Full wwPDB EM Validation Report (i)

Sep 16, 2026 – 12:42 PM JST

PDB ID	:	7D6Z / pdb_00007d6z
EMDB ID	:	EMD-30598
Title	:	Molecular model of the cryo-EM structure of 70S ribosome in complex with peptide deformylase and trigger factor
Authors	:	Akbar, S.; Bhakta, S.; Sengupta, J.
Deposited on	:	2020-10-02
Resolution	:	3.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

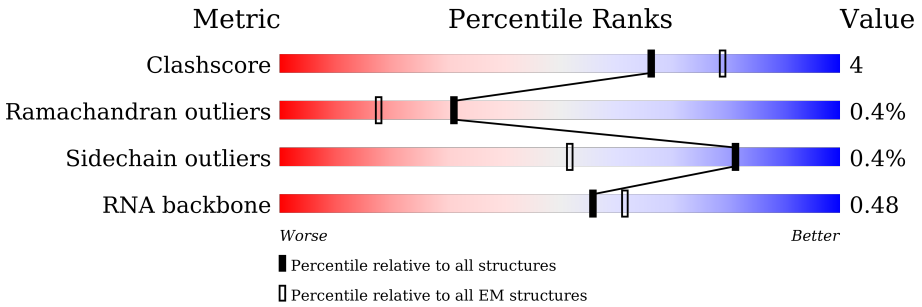
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

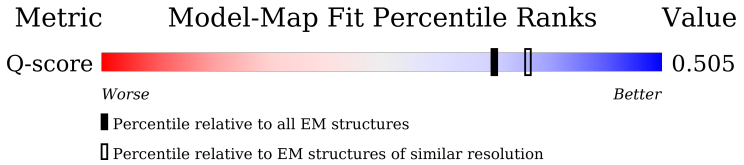
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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 <=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	0	87	79% 18% •
2	1	71	49% 21% • 28%
3	2	73	52% 27% 10% 11%

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Mol	Chain	Length	Quality of chain
4	3	77	66% 23% • 9%
5	4	76	50% 57% 25% 5% 13%
6	6	70	10% 83% 11% 6%
7	A	2903	77% 21% •
8	B	118	79% 19% •
9	C	273	83% 16% •
10	D	209	90% 10%
11	E	201	89% 11%
12	F	179	83% 16% •
13	G	177	• 82% 16% ••
14	H	149	27% 5% 68%
15	I	142	20% 73% 26% •
16	J	142	92% 8%
17	K	123	84% 15% •
18	L	144	85% 14% ••
19	M	136	87% 11% •
20	N	127	86% 9% 6%
21	O	117	80% 19% •
22	P	115	83% 16% •
23	Q	118	91% 8% •
24	R	103	88% 12%
25	S	110	92% 8%
26	T	59	85% 14% •
27	U	104	83% 14% ••
28	V	94	94% 6%

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Mol	Chain	Length	Quality of chain
29	W	85	81% 7% 12%
30	X	78	85% 14%
31	Y	63	73% 27%
32	Z	100	71% 25%
33	a	57	79% 18%
34	b	55	75% 16% 9%
35	c	46	85% 15%
36	d	65	83% 11% 5%
37	e	38	79% 18%
38	f	1539	73% 24%
39	g	169	83% 16%
40	h	118	79% 82% 18%
41	i	241	76% 14% 10%
42	j	233	73% 16% 12%
43	k	206	70% 30%
44	l	167	75% 14% 10%
45	m	135	55% 19% 26%
46	n	179	77% 8% 16%
47	o	130	89% 10%
48	p	130	82% 15%
49	q	103	79% 17% 5%
50	r	129	69% 22% 9%
51	s	124	77% 23%
52	t	118	86% 8%
53	u	101	80% 15% 5%

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Mol	Chain	Length	Quality of chain
54	v	89	84% 15%
55	w	82	85% 15%
56	x	84	71% 21% 5%
57	y	75	67% 7% 27%
58	z	92	62% 24% 14%

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 148863 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 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	85	665	411	137	114	3	0	0

- Molecule 2 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	51	425	265	86	73	1	0	0

- Molecule 3 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	2	65	1392	621	258	449	64	0	0

- Molecule 4 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	3	70	1496	665	267	494	70	0	0

- Molecule 5 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	4	66	1406	629	255	457	65	0	0

- Molecule 6 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	66	522	323	99	94	6	0	0

- Molecule 7 is a RNA chain called 23S ribosomal rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	A	2903	62317	27801	11467	20147	2902	0	0

- Molecule 8 is a RNA chain called 5S ribosomal rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	B	118	2529	1126	464	821	118	0	0

- Molecule 9 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	C	271	2082	1288	423	364	7	0	0

- Molecule 10 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	D	209	1565	979	288	294	4	0	0

- Molecule 11 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	E	201	1552	974	283	290	5	0	0

- Molecule 12 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	F	177	1410	899	249	256	6	0	0

- Molecule 13 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	G	176	1323	832	243	246	2	0	0

- Molecule 14 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	H	47	359	233	62	63	1	0	0

- Molecule 15 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	I	141	1032	651	179	196	6	0	0

- Molecule 16 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	J	142	1129	714	212	199	4	0	0

- Molecule 17 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	K	122	938	587	180	165	6	0	0

- Molecule 18 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	L	143	1045	649	206	189	1	0	0

- Molecule 19 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	M	136	1074	686	205	177	6	0	0

- Molecule 20 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	N	120	960	593	196	166	5	0	0

- Molecule 21 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	O	116	892	552	178	162	0	0

- Molecule 22 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	P	114	917	574	179	163	1	0	0

- Molecule 23 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	Q	117	947	604	192	151	0	0

- Molecule 24 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	R	103	816	516	153	145	2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	S	110	857	532	166	156	3	0	0

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	T	58	449	281	87	79	2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	U	102	779	492	146	141	0	0

- Molecule 28 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	V	94	753	479	137	134	3	0	0

- Molecule 29 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	W	75	569	353	113	102	1	0	0

- Molecule 30 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	X	77	625	388	129	106	2	0	0

- Molecule 31 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Y	63	509	313	99	95	2	0	0

- Molecule 32 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Z	96	764	484	142	136	2	0	0

- Molecule 33 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	a	56	444	269	94	80	1	0	0

- Molecule 34 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	b	50	409	263	75	71	0	0

- Molecule 35 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	c	46	377	228	90	57	2	0	0

- Molecule 36 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	d	64	504	323	105	74	2	0	0

- Molecule 37 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	e	38	302	185	65	48	4	0	0

- Molecule 38 is a RNA chain called 16S ribosomal rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
38	f	1539	33015	14725	6052	10699	1539	0	0

- Molecule 39 is a protein called Peptide deformylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	g	168	1346	844	241	255	6	0	0

- Molecule 40 is a protein called Trigger factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	h	118	919	583	157	176	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	0	HIS	-	expression tag	UNP P0A850

- Molecule 41 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	i	218	1704	1081	305	311	7	0	0

- Molecule 42 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	j	206	1624	1028	305	288	3	0	0

- Molecule 43 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	k	205	1643	1026	315	298	4	0	0

- Molecule 44 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	l	150	1105	687	211	201	6	0	0

- Molecule 45 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	m	100	817	515	148	148	6	0	0

- Molecule 46 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	n	151	1181	735	227	215	4	0	0

- Molecule 47 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	o	129	979	616	173	184	6	0	0

- Molecule 48 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	p	127	1022	634	206	179	3	0	0

- Molecule 49 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	q	98	786	493	150	142	1	0	0

- Molecule 50 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	r	117	877	540	174	160	3	0	0

- Molecule 51 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	s	123	955	590	196	165	4	0	0

- Molecule 52 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	t	114	883	546	178	156	3	0	0

- Molecule 53 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	u	96	774	483	160	128	3	0	0

- Molecule 54 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	v	88	710	437	143	129	1	0	0

- Molecule 55 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	w	82	649	406	128	114	1	0	0

- Molecule 56 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	x	80	648	411	121	113	3	0	0

- Molecule 57 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
57	y	55	455	288	86	81	0	0

- Molecule 58 is a protein called 30S ribosomal protein S19.

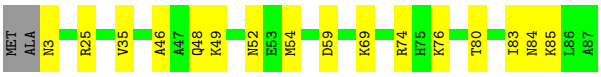
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	z	79	637	408	120	107	2	0	0

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: 30S ribosomal protein S20

Chain 0:

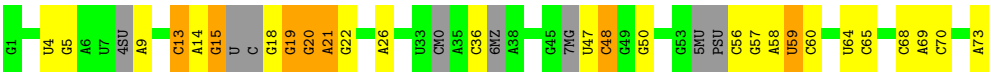


- Molecule 2: 30S ribosomal protein S21

Chain 1:

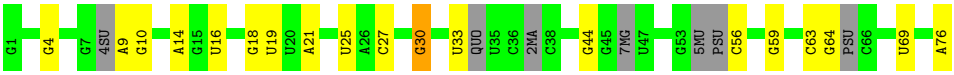
- Molecule 3: E-site tRNA

Chain 2:



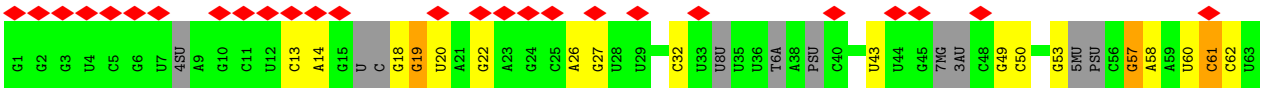
- Molecule 4: P-site tRNA

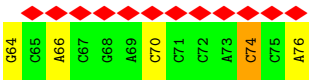
Chain 3:



- Molecule 5: A-site tRNA

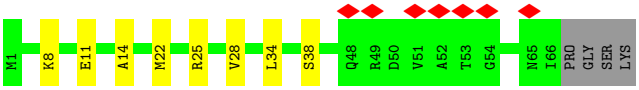
Chain 4:





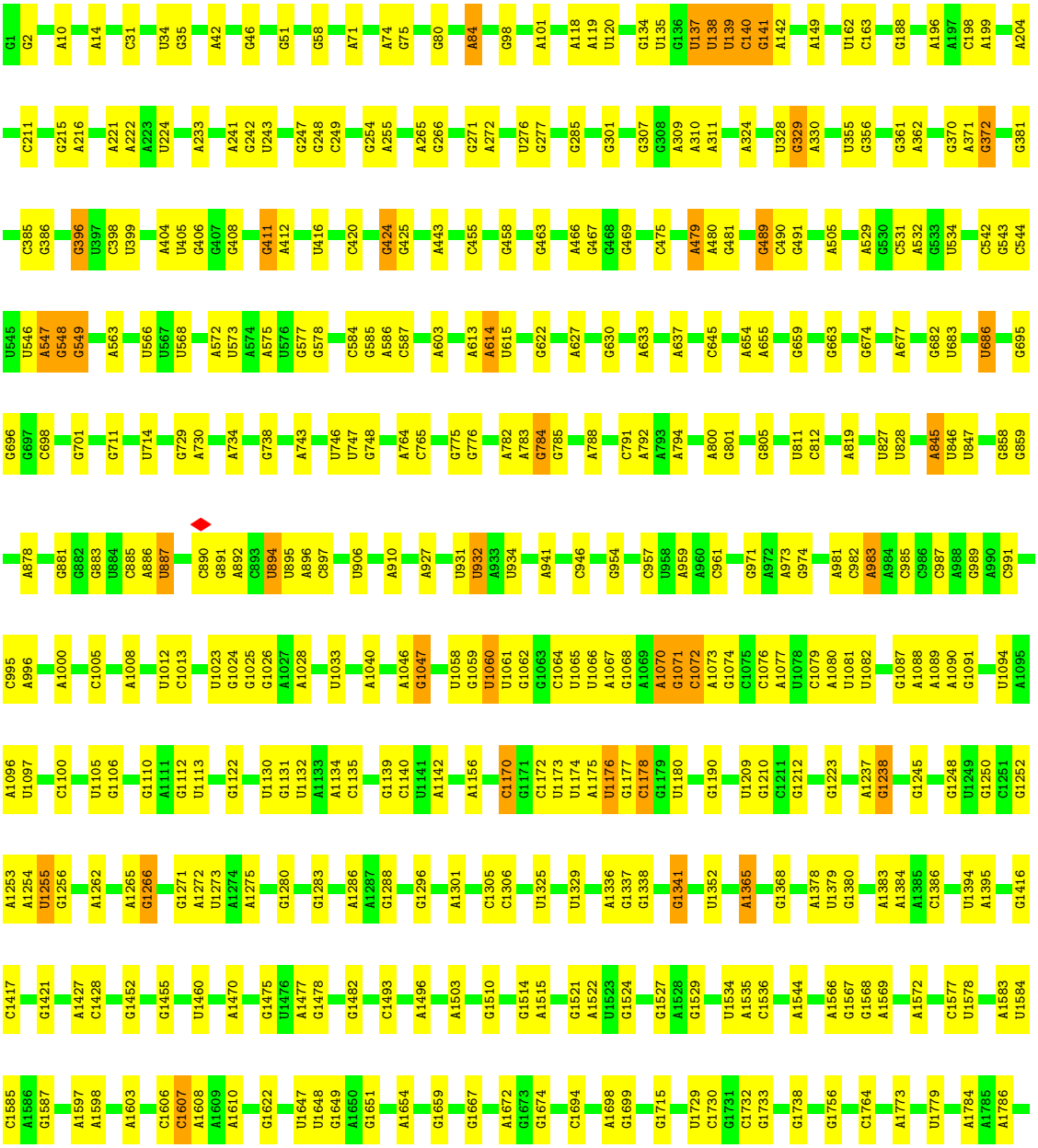
• Molecule 6: 50S ribosomal protein L31

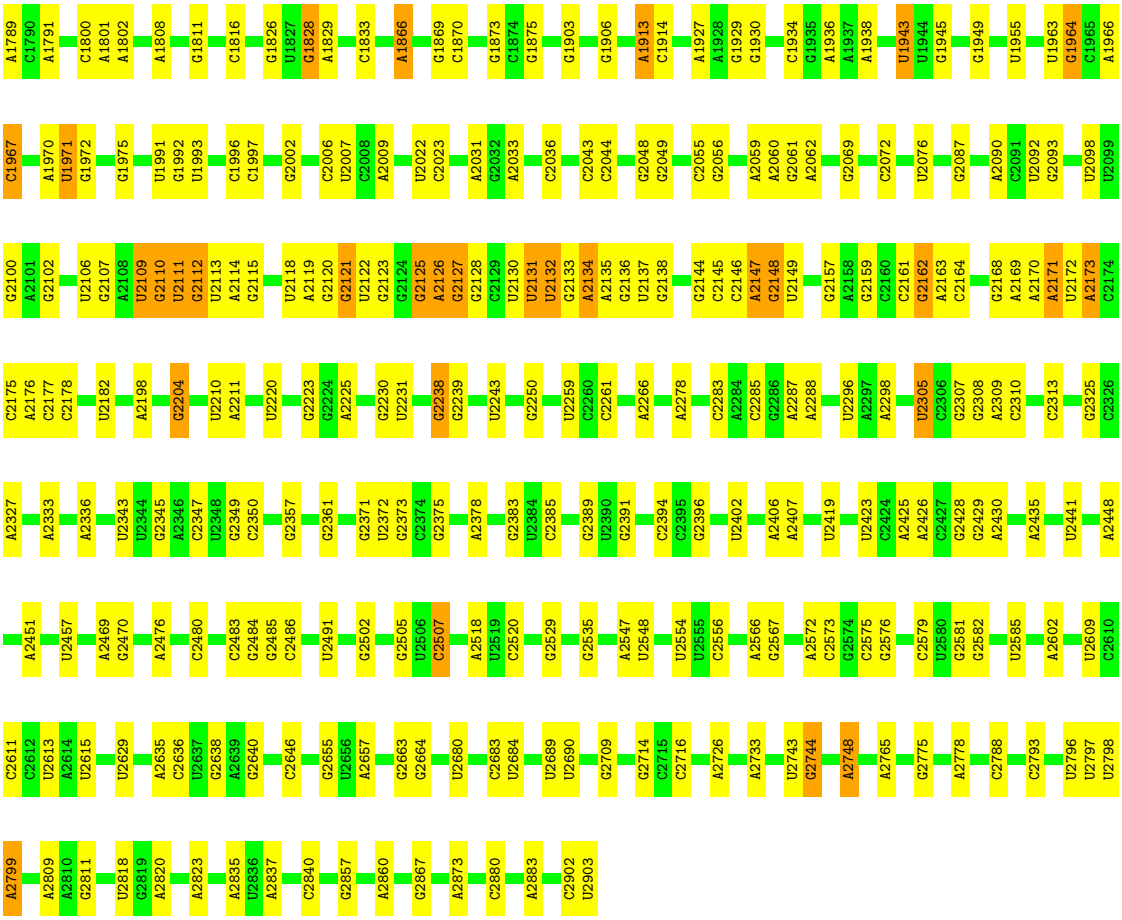
Chain 6:



• Molecule 7: 23S ribosomal rRNA

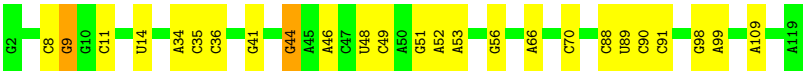
Chain A:





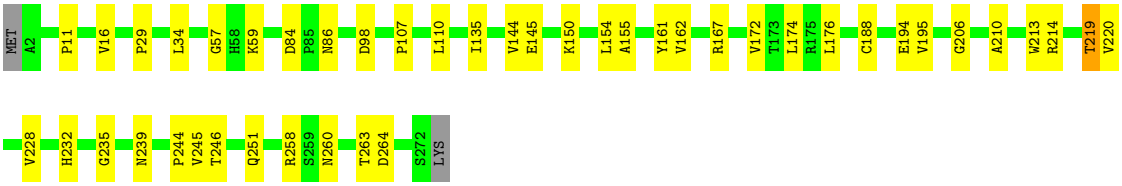
- Molecule 8: 5S ribosomal rRNA

Chain B:



