:ARG:NH2	2.29	0.66
33:a:553:C:OP1	37:e:54:LYS:NZ	2.29	0.65
42:j:14:ARG:NE	42:j:79:GLN:OE1	2.28	0.65
33:a:697:C:OP1	44:l:29:ASN:ND2	2.29	0.65
10:A:2098:A:N3	61:A:3224:HOH:O	2.29	0.65
10:A:2337:A:N6	17:J:76:THR:OG1	2.30	0.64
33:a:530:C:OP2	45:m:79:TYR:OH	2.15	0.64
39:g:23:VAL:O	39:g:27:ASN:ND2	2.29	0.64
10:A:1021:G:OP2	61:A:3207:HOH:O	2.15	0.64
3:3:39:ASP:OD2	3:3:44:ARG:NH2	2.31	0.64
33:a:90:C:O2'	33:a:91:U:OP2	2.17	0.63
10:A:620:G:O2'	10:A:1292:A:OP1	2.16	0.63
10:A:1582:U:O2'	10:A:1583:G:O5'	2.16	0.63
35:c:83:GLU:OE1	35:c:83:GLU:N	2.31	0.63
10:A:1823:U:H2'	10:A:1824:C:C6	2.34	0.62
33:a:130:A:O2'	33:a:131:C:OP1	2.18	0.62
49:q:54:GLU:N	49:q:54:GLU:OE1	2.30	0.62
21:O:87:ASP:OD1	21:O:87:ASP:N	2.32	0.62
36:d:180:ASP:OD2	36:d:203:ARG:NH2	2.32	0.62
39:g:15:GLU:OE1	39:g:15:GLU:N	2.32	0.62
51:s:40:GLU:OE1	51:s:40:GLU:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:1387:A:N3	40:h:3:ARG:NH2	2.48	0.62
33:a:951:G:N2	42:j:128:GLN:OE1	2.31	0.62
33:a:1114:C:OP1	35:c:95:ARG:NH2	2.33	0.61
10:A:1520:A:O2'	10:A:1521:A:OP2	2.18	0.61
10:A:1457:U:O2	10:A:1457:U:O2'	2.17	0.61
33:a:1370:A:OP2	47:o:35:ARG:NH2	2.34	0.61
37:e:143:GLU:N	37:e:143:GLU:OE1	2.34	0.60
10:A:830:U:H2'	10:A:831:C:C6	2.36	0.60
33:a:777:G:H4'	33:a:1524:A:H4'	1.82	0.60
17:J:101:ASP:OD1	17:J:102:LYS:N	2.34	0.60
10:A:2334:G:O6	17:J:41:GLY:N	2.35	0.60
10:A:2479:C:O2	61:A:3208:HOH:O	2.16	0.60
33:a:324:C:OP2	33:a:359:G:O2'	2.20	0.60
10:A:618:A:OP2	10:A:2526:C:O2'	2.20	0.60
13:E:491:GLN:N	13:E:491:GLN:OE1	2.35	0.60
33:a:272:C:O2'	50:r:68:PRO:O	2.20	0.60
42:j:29:ASN:N	42:j:64:ASP:OD1	2.34	0.59
10:A:312:A:O2'	10:A:313:U:O5'	2.16	0.59
33:a:509:C:OP1	45:m:127:ARG:NH2	2.35	0.59
10:A:856:U:OP1	61:A:3209:HOH:O	2.17	0.59
10:A:2817:A:O2'	10:A:2818:A:O4'	2.18	0.59
33:a:1159:C:OP2	42:j:13:ARG:NH2	2.36	0.59
41:i:26:GLU:OE1	41:i:26:GLU:N	2.36	0.58
10:A:1966:5MU:OP1	10:A:2631:U:O2'	2.21	0.58
31:Y:7:ILE:HD11	31:Y:65:VAL:HA	1.86	0.58
10:A:2715:G:OP1	10:A:2740:A:N6	2.37	0.58
33:a:1085:G:OP1	38:f:69:LYS:NZ	2.36	0.58
13:E:268:GLN:OE1	13:E:268:GLN:N	2.35	0.58
10:A:166:A:HO2'	10:A:167:U:H6	1.49	0.58
53:u:41:ASN:O	53:u:41:ASN:ND2	2.37	0.58
19:M:18:VAL:HG23	19:M:138:PRO:HB2	1.85	0.58
10:A:1806:U:H5	10:A:1811:A:N7	2.02	0.57
38:f:151:GLU:N	38:f:151:GLU:OE1	2.35	0.57
10:A:1582:U:O2'	10:A:1583:G:O4'	2.23	0.57
18:K:40:ARG:NH1	18:K:61:ASP:OD1	2.37	0.57
40:h:51:GLU:OE1	40:h:58:ALA:N	2.38	0.57
24:R:60:ASP:OD1	24:R:61:SER:N	2.38	0.57
33:a:18:U:H2'	33:a:19:C:C6	2.40	0.57
37:e:178:ARG:NH2	37:e:184:GLU:OE2	2.38	0.57
43:k:4:GLN:N	43:k:4:GLN:OE1	2.38	0.57
33:a:1135:G:N2	33:a:1136:U:O4	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:d:87:ARG:O	36:d:91:ASN:ND2	2.38	0.56
13:E:343:ASN:O	13:E:347:GLY:N	2.38	0.56
10:A:12:U:H2'	10:A:12:U:O2	2.05	0.56
10:A:160:G:O2'	10:A:168:A:N6	2.35	0.56
10:A:1817:C:H2'	10:A:1818:A:C5	2.40	0.56
12:F:16:C:OP1	12:F:17:C:N4	2.37	0.56
45:m:81:PRO:O	45:m:112:ARG:NH1	2.36	0.55
33:a:1534:G:OP1	44:l:128:ARG:NH2	2.40	0.55
10:A:788:A:O2'	10:A:1703:U:OP1	2.22	0.55
33:a:1287:C:O2'	33:a:1289:A:N7	2.39	0.55
6:6:1:MET:N	10:A:2312:C:OP2	2.33	0.55
10:A:2318:U:OP1	10:A:2407:A:O2'	2.24	0.55
33:a:1445:G:H2'	33:a:1446:C:C6	2.42	0.55
11:B:12:U:OP2	11:B:68:U:O2'	2.23	0.55
13:E:145:GLU:N	13:E:145:GLU:OE1	2.40	0.55
10:A:1038:C:OP1	26:T:53:ARG:NH2	2.40	0.54
33:a:409:C:OP2	37:e:66:ARG:NH1	2.39	0.54
33:a:461:C:O2'	49:q:73:ASN:OD1	2.20	0.54
10:A:2318:U:H2'	10:A:2319:U:C6	2.42	0.54
33:a:555:A:O5'	37:e:3:ARG:NH2	2.40	0.54
35:c:44:GLN:OE1	35:c:44:GLN:N	2.35	0.54
13:E:464:ARG:NH1	59:E:703:WUX:O6	2.41	0.54
51:s:42:GLY:O	51:s:68:ARG:NH2	2.38	0.54
33:a:1527:G:N1	33:a:1530:MA6:OP2	2.40	0.54
23:Q:121:LEU:O	23:Q:122:VAL:HB	2.08	0.54
10:A:631:U:H2'	10:A:632:U:C6	2.43	0.53
10:A:1357:G:C2	10:A:1366:U:H5''	2.43	0.53
33:a:222:G:O2'	33:a:223:C:OP2	2.25	0.53
10:A:858:U:H2'	10:A:859:C:C6	2.43	0.53
13:E:304:ASP:OD2	13:E:307:ALA:N	2.42	0.53
10:A:1074:G:OP2	22:P:128:LYS:NZ	2.39	0.53
10:A:2355:A:H2'	10:A:2356:A:C8	2.42	0.53
11:B:39:G:O2'	11:B:40:C:OP1	2.22	0.53
10:A:2353:U:O3'	61:A:3210:HOH:O	2.18	0.53
13:E:499:GLN:NE2	13:E:575:ASP:OD2	2.42	0.53
33:a:383:U:OP1	49:q:70:THR:OG1	2.23	0.53
10:A:593:U:OP2	27:U:64:LYS:NZ	2.33	0.53
10:A:1884:G:H2'	10:A:1885:G:O4'	2.10	0.52
10:A:2092:C:H4'	10:A:2278:OMG:HM22	1.90	0.52
33:a:721:G:H2'	33:a:722:G:C8	2.43	0.52
23:Q:26:ILE:HD11	23:Q:69:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Q:52:LYS:NZ	23:Q:96:ARG:O	2.42	0.52
10:A:164:A:O2'	10:A:165:C:O5'	2.26	0.52
27:U:54:GLU:N	27:U:54:GLU:OE1	2.41	0.52
16:I:20:SER:N	16:I:203:GLU:OE2	2.42	0.52
10:A:877:G:H2'	10:A:878:C:C6	2.45	0.52
10:A:2336:A:O2'	10:A:2337:A:OP1	2.19	0.52
33:a:381:A:C2	33:a:490:A:C6	2.97	0.52
33:a:1134:A:O2'	33:a:1135:G:H5'	2.10	0.52
10:A:340:C:OP1	30:X:90:LYS:NZ	2.42	0.52
33:a:80:A:O2'	33:a:81:A:O5'	2.25	0.52
28:V:65:ASN:ND2	28:V:67:ASP:OD2	2.43	0.52
10:A:787:U:H2'	10:A:788:A:C8	2.45	0.51
17:J:42:ASP:OD1	17:J:42:ASP:N	2.42	0.51
33:a:379:G:O2'	33:a:381:A:N7	2.39	0.51
33:a:1470:U:OP1	53:u:26:SER:OG	2.27	0.51
10:A:2091:C:H2'	10:A:2092:C:C6	2.45	0.51
18:K:64:ASN:HA	18:K:67:THR:HG22	1.92	0.51
33:a:1258:A:O2'	42:j:35:ARG:NH2	2.42	0.51
10:A:684:U:H2'	10:A:685:C:C6	2.45	0.51
33:a:1015:A:N7	33:a:1032:C:N4	2.59	0.51
10:A:1072:A:N6	10:A:1169:G:H2'	2.25	0.51
10:A:2354:A:H2'	10:A:2355:A:C8	2.44	0.51
40:h:118:ASP:O	40:h:122:ASN:ND2	2.39	0.51
10:A:841:C:H2'	10:A:842:U:C6	2.45	0.51
33:a:834:C:O2	41:i:16:ASN:ND2	2.44	0.51
4:4:33:GLU:OE2	4:4:47:ARG:NH2	2.44	0.51
10:A:2771:G:H1	10:A:2787:C:H5	1.58	0.51
33:a:1073:U:H2'	33:a:1074:C:C6	2.45	0.51
33:a:1524:A:H2'	33:a:1525:U:C6	2.45	0.51
10:A:285:U:O2'	10:A:287:G:OP1	2.26	0.51
10:A:2467:C:OP2	61:A:3211:HOH:O	2.19	0.51
10:A:688:A:N1	10:A:2396:A:O2'	2.42	0.51
10:A:1572:G:C6	10:A:1591:G:C6	2.99	0.51
33:a:29:G:O2'	33:a:304:U:OP1	2.23	0.51
33:a:722:G:H2'	33:a:723:A:C8	2.45	0.51
33:a:1484:G:H2'	33:a:1485:G:C8	2.46	0.51
10:A:2216:U:H3'	10:A:2217:G:H5''	1.93	0.50
10:A:1185:U:H4'	10:A:1186:A:O4'	2.11	0.50
10:A:1899:U:O2'	10:A:1900:G:O5'	2.25	0.50
10:A:2052:C:H2'	10:A:2053:U:C6	2.46	0.50
33:a:702:A:N1	33:a:795:A:O2'	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:955:A:H2'	10:A:956:A:C8	2.47	0.50
12:F:19:G:H4'	12:F:20:U:OP2	2.11	0.50
10:A:792:5MU:O2'	28:V:92:ARG:NH2	2.44	0.50
33:a:381:A:C2	33:a:382:A:C8	3.00	0.50
33:a:1378:A:OP1	43:k:64:GLN:NE2	2.43	0.50
10:A:1056:U:O2'	19:M:144:ARG:NH1	2.45	0.50
44:l:29:ASN:OD1	44:l:30:THR:N	2.44	0.50
10:A:2260:A:H2'	10:A:2261:G:C8	2.46	0.50
33:a:470:A:H2'	33:a:471:A:H8	1.77	0.50
10:A:856:U:H2'	21:O:21:ARG:HA	1.93	0.50
31:Y:7:ILE:C	31:Y:7:ILE:HD12	2.36	0.50
33:a:532:G:H2'	33:a:533:C:C6	2.46	0.50
1:1:14:THR:HG21	10:A:192:G:OP2	2.12	0.49
10:A:575:G:O2'	10:A:577:A:N7	2.43	0.49
10:A:1513:A:H2'	10:A:1514:A:C8	2.47	0.49
10:A:2584:G:H2'	10:A:2585:C:C6	2.47	0.49
10:A:194:A:H2'	10:A:195:C:C6	2.47	0.49
33:a:22:G:H2'	33:a:23:G:C8	2.47	0.49
33:a:954:G:C2	33:a:955:A:C8	3.01	0.49
33:a:958:A:N7	46:n:105:ASN:ND2	2.59	0.49
33:a:695:A:H1'	33:a:696:G:OP2	2.12	0.49
33:a:388:G:N1	33:a:392:G:O6	2.46	0.49
33:a:437:U:O2	33:a:438:A:C8	2.65	0.49
33:a:1327:C:O2'	33:a:1328:A:O4'	2.27	0.49
10:A:1700:C:H2'	10:A:1701:U:C6	2.48	0.49
10:A:2109:A:H2'	10:A:2110:G:O4'	2.13	0.49
33:a:529:G:OP2	45:m:64:LYS:NZ	2.46	0.49
10:A:579:U:H2'	10:A:580:C:C6	2.48	0.49
13:E:111:GLY:O	61:E:801:HOH:O	2.20	0.49
2:2:7:ARG:NH2	10:A:77:U:O2'	2.45	0.49
10:A:1463:A:H2'	10:A:1465:G:N7	2.28	0.49
10:A:2776:A:H1'	18:K:63:THR:HG22	1.95	0.49
13:E:442:ASP:O	13:E:446:GLY:N	2.44	0.49
33:a:1366:G:H2'	33:a:1367:A:C8	2.48	0.49
7:7:7:GLN:O	10:A:731:U:O2	2.30	0.48
10:A:527:G:O2'	10:A:552:A:N6	2.46	0.48
13:E:19:ILE:HD12	13:E:19:ILE:H	1.78	0.48
23:Q:75:ASP:OD1	23:Q:75:ASP:N	2.45	0.48
10:A:1391:A:H2'	10:A:1392:G:O4'	2.13	0.48
10:A:923:A:O2'	10:A:924:G:O5'	2.30	0.48
10:A:2232:A:H2'	10:A:2233:C:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2300:A:H2'	10:A:2301:A:C8	2.48	0.48
10:A:2313:A:H4'	10:A:2314:A:O4'	2.13	0.48
16:I:81:PRO:HB3	16:I:89:VAL:HG23	1.96	0.48
20:N:35:ILE:HG21	20:N:103:ALA:HB3	1.93	0.48
3:3:11:SER:OG	10:A:1033:G:OP2	2.32	0.48
10:A:1329:G:H2'	10:A:1330:U:C6	2.48	0.48
33:a:277:U:H2'	33:a:278:A:H8	1.79	0.48
33:a:332:G:N1	33:a:335:A:OP2	2.46	0.48
10:A:1238:U:H1'	26:T:4:VAL:HG22	1.95	0.48
48:p:24:SER:OG	48:p:26:GLU:OE1	2.31	0.48
18:K:45:GLN:NE2	18:K:46:GLU:O	2.47	0.48
33:a:99:U:H2'	33:a:100:A:C8	2.49	0.48
33:a:723:A:H2'	33:a:724:A:C8	2.48	0.48
5:5:9:SER:HB3	10:A:2047:A:H5'	1.96	0.48
10:A:1241:A:H2'	10:A:1242:A:C8	2.48	0.48
10:A:2347:A:H2'	10:A:2347:A:N3	2.29	0.48
33:a:627:U:O2	33:a:627:U:O5'	2.31	0.48
10:A:275:A:C2	10:A:305:A:O4'	2.66	0.48
10:A:2098:A:H2'	10:A:2099:G:C8	2.49	0.48
10:A:1473:G:H2'	10:A:1474:C:C6	2.49	0.47
10:A:1880:A:H2'	10:A:1881:A:C8	2.49	0.47
11:B:49:G:H2'	11:B:50:A:C8	2.49	0.47
33:a:9:A:OP2	37:e:200:ARG:NH2	2.47	0.47
33:a:169:C:O2'	33:a:170:U:H5'	2.13	0.47
33:a:1010:U:H2'	33:a:1011:U:C6	2.49	0.47
36:d:61:ASN:O	36:d:61:ASN:ND2	2.47	0.47
33:a:271:A:H2'	33:a:272:C:C5	2.49	0.47
33:a:1022:G:N2	33:a:1025:A:OP2	2.44	0.47
44:l:34:ILE:HD11	44:l:70:ALA:HB1	1.96	0.47
42:j:114:GLU:OE2	42:j:117:LYS:NZ	2.42	0.47
29:W:9:ARG:NH2	29:W:28:ASP:OD2	2.48	0.47
33:a:1232:G:OP2	33:a:1332:C:N4	2.42	0.47
15:H:100:GLU:O	15:H:103:GLN:HB2	2.14	0.47
33:a:130:A:HO2'	33:a:131:C:P	2.37	0.47
13:E:228:LYS:NZ	13:E:234:GLU:O	2.47	0.47
33:a:509:C:H2'	33:a:510:C:C6	2.49	0.47
14:G:267:ASP:OD1	14:G:268:LYS:N	2.48	0.47
33:a:155:U:H2'	33:a:156:C:C6	2.50	0.47
33:a:1330:C:O2	52:t:36:ARG:NH2	2.48	0.47
33:a:1441:C:H2'	33:a:1442:G:O4'	2.14	0.47
44:l:36:ASP:N	44:l:36:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:164:A:O2'	10:A:165:C:H6	1.98	0.47
10:A:1179:C:O2'	10:A:1180:G:OP1	2.29	0.47
10:A:1288:G:N7	21:O:18:ARG:NH2	2.63	0.47
11:B:23:U:H3'	11:B:24:C:H5''	1.96	0.47
14:G:79:ASP:N	14:G:93:LEU:O	2.47	0.47
33:a:147:G:H2'	33:a:148:G:C8	2.50	0.47
33:a:1167:A:C2	33:a:1191:G:C4	3.03	0.47
10:A:2348:G:H5'	10:A:2349:A:OP2	2.14	0.47
25:S:22:PHE:O	25:S:52:ARG:NH1	2.48	0.47
33:a:340:G:OP2	53:u:3:ASN:HA	2.14	0.47
10:A:349:U:H2'	10:A:350:G:O4'	2.15	0.47
10:A:1306:A:H2'	10:A:1307:G:O4'	2.15	0.47
10:A:2270:U:H2'	10:A:2271:U:C6	2.50	0.47
33:a:65:G:C6	33:a:99:U:O4	2.67	0.47
33:a:386:G:N1	33:a:394:C:N3	2.63	0.47
7:7:25:THR:HG21	61:A:3809:HOH:O	2.14	0.46
10:A:633:A:H2'	10:A:634:C:C6	2.50	0.46
10:A:759:U:O2'	10:A:761:A:N7	2.41	0.46
10:A:786:U:H2'	10:A:787:U:C6	2.51	0.46
10:A:901:G:H2'	10:A:902:A:C8	2.50	0.46
10:A:1959:A:H2'	10:A:1960:G:O4'	2.16	0.46
33:a:1322:G:N7	52:t:3:ARG:NH2	2.62	0.46
10:A:650:U:OP1	16:I:102:PRO:HA	2.16	0.46
10:A:1826:G:O2'	14:G:180:GLU:OE2	2.30	0.46
33:a:519:C:O2'	33:a:520:U:H5''	2.14	0.46
10:A:2457:A:H2'	10:A:2457:A:N3	2.30	0.46
14:G:221:ARG:NH2	61:G:304:HOH:O	2.48	0.46
10:A:69:C:H4'	10:A:75:G:N7	2.31	0.46
10:A:878:C:H2'	10:A:879:U:C6	2.49	0.46
10:A:2101:U:H2'	10:A:2102:U:C6	2.50	0.46
33:a:69:G:N2	33:a:152:A:O2'	2.48	0.46
33:a:480:G:N3	49:q:89:LYS:NZ	2.64	0.46
33:a:1170:G:C2	33:a:1171:C:C6	3.04	0.46
33:a:1289:A:N3	33:a:1289:A:H2'	2.31	0.46
10:A:2672:G:H4'	10:A:2759:G:O2'	2.14	0.46
33:a:469:U:H2'	33:a:470:A:C8	2.49	0.46
33:a:1312:U:O4	46:n:14:ARG:NH1	2.49	0.46
10:A:651:A:H2'	10:A:652:A:C8	2.51	0.46
10:A:1044:A:H2'	10:A:1045:A:C8	2.50	0.46
10:A:2056:G:N1	10:A:2060:A:OP2	2.35	0.46
33:a:1110:G:HO2'	33:a:1111:C:P	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:h:77:ALA:HA	40:h:86:GLN:HA	1.98	0.46
5:5:16:ARG:NH2	10:A:1302:G:OP1	2.45	0.46
10:A:1674:U:H2'	10:A:1675:G:O4'	2.15	0.46
33:a:47:G:O2'	33:a:373:U:H1'	2.15	0.46
46:n:34:LEU:HD21	46:n:41:ALA:HA	1.97	0.46
10:A:565:G:H2'	10:A:566:U:O4'	2.15	0.46
4:4:19:THR:HG22	4:4:19:THR:O	2.16	0.46
10:A:1220:A:O2'	10:A:1221:C:H5'	2.16	0.46
13:E:510:HIS:HB2	13:E:568:ASP:HB3	1.97	0.46
18:K:59:LYS:O	18:K:63:THR:HG23	2.16	0.46
33:a:6:U:H1'	33:a:7:G:OP2	2.16	0.46
33:a:456:A:OP2	33:a:493:G:N2	2.36	0.46
41:i:108:THR:HG22	41:i:109:SER:N	2.31	0.46
10:A:944:G:H3'	10:A:945:A:H5''	1.98	0.46
33:a:85:U:O2	33:a:86:G:N1	2.49	0.46
10:A:2488:C:H2'	10:A:2489:U:C6	2.51	0.45
33:a:160:A:H2'	33:a:161:A:O4'	2.16	0.45
10:A:2664:U:H2'	10:A:2665:G:O4'	2.16	0.45
11:B:39:G:H3'	11:B:40:C:H5'	1.97	0.45
24:R:25:THR:HG22	24:R:26:ALA:N	2.30	0.45
32:Z:41:GLY:N	32:Z:72:ASP:OD1	2.44	0.45
33:a:177:G:OP1	53:u:59:LYS:NZ	2.39	0.45
10:A:922:G:N2	10:A:944:G:OP2	2.48	0.45
27:U:10:LYS:NZ	27:U:23:GLU:OE2	2.46	0.45
33:a:392:G:H2'	33:a:393:C:C6	2.51	0.45
4:4:31:SER:HB2	4:4:46:ILE:HD13	1.98	0.45
10:A:680:C:O2'	10:A:684:U:OP1	2.32	0.45
10:A:2130:A:N6	10:A:2214:G:O6	2.49	0.45
33:a:382:A:C6	33:a:383:U:C4	3.05	0.45
33:a:459:A:O4'	33:a:460:A:C2	2.70	0.45
4:4:13:ILE:CD1	4:4:43:TYR:HB2	2.46	0.45
10:A:83:G:H21	10:A:102:A:H2	1.64	0.45
10:A:1700:C:H2'	10:A:1701:U:H6	1.81	0.45
10:A:1916:A:H2'	10:A:1917:A:C8	2.50	0.45
13:E:202:ASP:OD1	13:E:202:ASP:N	2.49	0.45
33:a:409:C:O2'	33:a:629:A:N3	2.46	0.45
10:A:942:C:H3'	10:A:943:C:H5''	1.99	0.45
33:a:612:G:H2'	33:a:613:U:O4'	2.16	0.45
33:a:955:A:H2'	33:a:956:G:C8	2.52	0.45
33:a:983:A:OP1	47:o:29:ARG:NH2	2.47	0.45
10:A:154:A:O2'	10:A:155:U:P	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:27:A:H2'	11:B:28:C:C6	2.52	0.45
33:a:271:A:H2'	33:a:272:C:C6	2.52	0.45
33:a:627:U:H5	37:e:127:ASP:HB3	1.81	0.45
10:A:2050:A:H2'	10:A:2051:C:C6	2.52	0.45
10:A:2822:C:H4'	10:A:2823:G:OP2	2.16	0.45
33:a:425:G:N2	33:a:548:G:O2'	2.50	0.45
41:i:115:ASP:OD2	41:i:119:ARG:NH2	2.46	0.45
46:n:100:GLN:N	46:n:100:GLN:OE1	2.50	0.45
10:A:522:G:H4'	10:A:547:A:N1	2.32	0.45
10:A:921:C:H2'	10:A:922:G:O4'	2.17	0.45
33:a:1242:U:OP1	42:j:128:GLN:NE2	2.50	0.45
46:n:34:LEU:O	46:n:37:ALA:O	2.35	0.45
10:A:2051:C:H2'	10:A:2052:C:C6	2.52	0.44
10:A:2130:A:C6	10:A:2214:G:C6	3.05	0.44
15:H:131:ILE:HD11	15:H:149:ARG:HA	1.99	0.44
33:a:1272:A:H2'	33:a:1273:A:O4'	2.17	0.44
10:A:250:G:H4'	10:A:432:G:C5	2.52	0.44
12:D:55:U:O2	12:D:55:U:O4'	2.35	0.44
12:F:55:U:O2'	12:F:57:A:N7	2.45	0.44
16:I:132:GLU:OE1	16:I:132:GLU:N	2.49	0.44
24:R:11:ARG:HD3	24:R:97:GLY:O	2.17	0.44
33:a:437:U:H4'	33:a:438:A:O5'	2.16	0.44
33:a:999:C:O2'	33:a:1000:U:H5'	2.16	0.44
33:a:1355:U:OP1	42:j:124:ARG:NH1	2.50	0.44
36:d:52:SER:OG	36:d:111:ASP:OD2	2.32	0.44
48:p:39:VAL:HG11	48:p:56:LEU:HB2	1.99	0.44
10:A:1829:A:H2'	10:A:1830:A:C8	2.52	0.44
10:A:2336:A:C2'	10:A:2337:A:OP1	2.65	0.44
10:A:2617:A:H2'	10:A:2618:C:C6	2.53	0.44
10:A:2618:C:H2'	10:A:2619:G:C8	2.52	0.44
23:Q:44:VAL:O	23:Q:48:ILE:HG12	2.17	0.44
33:a:10:G:OP2	38:f:126:LYS:NZ	2.34	0.44
33:a:377:C:H2'	33:a:378:C:C6	2.51	0.44
33:a:736:A:H2'	33:a:737:A:C8	2.52	0.44
33:a:1088:G:N2	33:a:1091:A:OP2	2.46	0.44
33:a:1479:A:H2'	33:a:1480:A:O4'	2.17	0.44
48:p:26:GLU:OE1	48:p:26:GLU:N	2.41	0.44
10:A:272:C:O2	10:A:272:C:H2'	2.17	0.44
10:A:1805:U:H2'	10:A:1811:A:N6	2.31	0.44
10:A:2238:U:O2'	10:A:2239:A:OP1	2.32	0.44
10:A:2482:G:H2'	10:A:2483:C:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:166:ILE:HB	13:E:174:ALA:HB3	1.99	0.44
33:a:356:G:N1	33:a:357:A:C5	2.85	0.44
33:a:1085:G:O2'	33:a:1112:A:N1	2.40	0.44
39:g:36:GLU:OE1	39:g:36:GLU:N	2.50	0.44
10:A:623:C:H2'	10:A:624:C:C6	2.52	0.44
10:A:638:U:H2'	10:A:639:U:C6	2.52	0.44
10:A:1836:A:H2'	10:A:1837:A:C8	2.53	0.44
10:A:1874:A:O2'	10:A:1875:A:C8	2.71	0.44
10:A:2383:C:H2'	10:A:2384:U:O4'	2.17	0.44
12:D:19:G:N2	12:D:57:A:N3	2.66	0.44
33:a:1327:C:O2'	33:a:1328:A:C5'	2.66	0.44
33:a:1529:MA6:H92	33:a:1530:MA6:H93	2.00	0.44
10:A:5:A:H2'	10:A:6:A:C8	2.53	0.44
10:A:615:A:H5''	10:A:616:G:OP2	2.17	0.44
10:A:725:A:OP1	10:A:821:C:N4	2.47	0.44
10:A:1071:A:C2	10:A:2515:A:H5'	2.53	0.44
10:A:1996:A:H5'	10:A:1997:A:OP1	2.18	0.44
10:A:2341:A:H2'	10:A:2342:U:C6	2.52	0.44
10:A:2507:C:H2'	10:A:2508:G:H5'	2.00	0.44
33:a:1014:C:O2	33:a:1014:C:O4'	2.34	0.44
44:l:15:ASN:OD1	44:l:15:ASN:N	2.51	0.44
10:A:637:U:H2'	10:A:638:U:C6	2.53	0.44
10:A:679:G:H2'	10:A:680:C:C6	2.53	0.44
10:A:2421:C:N3	12:D:76:A:O2'	2.41	0.44
10:A:2705:U:H2'	10:A:2706:A:C8	2.52	0.44
10:A:2886:G:C2	10:A:2888:A:H1'	2.53	0.44
33:a:1329:A:C8	33:a:1333:G:C5	3.06	0.44
46:n:11:ARG:HA	46:n:45:VAL:CG2	2.48	0.44