- Molecule 9: 50S ribosomal protein L2

Chain C:

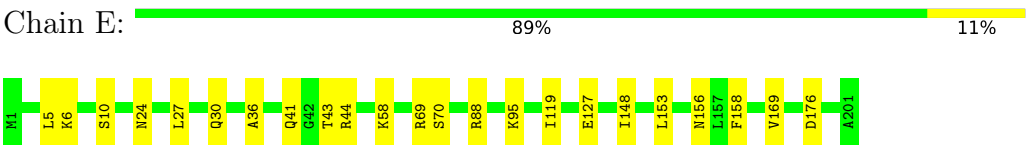


- Molecule 10: 50S ribosomal protein L3

Chain D:

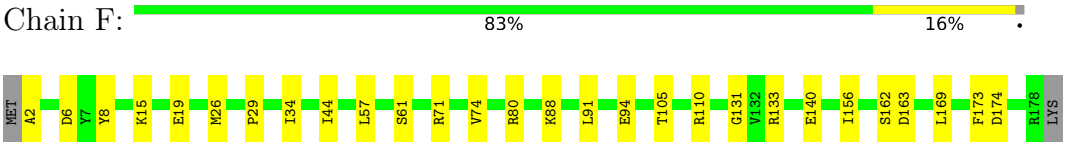
- Molecule 11: 50S ribosomal protein L4

Chain E:



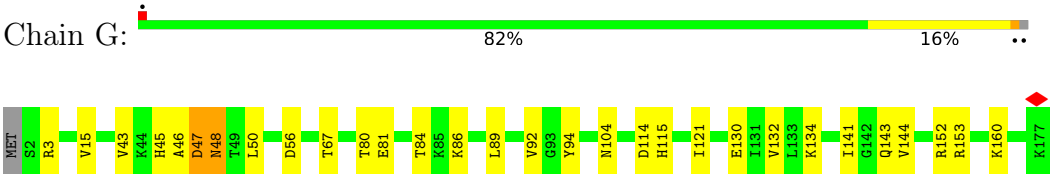
- Molecule 12: 50S ribosomal protein L5

Chain F:



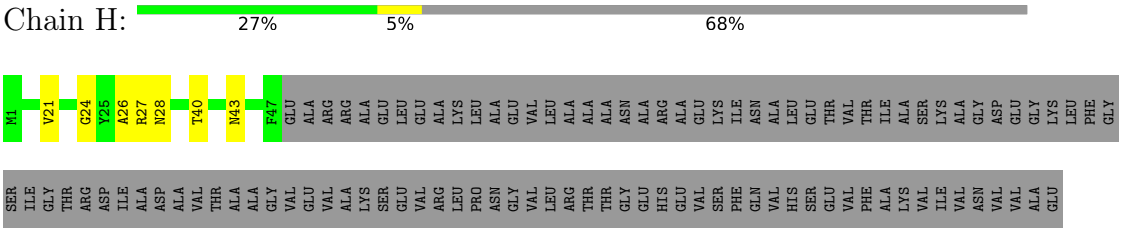
- Molecule 13: 50S ribosomal protein L6

Chain G:



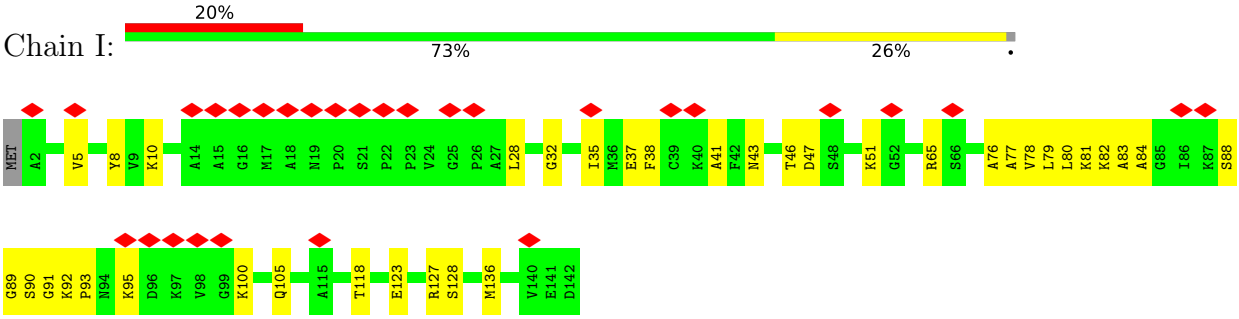
- Molecule 14: 50S ribosomal protein L9

Chain H:



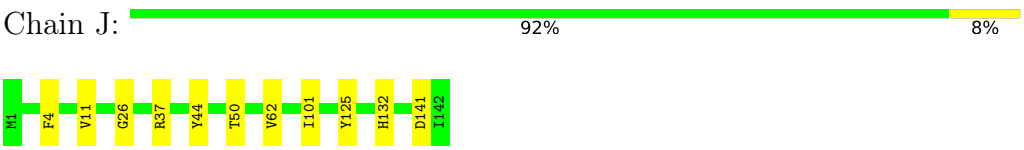
- Molecule 15: 50S ribosomal protein L11

Chain I:



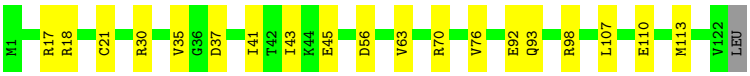
- Molecule 16: 50S ribosomal protein L13

Chain J:



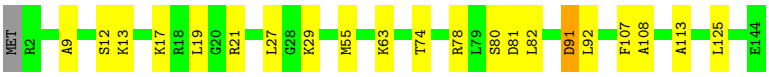
- Molecule 17: 50S ribosomal protein L14

Chain K: 84% 15%



• Molecule 18: 50S ribosomal protein L15

Chain L: 85% 14%



• Molecule 19: 50S ribosomal protein L16

Chain M: 87% 11%

• Molecule 20: 50S ribosomal protein L17

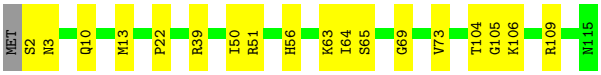
Chain N: 86% 9% 6%

• Molecule 21: 50S ribosomal protein L18

Chain O: 80% 19%

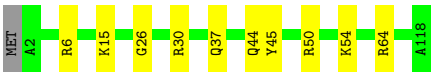
• Molecule 22: 50S ribosomal protein L19

Chain P: 83% 16%



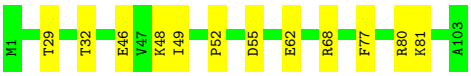
• Molecule 23: 50S ribosomal protein L20

Chain Q: 91% 8%



• Molecule 24: 50S ribosomal protein L21

Chain R: 88% 12%

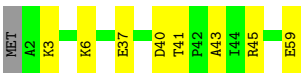


- Molecule 25: 50S ribosomal protein L22

Chain S: 92% 8%

- Molecule 26: 50S ribosomal protein L30

Chain T: 85% 14%



- Molecule 27: 50S ribosomal protein L24

Chain U: 83% 14%

- Molecule 28: 50S ribosomal protein L25

Chain V: 94% 6%

- Molecule 29: 50S ribosomal protein L27

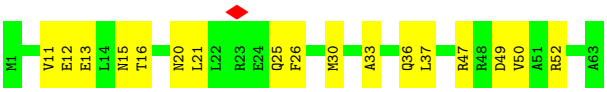
Chain W: 81% 7% 12%

- Molecule 30: 50S ribosomal protein L28

Chain X: 85% 14%

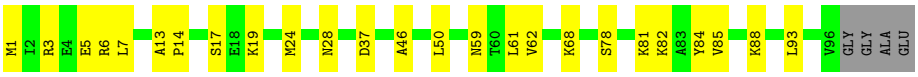
- Molecule 31: 50S ribosomal protein L29

Chain Y: 73% 27%



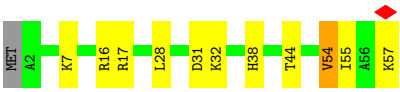
• Molecule 32: 50S ribosomal protein L23

Chain Z: 71% 25%



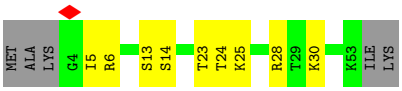
• Molecule 33: 50S ribosomal protein L32

Chain a: 79% 18%



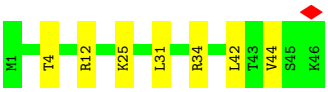
• Molecule 34: 50S ribosomal protein L33

Chain b: 75% 16% 9%



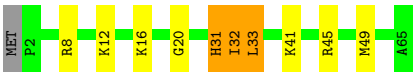
• Molecule 35: 50S ribosomal protein L34

Chain c: 85% 15%



• Molecule 36: 50S ribosomal protein L35

Chain d: 83% 11% 5%

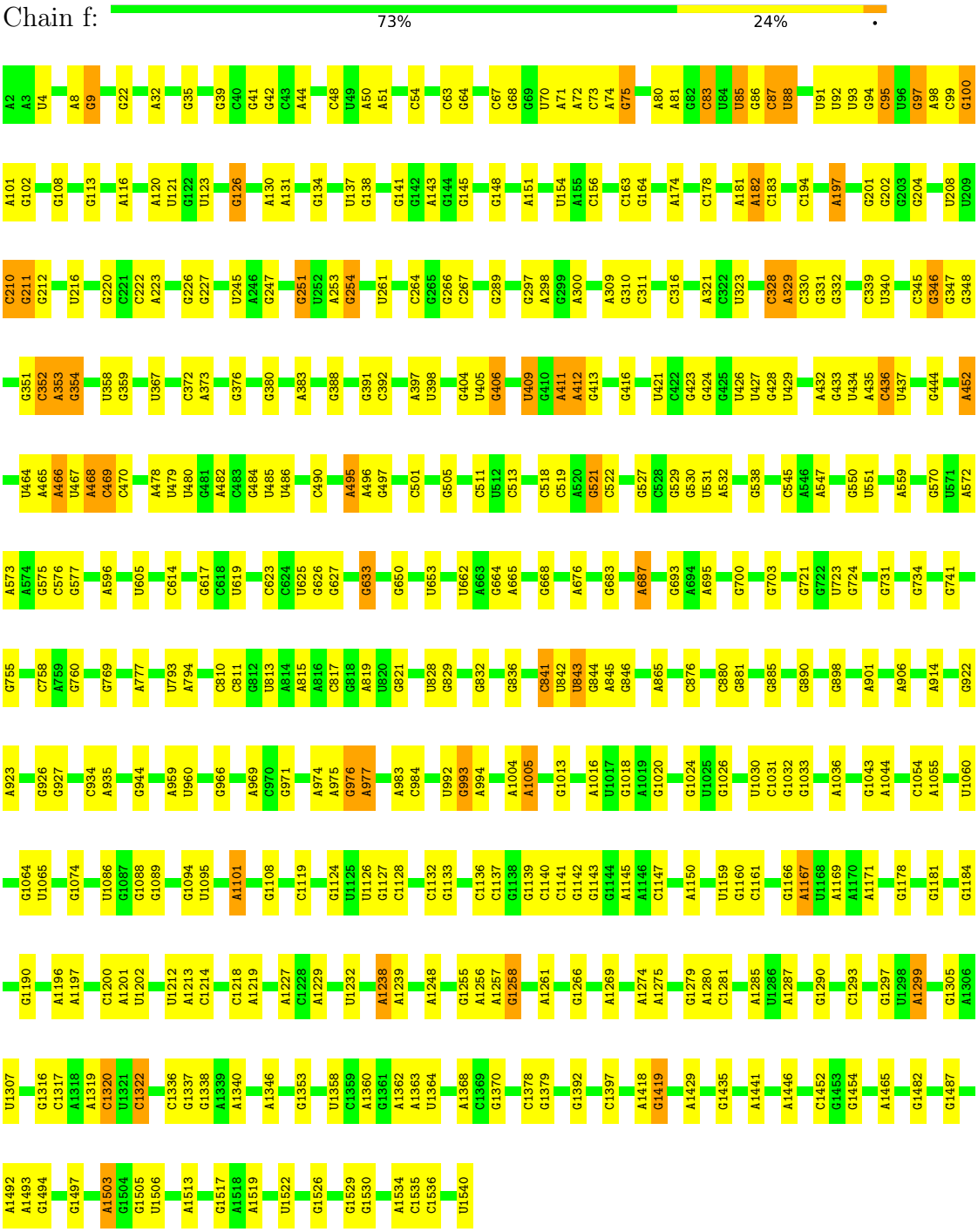


• Molecule 37: 50S ribosomal protein L36

Chain e: 79% 18%

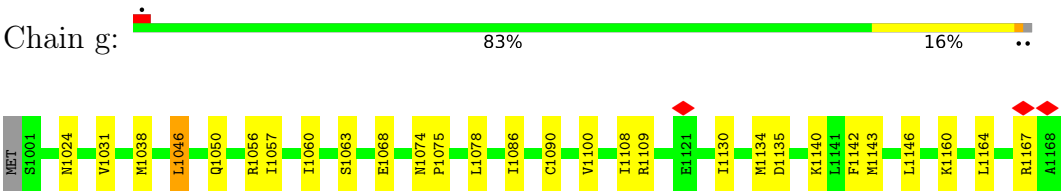
• Molecule 38: 16S ribosomal rRNA

Chain f:



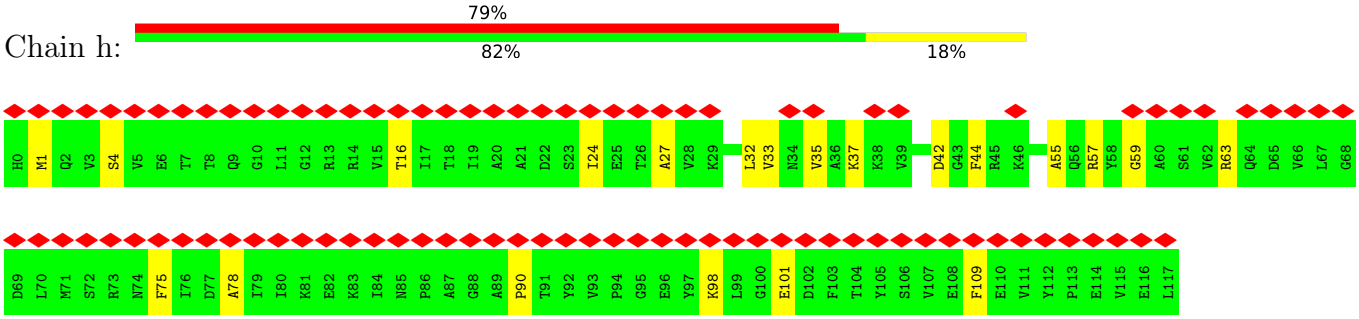
• Molecule 39: Peptide deformylase

Chain g:



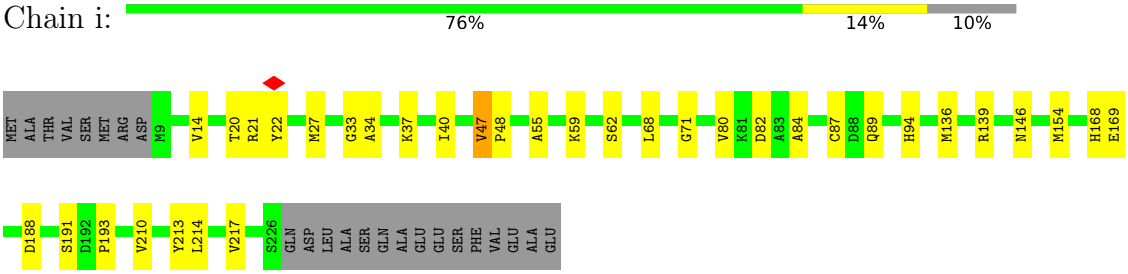
• Molecule 40: Trigger factor

Chain h:



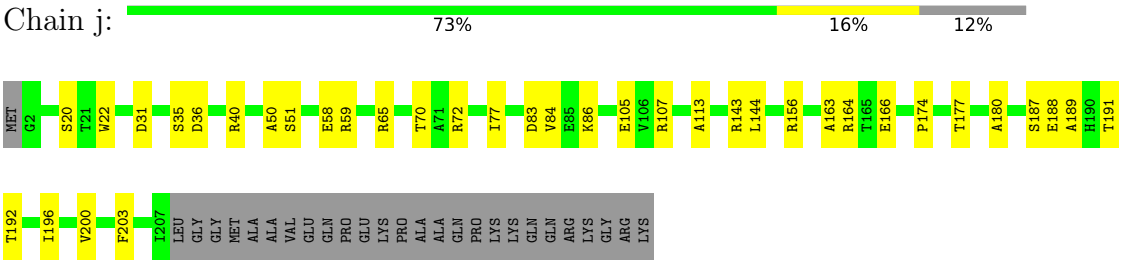
- Molecule 41: 30S ribosomal protein S2

Chain i:



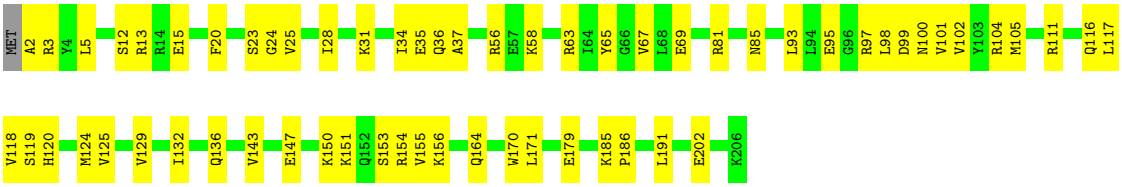
- Molecule 42: 30S ribosomal protein S3

Chain j:



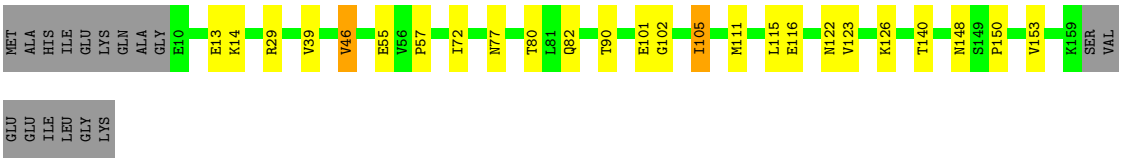
- Molecule 43: 30S ribosomal protein S4

Chain k:



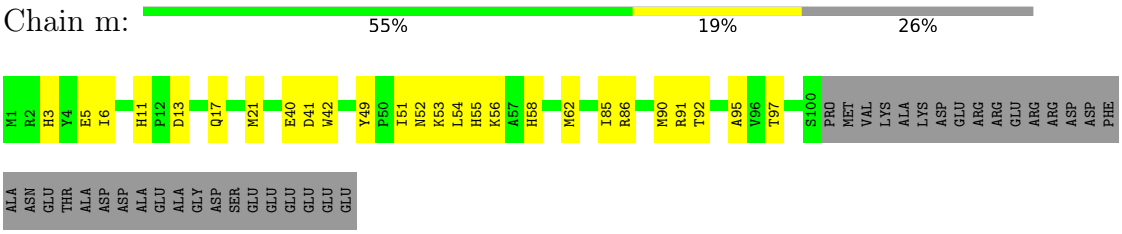
- Molecule 44: 30S ribosomal protein S5

Chain l:



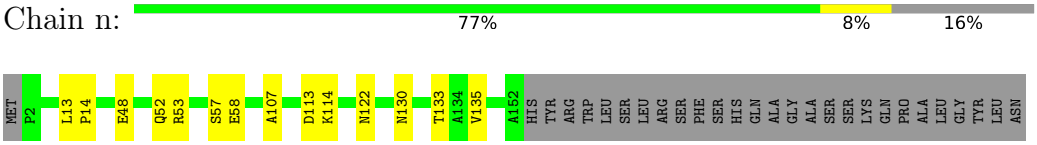
- Molecule 45: 30S ribosomal protein S6, fully modified isoform

Chain m:



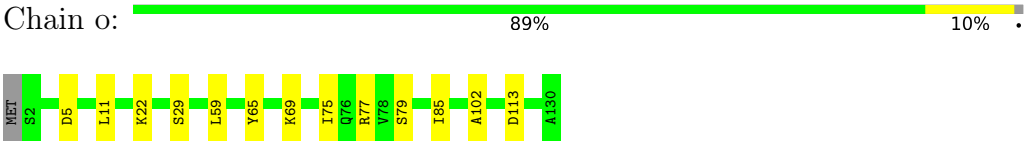
- Molecule 46: 30S ribosomal protein S7

Chain n:



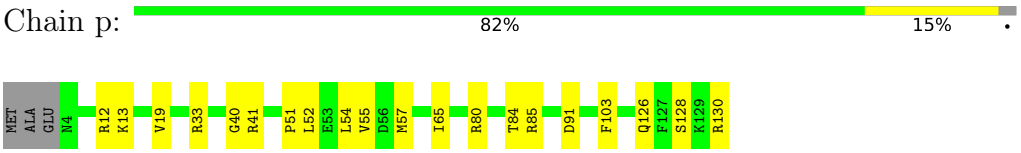
- Molecule 47: 30S ribosomal protein S8

Chain o:



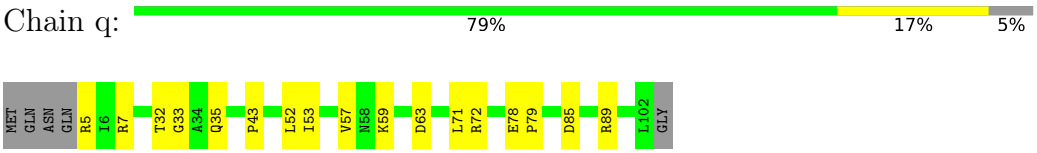
- Molecule 48: 30S ribosomal protein S9

Chain p:



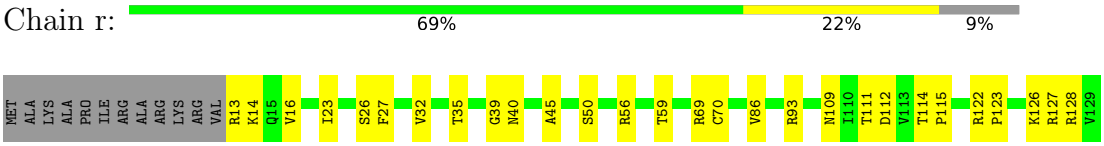
- Molecule 49: 30S ribosomal protein S10

Chain q:



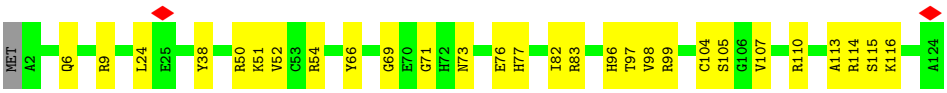
- Molecule 50: 30S ribosomal protein S11

Chain r:



- Molecule 51: 30S ribosomal protein S12

Chain s:



- Molecule 52: 30S ribosomal protein S13

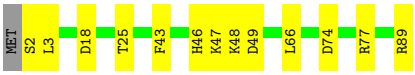
Chain t:

- Molecule 53: 30S ribosomal protein S14

Chain u:

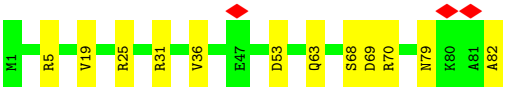
- Molecule 54: 30S ribosomal protein S15

Chain v:



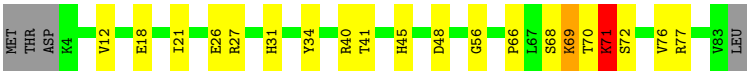
- Molecule 55: 30S ribosomal protein S16

Chain w:



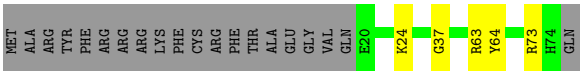
- Molecule 56: 30S ribosomal protein S17

Chain x:



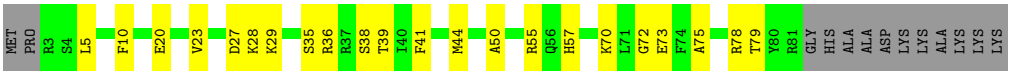
- Molecule 57: 30S ribosomal protein S18

Chain y:



- Molecule 58: 30S ribosomal protein S19

Chain z:


MET
PRO
R3
S4
L5
F10
E20
V23
D27
K28
K29
S35
R36
R37
S38
T39
I40
F41
M44
A50
R55
Q56
H57
K70
L71
G72
E73
F74
A75
R78
T79
Y80
R81
GLY
HIS
ALA
ALA
ASP
LYS
LYS
ALA
LYS
LYS
LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	194157	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	32.57	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	25.576	Depositor
Minimum map value	-14.991	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	441.6, 441.6, 441.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0	0.21	0/671	0.54	0/888
2	1	0.31	0/430	0.89	4/570 (0.7%)
3	2	0.14	0/1551	0.27	0/2404
4	3	0.20	0/1664	0.26	0/2577
5	4	0.13	0/1565	0.29	0/2421
6	6	0.18	0/531	0.48	0/709
7	A	0.42	0/69796	0.37	1/108888 (0.0%)
8	B	0.32	0/2828	0.30	0/4410
9	C	0.45	0/2121	0.60	0/2852
10	D	0.42	0/1586	0.53	0/2134
11	E	0.39	0/1571	0.47	0/2113
12	F	0.26	0/1434	0.46	0/1926
13	G	0.27	0/1343	0.47	0/1816
14	H	0.31	0/364	0.70	0/490
15	I	0.20	0/1046	0.55	0/1410
16	J	0.40	0/1152	0.45	0/1551
17	K	0.42	0/947	0.66	1/1268 (0.1%)
18	L	0.43	0/1054	0.66	0/1403
19	M	0.38	0/1093	0.57	0/1460
20	N	0.44	0/973	0.69	2/1301 (0.2%)
21	O	0.31	0/902	0.50	0/1209
22	P	0.38	0/929	0.54	0/1242
23	Q	0.49	0/960	0.53	0/1278
24	R	0.38	0/829	0.55	0/1107
25	S	0.39	0/864	0.50	0/1156
26	T	0.40	0/453	0.54	0/605
27	U	0.35	0/787	0.65	0/1051
28	V	0.32	0/766	0.47	0/1025
29	W	0.39	0/576	0.48	0/762
30	X	0.40	0/635	0.47	0/848
31	Y	0.33	0/510	0.42	0/677
32	Z	0.35	0/771	0.63	0/1031
33	a	0.40	0/450	0.71	0/599
34	b	0.27	0/416	0.42	0/554

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	c	0.48	0/380	0.51	0/498
36	d	0.42	0/513	0.72	1/676 (0.1%)
37	e	0.39	0/303	0.58	0/397
38	f	0.28	0/36966	0.31	0/57666
39	g	0.19	0/1361	0.53	0/1830
40	h	0.18	0/933	0.47	0/1261
41	i	0.26	0/1735	0.53	0/2338
42	j	0.27	0/1651	0.52	0/2225
43	k	0.25	0/1665	0.61	0/2227
44	l	0.33	0/1118	0.68	0/1504
45	m	0.28	0/835	0.70	1/1128 (0.1%)
46	n	0.23	0/1195	0.47	0/1602
47	o	0.29	0/989	0.43	0/1326
48	p	0.25	0/1034	0.57	0/1375
49	q	0.27	0/796	0.61	0/1077
50	r	0.29	0/893	0.54	0/1205
51	s	0.28	0/969	0.61	0/1300
52	t	0.24	0/892	0.58	1/1193 (0.1%)
53	u	0.26	0/785	0.57	0/1043
54	v	0.28	0/718	0.52	0/959
55	w	0.22	0/659	0.51	0/884
56	x	0.27	0/657	0.73	1/881 (0.1%)
57	y	0.29	0/462	0.49	0/621
58	z	0.22	0/652	0.44	0/877
All	All	0.36	0/161729	0.41	12/241828 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	D	0	1
12	F	0	1
13	G	0	2
17	K	0	1
18	L	0	1
19	M	0	2
20	N	0	1
27	U	0	2
33	a	0	1
36	d	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
37	e	0	1
41	i	0	1
43	k	0	1
44	l	0	2
45	m	0	2
48	p	0	1
51	s	0	1
52	t	0	1
56	x	0	2
All	All	0	25

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	37	PHE	CA-C-N	6.71	134.36	121.54
2	1	37	PHE	C-N-CA	6.71	134.36	121.54
36	d	32	ILE	N-CA-C	6.37	122.58	109.34
45	m	54	LEU	CA-CB-CG	5.76	136.46	116.30
17	K	35	VAL	N-CA-C	-5.54	107.88	113.20
2	1	24	GLU	CA-C-N	5.44	131.92	121.54
2	1	24	GLU	C-N-CA	5.44	131.92	121.54
7	A	1913	A	P-O3'-C3'	5.34	128.21	120.20
52	t	67	GLY	N-CA-C	5.19	125.47	113.18
56	x	71	LYS	CA-CB-CG	5.11	124.32	114.10
20	N	69	ARG	CA-C-N	5.02	131.13	121.54
20	N	69	ARG	C-N-CA	5.02	131.13	121.54

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	D	151	THR	Peptide
12	F	174	ASP	Peptide
13	G	46	ALA	Peptide
13	G	47	ASP	Peptide
17	K	92	GLU	Peptide
18	L	55	MET	Peptide
19	M	57	VAL	Peptide
19	M	58	LYS	Peptide
20	N	2	ARG	Peptide