10:A:365:A:OP1	16:I:168:ARG:HD2	2.18	0.44
10:A:837:G:H4'	10:A:838:A:C4	2.53	0.44
10:A:881:G:H2'	10:A:882:C:C6	2.52	0.44
10:A:1823:U:H2'	10:A:1824:C:H6	1.77	0.44
12:D:42:G:OP1	40:h:143:LYS:CE	2.64	0.44
13:E:138:ASP:OD2	13:E:260:THR:OG1	2.31	0.44
33:a:712:A:C4	33:a:713:G:C8	3.06	0.44
33:a:1079:G:OP1	33:a:1397:G:O2'	2.35	0.44
10:A:2570:G:H2'	10:A:2571:G:C8	2.53	0.44
33:a:715:U:H4'	44:l:22:HIS:CD2	2.52	0.44
33:a:716:A:O2'	33:a:717:U:O5'	2.34	0.44
33:a:1025:A:O2'	33:a:1227:U:O2'	2.36	0.44
33:a:1507:C:H2'	33:a:1508:G:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:21:LYS:NZ	6:6:28:GLU:O	2.51	0.43
10:A:2439:A:H2'	10:A:2440:G:O4'	2.18	0.43
24:R:41:TYR:CD1	24:R:41:TYR:N	2.86	0.43
33:a:1503:A:H5'	33:a:1504:A:OP2	2.18	0.43
36:d:11:ARG:NH2	36:d:176:THR:O	2.49	0.43
52:t:50:ALA:HB1	52:t:57:HIS:HB3	1.99	0.43
10:A:221:G:H22	10:A:238:U:H4'	1.84	0.43
29:W:19:ALA:HB1	29:W:24:LYS:HB2	2.00	0.43
33:a:1401:U:H2'	33:a:1402:G:C8	2.54	0.43
41:i:18:ASN:ND2	41:i:74:ILE:O	2.51	0.43
4:4:28:THR:O	4:4:30:THR:HG23	2.18	0.43
10:A:1314:A:H2'	10:A:1315:C:C6	2.53	0.43
10:A:2332:U:O2'	10:A:2333:U:P	2.77	0.43
28:V:82:LEU:HB2	28:V:98:LYS:HB2	2.00	0.43
33:a:74:G:O2'	33:a:95:A:N6	2.48	0.43
33:a:498:U:H2'	33:a:499:A:H8	1.83	0.43
33:a:1011:U:O2'	33:a:1012:G:H5'	2.18	0.43
10:A:2322:C:O2'	10:A:2323:U:H5'	2.18	0.43
10:A:2716:U:H5	61:A:3364:HOH:O	2.01	0.43
33:a:379:G:N3	33:a:381:A:N6	2.66	0.43
49:q:9:ARG:C	49:q:10:LEU:HD12	2.43	0.43
4:4:71:VAL:O	4:4:75:ASN:ND2	2.51	0.43
10:A:305:A:N6	10:A:410:G:H22	2.15	0.43
10:A:926:G:O6	10:A:928:C:N4	2.51	0.43
12:D:35:A:N1	34:b:14:A:C2	2.87	0.43
27:U:57:THR:O	27:U:101:ASN:N	2.41	0.43
33:a:1136:U:O2	33:a:1137:U:O2'	2.31	0.43
33:a:1282:U:H2'	33:a:1283:C:C6	2.53	0.43
10:A:92:G:H2'	10:A:93:U:C6	2.53	0.43
10:A:2319:U:H2'	10:A:2320:C:C6	2.53	0.43
18:K:126:GLU:N	18:K:126:GLU:OE1	2.51	0.43
33:a:563:C:H2'	33:a:564:C:C6	2.54	0.43
10:A:1423:C:H2'	10:A:1424:A:C8	2.53	0.43
10:A:2333:U:H2'	10:A:2334:G:N2	2.34	0.43
33:a:358:G:O2'	33:a:359:G:H5'	2.19	0.43
33:a:1366:G:H2'	33:a:1367:A:H8	1.83	0.43
10:A:154:A:H2'	10:A:155:U:O4'	2.18	0.43
10:A:2829:A:H2'	10:A:2830:A:C8	2.53	0.43
43:k:34:ALA:HB2	43:k:83:THR:HG21	2.00	0.43
10:A:872:U:OP2	61:A:3213:HOH:O	2.21	0.43
10:A:2077:C:OP1	61:A:3214:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:552:G:OP1	37:e:55:GLN:NE2	2.38	0.43
33:a:1136:U:C2	33:a:1138:G:C8	3.06	0.43
35:c:77:GLN:NE2	35:c:93:ASN:O	2.51	0.43
40:h:16:PRO:HA	42:j:48:LEU:HD22	2.00	0.43
10:A:346:A:H2'	10:A:347:U:C6	2.54	0.43
10:A:745:G:O2'	10:A:1676:A:N3	2.44	0.43
33:a:33:A:H2'	33:a:34:A:C8	2.54	0.43
38:f:15:VAL:O	38:f:15:VAL:HG23	2.18	0.43
41:i:20:VAL:HG12	41:i:20:VAL:O	2.19	0.43
48:p:19:GLU:O	48:p:20:THR:OG1	2.24	0.43
33:a:931:G:H2'	33:a:932:A:C8	2.54	0.42
33:a:1298:A:H2'	33:a:1299:A:O4'	2.19	0.42
35:c:118:GLU:OE2	35:c:152:ARG:NH2	2.52	0.42
39:g:28:GLY:O	39:g:32:THR:HG23	2.19	0.42
10:A:127:C:H2'	10:A:128:C:C6	2.53	0.42
10:A:1070:A:OP2	10:A:1178:C:O2'	2.29	0.42
10:A:1831:A:OP2	14:G:261:ARG:NH1	2.48	0.42
33:a:212:A:N6	33:a:229:C:H4'	2.34	0.42
33:a:693:G:O2'	33:a:694:U:H5'	2.18	0.42
33:a:1110:G:C2'	33:a:1111:C:O5'	2.67	0.42
10:A:942:C:O2	10:A:944:G:N2	2.53	0.42
10:A:1114:A:N7	10:A:1140:A:O2'	2.51	0.42
10:A:2672:G:C3'	10:A:2673:C:H5'	2.48	0.42
33:a:550:U:OP1	37:e:10:LYS:NZ	2.50	0.42
33:a:1287:C:O2'	33:a:1289:A:C8	2.73	0.42
33:a:1306:C:H4'	33:a:1312:U:O4	2.19	0.42
10:A:903:G:N3	10:A:2295:A:H2'	2.34	0.42
10:A:923:A:O2'	10:A:924:G:P	2.77	0.42
10:A:1208:A:H2'	10:A:1209:U:C6	2.54	0.42
10:A:1624:C:H2'	10:A:1625:U:C1'	2.49	0.42
10:A:1632:A:O2'	10:A:1633:A:H5'	2.19	0.42
10:A:2822:C:H3'	10:A:2823:G:H21	1.85	0.42
12:D:32:C:O2	12:D:32:C:O4'	2.36	0.42
13:E:673:ASP:OD2	13:E:674:HIS:ND1	2.40	0.42
45:m:98:GLY:O	45:m:109:HIS:ND1	2.47	0.42
10:A:1072:A:H2'	10:A:1073:A:C8	2.54	0.42
10:A:1680:U:H2'	10:A:1681:U:C6	2.54	0.42
10:A:2672:G:H3'	10:A:2673:C:H5'	2.00	0.42
13:E:315:LYS:HB3	13:E:327:PHE:HB2	2.01	0.42
26:T:58:ARG:HA	26:T:61:TRP:CE3	2.54	0.42
33:a:57:U:H2'	33:a:58:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:381:A:C2	33:a:382:A:N7	2.87	0.42
33:a:1030:G:O6	33:a:1032:C:N4	2.53	0.42
10:A:650:U:C5	10:A:665:G:C5	3.08	0.42
10:A:1222:A:H2'	10:A:1223:A:C8	2.54	0.42
10:A:2601:G:O2'	15:H:156:MET:HB3	2.19	0.42
10:A:2811:U:H2'	10:A:2812:U:C6	2.55	0.42
10:A:2820:U:O2	10:A:2820:U:O4'	2.36	0.42
33:a:407:G:H2'	33:a:408:C:C6	2.55	0.42
33:a:1422:C:H2'	33:a:1423:A:C8	2.55	0.42
50:r:29:THR:O	50:r:42:TYR:N	2.49	0.42
10:A:254:A:H2'	10:A:255:G:O4'	2.20	0.42
10:A:1453:G:H2'	10:A:1454:U:O4'	2.19	0.42
20:N:97:ARG:NH1	33:a:347:C:OP2	2.49	0.42
33:a:39:G:H22	33:a:405:A:H5'	1.85	0.42
33:a:376:U:O2	33:a:376:U:O4'	2.38	0.42
33:a:1010:U:H2'	33:a:1011:U:H6	1.85	0.42
10:A:768:A:H2'	10:A:769:U:O4'	2.20	0.42
33:a:244:G:H2'	33:a:245:C:O4'	2.18	0.42
33:a:1525:U:H2'	33:a:1526:C:C6	2.55	0.42
45:m:48:THR:N	45:m:67:ARG:O	2.53	0.42
10:A:56:A:H2'	10:A:57:C:O4'	2.20	0.42
10:A:165:C:O2'	10:A:166:A:H5'	2.19	0.42
11:B:62:U:O2'	11:B:63:U:H5'	2.20	0.42
15:H:55:ASP:OD1	15:H:85:LYS:NZ	2.53	0.42
33:a:34:A:H2'	33:a:35:C:C6	2.55	0.42
33:a:130:A:O2'	33:a:131:C:P	2.78	0.42
33:a:254:A:C2	33:a:290:A:C5	3.08	0.42
33:a:1021:A:H3'	33:a:1022:G:H5''	2.01	0.42
37:e:127:ASP:OD1	37:e:127:ASP:O	2.38	0.42
10:A:702:U:H2'	10:A:703:A:C8	2.55	0.42
10:A:1675:G:H1'	10:A:1679:A:N6	2.35	0.42
33:a:440:A:C4	33:a:441:A:C8	3.08	0.42
33:a:499:A:H2'	33:a:500:A:H8	1.85	0.42
33:a:1497:G:H2'	33:a:1498:G:C8	2.55	0.42
46:n:90:ARG:NE	46:n:96:PRO:O	2.50	0.42
10:A:160:G:H21	10:A:168:A:H2	1.68	0.41
10:A:464:U:H2'	10:A:465:C:C6	2.55	0.41
10:A:699:U:O2'	10:A:700:A:O5'	2.36	0.41
10:A:1161:A:O2'	10:A:1162:C:H5'	2.20	0.41
10:A:2704:A:H2'	10:A:2705:U:C6	2.54	0.41
23:Q:22:THR:HG21	23:Q:67:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:32:G:O2'	33:a:49:C:N4	2.52	0.41
33:a:384:G:H5''	49:q:6:ARG:HB2	2.02	0.41
33:a:439:A:C4	33:a:440:A:C8	3.07	0.41
33:a:885:A:H2'	33:a:886:C:C6	2.55	0.41
4:4:10:HIS:NE2	4:4:30:THR:HG22	2.34	0.41
10:A:302:A:H2'	10:A:303:G:C8	2.55	0.41
10:A:1031:C:H2'	10:A:1032:A:O4'	2.20	0.41
10:A:1280:U:H2'	10:A:1281:U:C6	2.56	0.41
13:E:572:HIS:N	13:E:576:SER:OG	2.49	0.41
12:F:33:U:OP2	42:j:132:ARG:NH2	2.45	0.41
19:M:143:LEU:O	19:M:144:ARG:HB2	2.20	0.41
33:a:36:G:H2'	33:a:37:C:C6	2.56	0.41
33:a:397:A:H3'	33:a:398:C:H6	1.84	0.41
33:a:547:A:H2'	33:a:548:G:C8	2.55	0.41
33:a:643:A:H2'	33:a:644:U:C6	2.55	0.41
33:a:1092:G:N7	38:f:52:LYS:NZ	2.68	0.41
33:a:1248:A:H2	33:a:1251:G:N3	2.18	0.41
4:4:13:ILE:HD12	4:4:43:TYR:HB2	2.02	0.41
10:A:165:C:H2'	10:A:166:A:C5'	2.50	0.41
10:A:892:U:C5	10:A:977:A:N1	2.89	0.41
10:A:973:A:H2'	10:A:974:U:C6	2.56	0.41
10:A:1356:G:O2'	10:A:1357:G:H5'	2.21	0.41
12:D:6:G:O2'	12:D:7:G:H5'	2.20	0.41
13:E:14:GLY:HA3	13:E:99:LEU:HD13	2.01	0.41
33:a:108:A:C6	33:a:335:A:C6	3.08	0.41
33:a:200:U:H2'	33:a:201:U:C6	2.55	0.41
4:4:48:LEU:HD21	17:J:106:VAL:HG22	2.03	0.41
10:A:1089:C:N4	10:A:1155:A:O2'	2.53	0.41
10:A:1519:U:O2'	10:A:1520:A:H5'	2.20	0.41
13:E:147:SER:O	13:E:150:THR:OG1	2.30	0.41
33:a:9:A:H5'	38:f:125:SER:O	2.19	0.41
33:a:363:C:C4	33:a:364:A:N7	2.88	0.41
33:a:877:C:H2'	33:a:878:A:O4'	2.21	0.41
10:A:922:G:N7	10:A:943:C:N4	2.69	0.41
10:A:1195:A:H2'	10:A:1196:C:O4'	2.21	0.41
10:A:1524:C:H2'	10:A:1525:U:O4'	2.19	0.41
33:a:50:U:O4	33:a:373:U:H5	2.03	0.41
33:a:262:G:C6	33:a:281:A:C6	3.09	0.41
41:i:108:THR:HG23	41:i:124:GLY:O	2.21	0.41
53:u:63:SER:O	53:u:64:ASN:HB2	2.21	0.41
10:A:1065:A:N3	10:A:1065:A:H3'	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1584:U:O2'	10:A:1585:G:O5'	2.36	0.41
33:a:9:A:N6	37:e:200:ARG:O	2.54	0.41
33:a:681:G:H2'	33:a:682:G:C8	2.56	0.41
33:a:1014:C:O2'	33:a:1015:A:O5'	2.31	0.41
35:c:186:ILE:O	35:c:186:ILE:HG22	2.21	0.41
4:4:31:SER:O	4:4:44:PRO:HB3	2.21	0.41
10:A:538:G:H2'	10:A:539:G:O4'	2.20	0.41
10:A:892:U:H5	10:A:977:A:N1	2.18	0.41
13:E:84:GLY:O	13:E:115:GLN:NE2	2.52	0.41
33:a:513:G:OP2	33:a:542:U:H2'	2.21	0.41
33:a:1022:G:N1	33:a:1025:A:OP2	2.50	0.41
10:A:65:A:H2'	10:A:66:C:C6	2.56	0.41
10:A:75:G:H22	10:A:110:A:H2	1.69	0.41
10:A:643:G:H2'	10:A:644:C:C6	2.56	0.41
10:A:1045:A:H2'	10:A:1046:G:O4'	2.21	0.41
10:A:1368:C:H2'	10:A:1370:C:C5	2.56	0.41
10:A:1457:U:O2'	10:A:1458:A:O5'	2.22	0.41
10:A:1844:G:H2'	10:A:1845:U:H5'	2.03	0.41
10:A:2043:U:H2'	10:A:2044:C:C6	2.56	0.41
10:A:2265:G:N3	10:A:2265:G:H2'	2.36	0.41
10:A:2817:A:H2'	10:A:2818:A:H8	1.86	0.41
13:E:36:ARG:O	13:E:37:ILE:C	2.63	0.41
13:E:502:GLY:HA2	34:b:17:U:O2	2.20	0.41
18:K:18:THR:HG23	18:K:25:THR:HG23	2.02	0.41
18:K:69:ARG:HD3	18:K:69:ARG:C	2.45	0.41
28:V:48:GLU:O	28:V:52:MET:HG2	2.21	0.41
33:a:366:U:N3	33:a:367:A:N7	2.68	0.41
33:a:513:G:H2'	33:a:514:G:C8	2.56	0.41
33:a:990:U:OP2	33:a:991:U:O2'	2.23	0.41
33:a:1450:U:H2'	33:a:1451:G:O4'	2.21	0.41
37:e:85:ASN:HA	37:e:88:ILE:HG12	2.02	0.41
38:f:105:VAL:O	38:f:105:VAL:HG13	2.20	0.41
46:n:32:LYS:O	46:n:35:GLU:HG2	2.20	0.41
10:A:805:G:H2'	10:A:806:A:O4'	2.21	0.41
15:H:139:GLY:HA3	15:H:147:PHE:O	2.21	0.41
18:K:121:ILE:HG21	18:K:144:LEU:HD13	2.02	0.41
24:R:11:ARG:HG3	24:R:99:TYR:CE1	2.56	0.41
33:a:90:C:HO2'	33:a:91:U:P	2.41	0.41
33:a:227:C:C2	33:a:228:A:C8	3.09	0.41
33:a:499:A:C2	33:a:500:A:C5	3.08	0.41
33:a:1102:U:C2	33:a:1106:U:C4	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:577:A:H4'	10:A:578:G:C8	2.56	0.40
10:A:1220:A:C2'	10:A:1221:C:H5'	2.51	0.40
10:A:1378:U:H1'	29:W:54:ASN:HB3	2.03	0.40
13:E:505:GLN:HG3	13:E:580:ALA:HB2	2.02	0.40
33:a:476:C:O2	33:a:476:C:O4'	2.38	0.40
46:n:23:TYR:O	46:n:65:VAL:HB	2.21	0.40
48:p:9:ASN:HA	48:p:12:ILE:HG12	2.03	0.40
7:7:25:THR:HG22	7:7:27:ASN:H	1.86	0.40
10:A:617:A:N6	10:A:2061:U:OP1	2.53	0.40
10:A:1546:A:H2'	10:A:1547:C:C6	2.56	0.40
10:A:1597:U:H2'	10:A:1598:U:C6	2.56	0.40
10:A:1651:C:H4'	10:A:1652:A:H5''	2.04	0.40
11:B:39:G:HO2'	11:B:40:C:P	2.40	0.40
15:H:189:ASP:HB3	15:H:194:VAL:HG23	2.03	0.40
33:a:182:A:H2'	33:a:183:U:H5'	2.03	0.40
33:a:184:A:N3	33:a:184:A:H2'	2.37	0.40
33:a:1157:C:O2	42:j:20:ARG:NH1	2.41	0.40
33:a:1287:C:H2'	33:a:1288:A:H5''	2.02	0.40
35:c:67:VAL:O	35:c:89:GLN:HB3	2.21	0.40
35:c:93:ASN:OD1	35:c:93:ASN:N	2.54	0.40
40:h:76:LYS:O	40:h:87:VAL:HG12	2.20	0.40
10:A:683:G:H2'	10:A:684:U:C6	2.56	0.40
10:A:748:U:H2'	10:A:749:G:O4'	2.21	0.40
10:A:1442:C:H2'	10:A:1443:A:C8	2.56	0.40
10:A:1539:A:H2'	10:A:1541:C:C5	2.56	0.40
10:A:2714:U:H2'	10:A:2715:G:O4'	2.20	0.40
33:a:302:C:OP1	33:a:618:G:O2'	2.32	0.40
33:a:388:G:C2	33:a:392:G:C6	3.10	0.40
33:a:445:U:O2'	33:a:446:G:H5'	2.22	0.40
33:a:771:G:H2'	33:a:772:C:C6	2.56	0.40
33:a:922:A:H4'	33:a:923:A:OP1	2.22	0.40
33:a:1444:A:H2'	33:a:1445:G:O4'	2.22	0.40
37:e:139:ILE:N	37:e:139:ILE:HD12	2.36	0.40
10:A:489:A:H1'	10:A:1240:U:O4'	2.21	0.40
10:A:604:G:O4'	26:T:48:ARG:NH2	2.55	0.40
10:A:996:G:C6	10:A:1010:G:C6	3.09	0.40
10:A:1476:G:H2'	10:A:1477:U:C6	2.55	0.40
10:A:2916:U:H2'	10:A:2917:U:C6	2.56	0.40
12:D:58:A:O2'	12:D:60:U:OP2	2.32	0.40
25:S:51:LYS:HG3	25:S:98:LYS:HE3	2.03	0.40
33:a:95:A:H8	33:a:95:A:O5'	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:146:G:C2	33:a:177:G:C5	3.10	0.40
37:e:182:ARG:NH2	37:e:186:PRO:O	2.52	0.40
10:A:164:A:O2'	10:A:165:C:P	2.79	0.40
10:A:326:A:H2'	10:A:327:G:O4'	2.20	0.40
10:A:2539:C:H2'	10:A:2540:A:O4'	2.21	0.40
12:D:23:C:C2	12:D:24:U:C5	3.09	0.40
12:D:65:C:C2'	12:D:66:C:H5'	2.52	0.40
13:E:251:VAL:HG12	13:E:251:VAL:O	2.22	0.40
33:a:459:A:H4'	33:a:460:A:O5'	2.21	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	1	59/62 (95%)	59 (100%)	0	0	100	100
2	2	63/69 (91%)	63 (100%)	0	0	100	100
3	3	54/59 (92%)	52 (96%)	2 (4%)	0	100	100
4	4	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
5	5	51/57 (90%)	49 (96%)	2 (4%)	0	100	100
6	6	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
7	7	41/45 (91%)	41 (100%)	0	0	100	100
8	8	62/66 (94%)	60 (97%)	2 (3%)	0	100	100
9	9	35/37 (95%)	35 (100%)	0	0	100	100
13	E	666/693 (96%)	649 (97%)	16 (2%)	1 (0%)	43	53
14	G	271/277 (98%)	265 (98%)	6 (2%)	0	100	100
15	H	214/220 (97%)	204 (95%)	10 (5%)	0	100	100
16	I	202/207 (98%)	200 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	J	174/179 (97%)	168 (97%)	6 (3%)	0	100	100
18	K	174/178 (98%)	169 (97%)	5 (3%)	0	100	100
19	M	142/145 (98%)	141 (99%)	1 (1%)	0	100	100
20	N	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
21	O	143/146 (98%)	138 (96%)	5 (4%)	0	100	100
22	P	134/144 (93%)	131 (98%)	3 (2%)	0	100	100
23	Q	118/122 (97%)	116 (98%)	2 (2%)	0	100	100
24	R	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
25	S	112/116 (97%)	110 (98%)	2 (2%)	0	100	100
26	T	114/118 (97%)	114 (100%)	0	0	100	100
27	U	99/102 (97%)	98 (99%)	1 (1%)	0	100	100
28	V	109/117 (93%)	108 (99%)	1 (1%)	0	100	100
29	W	87/91 (96%)	86 (99%)	1 (1%)	0	100	100
30	X	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
31	Y	92/217 (42%)	91 (99%)	1 (1%)	0	100	100
32	Z	82/94 (87%)	79 (96%)	3 (4%)	0	100	100
35	c	219/255 (86%)	210 (96%)	9 (4%)	0	100	100
36	d	202/217 (93%)	197 (98%)	5 (2%)	0	100	100
37	e	197/200 (98%)	194 (98%)	3 (2%)	0	100	100
38	f	154/166 (93%)	149 (97%)	5 (3%)	0	100	100
39	g	91/98 (93%)	85 (93%)	6 (7%)	0	100	100
40	h	144/156 (92%)	141 (98%)	3 (2%)	0	100	100
41	i	129/132 (98%)	124 (96%)	5 (4%)	0	100	100
42	j	126/132 (96%)	124 (98%)	2 (2%)	0	100	100
43	k	97/102 (95%)	94 (97%)	3 (3%)	0	100	100
44	l	116/129 (90%)	108 (93%)	8 (7%)	0	100	100
45	m	133/137 (97%)	128 (96%)	5 (4%)	0	100	100
46	n	111/121 (92%)	107 (96%)	3 (3%)	1 (1%)	14	16
47	o	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
48	p	84/89 (94%)	81 (96%)	3 (4%)	0	100	100
49	q	88/91 (97%)	84 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	r	78/87 (90%)	76 (97%)	2 (3%)	0	100	100
51	s	61/80 (76%)	61 (100%)	0	0	100	100
52	t	78/92 (85%)	76 (97%)	2 (3%)	0	100	100
53	u	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
All	All	6003/6468 (93%)	5848 (97%)	153 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
46	n	38	ASN
13	E	251	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	51/52 (98%)	51 (100%)	0	100	100
2	2	59/62 (95%)	59 (100%)	0	100	100
3	3	51/53 (96%)	51 (100%)	0	100	100
4	4	71/75 (95%)	65 (92%)	6 (8%)	10	11
5	5	48/50 (96%)	48 (100%)	0	100	100
6	6	46/47 (98%)	45 (98%)	1 (2%)	45	59
7	7	39/40 (98%)	38 (97%)	1 (3%)	40	53
8	8	55/57 (96%)	55 (100%)	0	100	100
9	9	35/35 (100%)	35 (100%)	0	100	100
13	E	559/579 (96%)	551 (99%)	8 (1%)	59	70
14	G	220/224 (98%)	219 (100%)	1 (0%)	81	87
15	H	174/177 (98%)	173 (99%)	1 (1%)	78	85
16	I	168/169 (99%)	168 (100%)	0	100	100
17	J	155/158 (98%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	K	153/155 (99%)	151 (99%)	2 (1%)	61	72
19	M	123/123 (100%)	123 (100%)	0	100	100
20	N	100/100 (100%)	100 (100%)	0	100	100
21	O	111/112 (99%)	109 (98%)	2 (2%)	51	64
22	P	113/119 (95%)	112 (99%)	1 (1%)	70	80
23	Q	101/102 (99%)	100 (99%)	1 (1%)	68	77
24	R	95/95 (100%)	95 (100%)	0	100	100
25	S	100/102 (98%)	100 (100%)	0	100	100
26	T	96/98 (98%)	96 (100%)	0	100	100
27	U	86/86 (100%)	85 (99%)	1 (1%)	63	74
28	V	90/94 (96%)	89 (99%)	1 (1%)	65	75
29	W	80/82 (98%)	80 (100%)	0	100	100
30	X	87/90 (97%)	85 (98%)	2 (2%)	44	57
31	Y	83/190 (44%)	83 (100%)	0	100	100
32	Z	65/75 (87%)	65 (100%)	0	100	100
35	c	192/221 (87%)	190 (99%)	2 (1%)	68	77
36	d	166/175 (95%)	163 (98%)	3 (2%)	51	64
37	e	174/175 (99%)	173 (99%)	1 (1%)	78	85
38	f	122/131 (93%)	122 (100%)	0	100	100
39	g	81/86 (94%)	80 (99%)	1 (1%)	63	74
40	h	126/132 (96%)	122 (97%)	4 (3%)	34	46
41	i	112/113 (99%)	108 (96%)	4 (4%)	31	42
42	j	106/109 (97%)	104 (98%)	2 (2%)	50	63
43	k	89/91 (98%)	88 (99%)	1 (1%)	65	75
44	l	94/104 (90%)	91 (97%)	3 (3%)	34	46
45	m	117/119 (98%)	117 (100%)	0	100	100
46	n	98/104 (94%)	93 (95%)	5 (5%)	21	29
47	o	52/53 (98%)	51 (98%)	1 (2%)	50	63
48	p	79/81 (98%)	77 (98%)	2 (2%)	42	54
49	q	76/77 (99%)	73 (96%)	3 (4%)	28	40
50	r	75/82 (92%)	75 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	s	56/68 (82%)	55 (98%)	1 (2%)	51	64
52	t	70/80 (88%)	69 (99%)	1 (1%)	59	70
53	u	67/69 (97%)	65 (97%)	2 (3%)	36	48
All	All	5166/5471 (94%)	5102 (99%)	64 (1%)	61	74