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Mol	Chain	Res	Type	Group
27	U	6	ARG	Peptide
27	U	89	ASP	Peptide
33	a	54	VAL	Peptide
36	d	31	HIS	Peptide
37	e	20	ASP	Peptide
41	i	34	ALA	Peptide
43	k	28	ILE	Peptide
44	l	102	GLY	Peptide
44	l	105	ILE	Peptide
45	m	52	ASN	Peptide
45	m	53	LYS	Peptide
48	p	55	VAL	Peptide
51	s	24	LEU	Peptide
52	t	66	GLU	Peptide
56	x	69	LYS	Peptide
56	x	70	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	665	0	714	12	0
2	1	425	0	449	12	0
3	2	1392	0	714	16	0
4	3	1496	0	764	8	0
5	4	1406	0	722	6	0
6	6	522	0	522	6	0
7	A	62317	0	31345	195	0
8	B	2529	0	1281	10	0
9	C	2082	0	2154	26	0
10	D	1565	0	1616	13	0
11	E	1552	0	1619	15	0
12	F	1410	0	1444	19	0
13	G	1323	0	1371	17	0
14	H	359	0	381	5	0
15	I	1032	0	1085	25	0
16	J	1129	0	1162	7	0
17	K	938	0	1012	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	L	1045	0	1117	17	0
19	M	1074	0	1157	13	0
20	N	960	0	1000	6	0
21	O	892	0	923	16	0
22	P	917	0	962	11	0
23	Q	947	0	1019	8	0
24	R	816	0	839	9	0
25	S	857	0	922	6	0
26	T	449	0	488	5	0
27	U	779	0	831	8	0
28	V	753	0	780	4	0
29	W	569	0	581	5	0
30	X	625	0	652	8	0
31	Y	509	0	543	20	0
32	Z	764	0	829	28	0
33	a	444	0	458	7	0
34	b	409	0	440	5	0
35	c	377	0	418	5	0
36	d	504	0	572	7	0
37	e	302	0	343	5	0
38	f	33015	0	16617	154	0
39	g	1346	0	1391	17	0
40	h	919	0	938	13	0
41	i	1704	0	1732	18	0
42	j	1624	0	1696	20	0
43	k	1643	0	1707	46	0
44	l	1105	0	1148	15	0
45	m	817	0	808	15	0
46	n	1181	0	1238	9	0
47	o	979	0	1031	7	0
48	p	1022	0	1070	11	0
49	q	786	0	828	11	0
50	r	877	0	887	20	0
51	s	955	0	1016	21	0
52	t	883	0	941	9	0
53	u	774	0	824	12	0
54	v	710	0	728	8	0
55	w	649	0	666	11	0
56	x	648	0	691	12	0
57	y	455	0	478	5	0
58	z	637	0	665	14	0
All	All	148863	0	100329	855	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (855) 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)
31:Y:21:LEU:CD1	32:Z:5:GLU:OE2	1.82	1.28
31:Y:21:LEU:HD13	32:Z:5:GLU:OE2	1.33	1.25
31:Y:21:LEU:HD11	32:Z:5:GLU:OE2	1.70	0.91
31:Y:33:ALA:CB	32:Z:13:ALA:HB1	2.03	0.88
38:f:64:G:O6	38:f:101:A:N6	2.19	0.76
7:A:138:U:H5'	32:Z:1:MET:HE3	1.67	0.76
31:Y:33:ALA:HB2	32:Z:13:ALA:CB	2.18	0.74
31:Y:33:ALA:HB1	32:Z:13:ALA:HB1	1.71	0.71
7:A:1071:G:H22	7:A:1090:A:H62	1.37	0.71
7:A:1047:G:HO2'	7:A:1110:G:H1	1.37	0.70
38:f:664:G:H22	38:f:741:G:H1	1.41	0.69
7:A:1341:G:H21	32:Z:59:ASN:HD22	1.39	0.69
32:Z:17:SER:O	40:h:44:PHE:CE1	2.46	0.68
38:f:409:U:H3	38:f:433:G:H1	1.41	0.68
31:Y:33:ALA:HB2	32:Z:13:ALA:HB1	1.74	0.66
41:i:87:CYS:H	41:i:89:GLN:HE21	1.43	0.66
43:k:34:ILE:HG13	43:k:35:GLU:HG2	1.78	0.66
7:A:1059:G:H21	15:I:128:SER:HA	1.61	0.65
38:f:99:C:H6	38:f:99:C:O5'	1.80	0.65
47:o:29:SER:HB3	47:o:59:LEU:HB2	1.78	0.65
23:Q:44:GLN:HE21	24:R:77:PHE:HB3	1.62	0.65
38:f:1124:G:O2'	38:f:1145:A:N6	2.30	0.64
45:m:51:ILE:HD11	45:m:85:ILE:HD12	1.79	0.64
10:D:110:THR:HG21	10:D:169:ARG:HH11	1.62	0.64
7:A:2336:A:H61	29:W:43:THR:HG21	1.63	0.64
38:f:71:A:C5	38:f:100:G:C6	2.86	0.64
38:f:501:C:OP1	51:s:114:ARG:NH2	2.31	0.64
38:f:959:A:HO2'	38:f:984:C:HO2'	1.43	0.64
16:J:62:VAL:HG11	16:J:101:ILE:HD11	1.80	0.63
3:2:5:G:N2	3:2:68:C:N3	2.45	0.63
40:h:98:LYS:HB2	40:h:101:GLU:HB2	1.81	0.63
44:l:115:LEU:HD13	44:l:123:VAL:HG11	1.79	0.63
18:L:74:THR:HG22	18:L:107:PHE:HB2	1.80	0.63
48:p:12:ARG:HD3	48:p:13:LYS:HG2	1.80	0.63
5:4:19:G:H1	5:4:57:G:H21	1.46	0.62
7:A:2126:A:H62	7:A:2171:A:H5"	1.64	0.62
44:l:77:ASN:HB2	44:l:82:GLN:HG2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1365:A:OP1	30:X:3:ARG:NH2	2.34	0.61
43:k:153:SER:HA	43:k:156:LYS:HG2	1.81	0.61
3:2:4:U:H3	3:2:70:C:H42	1.45	0.61
11:E:5:LEU:HD12	11:E:10:SER:HB2	1.82	0.61
38:f:434:U:H2'	38:f:435:A:H8	1.65	0.61
38:f:495:A:N1	43:k:120:HIS:NE2	2.49	0.61
2:1:34:ARG:NE	50:r:126:LYS:O	2.33	0.61
52:t:67:GLY:HA2	52:t:70:ARG:HD3	1.82	0.61
38:f:1178:G:N2	38:f:1181:G:OP2	2.34	0.61
38:f:519:C:N4	38:f:529:G:O2'	2.33	0.61
7:A:243:U:OP2	36:d:8:ARG:NH1	2.34	0.60
32:Z:24:MET:HG2	32:Z:93:LEU:HD21	1.83	0.60
38:f:101:A:H2'	38:f:102:G:C8	2.36	0.60
2:1:41:PRO:HA	2:1:44:GLU:HB3	1.82	0.60
38:f:1150:A:H4'	49:q:43:PRO:HG3	1.83	0.60
43:k:170:TRP:HD1	43:k:171:LEU:HG	1.67	0.60
30:X:19:SER:OG	30:X:20:HIS:N	2.35	0.60
7:A:1607:C:N4	7:A:1622:G:OP2	2.35	0.60
2:1:10:GLU:HG2	2:1:11:PRO:HD3	1.82	0.59
42:j:35:SER:OG	42:j:59:ARG:NH2	2.35	0.59
3:2:20:G:O2'	3:2:48:C:N4	2.35	0.59
4:3:56:C:N3	12:F:80:ARG:NH2	2.51	0.59
22:P:63:LYS:HE3	22:P:65:SER:HB2	1.84	0.59
15:I:37:GLU:HA	15:I:41:ALA:HB3	1.82	0.59
31:Y:21:LEU:HD13	32:Z:5:GLU:CD	2.24	0.59
38:f:8:A:N6	43:k:202:GLU:O	2.35	0.59
45:m:5:GLU:OE2	57:y:24:LYS:NZ	2.35	0.59
32:Z:3:ARG:NE	32:Z:3:ARG:O	2.36	0.59
7:A:2121:G:N2	7:A:2176:A:N1	2.50	0.59
13:G:86:LYS:HG2	13:G:132:VAL:HG22	1.85	0.58
38:f:522:C:H41	51:s:50:ARG:HH22	1.50	0.58
25:S:59:GLU:HB2	25:S:66:ILE:HD11	1.85	0.58
38:f:251:G:N2	38:f:253:A:N7	2.50	0.58
38:f:412:A:N6	38:f:432:A:N3	2.51	0.58
9:C:29:PRO:HG2	9:C:34:LEU:HD11	1.85	0.58
7:A:2204:G:H4'	9:C:150:LYS:HD3	1.85	0.58
38:f:75:G:H22	38:f:95:C:H42	1.52	0.58
7:A:2109:U:O2	7:A:2110:G:N2	2.37	0.58
9:C:235:GLY:O	9:C:239:ASN:ND2	2.36	0.58
48:p:84:THR:HG21	48:p:103:PHE:HB3	1.86	0.58
50:r:35:THR:OG1	50:r:40:ASN:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Y:33:ALA:HB2	32:Z:13:ALA:HB2	1.86	0.58
43:k:15:GLU:OE2	43:k:63:ARG:NH1	2.36	0.58
9:C:258:ARG:NH1	9:C:264:ASP:OD1	2.37	0.57
38:f:495:A:N6	43:k:116:GLN:OE1	2.37	0.57
38:f:976:G:N2	38:f:1362:A:O2'	2.37	0.57
39:g:1100:VAL:HG21	39:g:1142:PHE:HB2	1.86	0.57
13:G:104:ASN:ND2	13:G:114:ASP:OD1	2.38	0.57
43:k:186:PRO:HB2	43:k:191:LEU:HB2	1.85	0.57
49:q:52:LEU:HD11	49:q:59:LYS:HA	1.86	0.57
7:A:883:G:N2	7:A:894:U:O2'	2.37	0.57
38:f:550:G:O2'	51:s:116:LYS:NZ	2.37	0.57
7:A:2296:U:O4	21:O:9:ARG:NH2	2.36	0.57
7:A:2484:G:OP1	19:M:44:ARG:NH2	2.36	0.57
19:M:69:PRO:HA	19:M:94:ALA:HB2	1.86	0.57
42:j:20:SER:OG	42:j:40:ARG:NH2	2.37	0.57
38:f:405:U:O4	43:k:2:ALA:N	2.37	0.57
43:k:124:MET:HG2	43:k:129:VAL:HG23	1.86	0.57
58:z:36:ARG:NH2	58:z:72:GLY:O	2.38	0.57
7:A:698:C:O2'	7:A:734:A:N6	2.38	0.57
7:A:1337:G:O2'	40:h:42:ASP:O	2.23	0.57
7:A:2744:G:H21	13:G:143:GLN:HE22	1.53	0.57
38:f:81:A:N7	38:f:83:C:N4	2.53	0.57
46:n:113:ASP:OD2	46:n:122:ASN:ND2	2.37	0.57
7:A:370:G:O2'	7:A:424:G:OP1	2.22	0.57
26:T:6:LYS:HG2	26:T:37:GLU:HB3	1.87	0.57
39:g:1056:ARG:NH1	39:g:1074:ASN:OD1	2.38	0.57
7:A:1173:U:O2	7:A:1176:U:N3	2.38	0.57
55:w:68:SER:OG	55:w:69:ASP:N	2.37	0.57
7:A:2796:U:H3	7:A:2799:A:H61	1.53	0.56
38:f:100:G:H2'	38:f:101:A:H5'	1.87	0.56
38:f:1013:G:N2	38:f:1016:A:OP2	2.38	0.56
50:r:23:ILE:HD11	50:r:86:VAL:HG22	1.87	0.56
31:Y:26:PHE:CZ	32:Z:50:LEU:HD23	2.40	0.56
7:A:2349:G:OP1	36:d:45:ARG:NH2	2.38	0.56
18:L:91:ASP:OD1	18:L:91:ASP:N	2.38	0.56
20:N:22:ARG:HG3	20:N:70:THR:HA	1.87	0.56
21:O:31:THR:O	21:O:102:ARG:NH1	2.38	0.56
38:f:406:G:H5'	43:k:5:LEU:HD21	1.86	0.56
38:f:436:C:O2	43:k:154:ARG:NH2	2.38	0.56
43:k:125:VAL:HG12	43:k:143:VAL:HG22	1.86	0.56
58:z:50:ALA:HB1	58:z:57:HIS:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:56:C:O2	7:A:2112:G:N2	2.38	0.56
43:k:98:LEU:HB3	43:k:118:VAL:HG21	1.87	0.56
44:l:13:GLU:HB3	44:l:39:VAL:HG12	1.87	0.56
7:A:1791:A:N6	7:A:1828:G:O2'	2.39	0.56
7:A:1936:A:H2	7:A:1943:U:H3	1.52	0.56
7:A:2305:U:H5"	12:F:131:GLY:HA3	1.87	0.56
7:A:2857:G:N2	7:A:2860:A:OP2	2.36	0.56
9:C:161:TYR:HB3	9:C:194:GLU:HB2	1.87	0.56
52:t:89:LEU:HD23	52:t:92:ARG:HD3	1.87	0.56
38:f:101:A:H2'	38:f:102:G:H8	1.70	0.56
16:J:125:TYR:OH	16:J:132:HIS:NE2	2.35	0.56
17:K:98:ARG:NH2	38:f:340:U:OP2	2.38	0.56
43:k:13:ARG:NH1	43:k:37:ALA:O	2.39	0.56
7:A:682:G:O6	7:A:794:A:N6	2.38	0.56
5:4:18:G:O6	5:4:61:C:N4	2.39	0.55
5:4:76:A:HO3'	7:A:2451:A:HO2'	1.54	0.55
12:F:2:ALA:N	12:F:94:GLU:OE2	2.39	0.55
43:k:143:VAL:HB	43:k:179:GLU:HA	1.87	0.55
2:1:6:VAL:O	50:r:109:ASN:ND2	2.39	0.55
7:A:729:G:N2	9:C:11:PRO:O	2.39	0.55
51:s:69:GLY:HA3	51:s:107:VAL:HG11	1.87	0.55
15:I:123:GLU:O	15:I:127:ARG:NH1	2.39	0.55
38:f:693:G:OP1	50:r:127:ARG:NH2	2.39	0.55
38:f:1064:G:O2'	38:f:1190:G:N2	2.38	0.55
38:f:1126:U:OP1	49:q:7:ARG:NH2	2.40	0.55
32:Z:6:ARG:NH2	32:Z:37:ASP:OD1	2.39	0.55
38:f:444:G:N2	38:f:490:C:O2	2.39	0.55
41:i:55:ALA:O	41:i:59:LYS:NZ	2.40	0.55
43:k:93:LEU:HG	43:k:136:GLN:HE22	1.71	0.55
7:A:466:A:OP1	35:c:34:ARG:NH1	2.39	0.55
42:j:164:ARG:NH1	42:j:166:GLU:OE1	2.40	0.55
7:A:2134:A:O2'	7:A:2159:G:N3	2.39	0.55
38:f:880:C:OP1	51:s:9:ARG:NH2	2.40	0.55
38:f:1127:G:H1	38:f:1145:A:H61	1.55	0.55
7:A:2575:C:OP1	10:D:149:ASN:ND2	2.40	0.55
38:f:890:G:O2'	38:f:906:A:N6	2.39	0.55
50:r:13:ARG:HG2	50:r:14:LYS:HG2	1.88	0.55
7:A:301:G:OP2	27:U:82:ARG:NH1	2.39	0.55
15:I:81:LYS:HA	15:I:136:MET:HE1	1.87	0.55
22:P:2:SER:OG	22:P:3:ASN:N	2.38	0.55
24:R:46:GLU:OE2	24:R:48:LYS:NZ	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:f:426:U:OP1	43:k:36:GLN:NE2	2.40	0.55
38:f:1248:A:H4'	48:p:33:ARG:HH12	1.71	0.55
41:i:168:HIS:ND1	41:i:169:GLU:OE2	2.39	0.55
53:u:30:ILE:O	53:u:35:ASN:ND2	2.40	0.55
53:u:41:ARG:NH1	53:u:42:TRP:O	2.40	0.55
11:E:6:LYS:HG3	11:E:119:ILE:HG23	1.87	0.55
38:f:94:G:N2	38:f:98:A:C6	2.75	0.55
51:s:99:ARG:NE	51:s:104:CYS:SG	2.80	0.55
7:A:1170:C:N3	7:A:1178:C:N4	2.55	0.54
28:V:77:VAL:HG23	28:V:89:ILE:HG12	1.88	0.54
38:f:210:C:OP1	38:f:211:G:N2	2.40	0.54
54:v:18:ASP:OD1	54:v:18:ASP:N	2.38	0.54
9:C:210:ALA:O	9:C:214:ARG:NH1	2.40	0.54
11:E:176:ASP:N	11:E:176:ASP:OD1	2.37	0.54
30:X:12:PRO:HB3	30:X:30:LEU:HD23	1.88	0.54
45:m:86:ARG:NH1	57:y:64:TYR:O	2.41	0.54
7:A:1336:A:OP2	32:Z:68:LYS:NZ	2.38	0.54
38:f:70:U:O2	38:f:71:A:N6	2.40	0.54
49:q:85:ASP:O	49:q:89:ARG:NH1	2.41	0.54
50:r:50:SER:OG	50:r:69:ARG:NH1	2.39	0.54
38:f:662:U:O2'	38:f:836:G:OP1	2.24	0.54
9:C:135:ILE:O	9:C:167:ARG:NH1	2.40	0.54
38:f:668:G:H21	54:v:46:HIS:HE1	1.55	0.54
42:j:105:GLU:OE1	42:j:107:ARG:NH1	2.40	0.54
50:r:93:ARG:NH2	50:r:112:ASP:OD2	2.41	0.54
7:A:1341:G:H21	32:Z:59:ASN:ND2	2.04	0.54
7:A:2092:U:OP2	14:H:27:ARG:NH2	2.40	0.54
32:Z:7:LEU:HD12	32:Z:46:ALA:HA	1.89	0.54
41:i:47:VAL:HG23	41:i:48:PRO:HD3	1.90	0.54
3:2:4:U:O4	3:2:69:A:N6	2.41	0.54
7:A:2483:C:N3	19:M:123:LYS:NZ	2.53	0.54
17:K:70:ARG:HG2	17:K:76:VAL:HG12	1.90	0.54
32:Z:61:LEU:HD21	32:Z:82:LYS:HD2	1.90	0.54
54:v:2:SER:OG	54:v:3:LEU:N	2.41	0.54
7:A:138:U:H4'	7:A:140:C:H42	1.73	0.53
7:A:987:C:O2'	7:A:1000:A:N3	2.39	0.53
7:A:2298:A:OP1	12:F:71:ARG:NH2	2.40	0.53
38:f:1322:C:OP1	58:z:78:ARG:NH2	2.39	0.53
7:A:138:U:H5'	32:Z:1:MET:CE	2.37	0.53
11:E:153:LEU:HD11	11:E:158:PHE:HB2	1.90	0.53
31:Y:49:ASP:OD1	31:Y:52:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:k:58:LYS:NZ	43:k:69:GLU:OE1	2.41	0.53
45:m:11:HIS:ND1	45:m:13:ASP:OD1	2.41	0.53
54:v:74:ASP:OD2	54:v:77:ARG:NH1	2.41	0.53
9:C:16:VAL:HG22	9:C:206:GLY:HA3	1.90	0.53
13:G:121:ILE:HD12	13:G:141:ILE:HG22	1.89	0.53
38:f:182:A:N1	38:f:223:A:O2'	2.41	0.53
38:f:1435:G:O6	38:f:1465:A:N6	2.42	0.53
54:v:25:THR:HG23	54:v:66:LEU:HD12	1.91	0.53
22:P:51:ARG:NH1	22:P:56:HIS:O	2.42	0.53
37:e:23:ILE:HB	37:e:38:GLY:HA3	1.89	0.53
38:f:570:G:O6	38:f:865:A:N6	2.41	0.53
7:A:2006:C:O2'	7:A:2823:A:N3	2.41	0.53
17:K:63:VAL:HG12	17:K:107:LEU:HD11	1.89	0.53
38:f:923:A:N6	38:f:1392:G:O6	2.42	0.53
38:f:1060:U:H4'	49:q:53:ILE:HG23	1.91	0.53
15:I:80:LEU:HD22	15:I:84:ALA:HB2	1.90	0.53
27:U:74:ASN:ND2	27:U:81:ASP:OD2	2.42	0.53
38:f:227:G:O2'	55:w:63:GLN:NE2	2.39	0.53
7:A:2840:C:H5"	20:N:53:THR:HG21	1.89	0.53
27:U:51:ALA:O	27:U:54:GLN:NE2	2.42	0.53
38:f:416:G:H1	38:f:427:U:H3	1.57	0.53
55:w:69:ASP:N	55:w:69:ASP:OD1	2.39	0.53
7:A:572:A:OP2	24:R:80:ARG:NH2	2.42	0.53
7:A:2122:U:H3	7:A:2177:C:H1'	1.73	0.53
7:A:2635:A:O2'	10:D:49:GLN:NE2	2.42	0.53
28:V:51:GLN:OE1	28:V:57:TYR:OH	2.27	0.53
38:f:551:U:O2'	51:s:83:ARG:NH1	2.42	0.53
38:f:1307:U:OP1	52:t:100:GLN:NE2	2.42	0.53
38:f:683:G:N2	50:r:39:GLY:O	2.42	0.53
49:q:5:ARG:HE	49:q:79:PRO:HG3	1.74	0.53
53:u:90:ARG:NH1	53:u:92:GLU:OE1	2.42	0.53
7:A:981:A:OP2	7:A:982:C:N4	2.42	0.53
7:A:2485:G:OP1	19:M:45:GLN:NE2	2.39	0.53
12:F:34:ILE:HG12	12:F:156:ILE:HG12	1.90	0.53
13:G:86:LYS:NZ	13:G:130:GLU:OE2	2.42	0.53
17:K:110:GLU:H	17:K:113:MET:HE2	1.73	0.53
38:f:1255:G:O2'	38:f:1258:G:N3	2.41	0.53
43:k:147:GLU:HA	43:k:150:LYS:HB2	1.91	0.53
38:f:380:G:N2	38:f:383:A:OP2	2.41	0.52
38:f:1060:U:OP1	53:u:85:ARG:NH2	2.43	0.52
47:o:11:LEU:HD22	47:o:75:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2638:G:O2'	7:A:2775:G:N2	2.41	0.52
38:f:993:G:O2'	38:f:994:A:N7	2.42	0.52
41:i:71:GLY:HA3	41:i:80:VAL:HG21	1.90	0.52
7:A:443:A:N6	11:E:36:ALA:O	2.41	0.52
38:f:254:G:N2	56:x:18:GLU:OE1	2.39	0.52
38:f:614:C:OP2	43:k:81:ARG:NH2	2.42	0.52
38:f:1005:A:N6	38:f:1024:G:O2'	2.43	0.52
4:3:63:C:H2'	4:3:64:G:H8	1.75	0.52
7:A:309:A:N3	7:A:329:G:O2'	2.41	0.52
7:A:1826:G:O2'	7:A:1971:U:OP2	2.27	0.52
21:O:8:ILE:O	21:O:12:THR:OG1	2.27	0.52
22:P:106:LYS:O	22:P:109:ARG:NH2	2.37	0.52
48:p:51:PRO:HD3	48:p:80:ARG:HG3	1.90	0.52
30:X:2:SER:OG	30:X:3:ARG:N	2.41	0.52
38:f:123:U:OP1	38:f:311:C:O2'	2.28	0.52
40:h:90:PRO:HB3	40:h:109:PHE:HB3	1.92	0.52
4:3:27:C:O2	4:3:44:G:N2	2.42	0.52
15:I:78:VAL:O	15:I:82:LYS:NZ	2.43	0.52
19:M:55:ARG:O	19:M:55:ARG:NH2	2.42	0.52
26:T:41:THR:HG23	26:T:43:ALA:H	1.74	0.52
38:f:841:C:H2'	38:f:843:U:H5"	1.92	0.52
42:j:83:ASP:HA	42:j:86:LYS:HG2	1.91	0.52
2:1:7:ARG:NH1	2:1:8:GLU:O	2.43	0.52
7:A:2743:U:O2'	13:G:153:ARG:NH1	2.43	0.52
16:J:11:VAL:HG21	16:J:50:THR:HG22	1.92	0.52
46:n:130:ASN:HA	46:n:135:VAL:HG21	1.92	0.52
7:A:1252:G:H22	23:Q:37:GLN:HE21	1.57	0.52
38:f:404:G:H5'	43:k:119:SER:HB2	1.90	0.52
44:l:55:GLU:HG3	44:l:57:PRO:HD2	1.90	0.52
46:n:53:ARG:NH1	46:n:122:ASN:OD1	2.43	0.52
38:f:1297:G:O2'	46:n:114:LYS:NZ	2.43	0.52
7:A:396:G:OP2	30:X:10:LYS:NZ	2.42	0.51
7:A:2144:G:O2'	7:A:2147:A:N6	2.42	0.51
50:r:26:SER:OG	50:r:27:PHE:N	2.42	0.51
7:A:1245:G:OP1	18:L:13:LYS:NZ	2.43	0.51
7:A:2285:C:OP2	34:b:6:ARG:NH1	2.42	0.51
38:f:134:G:O6	55:w:25:ARG:NH1	2.43	0.51
9:C:219:THR:O	9:C:219:THR:OG1	2.25	0.51
43:k:85:ASN:ND2	44:l:101:GLU:O	2.44	0.51
35:c:31:LEU:HD22	35:c:42:LEU:HD23	1.93	0.51
38:f:881:G:OP2	51:s:6:GLN:NE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:m:40:GLU:OE1	45:m:42:TRP:NE1	2.39	0.51
51:s:52:VAL:HG12	51:s:66:TYR:HA	1.93	0.51
3:2:18:G:O2'	3:2:57:G:O6	2.28	0.51
7:A:2788:C:O2'	7:A:2809:A:N3	2.37	0.51
38:f:80:A:N6	38:f:88:U:O4	2.44	0.51
38:f:617:G:H1	38:f:623:C:H42	1.58	0.51
40:h:55:ALA:HA	40:h:59:GLY:HA3	1.91	0.51
43:k:65:TYR:HB2	43:k:67:VAL:HG23	1.91	0.51
7:A:585:G:N7	23:Q:6:ARG:NH1	2.58	0.51
7:A:1113:U:H5'	13:G:3:ARG:HH12	1.75	0.51
11:E:41:GLN:NE2	11:E:43:THR:OG1	2.42	0.51
13:G:80:THR:OG1	13:G:81:GLU:OE1	2.28	0.51
1:0:49:LYS:O	1:0:49:LYS:NZ	2.37	0.51
7:A:1527:G:N1	7:A:1544:A:OP2	2.38	0.51
13:G:84:THR:HG22	13:G:134:LYS:HG2	1.93	0.51
38:f:522:C:H5	51:s:50:ARG:HH12	1.58	0.51
39:g:1164:LEU:O	39:g:1167:ARG:NH1	2.38	0.51
58:z:35:SER:HG	58:z:38:SER:HG	1.57	0.51
2:1:4:ILE:HG21	57:y:73:ARG:HH22	1.74	0.51
5:4:74:C:N4	7:A:2507:C:O2'	2.43	0.51
7:A:1866:A:N6	7:A:1875:G:O2'	2.44	0.51
38:f:468:A:OP2	38:f:470:C:N4	2.44	0.51
56:x:21:ILE:HB	56:x:48:ASP:HB2	1.93	0.51
38:f:927:G:O2'	38:f:1503:A:N7	2.42	0.51
38:f:1397:C:OP2	44:l:29:ARG:NH2	2.39	0.51
41:i:33:GLY:H	41:i:40:ILE:HG13	1.76	0.51
7:A:211:C:OP1	35:c:25:LYS:NZ	2.35	0.51
38:f:1232:U:OP1	48:p:126:GLN:NE2	2.40	0.51
43:k:151:LYS:HG3	43:k:155:VAL:HG11	1.93	0.51
46:n:48:GLU:O	46:n:52:GLN:NE2	2.44	0.51
14:H:24:GLY:O	14:H:28:ASN:ND2	2.42	0.50
7:A:1667:G:N2	7:A:1992:G:OP2	2.41	0.50
7:A:2680:U:H5'	10:D:194:PRO:HA	1.92	0.50
9:C:145:GLU:HB2	9:C:188:CYS:HB3	1.93	0.50
10:D:39:ASP:N	10:D:39:ASP:OD1	2.44	0.50
38:f:1119:C:OP1	48:p:85:ARG:NH2	2.44	0.50
56:x:68:SER:OG	56:x:69:LYS:O	2.26	0.50
7:A:2576:G:O2'	7:A:2579:C:OP2	2.27	0.50
42:j:113:ALA:HB1	42:j:200:VAL:HG13	1.93	0.50
7:A:1070:A:H1'	15:I:10:LYS:HD2	1.94	0.50
7:A:1266:G:OP2	33:a:17:ARG:NE	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:98:G:H1	28:V:14:LYS:HB3	1.77	0.50
55:w:36:VAL:HG13	55:w:53:ASP:HB3	1.94	0.50
7:A:411:G:OP2	7:A:2406:A:O2'	2.29	0.50
7:A:547:A:H8	7:A:548:G:H5'	1.76	0.50
8:B:11:C:OP1	29:W:72:LYS:NZ	2.41	0.50
18:L:17:LYS:HE3	18:L:27:LEU:HD21	1.94	0.50
34:b:25:LYS:NZ	34:b:30:LYS:O	2.44	0.50
38:f:406:G:O2'	43:k:116:GLN:NE2	2.43	0.50
38:f:880:C:H2'	38:f:881:G:H8	1.77	0.50
45:m:49:TYR:OH	57:y:63:ARG:O	2.27	0.50
2:1:4:ILE:HG23	50:r:112:ASP:HB3	1.93	0.50
22:P:22:PRO:HD3	22:P:50:ILE:HD12	1.92	0.50
32:Z:62:VAL:HG22	32:Z:81:LYS:HG3	1.93	0.50
6:6:14:ALA:HB3	6:6:22:MET:HG3	1.94	0.50
7:A:2144:G:N2	7:A:2148:G:O6	2.45	0.50
24:R:55:ASP:OD1	24:R:55:ASP:N	2.44	0.50
42:j:58:GLU:HG3	42:j:65:ARG:HB3	1.93	0.50
58:z:36:ARG:NH2	58:z:75:ALA:O	2.44	0.50
58:z:39:THR:HG22	58:z:70:LYS:HG2	1.92	0.50
7:A:568:U:O4	24:R:81:LYS:NZ	2.44	0.50
38:f:148:G:H1	38:f:174:A:H61	1.60	0.50
58:z:41:PHE:HB2	58:z:44:MET:HE3	1.94	0.50
1:0:80:THR:O	1:0:84:ASN:ND2	2.45	0.49
7:A:458:G:O2'	7:A:469:G:O6	2.28	0.49
32:Z:19:LYS:NZ	32:Z:84:TYR:OH	2.44	0.49
3:2:13:C:N4	3:2:48:C:O2	2.45	0.49
9:C:260:ASN:ND2	9:C:263:THR:OG1	2.39	0.49
41:i:20:THR:O	41:i:37:LYS:NZ	2.45	0.49
7:A:1394:U:H4'	7:A:1603:A:H4'	1.93	0.49
7:A:2123:G:O6	7:A:2125:G:N2	2.45	0.49
42:j:51:SER:HB3	42:j:72:ARG:HH21	1.77	0.49
57:y:37:GLY:O	57:y:63:ARG:NH2	2.42	0.49
58:z:20:GLU:HA	58:z:23:VAL:HG12	1.93	0.49
7:A:1223:G:OP1	24:R:68:ARG:NH2	2.45	0.49
9:C:107:PRO:HA	9:C:195:VAL:HA	1.94	0.49
21:O:28:VAL:HG11	21:O:103:VAL:HG13	1.95	0.49
38:f:181:A:O2'	38:f:194:C:N4	2.45	0.49
7:A:2130:U:H1'	7:A:2159:G:H1	1.77	0.49
19:M:25:ASP:N	19:M:25:ASP:OD1	2.44	0.49
21:O:16:ARG:NH2	21:O:19:GLN:OE1	2.46	0.49
49:q:63:ASP:OD2	53:u:85:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:54:THR:HA	19:M:57:VAL:HG12	1.94	0.49
38:f:898:G:N2	38:f:901:A:OP2	2.38	0.49
38:f:974:A:OP1	53:u:69:ARG:NH2	2.45	0.49
50:r:23:ILE:HG22	50:r:32:VAL:HG22	1.95	0.49
7:A:788:A:OP1	7:A:791:C:N4	2.40	0.49
7:A:1072:C:N4	7:A:1091:G:O6	2.45	0.49
15:I:88:SER:OG	15:I:89:GLY:N	2.45	0.49
19:M:42:THR:HG22	19:M:93:VAL:HG12	1.95	0.49
23:Q:26:GLY:O	23:Q:30:ARG:NH1	2.44	0.49
40:h:1:MET:HE2	40:h:78:ALA:HB2	1.95	0.49
3:2:21:A:N6	3:2:47:U:OP2	2.46	0.49
12:F:15:LYS:NZ	12:F:19:GLU:OE2	2.42	0.49
43:k:104:ARG:HD2	43:k:170:TRP:HE1	1.77	0.49
46:n:57:SER:OG	46:n:58:GLU:N	2.45	0.49
38:f:1261:A:N6	38:f:1274:A:O2'	2.45	0.48
6:6:34:LEU:HD23	12:F:110:ARG:HD2	1.95	0.48
7:A:659:G:O2'	11:E:95:LYS:O	2.30	0.48
7:A:1779:U:OP2	7:A:1784:A:N6	2.45	0.48
45:m:3:HIS:H	45:m:92:THR:HG23	1.78	0.48
34:b:5:ILE:O	34:b:28:ARG:NH2	2.46	0.48
38:f:202:G:H21	38:f:466:A:H61	1.60	0.48
7:A:1597:A:H5"	7:A:1598:A:H5'	1.95	0.48
7:A:577:G:O2'	7:A:1254:A:OP1	2.31	0.48
7:A:2261:C:OP1	29:W:19:LYS:NZ	2.44	0.48
16:J:37:ARG:NH2	16:J:44:TYR:OH	2.41	0.48
24:R:32:THR:HA	24:R:62:GLU:HA	1.95	0.48
31:Y:30:MET:SD	32:Z:14:PRO:HD3	2.54	0.48
38:f:977:A:OP1	53:u:61:ARG:NH2	2.42	0.48
43:k:25:VAL:O	43:k:164:GLN:NE2	2.47	0.48
50:r:35:THR:HG1	50:r:40:ASN:H	1.61	0.48
27:U:99:ASN:ND2	27:U:101:GLU:OE2	2.47	0.48
34:b:13:SER:OG	34:b:14:SER:N	2.46	0.48
38:f:201:G:N2	38:f:469:C:O2	2.42	0.48
38:f:1166:G:N1	38:f:1169:A:OP2	2.43	0.48
43:k:20:PHE:O	43:k:111:ARG:NH2	2.39	0.48
44:l:14:LYS:NZ	44:l:116:GLU:OE2	2.39	0.48
7:A:2683:C:OP1	22:P:51:ARG:NH2	2.39	0.48
11:E:127:GLU:O	11:E:156:ASN:ND2	2.46	0.48
15:I:90:SER:OG	15:I:91:GLY:N	2.46	0.48
17:K:30:ARG:NH2	17:K:37:ASP:OD2	2.47	0.48
32:Z:3:ARG:O	32:Z:5:GLU:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:j:31:ASP:OD1	42:j:31:ASP:N	2.39	0.48
48:p:19:VAL:HA	48:p:65:ILE:HG22	1.96	0.48
4:3:4:G:H1	4:3:69:U:H3	1.60	0.48
38:f:1055:A:N3	42:j:156:ARG:NH1	2.62	0.48
43:k:105:MET:HG3	43:k:171:LEU:HD13	1.94	0.48
39:g:1063:SER:OG	39:g:1068:GLU:OE1	2.32	0.48
55:w:79:ASN:HB3	55:w:82:ALA:HB3	1.95	0.48
39:g:1078:LEU:HD21	39:g:1109:ARG:HG2	1.95	0.47
41:i:188:ASP:H	41:i:191:SER:HB2	1.79	0.47
42:j:187:SER:OG	42:j:188:GLU:N	2.46	0.47
45:m:91:ARG:NH1	45:m:92:THR:O	2.47	0.47
7:A:396:G:N2	7:A:2231:U:O2'	2.47	0.47
7:A:2137:U:H2'	7:A:2138:G:H8	1.78	0.47
7:A:2250:G:OP1	19:M:84:LYS:NZ	2.47	0.47
7:A:2581:G:N2	7:A:2581:G:OP2	2.47	0.47
7:A:2657:A:O2'	13:G:160:LYS:NZ	2.47	0.47
11:E:58:LYS:NZ	11:E:70:SER:O	2.46	0.47
13:G:152:ARG:HA	13:G:152:ARG:HD3	1.74	0.47
15:I:83:ALA:HB3	15:I:105:GLN:HG3	1.96	0.47
18:L:78:ARG:NH2	18:L:80:SER:OG	2.47	0.47
21:O:31:THR:OG1	21:O:34:HIS:O	2.32	0.47
38:f:1360:A:OP2	53:u:75:ARG:NH2	2.47	0.47
4:3:10:G:H1	4:3:25:U:H3	1.62	0.47
9:C:232:HIS:HE2	9:C:244:PRO:HA	1.79	0.47
12:F:57:LEU:O	12:F:61:SER:OG	2.31	0.47
12:F:61:SER:HB2	12:F:91:LEU:HD21	1.95	0.47
41:i:82:ASP:OD1	41:i:84:ALA:N	2.43	0.47
50:r:56:ARG:O	50:r:59:THR:OG1	2.27	0.47
54:v:46:HIS:O	54:v:48:LYS:N	2.47	0.47
5:4:58:A:O2'	5:4:60:U:OP2	2.30	0.47
7:A:1070:A:N7	7:A:1096:A:O2'	2.41	0.47
7:A:1105:U:H2'	7:A:1106:G:H8	1.80	0.47
38:f:297:G:N2	38:f:300:A:OP2	2.37	0.47
52:t:8:ASN:ND2	52:t:66:GLU:OE2	2.47	0.47
7:A:906:U:O2'	19:M:66:ARG:NH2	2.47	0.47
7:A:1568:G:H4'	9:C:59:LYS:HG2	1.96	0.47
7:A:2131:U:H5'	7:A:2132:U:H5"	1.96	0.47
15:I:28:LEU:HD13	15:I:38:PHE:HZ	1.79	0.47
38:f:35:G:N3	51:s:115:SER:OG	2.47	0.47
55:w:68:SER:OG	55:w:69:ASP:OD1	2.33	0.47
8:B:34:A:N6	8:B:44:G:O2'	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:107:PRO:HD2	9:C:110:LEU:HD22	1.96	0.47
9:C:245:VAL:HG12	9:C:251:GLN:HA	1.96	0.47
14:H:40:THR:OG1	14:H:43:ASN:ND2	2.47	0.47
38:f:352:C:O2'	38:f:354:G:OP1	2.30	0.47
43:k:119:SER:O	43:k:119:SER:OG	2.31	0.47
7:A:630:G:N2	7:A:633:A:OP2	2.44	0.47
7:A:714:U:H3'	54:v:89:ARG:HH22	1.79	0.47
7:A:1262:A:N3	33:a:7:LYS:NZ	2.62	0.47
7:A:2125:G:H2'	7:A:2173:A:H61	1.80	0.47
15:I:92:LYS:HB3	15:I:95:LYS:HD2	1.96	0.47
38:f:976:G:OP2	38:f:1358:U:O2'	2.33	0.47
38:f:1239:A:H62	38:f:1299:A:N6	2.13	0.47
45:m:17:GLN:O	45:m:21:MET:N	2.44	0.47
52:t:23:TYR:HB3	52:t:66:GLU:HG2	1.96	0.47
58:z:39:THR:HA	58:z:70:LYS:HA	1.96	0.47
33:a:31:ASP:OD1	33:a:32:LYS:N	2.48	0.47
38:f:197:A:N1	38:f:220:G:O2'	2.39	0.47
38:f:216:U:H4'	38:f:464:U:H4'	1.97	0.47
48:p:128:SER:OG	48:p:130:ARG:O	2.32	0.47
4:3:16:U:O4'	4:3:59:G:N2	2.48	0.47
40:h:75:PHE:HA	40:h:78:ALA:HB3	1.97	0.47
41:i:136:MET:HA	41:i:139:ARG:HG2	1.96	0.47
45:m:5:GLU:HB3	45:m:90:MET:HB2	1.97	0.47
3:2:47:U:O2'	3:2:50:G:OP1	2.29	0.47
7:A:784:G:C6	9:C:228:VAL:HG21	2.49	0.47
12:F:8:TYR:HB2	12:F:173:PHE:HZ	1.80	0.47
2:1:24:GLU:HB2	2:1:27:GLY:H	1.79	0.46
23:Q:50:ARG:O	23:Q:54:LYS:NZ	2.46	0.46
7:A:1077:A:H1'	15:I:93:PRO:HG2	1.97	0.46
7:A:2394:C:H5"	18:L:63:LYS:HE2	1.97	0.46
17:K:43:ILE:HD12	17:K:56:ASP:HB2	1.98	0.46
38:f:1266:G:N2	38:f:1269:A:OP2	2.44	0.46
41:i:68:LEU:HD22	41:i:154:MET:HE1	1.97	0.46
51:s:71:GLY:O	51:s:99:ARG:NH1	2.42	0.46
3:2:19:G:N3	3:2:57:G:N2	2.54	0.46
27:U:27:ASN:OD1	27:U:27:ASN:N	2.46	0.46
37:e:20:ASP:O	37:e:22:VAL:N	2.47	0.46
38:f:9:G:OP2	44:l:126:LYS:NZ	2.39	0.46
3:2:19:G:H1	7:A:2112:G:H2'	1.81	0.46
3:2:20:G:N2	3:2:22:G:O4'	2.49	0.46
3:2:50:G:N2	3:2:64:U:O2'	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:f:1088:G:H21	38:f:1167:A:H62	1.63	0.46
53:u:64:CYS:HB3	53:u:69:ARG:H	1.80	0.46
7:A:1296:G:OP1	7:A:2709:G:O2'	2.31	0.46
7:A:1949:G:HO2'	38:f:1419:G:HO2'	1.61	0.46
9:C:167:ARG:HG3	9:C:172:VAL:HG22	1.97	0.46
15:I:76:ALA:HA	15:I:79:LEU:HB2	1.98	0.46
38:f:145:G:N2	38:f:178:C:N3	2.63	0.46
42:j:22:TRP:NE1	42:j:36:ASP:OD2	2.44	0.46
7:A:58:G:OP1	32:Z:78:SER:HB2	2.16	0.46
7:A:463:G:N2	7:A:466:A:OP2	2.43	0.46
38:f:842:U:O2'	38:f:845:A:OP2	2.33	0.46
50:r:111:THR:OG1	50:r:112:ASP:N	2.49	0.46
58:z:5:LEU:HD11	58:z:10:PHE:HB2	1.96	0.46
7:A:1082:U:H1'	15:I:118:THR:HB	1.98	0.46
10:D:77:ARG:NH1	10:D:200:ASP:OD1	2.48	0.46
31:Y:36:GLN:HE21	40:h:57:ARG:HH22	1.63	0.46
48:p:40:GLY:O	48:p:41:ARG:NE	2.49	0.46
49:q:52:LEU:HB2	53:u:81:ARG:HD2	1.96	0.46
7:A:2798:U:H4'	7:A:2799:A:H5'	1.97	0.46
31:Y:13:GLU:HA	31:Y:16:THR:HG22	1.98	0.46
31:Y:20:ASN:HB3	31:Y:50:VAL:HG12	1.97	0.46
38:f:71:A:C6	38:f:100:G:C5	3.04	0.46
38:f:373:A:H61	38:f:391:G:H1'	1.81	0.46
58:z:28:LYS:HG3	58:z:29:LYS:HG3	1.97	0.46
4:3:9:A:O2'	4:3:10:G:N7	2.49	0.46
7:A:381:G:OP1	30:X:18:ARG:NH1	2.48	0.46
7:A:663:G:H5"	18:L:17:LYS:HD3	1.97	0.46
7:A:971:G:O2'	7:A:983:A:N3	2.43	0.46
7:A:1080:A:O2'	15:I:127:ARG:NE	2.49	0.46
7:A:2313:C:H5"	12:F:88:LYS:HD2	1.97	0.46
18:L:108:ALA:HB3	18:L:125:LEU:HG	1.98	0.46
20:N:106:ASP:N	20:N:106:ASP:OD1	2.49	0.46
1:0:48:GLN:OE1	1:0:52:ASN:ND2	2.49	0.46
6:6:11:GLU:HA	6:6:25:ARG:HA	1.97	0.46
7:A:1081:U:O5'	15:I:127:ARG:NH2	2.49	0.46
8:B:8:C:O3'	21:O:25:ARG:NH1	2.49	0.46
12:F:6:ASP:OD1	12:F:6:ASP:N	2.48	0.46
32:Z:28:ASN:ND2	32:Z:88:LYS:O	2.49	0.46
7:A:1964:G:O2'	7:A:1967:C:OP2	2.29	0.45
7:A:2114:A:H62	7:A:2115:G:H21	1.64	0.45
8:B:36:C:N4	8:B:49:C:O2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:f:81:A:N6	38:f:87:C:N3	2.60	0.45
44:l:111:MET:HG3	44:l:140:THR:HG21	1.99	0.45
29:W:56:ASP:OD1	29:W:56:ASP:N	2.44	0.45
31:Y:11:VAL:O	31:Y:15:ASN:ND2	2.49	0.45
53:u:33:ASP:HB3	53:u:35:ASN:HD21	1.82	0.45
7:A:84:A:N1	7:A:98:G:O2'	2.41	0.45
7:A:811:U:H2'	18:L:21:ARG:HA	1.98	0.45
7:A:1288:G:OP2	7:A:1288:G:N2	2.44	0.45
35:c:12:ARG:HD2	35:c:44:VAL:HG21	1.99	0.45
43:k:3:ARG:HH12	43:k:116:GLN:HE21	1.64	0.45
7:A:743:A:O2'	7:A:1659:G:OP1	2.34	0.45
7:A:2106:U:H2'	7:A:2107:G:H8	1.81	0.45
38:f:310:G:H5"	55:w:31:ARG:HB2	1.98	0.45
51:s:110:ARG:HH21	51:s:113:ALA:HB3	1.80	0.45
7:A:2009:A:OP1	25:S:41:LYS:NZ	2.50	0.45
49:q:32:THR:OG1	49:q:33:GLY:N	2.50	0.45
7:A:2127:G:N2	7:A:2162:G:O5'	2.50	0.45
38:f:944:G:N1	38:f:1338:G:OP2	2.42	0.45
39:g:1130:ILE:HG22	39:g:1134:MET:HE2	1.98	0.45
43:k:95:GLU:HB3	43:k:185:LYS:HE3	1.99	0.45
7:A:475:C:O2	7:A:479:A:N6	2.47	0.45
9:C:98:ASP:OD1	9:C:98:ASP:N	2.40	0.45
22:P:64:ILE:HA	22:P:69:GLY:HA2	1.99	0.45
25:S:59:GLU:HA	25:S:64:ALA:HA	1.98	0.45
7:A:247:G:O6	36:d:12:LYS:NZ	2.43	0.45
38:f:83:C:O2'	38:f:85:U:N3	2.40	0.45
40:h:27:ALA:HB3	40:h:63:ARG:HH22	1.82	0.45
56:x:27:ARG:HG3	56:x:40:ARG:HB3	1.99	0.45
1:0:59:ASP:OD2	1:0:76:LYS:NZ	2.43	0.45
7:A:578:G:OP1	7:A:1255:U:O2'	2.28	0.45
9:C:144:VAL:HG11	9:C:174:LEU:HD21	1.99	0.45
38:f:97:G:H2'	38:f:98:A:O4'	2.17	0.45
22:P:39:ARG:NH1	38:f:346:G:OP1	2.50	0.45
38:f:126:G:OP1	38:f:605:U:O2'	2.26	0.45
42:j:174:PRO:O	42:j:177:THR:OG1	2.35	0.45
7:A:959:A:N3	7:A:2457:U:O2'	2.44	0.44
7:A:1306:C:H41	7:A:1606:C:H2'	1.83	0.44
7:A:1266:G:OP1	33:a:16:ARG:NE	2.50	0.44
7:A:1945:G:N2	7:A:1963:U:O4	2.50	0.44
13:G:45:HIS:HA	13:G:50:LEU:HD23	1.98	0.44
44:l:80:THR:HB	44:l:122:ASN:HD22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:74:ARG:NH2	38:f:261:U:OP2	2.50	0.44
7:A:372:G:H2'	30:X:58:VAL:HG12	1.99	0.44
38:f:495:A:H62	43:k:154:ARG:HH12	1.65	0.44
1:0:85:LYS:HB2	1:0:85:LYS:HE2	1.75	0.44
7:A:2076:U:OP2	7:A:2238:G:N2	2.46	0.44
7:A:2111:U:O3'	7:A:2118:U:O2'	2.35	0.44
7:A:2375:G:N2	7:A:2378:A:OP2	2.45	0.44
8:B:46:A:H5"	21:O:3:LYS:HE2	1.99	0.44
13:G:48:ASN:OD1	13:G:48:ASN:N	2.51	0.44
18:L:78:ARG:HB3	18:L:113:ALA:HB3	1.99	0.44
38:f:687:A:N1	38:f:700:G:O2'	2.47	0.44
41:i:27:MET:HE3	41:i:193:PRO:HD3	2.00	0.44
48:p:91:ASP:OD1	48:p:91:ASP:N	2.49	0.44
52:t:12:HIS:H	52:t:45:ILE:HG22	1.83	0.44
7:A:534:U:O2'	23:Q:45:TYR:O	2.35	0.44
7:A:566:U:H5"	18:L:29:LYS:HE3	1.99	0.44
7:A:2343:U:O2'	7:A:2373:G:O2'	2.35	0.44
38:f:227:G:N2	55:w:63:GLN:O	2.38	0.44
38:f:436:C:O5'	43:k:153:SER:OG	2.32	0.44
7:A:1064:C:N4	7:A:1070:A:OP2	2.50	0.44
12:F:29:PRO:HB2	12:F:169:LEU:HD22	1.99	0.44
14:H:21:VAL:HG21	14:H:26:ALA:HB2	1.99	0.44
31:Y:21:LEU:CD1	32:Z:5:GLU:CD	2.80	0.44
43:k:116:GLN:HA	43:k:119:SER:HB3	1.99	0.44
58:z:55:ARG:HH21	58:z:79:THR:HG21	1.83	0.44
3:2:15:G:H2'	3:2:59:U:H3	1.83	0.44
7:A:587:C:OP2	18:L:21:ARG:NH2	2.50	0.44
7:A:1475:G:O2'	7:A:1514:G:O6	2.30	0.44
7:A:1477:A:N6	7:A:1514:G:O2'	2.50	0.44
8:B:48:U:H4'	21:O:100:HIS:HD2	1.81	0.44
11:E:88:ARG:HA	11:E:88:ARG:HD3	1.72	0.44
15:I:32:GLY:O	15:I:65:ARG:NH2	2.47	0.44