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	4	27	SER
4	4	33	GLU
4	4	43	TYR
4	4	71	VAL
4	4	76	LYS
4	4	77	LYS
6	6	1	MET
7	7	44	SER
13	E	68	THR
13	E	423	MET
13	E	429	LYS
13	E	431	GLN
13	E	436	THR
13	E	495	LYS
13	E	500	SER
13	E	577	SER
14	G	65	ILE
15	H	200	ASN
18	K	25	THR
18	K	176	THR
21	O	87	ASP
21	O	145	VAL
22	P	77	LYS
23	Q	75	ASP
27	U	57	THR
28	V	11	ARG
30	X	70	LEU
30	X	101	ILE
35	c	83	GLU
35	c	151	ILE
36	d	57	GLU
36	d	195	LEU
36	d	197	VAL

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Mol	Chain	Res	Type
37	e	3	ARG
39	g	66	LYS
40	h	75	VAL
40	h	78	ARG
40	h	84	ASN
40	h	89	VAL
41	i	25	LEU
41	i	53	GLU
41	i	54	ASP
41	i	77	LEU
42	j	70	HIS
42	j	93	ASP
43	k	14	ASP
44	l	36	ASP
44	l	119	ASN
44	l	129	VAL
46	n	3	ARG
46	n	13	LYS
46	n	43	THR
46	n	48	LEU
46	n	49	THR
47	o	57	ARG
48	p	29	ILE
48	p	73	LYS
49	q	14	ARG
49	q	82	LYS
49	q	83	LYS
51	s	61	THR
52	t	18	LYS
53	u	3	ASN
53	u	28	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	36	GLN
4	4	75	ASN
13	E	122	GLN
13	E	357	GLN
13	E	359	HIS
13	E	447	GLN
13	E	640	GLN

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Mol	Chain	Res	Type
14	G	61	GLN
14	G	134	ASN
14	G	153	GLN
14	G	163	GLN
14	G	194	GLN
15	H	103	GLN
15	H	134	HIS
15	H	181	GLN
16	I	141	ASN
16	I	188	ASN
17	J	37	ASN
18	K	38	ASN
18	K	64	ASN
20	N	72	ASN
26	T	108	GLN
27	U	63	ASN
30	X	8	ASN
30	X	76	ASN
32	Z	86	GLN
36	d	61	ASN
36	d	99	HIS
36	d	101	ASN
37	e	158	ASN
39	g	27	ASN
40	h	19	ASN
41	i	48	ASN
44	l	77	HIS
46	n	91	HIS
46	n	105	ASN
48	p	46	HIS
53	u	69	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	2841/2923 (97%)	321 (11%)	14 (0%)
11	B	112/115 (97%)	18 (16%)	0
12	D	76/77 (98%)	18 (23%)	0
12	F	75/77 (97%)	9 (12%)	0
33	a	1523/1555 (97%)	228 (14%)	0
34	b	7/24 (29%)	3 (42%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4634/4771 (97%)	597 (12%)	14 (0%)

All (597) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	34	U
10	A	63	U
10	A	64	A
10	A	71	A
10	A	75	G
10	A	89	U
10	A	90	A
10	A	117	A
10	A	118	A
10	A	119	U
10	A	155	U
10	A	164	A
10	A	165	C
10	A	167	U
10	A	168	A
10	A	176	A
10	A	199	A
10	A	218	G
10	A	219	A
10	A	224	A
10	A	225	A
10	A	232	U
10	A	251	G
10	A	255	G
10	A	261	C
10	A	269	G
10	A	284	C
10	A	285	U
10	A	286	U
10	A	289	U
10	A	312	A
10	A	313	U
10	A	314	A
10	A	315	C
10	A	321	U
10	A	324	A
10	A	327	G

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Mol	Chain	Res	Type
10	A	354	A
10	A	373	A
10	A	404	U
10	A	410	G
10	A	411	A
10	A	432	G
10	A	457	G
10	A	458	A
10	A	497	U
10	A	502	C
10	A	527	G
10	A	550	A
10	A	553	A
10	A	575	G
10	A	576	U
10	A	577	A
10	A	578	G
10	A	583	A
10	A	590	U
10	A	592	A
10	A	593	U
10	A	594	G
10	A	606	G
10	A	616	G
10	A	618	A
10	A	630	G
10	A	646	A
10	A	650	U
10	A	682	A
10	A	683	G
10	A	690	U
10	A	699	U
10	A	700	A
10	A	731	U
10	A	762	C
10	A	767	A
10	A	774	G
10	A	775	A
10	A	792	5MU
10	A	809	A
10	A	810	A
10	A	820	G

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Mol	Chain	Res	Type
10	A	827	A
10	A	829	U
10	A	835	U
10	A	837	G
10	A	850	G
10	A	857	C
10	A	872	U
10	A	873	U
10	A	904	G
10	A	911	A
10	A	919	G
10	A	923	A
10	A	924	G
10	A	925	G
10	A	927	G
10	A	941	A
10	A	943	C
10	A	945	A
10	A	955	A
10	A	970	U
10	A	971	U
10	A	972	A
10	A	985	A
10	A	989	A
10	A	990	G
10	A	1005	G
10	A	1018	A
10	A	1027	A
10	A	1040	A
10	A	1049	C
10	A	1056	U
10	A	1057	A
10	A	1066	G
10	A	1070	A
10	A	1077	U
10	A	1090	A
10	A	1091	G
10	A	1111	A
10	A	1114	A
10	A	1119	C
10	A	1121	A
10	A	1128	A