15:I:46:THR:HB	15:I:51:LYS:HE3	1.99	0.44
38:f:409:U:H5'	43:k:24:GLY:HA2	2.00	0.44
7:A:2:G:N2	7:A:2902:C:O2'	2.51	0.44
7:A:1280:G:OP1	33:a:57:LYS:NZ	2.50	0.44
15:I:79:LEU:HD22	15:I:105:GLN:HE22	1.83	0.44
26:T:40:ASP:OD1	26:T:45:ARG:NE	2.48	0.44
39:g:1086:ILE:HD12	39:g:1086:ILE:HA	1.90	0.44
41:i:214:LEU:HA	41:i:217:VAL:HG12	2.00	0.44
44:l:126:LYS:HD2	44:l:126:LYS:HA	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:s:82:ILE:HG22	51:s:97:THR:HG22	1.99	0.44
7:A:1105:U:H2'	7:A:1106:G:C8	2.53	0.44
18:L:19:LEU:HG	18:L:27:LEU:HD23	1.99	0.44
47:o:5:ASP:OD2	47:o:77:ARG:NH1	2.51	0.44
56:x:40:ARG:HA	56:x:40:ARG:HD3	1.80	0.44
6:6:8:LYS:HA	6:6:8:LYS:HD2	1.87	0.43
7:A:1496:A:N3	7:A:1577:C:O2'	2.43	0.43
13:G:89:LEU:HD23	13:G:94:TYR:HB3	2.00	0.43
30:X:16:ASN:HD22	30:X:24:ALA:HB1	1.82	0.43
53:u:6:MET:HE3	53:u:6:MET:HB3	1.88	0.43
7:A:932:U:O2'	7:A:934:U:O4	2.35	0.43
7:A:1060:U:H4'	15:I:77:ALA:HB2	2.00	0.43
8:B:14:U:OP2	8:B:70:C:O2'	2.35	0.43
34:b:23:THR:OG1	34:b:24:THR:N	2.51	0.43
7:A:398:C:OP1	7:A:2090:A:O2'	2.33	0.43
7:A:2655:G:O2'	7:A:2664:G:O6	2.32	0.43
15:I:78:VAL:HA	15:I:81:LYS:HB2	1.99	0.43
17:K:21:CYS:HA	17:K:41:ILE:HG22	2.00	0.43
38:f:54:C:H41	38:f:352:C:H3'	1.83	0.43
38:f:72:A:H61	38:f:98:A:H2	1.66	0.43
38:f:126:G:H5'	38:f:633:G:H22	1.83	0.43
38:f:376:G:H5"	55:w:5:ARG:HB2	1.99	0.43
38:f:676:A:H5"	50:r:115:PRO:HB3	2.00	0.43
38:f:811:C:O2'	38:f:901:A:N1	2.51	0.43
39:g:1143:MET:HE3	39:g:1143:MET:HB2	1.86	0.43
45:m:6:ILE:HB	45:m:62:MET:HB2	2.00	0.43
3:2:20:G:N2	3:2:21:A:O2'	2.51	0.43
7:A:887:U:OP1	52:t:92:ARG:NE	2.51	0.43
17:K:76:VAL:HG22	22:P:73:VAL:HG22	1.99	0.43
38:f:222:C:H2'	38:f:223:A:C8	2.53	0.43
38:f:452:A:H62	38:f:480:U:H3	1.66	0.43
38:f:1522:U:OP1	50:r:128:ARG:NH2	2.48	0.43
6:6:38:SER:HB3	12:F:105:THR:HA	2.01	0.43
7:A:1789:A:H5'	9:C:220:VAL:HG22	2.00	0.43
13:G:115:HIS:HE1	13:G:144:VAL:HG13	1.84	0.43
38:f:1238:A:H5'	38:f:1336:C:H41	1.82	0.43
40:h:32:LEU:HA	40:h:35:VAL:HG12	2.00	0.43
46:n:13:LEU:HD12	46:n:14:PRO:HD2	2.00	0.43
5:4:27:G:H1	5:4:43:U:H3	1.65	0.43
7:A:954:G:OP2	19:M:16:ARG:NH1	2.52	0.43
11:E:24:ASN:HB3	11:E:27:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:8:TYR:HE2	15:I:10:LYS:HE3	1.83	0.43
25:S:109:ASP:OD1	25:S:109:ASP:N	2.50	0.43
38:f:264:C:O2'	56:x:66:PRO:O	2.32	0.43
41:i:21:ARG:HG3	41:i:22:TYR:CD2	2.54	0.43
43:k:23:SER:OG	43:k:24:GLY:N	2.52	0.43
9:C:57:GLY:HA2	9:C:213:TRP:HA	2.00	0.43
9:C:155:ALA:HB2	9:C:162:VAL:HG23	2.00	0.43
10:D:130:GLN:NE2	10:D:139:SER:OG	2.52	0.43
33:a:28:LEU:HD23	33:a:28:LEU:HA	1.86	0.43
40:h:4:SER:O	40:h:16:THR:OG1	2.31	0.43
6:6:28:VAL:HG22	12:F:140:GLU:HA	2.00	0.43
17:K:18:ARG:HB3	17:K:45:GLU:HB2	2.00	0.43
29:W:59:LEU:HD12	29:W:80:ILE:HD12	2.00	0.43
38:f:358:U:H2'	38:f:359:G:H8	1.84	0.43
7:A:1140:C:H5'	16:J:26:GLY:HA3	2.01	0.43
39:g:1075:PRO:HB3	39:g:1108:ILE:HD11	2.01	0.43
42:j:189:ALA:HB3	42:j:196:ILE:HB	2.00	0.43
7:A:686:U:O2'	35:c:4:THR:O	2.33	0.43
7:A:2579:C:O2'	10:D:136:ASN:OD1	2.37	0.43
16:J:141:ASP:OD1	16:J:141:ASP:N	2.44	0.43
39:g:1038:MET:HG3	39:g:1046:LEU:HB2	2.01	0.43
2:1:23:CYS:SG	2:1:24:GLU:N	2.89	0.42
2:1:24:GLU:H	2:1:24:GLU:HG3	1.67	0.42
7:A:31:C:O2'	7:A:1238:G:OP1	2.36	0.42
7:A:489:G:H5"	39:g:1160:LYS:HE3	2.01	0.42
7:A:1417:C:HO2'	7:A:1587:G:HO2'	1.65	0.42
10:D:199:SER:OG	10:D:200:ASP:N	2.52	0.42
31:Y:12:GLU:HA	31:Y:15:ASN:HD21	1.84	0.42
36:d:16:LYS:HE2	36:d:20:GLY:HA2	2.01	0.42
37:e:25:VAL:HB	37:e:35:GLN:HB2	2.01	0.42
38:f:1316:G:N1	38:f:1319:A:OP2	2.51	0.42
44:l:105:ILE:HD12	44:l:105:ILE:HA	1.90	0.42
45:m:97:THR:O	45:m:97:THR:OG1	2.35	0.42
46:n:107:ALA:HB1	46:n:133:THR:HG23	2.00	0.42
49:q:35:GLN:HB2	49:q:78:GLU:HG2	1.99	0.42
52:t:90:ARG:HB3	52:t:97:VAL:HG22	2.00	0.42
7:A:2636:C:O2'	10:D:45:TYR:OH	2.37	0.42
7:A:2748:A:H1'	13:G:67:THR:HG22	2.01	0.42
24:R:49:ILE:HB	24:R:52:PRO:HA	2.01	0.42
38:f:113:G:N3	38:f:353:A:O2'	2.51	0.42
45:m:3:HIS:HB3	45:m:95:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:o:79:SER:HB2	47:o:85:ILE:H	1.83	0.42
51:s:38:TYR:OH	51:s:54:ARG:NE	2.49	0.42
51:s:76:GLU:O	51:s:77:HIS:ND1	2.52	0.42
1:0:3:ASN:ND2	38:f:331:G:O3'	2.51	0.42
7:A:746:U:O2'	7:A:2611:C:O2'	2.34	0.42
7:A:1209:U:O2'	7:A:1237:A:N1	2.51	0.42
7:A:1283:G:N1	7:A:1286:A:OP2	2.52	0.42
15:I:43:ASN:ND2	15:I:47:ASP:OD2	2.53	0.42
21:O:95:SER:O	21:O:95:SER:OG	2.30	0.42
36:d:31:HIS:O	36:d:33:LEU:N	2.51	0.42
38:f:1128:C:H1'	38:f:1147:C:H42	1.84	0.42
42:j:143:ARG:HG3	42:j:144:LEU:HD12	2.00	0.42
12:F:162:SER:OG	12:F:163:ASP:N	2.45	0.42
21:O:27:VAL:HG21	21:O:40:ILE:HD12	2.00	0.42
26:T:6:LYS:HB3	26:T:6:LYS:HE2	1.83	0.42
38:f:1279:G:O2'	38:f:1281:C:OP2	2.36	0.42
39:g:1024:ASN:OD1	39:g:1024:ASN:N	2.52	0.42
43:k:100:ASN:HD21	43:k:104:ARG:HE	1.67	0.42
51:s:73:ASN:ND2	51:s:105:SER:OG	2.51	0.42
15:I:100:LYS:HA	15:I:100:LYS:HD3	1.84	0.42
21:O:67:ASN:OD1	21:O:70:ALA:N	2.48	0.42
23:Q:15:LYS:HB3	23:Q:15:LYS:HE2	1.81	0.42
38:f:411:A:H2'	43:k:31:LYS:HD3	2.02	0.42
42:j:77:ILE:HA	42:j:84:VAL:HB	2.01	0.42
48:p:52:LEU:HD22	48:p:57:MET:HB3	2.02	0.42
20:N:117:ASP:OD1	20:N:117:ASP:N	2.47	0.42
38:f:137:U:H2'	38:f:138:G:H8	1.85	0.42
38:f:404:G:OP2	43:k:97:ARG:NH2	2.53	0.42
38:f:522:C:OP2	51:s:66:TYR:OH	2.34	0.42
51:s:83:ARG:HB2	51:s:98:VAL:HG23	2.01	0.42
7:A:137:U:O4	7:A:140:C:O2'	2.36	0.42
7:A:845:A:N6	7:A:847:U:O2	2.52	0.42
7:A:1047:G:O2'	7:A:1110:G:N1	2.43	0.42
7:A:2684:U:O4'	17:K:70:ARG:NH1	2.52	0.42
8:B:52:A:N7	21:O:64:TYR:OH	2.48	0.42
9:C:154:LEU:HD13	9:C:176:LEU:HD21	2.00	0.42
38:f:328:C:H4'	38:f:329:A:H5"	2.02	0.42
38:f:521:G:OP2	51:s:51:LYS:NZ	2.43	0.42
44:l:150:PRO:HA	44:l:153:VAL:HG12	2.00	0.42
50:r:45:ALA:HB3	50:r:70:CYS:HB2	2.02	0.42
1:0:25:ARG:NH2	38:f:323:U:OP1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:35:VAL:HG21	1:0:54:MET:HG2	2.02	0.42
7:A:1470:A:N6	7:A:1521:G:O2'	2.53	0.42
8:B:9:G:O2'	21:O:45:SER:OG	2.30	0.42
33:a:38:HIS:HB3	33:a:44:THR:HG22	2.02	0.42
38:f:1218:C:H2'	38:f:1219:A:C8	2.55	0.42
43:k:97:ARG:HG3	43:k:99:ASP:H	1.85	0.42
1:0:48:GLN:HE22	1:0:83:ILE:HD12	1.85	0.42
7:A:674:G:H1'	11:E:69:ARG:HD3	2.01	0.42
7:A:2419:U:OP1	36:d:41:LYS:NZ	2.53	0.42
21:O:34:HIS:HB3	21:O:53:THR:HB	2.01	0.42
25:S:69:LEU:HG	25:S:107:VAL:HG22	2.02	0.42
28:V:40:ILE:HD13	28:V:40:ILE:HA	1.91	0.42
47:o:102:ALA:HB3	47:o:113:ASP:HB3	2.01	0.42
50:r:122:ARG:HA	50:r:123:PRO:HD3	1.93	0.42
7:A:811:U:O4	18:L:21:ARG:NH1	2.53	0.41
7:A:1248:G:OP1	11:E:44:ARG:NH1	2.53	0.41
12:F:26:MET:HE3	12:F:26:MET:HB3	1.88	0.41
13:G:56:ASP:OD1	13:G:56:ASP:N	2.46	0.41
20:N:1:MET:HE2	20:N:1:MET:HB3	1.93	0.41
37:e:16:ILE:HD13	37:e:25:VAL:HG22	2.00	0.41
40:h:24:ILE:O	40:h:63:ARG:NH2	2.42	0.41
40:h:33:VAL:O	40:h:37:LYS:NZ	2.41	0.41
51:s:83:ARG:N	51:s:96:HIS:O	2.45	0.41
56:x:12:VAL:HB	56:x:56:GLY:H	1.85	0.41
7:A:881:G:N1	7:A:895:U:O2	2.48	0.41
20:N:28:LEU:HD23	20:N:48:VAL:HG11	2.02	0.41
41:i:210:VAL:HA	41:i:213:TYR:HD2	1.85	0.41
43:k:101:VAL:HG12	43:k:105:MET:HE2	2.02	0.41
7:A:1417:C:O2'	7:A:1587:G:O2'	2.30	0.41
7:A:2175:C:H2'	7:A:2176:A:C8	2.56	0.41
7:A:2547:A:H2'	7:A:2548:U:C6	2.56	0.41
9:C:84:ASP:OD1	9:C:86:ASN:ND2	2.52	0.41
38:f:41:G:H2'	38:f:42:G:H8	1.84	0.41
38:f:67:C:H2'	38:f:68:G:C8	2.56	0.41
38:f:1418:A:N6	38:f:1482:G:O2'	2.53	0.41
44:l:148:ASN:OD1	44:l:148:ASN:N	2.46	0.41
7:A:1378:A:O2'	7:A:1380:G:OP2	2.37	0.41
18:L:81:ASP:OD1	18:L:81:ASP:N	2.52	0.41
21:O:89:ASP:OD1	21:O:89:ASP:N	2.46	0.41
22:P:104:THR:OG1	22:P:105:GLY:N	2.53	0.41
25:S:86:MET:HE3	25:S:87:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:f:769:G:H4'	38:f:1513:A:H4'	2.03	0.41
39:g:1143:MET:HA	39:g:1146:LEU:HD12	2.03	0.41
56:x:45:HIS:HB2	56:x:71:LYS:HB3	2.01	0.41
4:3:30:G:OP1	38:f:1229:A:O2'	2.31	0.41
7:A:659:G:N2	11:E:30:GLN:OE1	2.48	0.41
7:A:1028:A:N3	7:A:2486:C:O2'	2.49	0.41
22:P:10:GLN:HA	22:P:13:MET:HG3	2.01	0.41
41:i:59:LYS:O	41:i:62:SER:OG	2.31	0.41
45:m:55:HIS:HD2	45:m:56:LYS:HG3	1.86	0.41
1:0:48:GLN:O	1:0:52:ASN:ND2	2.39	0.41
7:A:139:U:O2'	7:A:141:G:N2	2.47	0.41
19:M:127:LYS:HE3	19:M:127:LYS:HB2	1.83	0.41
41:i:94:HIS:CG	41:i:146:ASN:HB2	2.55	0.41
42:j:180:ALA:HB1	42:j:203:PHE:HE1	1.85	0.41
10:D:197:THR:O	10:D:197:THR:OG1	2.37	0.41
36:d:49:MET:HE3	36:d:49:MET:HB3	1.86	0.41
38:f:625:U:H2'	38:f:626:G:H8	1.86	0.41
3:2:9:A:N6	3:2:22:G:OP2	2.45	0.41
7:A:1058:U:H2'	7:A:1059:G:H8	1.85	0.41
12:F:133:ARG:HA	12:F:133:ARG:HD3	1.87	0.41
18:L:92:LEU:HD12	18:L:92:LEU:HA	1.91	0.41
24:R:29:THR:O	24:R:29:THR:OG1	2.36	0.41
39:g:1060:ILE:HG12	39:g:1130:ILE:HG13	2.02	0.41
39:g:1135:ASP:HB2	39:g:1140:LYS:HB2	2.03	0.41
49:q:71:LEU:O	49:q:72:ARG:NH1	2.39	0.41
2:1:29:LEU:HD22	50:r:114:THR:HG21	2.03	0.41
7:A:548:G:H4'	7:A:549:G:C4	2.56	0.41
10:D:88:GLU:HB3	10:D:90:PHE:HE1	1.86	0.41
16:J:4:PHE:O	23:Q:64:ARG:NH2	2.45	0.41
18:L:9:ALA:O	18:L:12:SER:OG	2.32	0.41
27:U:49:VAL:O	27:U:54:GLN:NE2	2.41	0.41
37:e:20:ASP:OD1	37:e:20:ASP:N	2.51	0.41
38:f:316:C:OP2	38:f:351:G:O2'	2.36	0.41
38:f:1074:G:O2'	38:f:1101:A:N1	2.46	0.41
43:k:102:VAL:HG11	43:k:117:LEU:HB2	2.03	0.41
47:o:69:LYS:HB2	47:o:69:LYS:HE2	1.84	0.41
54:v:43:PHE:HE1	54:v:49:ASP:HB3	1.85	0.41
12:F:44:ILE:H	12:F:44:ILE:HG13	1.75	0.41
14:H:27:ARG:HH21	14:H:27:ARG:HD2	1.76	0.41
38:f:1128:C:O2'	38:f:1147:C:N3	2.44	0.41
52:t:8:ASN:OD1	52:t:8:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:w:70:ARG:HD2	55:w:70:ARG:HA	1.72	0.41
56:x:31:HIS:HD2	56:x:34:TYR:H	1.67	0.41
56:x:76:VAL:HG12	56:x:77:ARG:H	1.85	0.41
2:1:17:ARG:HE	2:1:20:LYS:HE2	1.85	0.40
7:A:242:G:O2'	7:A:254:G:O6	2.37	0.40
7:A:613:A:H5"	7:A:614:A:H8	1.86	0.40
26:T:3:LYS:NZ	26:T:59:GLU:OE1	2.42	0.40
31:Y:37:LEU:HD12	31:Y:37:LEU:HA	1.95	0.40
42:j:50:ALA:O	42:j:70:THR:OG1	2.40	0.40
42:j:191:THR:OG1	42:j:192:THR:N	2.54	0.40
56:x:72:SER:O	56:x:72:SER:OG	2.32	0.40
58:z:27:ASP:OD1	58:z:27:ASP:N	2.54	0.40
7:A:224:U:OP2	7:A:408:G:N2	2.44	0.40
27:U:17:LYS:HE3	27:U:17:LYS:HB3	1.86	0.40
39:g:1031:VAL:HG22	39:g:1057:ILE:HG21	2.01	0.40
10:D:48:ILE:HG23	10:D:84:LEU:HD21	2.03	0.40
17:K:17:ARG:HB3	17:K:45:GLU:HB3	2.03	0.40
43:k:56:ARG:HA	43:k:56:ARG:HD3	1.89	0.40
44:l:46:VAL:O	44:l:72:ILE:N	2.54	0.40
56:x:26:GLU:OE1	56:x:41:THR:OG1	2.38	0.40
1:0:46:ALA:HA	1:0:49:LYS:HB3	2.02	0.40
7:A:355:U:H2'	7:A:356:G:H8	1.86	0.40
7:A:1654:A:N1	7:A:2048:G:O2'	2.54	0.40
7:A:1992:G:N2	7:A:1996:C:O2'	2.46	0.40
11:E:148:ILE:HB	11:E:169:VAL:HG22	2.03	0.40
38:f:222:C:H2'	38:f:223:A:H8	1.87	0.40
38:f:1320:C:H1'	58:z:73:GLU:HG2	2.04	0.40
39:g:1050:GLN:NE2	39:g:1090:CYS:SG	2.95	0.40
41:i:20:THR:OG1	41:i:37:LYS:O	2.32	0.40
42:j:156:ARG:H	42:j:163:ALA:HA	1.86	0.40
46:n:130:ASN:HB2	46:n:135:VAL:HG11	2.02	0.40
47:o:22:LYS:O	47:o:65:TYR:OH	2.34	0.40
7:A:307:G:N2	7:A:310:A:OP2	2.51	0.40
19:M:34:LYS:HE3	19:M:34:LYS:HB2	1.95	0.40
27:U:13:VAL:HG21	27:U:39:ILE:HG21	2.02	0.40
31:Y:25:GLN:HE22	31:Y:47:ARG:HG2	1.86	0.40
38:f:143:A:H2	38:f:220:G:H1	1.69	0.40
43:k:12:SER:O	43:k:12:SER:OG	2.39	0.40
45:m:41:ASP:OD1	45:m:58:HIS:NE2	2.50	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	0	83/87 (95%)	77 (93%)	5 (6%)	1 (1%)	10	35
2	1	49/71 (69%)	34 (69%)	15 (31%)	0	100	100
6	6	64/70 (91%)	55 (86%)	9 (14%)	0	100	100
9	C	269/273 (98%)	241 (90%)	28 (10%)	0	100	100
10	D	207/209 (99%)	194 (94%)	12 (6%)	1 (0%)	24	54
11	E	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
12	F	175/179 (98%)	159 (91%)	16 (9%)	0	100	100
13	G	174/177 (98%)	160 (92%)	12 (7%)	2 (1%)	11	38
14	H	45/149 (30%)	35 (78%)	10 (22%)	0	100	100
15	I	139/142 (98%)	112 (81%)	27 (19%)	0	100	100
16	J	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
17	K	120/123 (98%)	101 (84%)	18 (15%)	1 (1%)	16	44
18	L	141/144 (98%)	122 (86%)	18 (13%)	1 (1%)	18	47
19	M	134/136 (98%)	123 (92%)	8 (6%)	3 (2%)	5	24
20	N	118/127 (93%)	103 (87%)	14 (12%)	1 (1%)	16	44
21	O	114/117 (97%)	106 (93%)	8 (7%)	0	100	100
22	P	112/115 (97%)	99 (88%)	13 (12%)	0	100	100
23	Q	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
24	R	101/103 (98%)	92 (91%)	9 (9%)	0	100	100
25	S	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
26	T	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
27	U	100/104 (96%)	85 (85%)	12 (12%)	3 (3%)	3	18
28	V	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
29	W	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
30	X	75/78 (96%)	71 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	Y	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
32	Z	94/100 (94%)	82 (87%)	12 (13%)	0	100	100
33	a	54/57 (95%)	49 (91%)	4 (7%)	1 (2%)	6	26
34	b	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
35	c	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
36	d	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	3	17
37	e	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	4	19
39	g	166/169 (98%)	158 (95%)	8 (5%)	0	100	100
40	h	116/118 (98%)	105 (90%)	11 (10%)	0	100	100
41	i	216/241 (90%)	185 (86%)	31 (14%)	0	100	100
42	j	204/233 (88%)	181 (89%)	23 (11%)	0	100	100
43	k	203/206 (98%)	167 (82%)	36 (18%)	0	100	100
44	l	148/167 (89%)	119 (80%)	29 (20%)	0	100	100
45	m	98/135 (73%)	85 (87%)	13 (13%)	0	100	100
46	n	149/179 (83%)	141 (95%)	8 (5%)	0	100	100
47	o	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
48	p	125/130 (96%)	106 (85%)	18 (14%)	1 (1%)	16	44
49	q	96/103 (93%)	82 (85%)	13 (14%)	1 (1%)	12	40
50	r	115/129 (89%)	99 (86%)	16 (14%)	0	100	100
51	s	121/124 (98%)	100 (83%)	21 (17%)	0	100	100
52	t	112/118 (95%)	103 (92%)	7 (6%)	2 (2%)	6	26
53	u	92/101 (91%)	78 (85%)	13 (14%)	1 (1%)	11	38
54	v	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	10	35
55	w	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
56	x	78/84 (93%)	67 (86%)	10 (13%)	1 (1%)	9	33
57	y	53/75 (71%)	48 (91%)	5 (9%)	0	100	100
58	z	77/92 (84%)	70 (91%)	7 (9%)	0	100	100
All	All	5864/6342 (92%)	5255 (90%)	585 (10%)	24 (0%)	31	59