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Mol	Chain	Res	Type
10	A	1129	A
10	A	1132	A
10	A	1134	U
10	A	1141	U
10	A	1156	G
10	A	1172	A
10	A	1176	U
10	A	1179	C
10	A	1180	G
10	A	1186	A
10	A	1199	A
10	A	1216	U
10	A	1218	G
10	A	1221	C
10	A	1222	A
10	A	1276	G
10	A	1291	A
10	A	1292	A
10	A	1294	G
10	A	1309	G
10	A	1310	A
10	A	1318	G
10	A	1337	A
10	A	1339	U
10	A	1402	A
10	A	1405	G
10	A	1415	A
10	A	1416	U
10	A	1421	A
10	A	1449	A
10	A	1455	U
10	A	1457	U
10	A	1458	A
10	A	1459	A
10	A	1463	A
10	A	1464	U
10	A	1471	A
10	A	1472	C
10	A	1477	U
10	A	1490	G
10	A	1497	A
10	A	1498	U

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Mol	Chain	Res	Type
10	A	1504	U
10	A	1507	A
10	A	1511	C
10	A	1518	G
10	A	1526	G
10	A	1530	A
10	A	1533	A
10	A	1536	C
10	A	1553	A
10	A	1560	A
10	A	1569	G
10	A	1578	A
10	A	1580	A
10	A	1581	U
10	A	1582	U
10	A	1583	G
10	A	1585	G
10	A	1587	C
10	A	1594	U
10	A	1606	C
10	A	1613	G
10	A	1616	A
10	A	1625	U
10	A	1630	A
10	A	1631	G
10	A	1642	C
10	A	1651	C
10	A	1652	A
10	A	1654	A
10	A	1690	A
10	A	1691	G
10	A	1692	C
10	A	1718	G
10	A	1740	G
10	A	1759	G
10	A	1772	G
10	A	1790	G
10	A	1791	G
10	A	1800	A
10	A	1803	G
10	A	1809	C
10	A	1818	A

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Mol	Chain	Res	Type
10	A	1827	C
10	A	1828	U
10	A	1843	U
10	A	1856	A
10	A	1899	U
10	A	1900	G
10	A	1909	C
10	A	1933	G
10	A	1934	G
10	A	1940	A
10	A	1941	C
10	A	1943	A
10	A	1956	G
10	A	1957	G
10	A	1963	A
10	A	1964	A
10	A	1965	A
10	A	1982	U
10	A	1994	C
10	A	1997	A
10	A	1998	A
10	A	1999	G
10	A	2020	U
10	A	2040	A
10	A	2050	A
10	A	2058	A
10	A	2059	G
10	A	2060	A
10	A	2070	C
10	A	2082	C
10	A	2083	G
10	A	2087	A
10	A	2088	G
10	A	2089	A
10	A	2096	G
10	A	2120	G
10	A	2123	A
10	A	2209	G
10	A	2215	U
10	A	2217	G
10	A	2225	A
10	A	2231	C

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Mol	Chain	Res	Type
10	A	2238	U
10	A	2239	A
10	A	2252	A
10	A	2265	G
10	A	2266	G
10	A	2295	A
10	A	2306	G
10	A	2310	C
10	A	2314	A
10	A	2333	U
10	A	2334	G
10	A	2335	G
10	A	2336	A
10	A	2337	A
10	A	2347	A
10	A	2349	A
10	A	2352	G
10	A	2361	U
10	A	2362	A
10	A	2374	C
10	A	2377	C
10	A	2406	G
10	A	2410	G
10	A	2412	C
10	A	2429	U
10	A	2433	C
10	A	2449	C
10	A	2450	U
10	A	2452	A
10	A	2455	G
10	A	2456	G
10	A	2457	A
10	A	2458	U
10	A	2462	A
10	A	2468	C
10	A	2475	A
10	A	2529	G
10	A	2532	G
10	A	2545	A
10	A	2556	G
10	A	2575	G
10	A	2581	U

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Mol	Chain	Res	Type
10	A	2593	A
10	A	2594	G
10	A	2600	C
10	A	2605	G
10	A	2613	C
10	A	2629	A
10	A	2637	C
10	A	2640	U
10	A	2657	G
10	A	2690	G
10	A	2692	A
10	A	2716	U
10	A	2718	C
10	A	2741	G
10	A	2753	U
10	A	2760	A
10	A	2775	A
10	A	2792	A
10	A	2793	G
10	A	2805	A
10	A	2818	A
10	A	2821	U
10	A	2823	G
10	A	2824	G
10	A	2827	A
10	A	2828	U
10	A	2852	U
10	A	2887	G
10	A	2892	G
10	A	2900	C
10	A	2903	A
10	A	2913	G
11	B	10	U
11	B	11	A
11	B	22	G
11	B	23	U
11	B	24	C
11	B	25	A
11	B	26	C
11	B	30	U
11	B	39	G
11	B	40	C

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Mol	Chain	Res	Type
11	B	41	C
11	B	43	A
11	B	54	U
11	B	55	A
11	B	85	U
11	B	87	C
11	B	88	G
11	B	106	G
12	D	4	G
12	D	8	U
12	D	11	A
12	D	16	C
12	D	17(A)	U
12	D	19	G
12	D	20	U
12	D	21	A
12	D	22	G
12	D	33	U
12	D	35	A
12	D	43	A
12	D	46	G
12	D	47	U
12	D	56	C
12	D	58	A
12	D	66	C
12	D	76	A
12	F	9	G
12	F	17(A)	U
12	F	19	G
12	F	21	A
12	F	43	A
12	F	47	U
12	F	48	C
12	F	58	A
12	F	76	A
33	a	6	U
33	a	7	G
33	a	10	G
33	a	14	U
33	a	33	A
33	a	40	G
33	a	48	C

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Mol	Chain	Res	Type
33	a	49	C
33	a	51	A
33	a	52	A
33	a	74	G
33	a	75	A
33	a	81	A
33	a	82	G
33	a	83	C
33	a	84	U
33	a	85	U
33	a	87	C
33	a	89	U
33	a	91	U
33	a	94	G
33	a	97	G
33	a	119	A
33	a	120	C
33	a	131	C
33	a	163	C
33	a	164	C
33	a	183	U
33	a	190	A
33	a	205	A
33	a	210	A
33	a	212	A
33	a	213	G
33	a	220	U
33	a	221	U
33	a	222	G
33	a	234	A
33	a	248	U
33	a	249	G
33	a	253	U
33	a	255	G
33	a	259	G
33	a	274	G
33	a	275	C
33	a	278	A
33	a	297	G
33	a	329	A
33	a	336	C
33	a	340	G

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Mol	Chain	Res	Type
33	a	355	G
33	a	356	G
33	a	360	C
33	a	362	G
33	a	375	U
33	a	376	U
33	a	380	C
33	a	381	A
33	a	392	G
33	a	405	A
33	a	414	G
33	a	417	U
33	a	419	A
33	a	420	U
33	a	421	G
33	a	429	U
33	a	432	G
33	a	437	U
33	a	438	A
33	a	447	U
33	a	456	A
33	a	460	A
33	a	461	C
33	a	466	G
33	a	468	G
33	a	486	C
33	a	490	A
33	a	492	G
33	a	493	G
33	a	503	A
33	a	505	A
33	a	517	A
33	a	519	C
33	a	520	U
33	a	526	C
33	a	529	G
33	a	533	C
33	a	534	C
33	a	535	G7M
33	a	540	A
33	a	541	A
33	a	555	A

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Mol	Chain	Res	Type
33	a	567	A
33	a	572	U
33	a	580	A
33	a	581	A
33	a	584	C
33	a	585	G
33	a	641	U
33	a	661	U
33	a	669	G
33	a	673	A
33	a	695	A
33	a	696	G
33	a	709	C
33	a	711	G
33	a	717	U
33	a	731	U
33	a	732	G
33	a	755	U
33	a	757	A
33	a	763	G
33	a	771	G
33	a	785	A
33	a	801	U
33	a	802	A
33	a	817	G
33	a	823	A
33	a	825	C
33	a	827	A
33	a	836	A
33	a	881	A
33	a	883	G
33	a	923	A
33	a	924	A
33	a	935	G
33	a	936	G
33	a	940	C
33	a	943	C
33	a	944	A
33	a	969	U
33	a	978	A
33	a	980	G
33	a	981	C

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Mol	Chain	Res	Type
33	a	984	A
33	a	985	G
33	a	986	A
33	a	992	A
33	a	993	C
33	a	1001	U
33	a	1002	G
33	a	1013	A
33	a	1015	A
33	a	1016	A
33	a	1017	C
33	a	1018	U
33	a	1019	C
33	a	1022	G
33	a	1026	U
33	a	1030	G
33	a	1035	C
33	a	1036	C
33	a	1046	G
33	a	1048	C
33	a	1050	A
33	a	1051	A
33	a	1056	C
33	a	1057	A
33	a	1076	U
33	a	1096	U
33	a	1105	G
33	a	1106	U
33	a	1111	C
33	a	1112	A
33	a	1113	A
33	a	1114	C
33	a	1134	A
33	a	1141	A
33	a	1143	C
33	a	1145	U
33	a	1149	G
33	a	1152	G
33	a	1156	A
33	a	1167	A
33	a	1168	C
33	a	1169	U

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Mol	Chain	Res	Type
33	a	1174	G
33	a	1175	U
33	a	1176	G
33	a	1177	A
33	a	1178	C
33	a	1179	A
33	a	1194	G
33	a	1197	G
33	a	1206	A
33	a	1207	A
33	a	1223	A
33	a	1229	U
33	a	1237	A
33	a	1248	A
33	a	1266	C
33	a	1267	A
33	a	1289	A
33	a	1290	A
33	a	1296	U
33	a	1297	A
33	a	1302	U
33	a	1303	G
33	a	1309	A
33	a	1310	G
33	a	1312	U
33	a	1328	A
33	a	1329	A
33	a	1330	C
33	a	1346	U
33	a	1348	G
33	a	1363	G
33	a	1374	U
33	a	1389	G
33	a	1398	U
33	a	1399	C
33	a	1404	A
33	a	1407	C
33	a	1408	A
33	a	1416	U
33	a	1452	G
33	a	1456	A
33	a	1460	U

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Mol	Chain	Res	Type
33	a	1463	U
33	a	1464	A
33	a	1503	A
33	a	1504	A
33	a	1505	G
33	a	1513	A
33	a	1517	U
33	a	1528	G
33	a	1540	G
33	a	1541	G
33	a	1543	U
34	b	13	A
34	b	14	A
34	b	19	G

All (14) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	130	A
10	A	154	A
10	A	312	A
10	A	809	A
10	A	827	A
10	A	1113	A
10	A	1179	C
10	A	1291	A
10	A	2336	A
10	A	2449	C
10	A	2457	A
10	A	2817	A
10	A	2822	C
10	A	2827	A

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

14 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
33	UR3	a	1509	33	19,22,23	0.30	0	26,32,35	0.30	0
33	2MG	a	975	33	23,26,27	0.27	0	33,38,41	0.32	0
10	5MU	A	1966	10	19,22,23	0.31	0	27,32,35	0.43	0
10	OMG	A	2278	55,10,12	23,26,27	0.44	0	32,38,41	0.38	0
33	MA6	a	1529	33	23,26,27	0.30	0	33,38,41	0.61	1 (3%)
33	G7M	a	535	33	23,26,27	0.34	0	34,39,42	0.79	2 (5%)
33	MA6	a	1530	33	23,26,27	0.30	0	33,38,41	0.59	1 (3%)
10	H2U	A	2476	10	18,21,22	0.30	0	19,30,33	0.44	0
10	2MA	A	2530	55,10	22,25,26	1.14	2 (9%)	32,37,40	1.41	3 (9%)
33	5MC	a	976	33	19,22,23	0.37	0	26,32,35	0.80	1 (3%)
10	2MG	A	2472	10	23,26,27	0.49	0	33,38,41	0.33	0
10	3TD	A	1942	10	19,22,23	0.54	0	23,32,35	0.59	0
33	4OC	a	1412	55,33	20,23,24	0.31	0	25,32,35	0.47	0
10	5MU	A	792	10	19,22,23	0.31	0	27,32,35	0.37	0

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
33	UR3	a	1509	33	-	0/7/25/26	0/2/2/2
33	2MG	a	975	33	-	0/9/27/28	0/3/3/3
10	5MU	A	1966	10	-	0/7/25/26	0/2/2/2
10	OMG	A	2278	55,10,12	-	0/9/27/28	0/3/3/3
33	MA6	a	1529	33	-	0/11/29/30	0/3/3/3
33	G7M	a	535	33	-	3/7/25/26	0/3/3/3
33	MA6	a	1530	33	-	3/11/29/30	0/3/3/3
10	H2U	A	2476	10	-	0/7/38/39	0/2/2/2
10	2MA	A	2530	55,10	-	2/7/25/26	0/3/3/3
33	5MC	a	976	33	-	0/7/25/26	0/2/2/2
10	2MG	A	2472	10	-	0/9/27/28	0/3/3/3
10	3TD	A	1942	10	-	0/7/25/26	0/2/2/2
33	4OC	a	1412	55,33	-	0/9/29/30	0/2/2/2
10	5MU	A	792	10	-	0/7/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2530	2MA	C6-N6	-4.20	1.23	1.34
10	A	2530	2MA	C2-N3	-2.09	1.30	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2530	2MA	N6-C6-N1	4.43	123.01	117.03
10	A	2530	2MA	C2-N1-C6	4.37	124.82	118.10
10	A	2530	2MA	C5-C6-N1	-4.09	112.54	118.90
33	a	535	G7M	O3'-C3'-C4'	2.87	119.33	111.08
33	a	976	5MC	O4'-C1'-N1	2.60	114.25	108.36
33	a	535	G7M	O3'-C3'-C2'	2.52	119.89	111.82
33	a	1530	MA6	C2-N1-C6	2.28	117.39	111.83
33	a	1529	MA6	C2-N1-C6	2.26	117.36	111.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	a	535	G7M	C3'-C4'-C5'-O5'
33	a	1530	MA6	O4'-C4'-C5'-O5'
33	a	535	G7M	O4'-C4'-C5'-O5'
33	a	1530	MA6	C3'-C4'-C5'-O5'
33	a	535	G7M	C4'-C5'-O5'-P
10	A	2530	2MA	O4'-C4'-C5'-O5'
10	A	2530	2MA	C4'-C5'-O5'-P
33	a	1530	MA6	C4'-C5'-O5'-P

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1966	5MU	1	0
10	A	2278	OMG	1	0
33	a	1529	MA6	1	0
33	a	1530	MA6	2	0
10	A	792	5MU	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 153 ligands modelled in this entry, 149 are monoatomic - leaving 4 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	WUX	E	703	-	42,43,43	0.46	0	52,68,68	0.69	0
58	GDP	E	701	55	29,30,30	0.44	0	45,47,47	0.42	0
56	SPD	A	3001	-	9,9,9	0.11	0	8,8,8	0.26	0
57	PUT	A	3002	-	5,5,5	0.13	0	4,4,4	0.09	0

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	WUX	E	703	-	-	3/16/99/99	0/5/5/5
58	GDP	E	701	55	-	3/16/32/32	0/3/3/3
56	SPD	A	3001	-	-	1/7/7/7	-
57	PUT	A	3002	-	-	1/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	E	701	GDP	C5'-O5'-PA-O3A
59	E	703	WUX	C23-C22-C29-O4
59	E	703	WUX	C23-C22-C29-O5
58	E	701	GDP	O4'-C4'-C5'-O5'
59	E	703	WUX	C22-C23-C24-C25
58	E	701	GDP	C3'-C4'-C5'-O5'
57	A	3002	PUT	C1-C2-C3-C4

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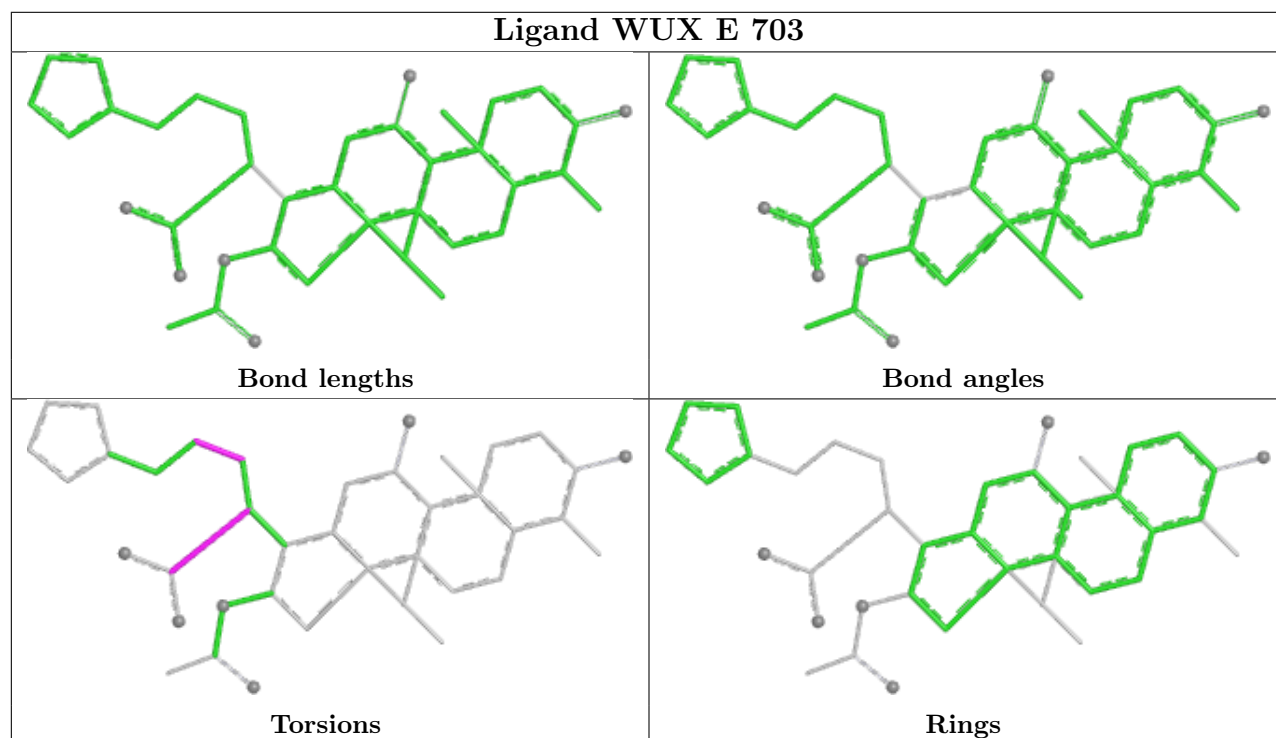
Mol	Chain	Res	Type	Atoms
56	A	3001	SPD	C8-C7-N6-C5

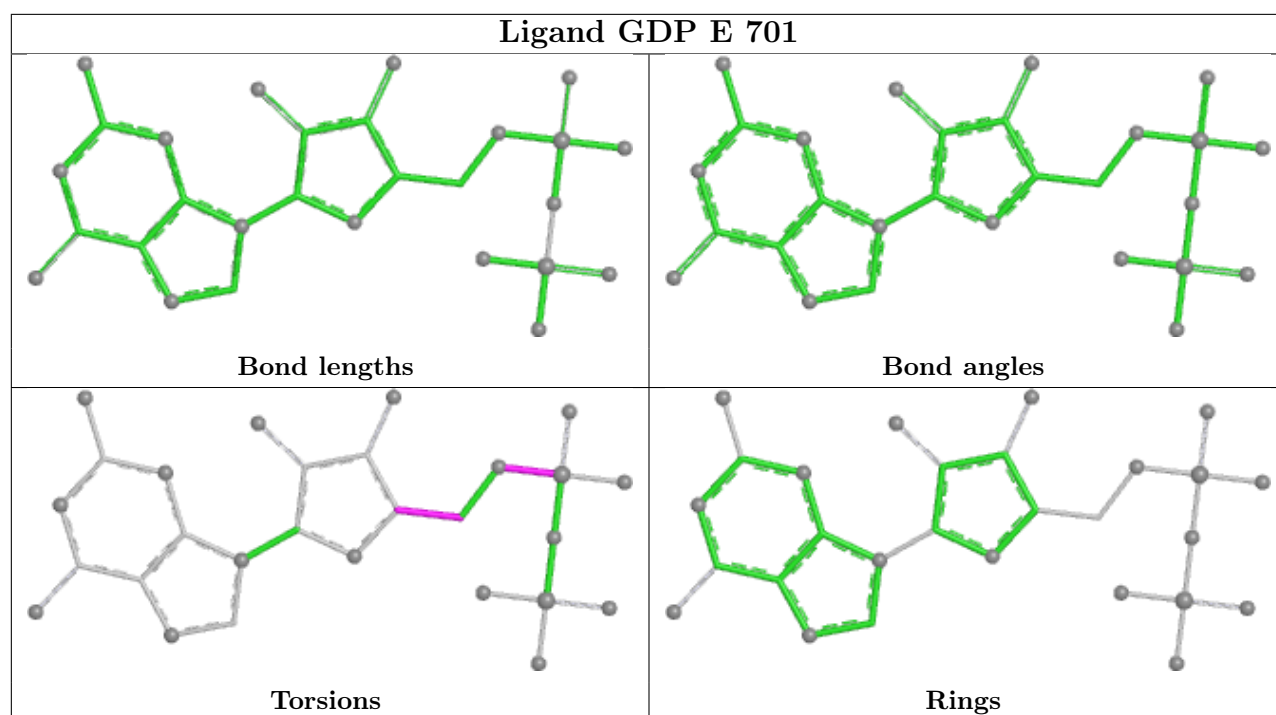
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	E	703	WUX	1	0

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.

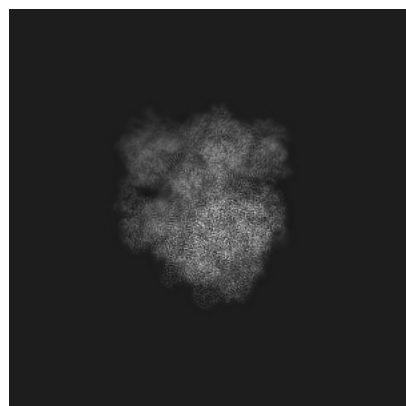
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17363. These allow visual inspection of the internal detail of the map and identification of artifacts.

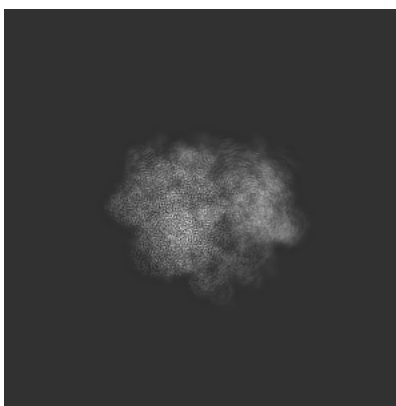
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

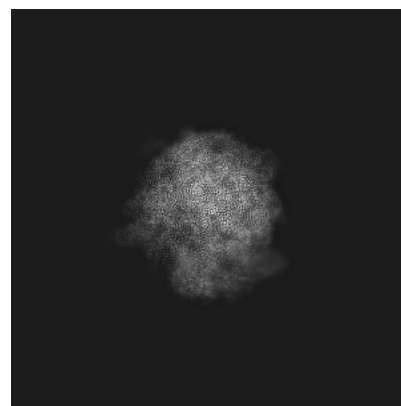
6.1.1 Primary map



X

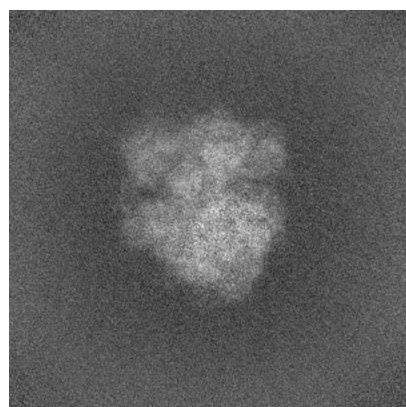


Y

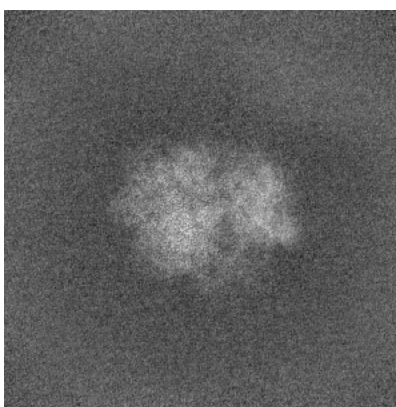


Z

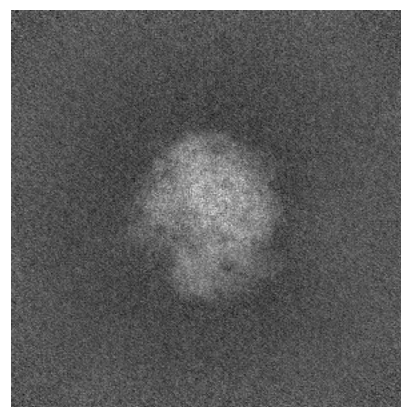
6.1.2 Raw map



X



Y



Z

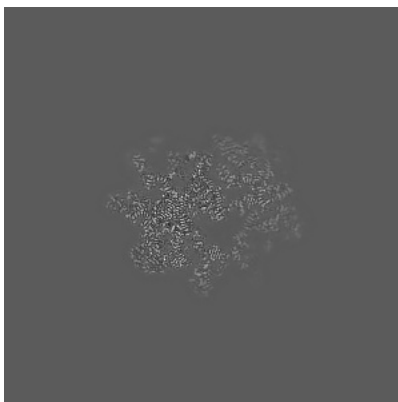
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 350

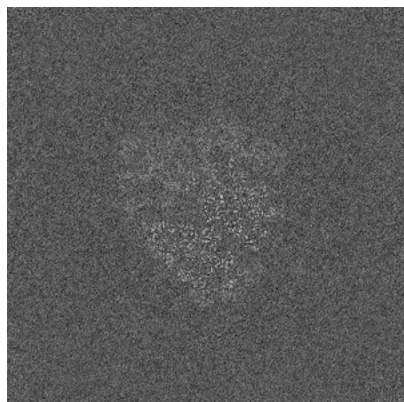


Y Index: 350

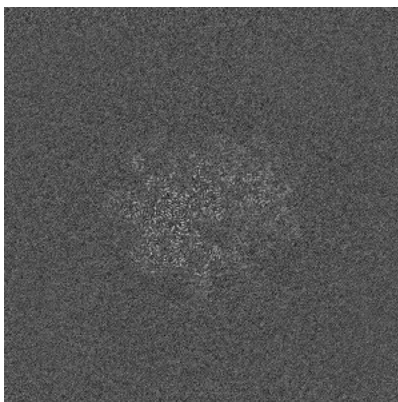


Z Index: 350

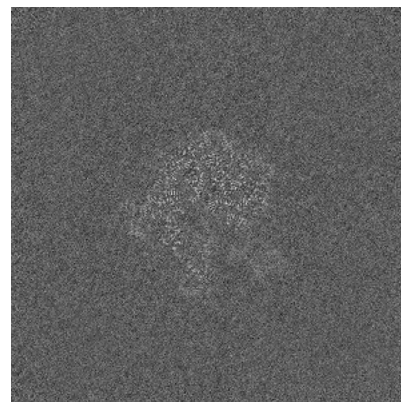
6.2.2 Raw map



X Index: 350



Y Index: 350

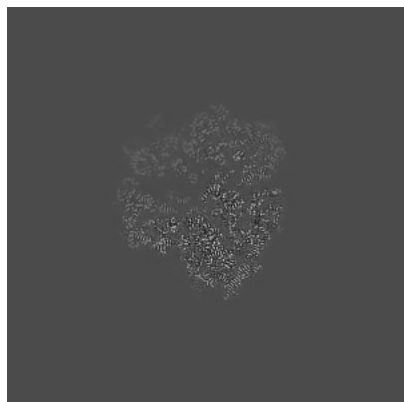


Z Index: 350

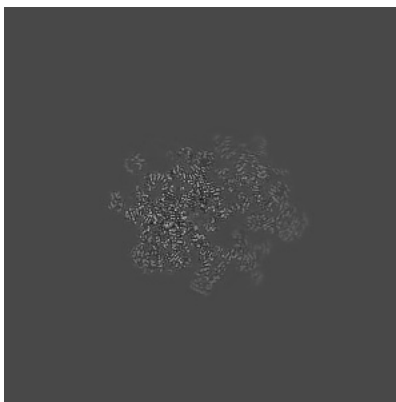
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 334

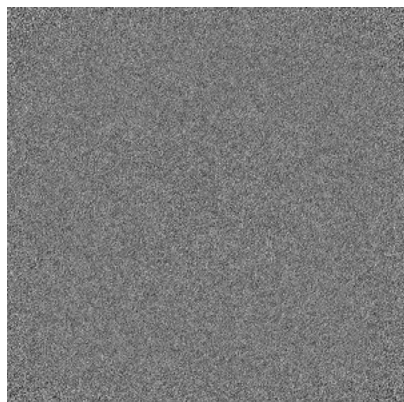


Y Index: 357

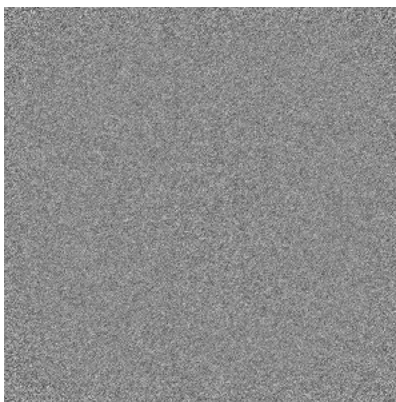


Z Index: 293

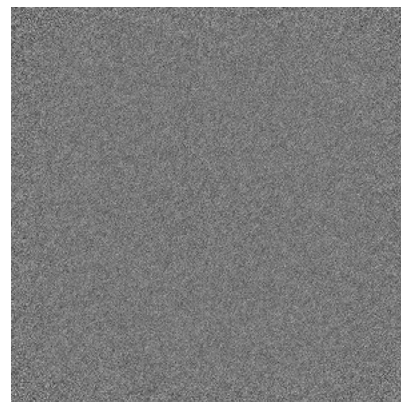
6.3.2 Raw map



X Index: 0



Y Index: 0

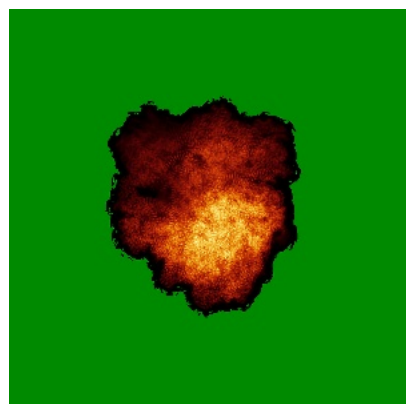


Z Index: 0

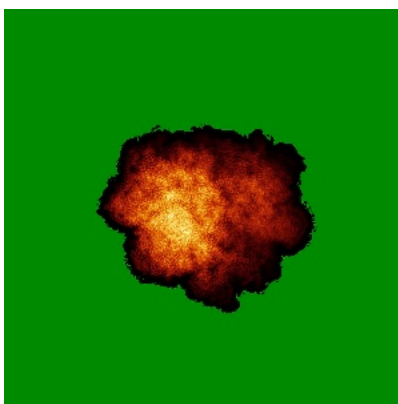
The images above show the largest variance slices of the map in three orthogonal directions.