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	G	48	ASN

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Mol	Chain	Res	Type
18	L	82	LEU
36	d	32	ILE
52	t	67	GLY
1	0	69	LYS
13	G	47	ASP
19	M	59	ARG
27	U	90	GLY
36	d	33	LEU
37	e	21	GLY
54	v	47	LYS
56	x	71	LYS
10	D	152	PRO
52	t	66	GLU
33	a	55	ILE
19	M	58	LYS
20	N	3	HIS
53	u	4	GLN
17	K	93	GLN
27	U	51	ALA
27	U	52	LEU
48	p	54	LEU
49	q	57	VAL
19	M	69	PRO

5.3.2 Protein sidechains (i)

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	0	65/66 (98%)	65 (100%)	0	100	100
2	1	44/61 (72%)	44 (100%)	0	100	100
6	6	59/62 (95%)	59 (100%)	0	100	100
9	C	216/218 (99%)	214 (99%)	2 (1%)	70	76
10	D	164/164 (100%)	164 (100%)	0	100	100
11	E	165/165 (100%)	165 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	F	148/150 (99%)	147 (99%)	1 (1%)	76	78
13	G	137/138 (99%)	134 (98%)	3 (2%)	45	63
14	H	38/114 (33%)	38 (100%)	0	100	100
15	I	109/110 (99%)	107 (98%)	2 (2%)	51	67
16	J	116/116 (100%)	116 (100%)	0	100	100
17	K	103/104 (99%)	103 (100%)	0	100	100
18	L	102/103 (99%)	101 (99%)	1 (1%)	68	75
19	M	109/109 (100%)	109 (100%)	0	100	100
20	N	100/103 (97%)	100 (100%)	0	100	100
21	O	86/87 (99%)	86 (100%)	0	100	100
22	P	99/100 (99%)	99 (100%)	0	100	100
23	Q	89/90 (99%)	89 (100%)	0	100	100
24	R	84/84 (100%)	84 (100%)	0	100	100
25	S	93/93 (100%)	93 (100%)	0	100	100
26	T	48/49 (98%)	48 (100%)	0	100	100
27	U	83/85 (98%)	83 (100%)	0	100	100
28	V	78/78 (100%)	78 (100%)	0	100	100
29	W	56/63 (89%)	56 (100%)	0	100	100
30	X	67/68 (98%)	67 (100%)	0	100	100
31	Y	55/55 (100%)	55 (100%)	0	100	100
32	Z	83/84 (99%)	82 (99%)	1 (1%)	63	72
33	a	47/48 (98%)	46 (98%)	1 (2%)	47	64
34	b	45/49 (92%)	45 (100%)	0	100	100
35	c	38/38 (100%)	38 (100%)	0	100	100
36	d	51/52 (98%)	51 (100%)	0	100	100
37	e	34/34 (100%)	34 (100%)	0	100	100
39	g	148/149 (99%)	147 (99%)	1 (1%)	76	78
40	h	100/100 (100%)	100 (100%)	0	100	100
41	i	180/199 (90%)	178 (99%)	2 (1%)	65	74
42	j	170/190 (90%)	170 (100%)	0	100	100
43	k	172/173 (99%)	171 (99%)	1 (1%)	78	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	l	113/126 (90%)	111 (98%)	2 (2%)	51	67
45	m	87/116 (75%)	87 (100%)	0	100	100
46	n	124/147 (84%)	124 (100%)	0	100	100
47	o	104/105 (99%)	104 (100%)	0	100	100
48	p	105/107 (98%)	105 (100%)	0	100	100
49	q	86/90 (96%)	86 (100%)	0	100	100
50	r	90/99 (91%)	89 (99%)	1 (1%)	65	74
51	s	103/104 (99%)	103 (100%)	0	100	100
52	t	92/96 (96%)	92 (100%)	0	100	100
53	u	79/84 (94%)	79 (100%)	0	100	100
54	v	75/77 (97%)	75 (100%)	0	100	100
55	w	65/65 (100%)	64 (98%)	1 (2%)	57	69
56	x	74/78 (95%)	74 (100%)	0	100	100
57	y	48/65 (74%)	48 (100%)	0	100	100
58	z	70/79 (89%)	70 (100%)	0	100	100
All	All	4896/5189 (94%)	4877 (100%)	19 (0%)	81	83