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

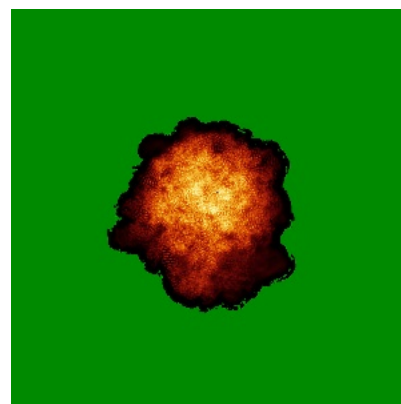
6.4.1 Primary map



X

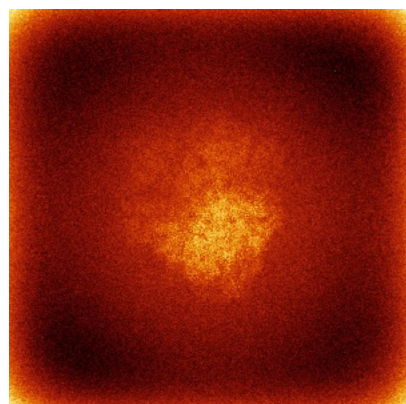


Y

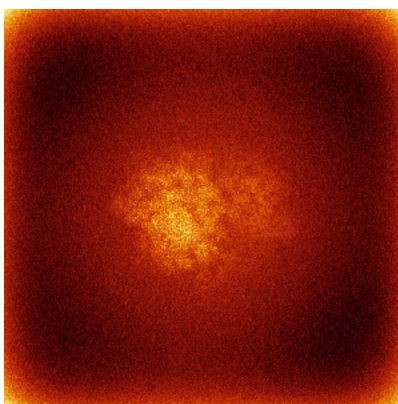


Z

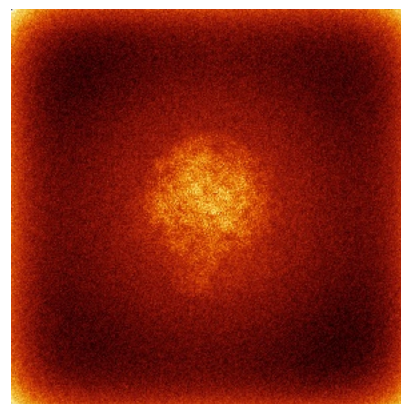
6.4.2 Raw map



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.

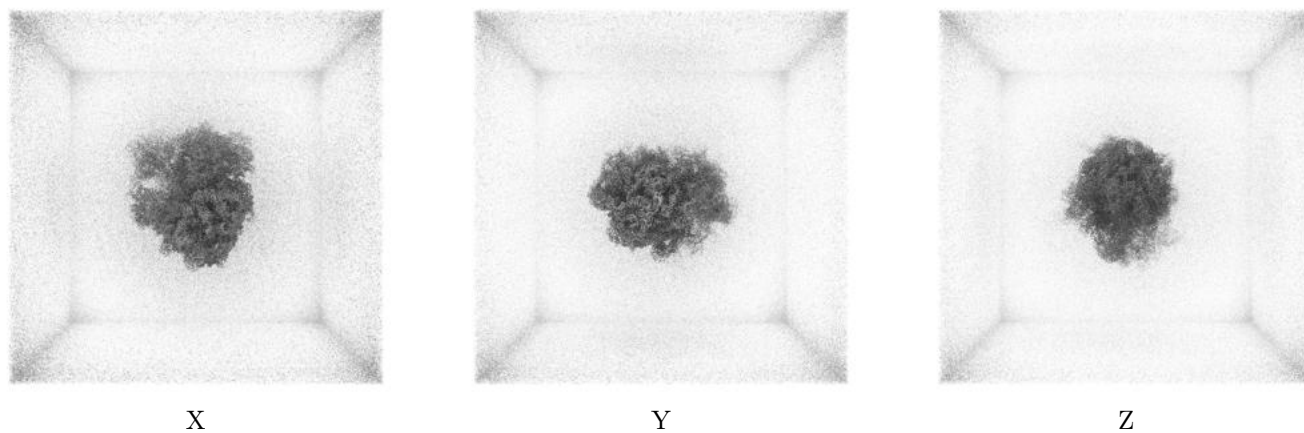
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

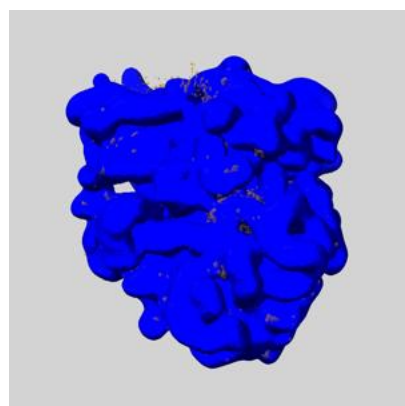
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

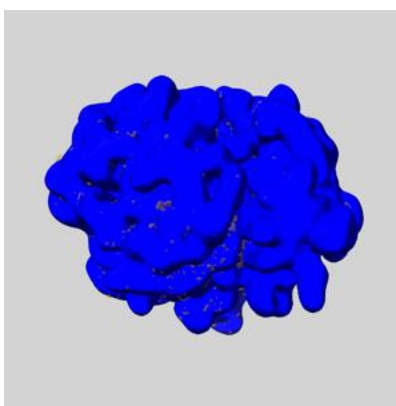
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

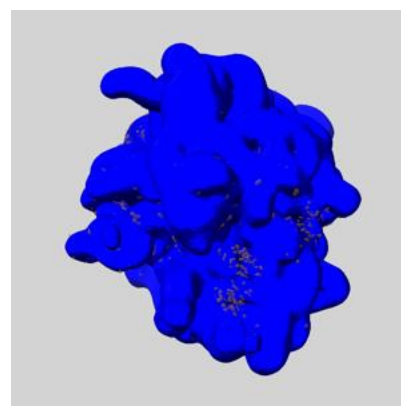
6.6.1 emd_17363_msk_1.map [i](#)



X



Y

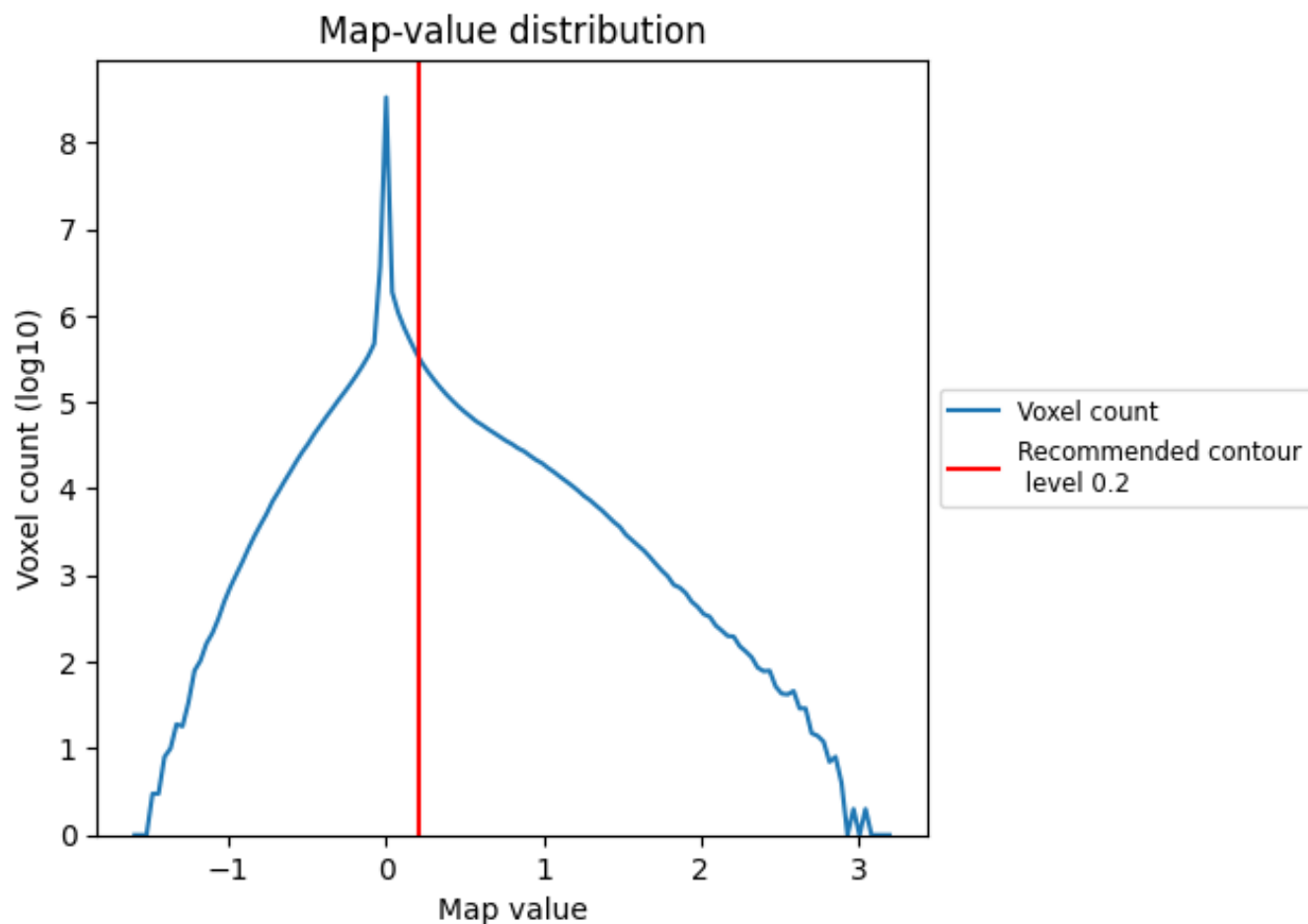


Z

7 Map analysis [i](#)

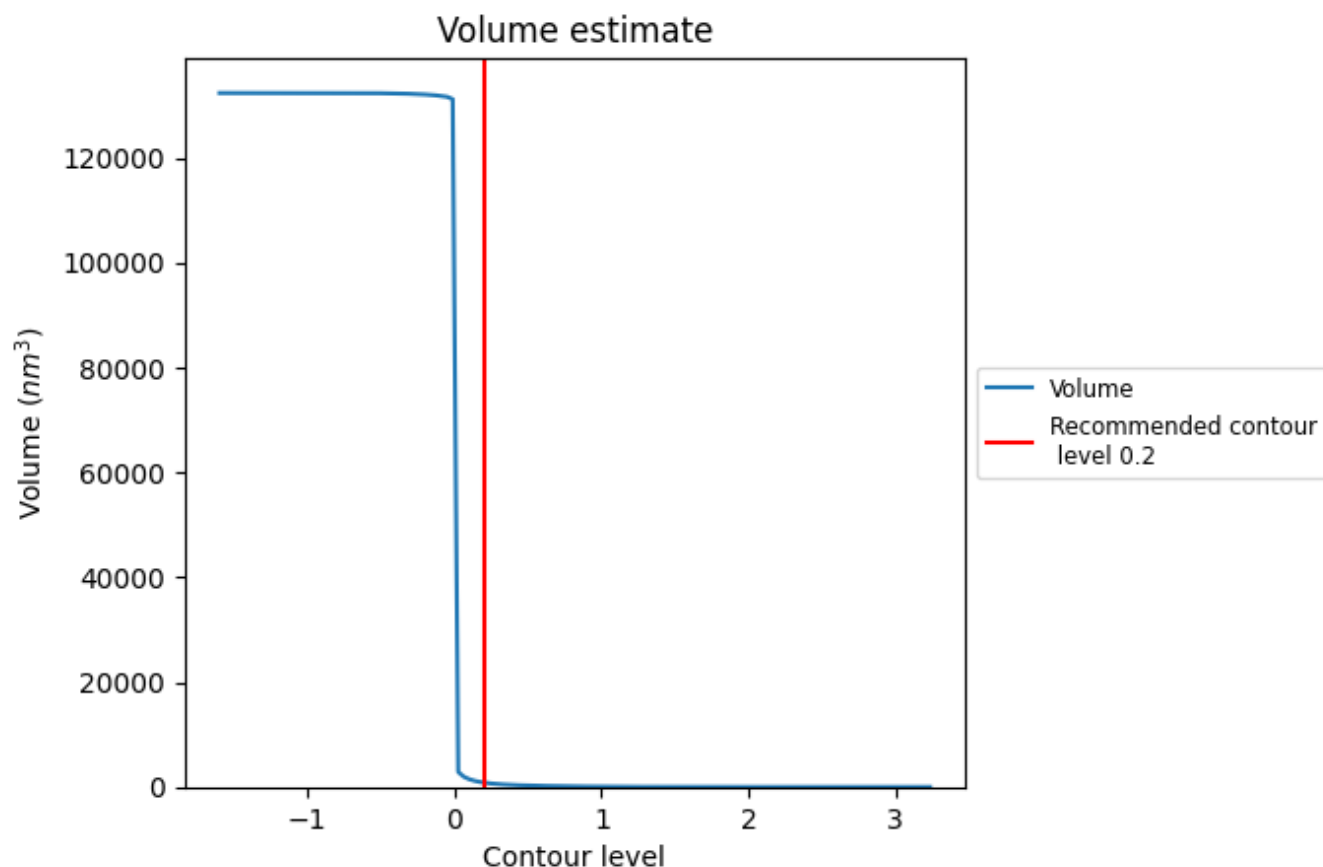
This section contains the results of statistical analysis of the map.

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.

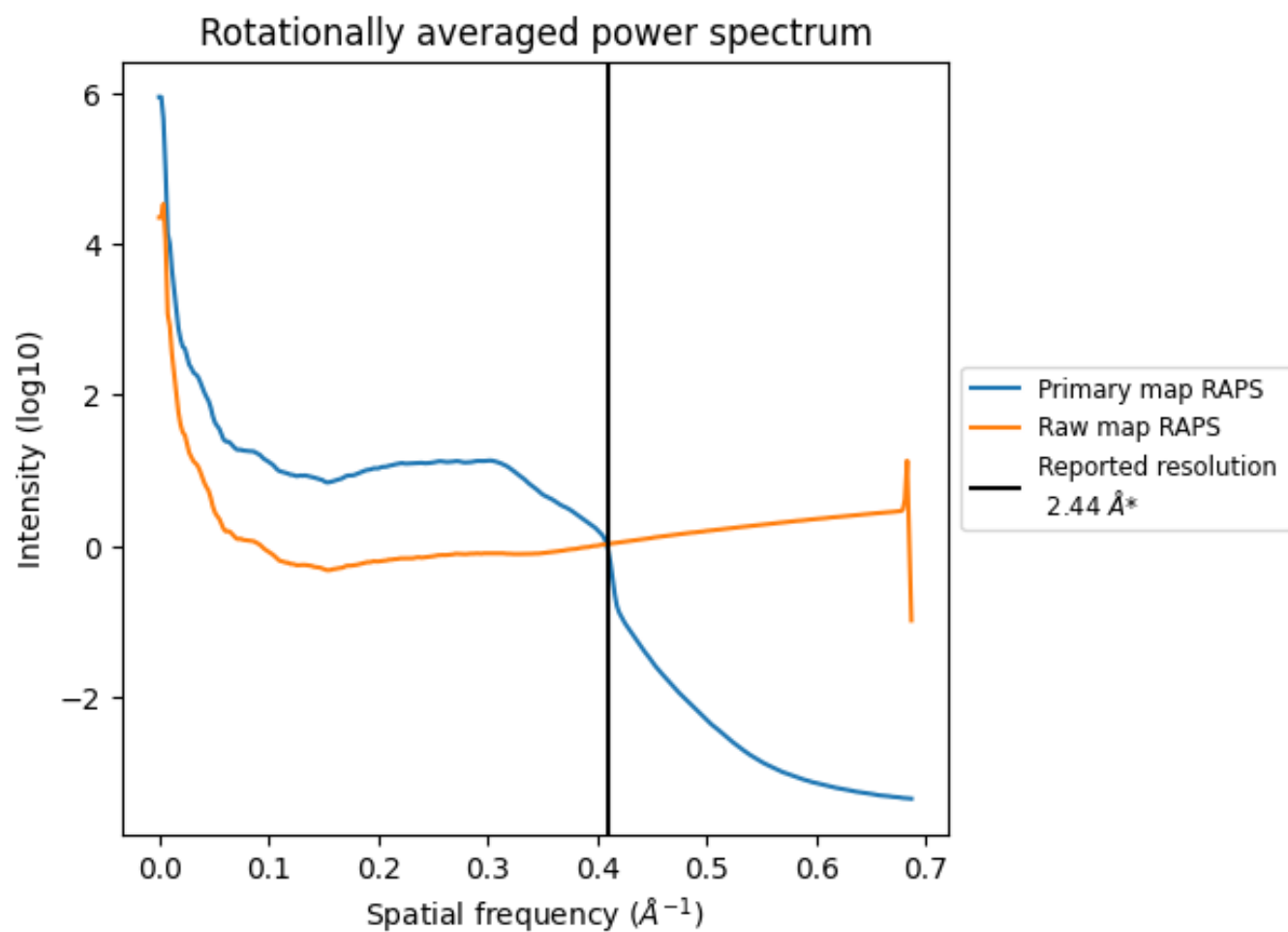
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 830 nm^3 ; this corresponds to an approximate mass of 749 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 ⓘ

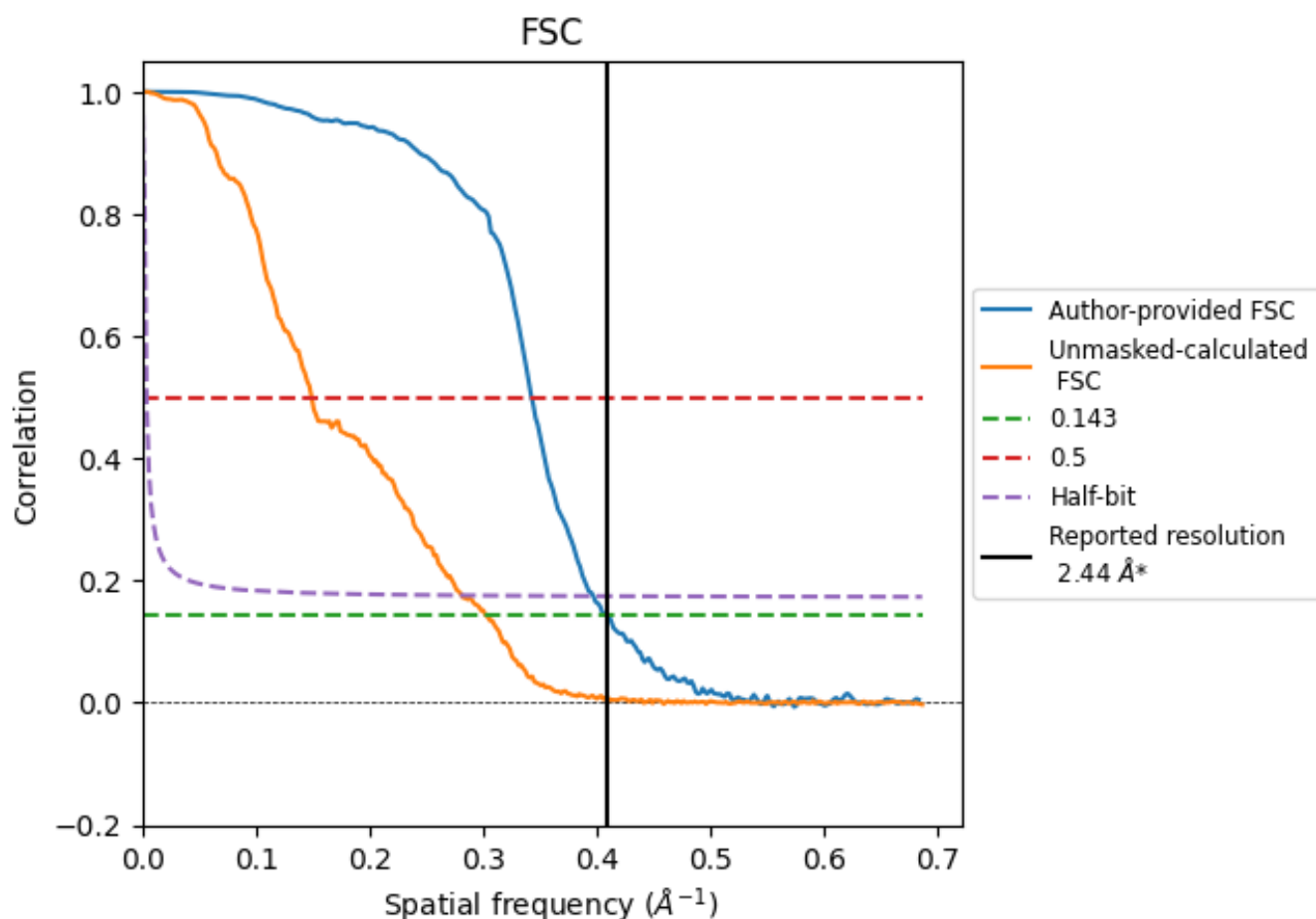


*Reported resolution corresponds to spatial frequency of 0.410 $\text{\AA}^{-1}$

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 $0.410 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

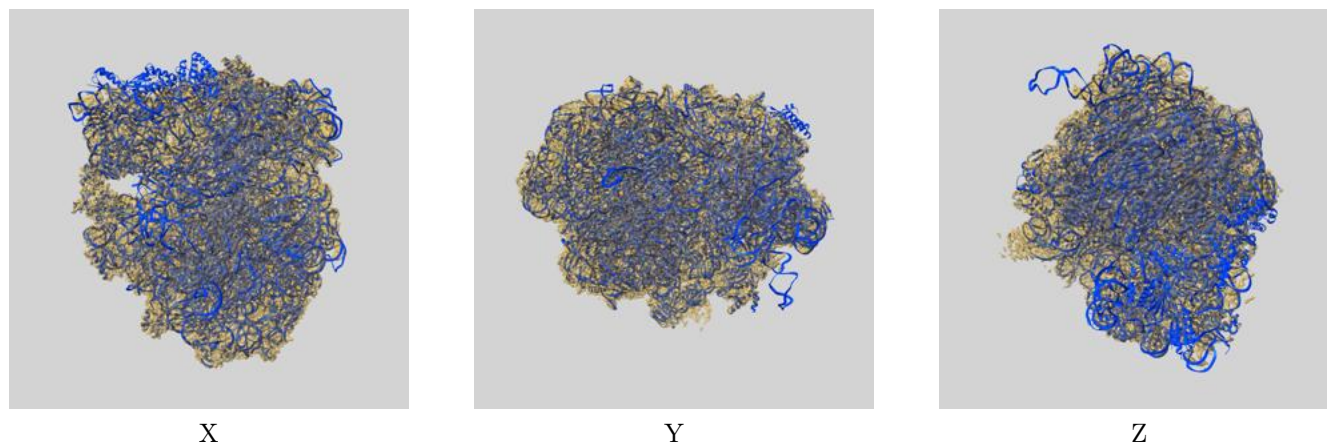
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.44	-	-
Author-provided FSC curve	2.44	2.92	2.52
Unmasked-calculated*	3.30	6.70	3.55

*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 3.30 differs from the reported value 2.44 by more than 10 %

9 Map-model fit [i](#)

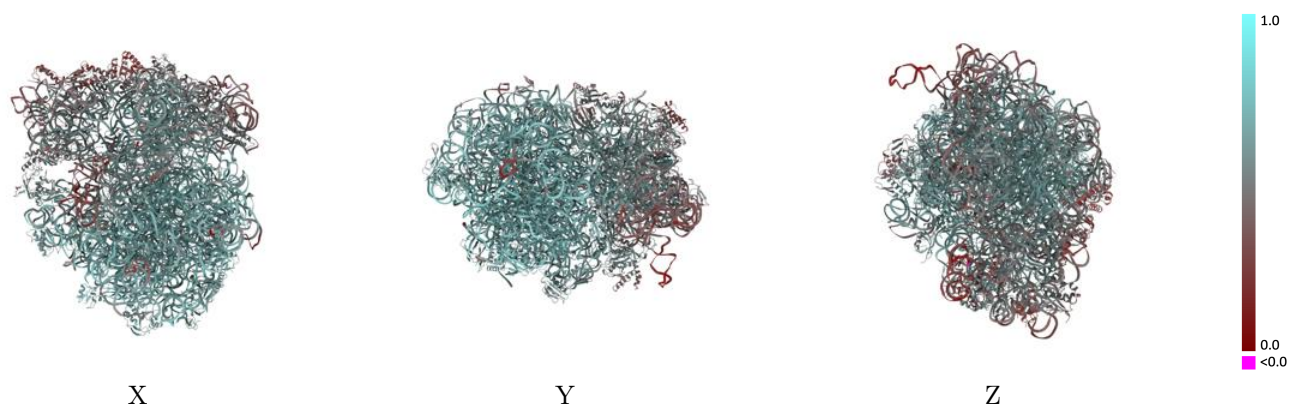
This section contains information regarding the fit between EMDB map EMD-17363 and PDB model 8P2F. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



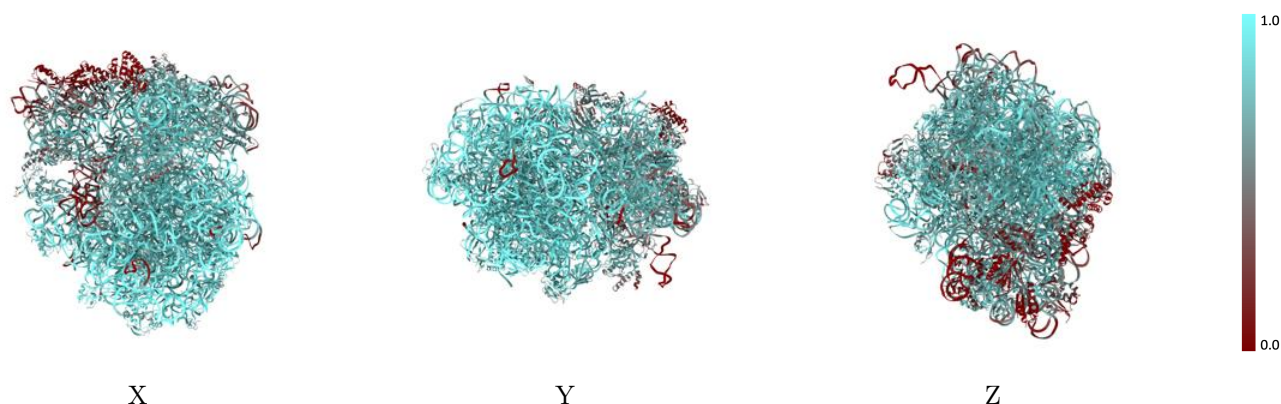
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



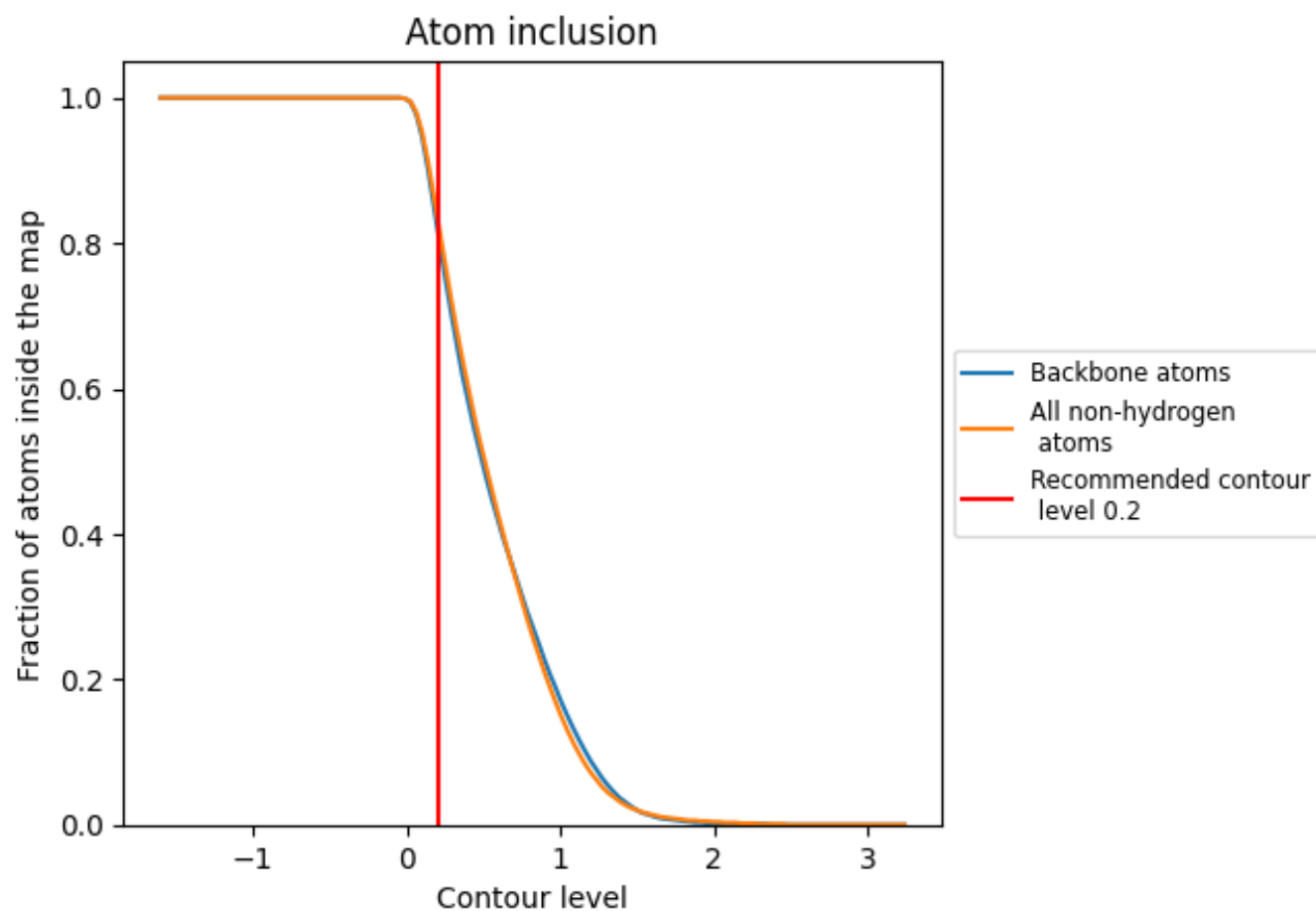
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 84% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8350	 0.5970
1	 0.9070	 0.6440
2	 0.8610	 0.6200
3	 0.9600	 0.6870
4	 0.5560	 0.4680
5	 0.9460	 0.6820
6	 0.8580	 0.6270
7	 0.9940	 0.7170
8	 0.9940	 0.7180
9	 0.9550	 0.6860
A	 0.9580	 0.6650
B	 0.9710	 0.6350
D	 0.3180	 0.3830
E	 0.6450	 0.5110
F	 0.8530	 0.5880
G	 0.9610	 0.6870
H	 0.9540	 0.6890
I	 0.9190	 0.6660
J	 0.8060	 0.5740
K	 0.7910	 0.5720
M	 0.9580	 0.6770
N	 0.9620	 0.6810
O	 0.9350	 0.6740
P	 0.9470	 0.6700
Q	 0.9500	 0.6860
R	 0.8770	 0.6090
S	 0.9360	 0.6630
T	 0.9710	 0.6970
U	 0.9440	 0.6730
V	 0.9580	 0.6820
W	 0.9320	 0.6520
X	 0.7940	 0.5880
Y	 0.7850	 0.5710
Z	 0.9610	 0.6870
a	 0.7810	 0.5230



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Chain	Atom inclusion	Q-score
b	 0.8240	 0.5390
c	 0.0690	 0.3530
d	 0.1980	 0.4310
e	 0.6390	 0.4890
f	 0.7690	 0.5620
g	 0.5530	 0.4630
h	 0.5840	 0.4760
i	 0.7700	 0.5520
j	 0.4470	 0.4630
k	 0.1880	 0.4080
l	 0.5590	 0.4300
m	 0.7990	 0.5720
n	 0.5250	 0.4590
o	 0.3700	 0.4740
p	 0.7690	 0.5340
q	 0.6120	 0.4340
r	 0.6700	 0.5060
s	 0.6550	 0.4910
t	 0.2180	 0.3320
u	 0.7160	 0.5100