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	C	219	THR
9	C	246	THR
12	F	74	VAL
13	G	15	VAL
13	G	43	VAL
13	G	92	VAL
15	I	5	VAL
15	I	35	ILE
18	L	91	ASP
32	Z	85	VAL
33	a	54	VAL
39	g	1046	LEU
41	i	14	VAL
41	i	47	VAL
43	k	132	ILE
44	l	46	VAL
44	l	90	THR

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Mol	Chain	Res	Type
50	r	16	VAL
55	w	19	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	48	GLN
1	0	52	ASN
1	0	61	GLN
1	0	68	HIS
1	0	70	ASN
1	0	84	ASN
6	6	33	ASN
6	6	61	ASN
9	C	143	ASN
9	C	226	ASN
10	D	32	ASN
10	D	49	GLN
10	D	58	ASN
11	E	9	GLN
11	E	41	GLN
11	E	136	GLN
12	F	5	HIS
12	F	27	GLN
13	G	20	ASN
13	G	104	ASN
13	G	115	HIS
13	G	143	GLN
14	H	43	ASN
15	I	34	ASN
15	I	43	ASN
16	J	47	HIS
17	K	9	ASN
17	K	88	ASN
20	N	3	HIS
21	O	116	GLN
23	Q	37	GLN
23	Q	44	GLN
23	Q	71	GLN
26	T	9	GLN
26	T	20	HIS
27	U	74	ASN

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Mol	Chain	Res	Type
28	V	49	ASN
30	X	16	ASN
31	Y	15	ASN
31	Y	25	GLN
31	Y	27	ASN
32	Z	59	ASN
32	Z	70	HIS
33	a	4	GLN
33	a	42	HIS
34	b	26	ASN
35	c	13	ASN
37	e	13	ASN
37	e	37	GLN
39	g	1050	GLN
39	g	1131	GLN
40	h	74	ASN
41	i	89	GLN
41	i	103	ASN
43	k	100	ASN
43	k	116	GLN
43	k	136	GLN
43	k	152	GLN
44	l	43	ASN
44	l	82	GLN
44	l	132	ASN
45	m	46	GLN
46	n	28	ASN
46	n	52	GLN
47	o	18	GLN
47	o	67	GLN
48	p	4	ASN
48	p	5	GLN
48	p	75	GLN
50	r	118	HIS
51	s	5	ASN
51	s	73	ASN
51	s	75	GLN
53	u	35	ASN
53	u	49	GLN
53	u	71	HIS
54	v	20	ASN
54	v	37	ASN

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Mol	Chain	Res	Type
54	v	46	HIS
55	w	26	ASN
55	w	29	ASN
55	w	63	GLN
56	x	31	HIS
57	y	52	GLN
58	z	43	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	2	58/73 (79%)	13 (22%)	1 (1%)
38	f	1538/1539 (99%)	262 (17%)	0
4	3	63/77 (81%)	7 (11%)	0
5	4	58/76 (76%)	17 (29%)	1 (1%)
7	A	2902/2903 (99%)	477 (16%)	7 (0%)
8	B	117/118 (99%)	14 (11%)	0
All	All	4736/4786 (98%)	790 (16%)	9 (0%)

All (790) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	2	13	C
3	2	14	A
3	2	15	G
3	2	19	G
3	2	20	G
3	2	21	A
3	2	26	A
3	2	36	C
3	2	48	C
3	2	59	U
3	2	60	C
3	2	65	C
3	2	73	A
4	3	14	A
4	3	18	G
4	3	19	U
4	3	21	A
4	3	30	G
4	3	33	U

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Mol	Chain	Res	Type
4	3	76	A
5	4	13	C
5	4	14	A
5	4	19	G
5	4	20	U
5	4	22	G
5	4	26	A
5	4	32	C
5	4	49	G
5	4	50	C
5	4	53	G
5	4	57	G
5	4	61	C
5	4	62	C
5	4	64	G
5	4	66	A
5	4	70	C
5	4	74	C
7	A	10	A
7	A	14	A
7	A	34	U
7	A	35	G
7	A	42	A
7	A	46	G
7	A	51	G
7	A	71	A
7	A	74	A
7	A	75	G
7	A	80	G
7	A	84	A
7	A	101	A
7	A	118	A
7	A	119	A
7	A	120	U
7	A	134	G
7	A	135	U
7	A	137	U
7	A	138	U
7	A	139	U
7	A	140	C
7	A	141	G
7	A	142	A

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Mol	Chain	Res	Type
7	A	149	A
7	A	162	U
7	A	163	C
7	A	188	G
7	A	196	A
7	A	198	C
7	A	199	A
7	A	204	A
7	A	215	G
7	A	216	A
7	A	221	A
7	A	222	A
7	A	233	A
7	A	241	A
7	A	248	G
7	A	249	C
7	A	255	A
7	A	265	A
7	A	266	G
7	A	271	G
7	A	272	A
7	A	276	U
7	A	277	G
7	A	285	G
7	A	311	A
7	A	324	A
7	A	328	U
7	A	329	G
7	A	330	A
7	A	361	G
7	A	362	A
7	A	371	A
7	A	372	G
7	A	385	C
7	A	386	G
7	A	396	G
7	A	399	U
7	A	405	U
7	A	406	G
7	A	411	G
7	A	412	A
7	A	416	U

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Mol	Chain	Res	Type
7	A	420	C
7	A	424	G
7	A	425	G
7	A	455	C
7	A	467	G
7	A	480	A
7	A	481	G
7	A	489	G
7	A	490	C
7	A	491	G
7	A	505	A
7	A	529	A
7	A	531	C
7	A	532	A
7	A	542	C
7	A	543	G
7	A	544	C
7	A	546	U
7	A	547	A
7	A	548	G
7	A	549	G
7	A	563	A
7	A	573	U
7	A	575	A
7	A	584	C
7	A	586	A
7	A	603	A
7	A	614	A
7	A	615	U
7	A	622	G
7	A	627	A
7	A	637	A
7	A	645	C
7	A	654	A
7	A	655	A
7	A	677	A
7	A	683	U
7	A	686	U
7	A	695	G
7	A	696	G
7	A	701	G
7	A	711	G

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Mol	Chain	Res	Type
7	A	730	A
7	A	738	G
7	A	747	U
7	A	748	G
7	A	764	A
7	A	765	C
7	A	775	G
7	A	776	G
7	A	782	A
7	A	783	A
7	A	784	G
7	A	785	G
7	A	792	A
7	A	800	A
7	A	801	G
7	A	805	G
7	A	812	C
7	A	819	A
7	A	827	U
7	A	828	U
7	A	845	A
7	A	846	U
7	A	858	G
7	A	859	G
7	A	878	A
7	A	885	C
7	A	886	A
7	A	887	U
7	A	890	C
7	A	891	G
7	A	892	A
7	A	894	U
7	A	896	A
7	A	897	C
7	A	910	A
7	A	927	A
7	A	931	U
7	A	932	U
7	A	941	A
7	A	946	C
7	A	957	C
7	A	961	C

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Mol	Chain	Res	Type
7	A	973	A
7	A	974	G
7	A	983	A
7	A	985	C
7	A	989	G
7	A	991	C
7	A	995	C
7	A	996	A
7	A	1005	C
7	A	1008	A
7	A	1012	U
7	A	1013	C
7	A	1023	U
7	A	1024	G
7	A	1025	G
7	A	1026	G
7	A	1033	U
7	A	1040	A
7	A	1046	A
7	A	1047	G
7	A	1060	U
7	A	1061	U
7	A	1062	G
7	A	1065	U
7	A	1066	U
7	A	1067	A
7	A	1068	G
7	A	1070	A
7	A	1071	G
7	A	1072	C
7	A	1073	A
7	A	1074	G
7	A	1076	C
7	A	1079	C
7	A	1087	G
7	A	1088	A
7	A	1089	A
7	A	1094	U
7	A	1097	U
7	A	1100	C
7	A	1112	G
7	A	1122	G

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Mol	Chain	Res	Type
7	A	1130	U
7	A	1131	G
7	A	1132	U
7	A	1134	A
7	A	1135	C
7	A	1139	G
7	A	1142	A
7	A	1156	A
7	A	1170	C
7	A	1172	C
7	A	1174	U
7	A	1175	A
7	A	1176	U
7	A	1177	G
7	A	1178	C
7	A	1180	U
7	A	1190	G
7	A	1210	G
7	A	1212	G
7	A	1238	G
7	A	1250	G
7	A	1253	A
7	A	1255	U
7	A	1256	G
7	A	1265	A
7	A	1266	G
7	A	1271	G
7	A	1272	A
7	A	1273	U
7	A	1275	A
7	A	1301	A
7	A	1305	C
7	A	1325	U
7	A	1329	U
7	A	1338	G
7	A	1341	G
7	A	1352	U
7	A	1365	A
7	A	1368	G
7	A	1379	U
7	A	1383	A
7	A	1384	A

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Mol	Chain	Res	Type
7	A	1386	C
7	A	1395	A
7	A	1416	G
7	A	1421	G
7	A	1427	A
7	A	1428	C
7	A	1452	G
7	A	1455	G
7	A	1460	U
7	A	1478	G
7	A	1482	G
7	A	1493	C
7	A	1503	A
7	A	1510	G
7	A	1515	A
7	A	1522	A
7	A	1524	G
7	A	1529	G
7	A	1534	U
7	A	1535	A
7	A	1536	C
7	A	1566	A
7	A	1567	G
7	A	1569	A
7	A	1572	A
7	A	1578	U
7	A	1583	A
7	A	1584	U
7	A	1585	C
7	A	1607	C
7	A	1608	A
7	A	1610	A
7	A	1647	U
7	A	1648	U
7	A	1649	G
7	A	1651	G
7	A	1672	A
7	A	1674	G
7	A	1694	C
7	A	1698	A
7	A	1699	G
7	A	1715	G

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Mol	Chain	Res	Type
7	A	1729	U
7	A	1730	C
7	A	1732	C
7	A	1733	G
7	A	1738	G
7	A	1756	G
7	A	1764	C
7	A	1773	A
7	A	1786	A
7	A	1800	C
7	A	1801	A
7	A	1802	A
7	A	1808	A
7	A	1811	G
7	A	1816	C
7	A	1828	G
7	A	1829	A
7	A	1833	C
7	A	1866	A
7	A	1869	G
7	A	1870	C
7	A	1873	G
7	A	1903	G
7	A	1906	G
7	A	1913	A
7	A	1914	C
7	A	1927	A
7	A	1929	G
7	A	1930	G
7	A	1934	C
7	A	1938	A
7	A	1943	U
7	A	1955	U
7	A	1964	G
7	A	1966	A
7	A	1967	C
7	A	1970	A
7	A	1971	U
7	A	1972	G
7	A	1975	G
7	A	1991	U
7	A	1993	U

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Mol	Chain	Res	Type
7	A	1997	C
7	A	2002	G
7	A	2007	U
7	A	2022	U
7	A	2023	C
7	A	2031	A
7	A	2033	A
7	A	2036	C
7	A	2043	C
7	A	2044	C
7	A	2049	G
7	A	2055	C
7	A	2056	G
7	A	2059	A
7	A	2060	A
7	A	2061	G
7	A	2062	A
7	A	2069	G
7	A	2072	C
7	A	2087	G
7	A	2093	G
7	A	2098	U
7	A	2100	G
7	A	2102	G
7	A	2109	U
7	A	2110	G
7	A	2111	U
7	A	2112	G
7	A	2113	U
7	A	2119	A
7	A	2120	G
7	A	2121	G
7	A	2125	G
7	A	2126	A
7	A	2127	G
7	A	2128	G
7	A	2131	U
7	A	2132	U
7	A	2133	G
7	A	2134	A
7	A	2135	A
7	A	2136	G

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Mol	Chain	Res	Type
7	A	2145	C
7	A	2146	C
7	A	2147	A
7	A	2148	G
7	A	2149	U
7	A	2157	G
7	A	2161	C
7	A	2162	G
7	A	2163	A
7	A	2164	C
7	A	2168	G
7	A	2169	A
7	A	2170	A
7	A	2171	A
7	A	2172	U
7	A	2173	A
7	A	2178	C
7	A	2182	U
7	A	2198	A
7	A	2204	G
7	A	2210	U
7	A	2211	A
7	A	2220	U
7	A	2223	G
7	A	2225	A
7	A	2230	G
7	A	2238	G
7	A	2239	G
7	A	2243	U
7	A	2259	U
7	A	2266	A
7	A	2278	A
7	A	2283	C
7	A	2287	A
7	A	2288	A
7	A	2305	U
7	A	2307	G
7	A	2308	G
7	A	2309	A
7	A	2310	C
7	A	2325	G
7	A	2327	A

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Mol	Chain	Res	Type
7	A	2333	A
7	A	2345	G
7	A	2347	C
7	A	2350	C
7	A	2357	G
7	A	2361	G
7	A	2371	G
7	A	2372	U
7	A	2383	G
7	A	2385	C
7	A	2389	G
7	A	2391	G
7	A	2396	G
7	A	2402	U
7	A	2407	A
7	A	2423	U
7	A	2425	A
7	A	2426	A
7	A	2428	G
7	A	2429	G
7	A	2430	A
7	A	2435	A
7	A	2441	U
7	A	2448	A
7	A	2469	A
7	A	2470	G
7	A	2476	A
7	A	2480	C
7	A	2491	U
7	A	2502	G
7	A	2505	G
7	A	2507	C
7	A	2518	A
7	A	2520	C
7	A	2529	G
7	A	2535	G
7	A	2554	U
7	A	2556	C
7	A	2566	A
7	A	2567	G
7	A	2572	A
7	A	2573	C

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Mol	Chain	Res	Type
7	A	2582	G
7	A	2585	U
7	A	2602	A
7	A	2609	U
7	A	2613	U
7	A	2615	U
7	A	2629	U
7	A	2640	G
7	A	2646	C
7	A	2663	G
7	A	2689	U
7	A	2690	U
7	A	2714	G
7	A	2716	C
7	A	2726	A
7	A	2733	A
7	A	2744	G
7	A	2748	A
7	A	2765	A
7	A	2778	A
7	A	2793	C
7	A	2797	U
7	A	2799	A
7	A	2811	G
7	A	2818	U
7	A	2820	A
7	A	2835	A
7	A	2837	A
7	A	2867	G
7	A	2873	A
7	A	2880	C
7	A	2883	A
7	A	2903	U
8	B	9	G
8	B	35	C
8	B	41	G
8	B	44	G
8	B	51	G
8	B	53	A
8	B	56	G
8	B	66	A
8	B	88	C

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Mol	Chain	Res	Type
8	B	89	U
8	B	90	C
8	B	91	C
8	B	99	A
8	B	109	A
38	f	4	U
38	f	9	G
38	f	22	G
38	f	32	A
38	f	39	G
38	f	44	A
38	f	48	C
38	f	50	A
38	f	51	A
38	f	63	C
38	f	73	C
38	f	74	A
38	f	75	G
38	f	83	C
38	f	85	U
38	f	86	G
38	f	87	C
38	f	88	U
38	f	91	U
38	f	92	U
38	f	93	U
38	f	95	C
38	f	97	G
38	f	100	G
38	f	108	G
38	f	116	A
38	f	120	A
38	f	121	U
38	f	126	G
38	f	130	A
38	f	131	A
38	f	141	G
38	f	151	A
38	f	154	U
38	f	156	C
38	f	163	C
38	f	164	G

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Mol	Chain	Res	Type
38	f	182	A
38	f	183	C
38	f	197	A
38	f	204	G
38	f	208	U
38	f	210	C
38	f	211	G
38	f	212	G
38	f	226	G
38	f	245	U
38	f	247	G
38	f	251	G
38	f	254	G
38	f	266	G
38	f	267	C
38	f	289	G
38	f	298	A
38	f	309	A
38	f	321	A
38	f	328	C
38	f	329	A
38	f	330	C
38	f	332	G
38	f	339	C
38	f	345	C
38	f	346	G
38	f	347	G
38	f	348	G
38	f	352	C
38	f	353	A
38	f	354	G
38	f	367	U
38	f	372	C
38	f	388	G
38	f	392	C
38	f	397	A
38	f	398	U
38	f	406	G
38	f	409	U
38	f	411	A
38	f	412	A
38	f	413	G

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Mol	Chain	Res	Type
38	f	421	U
38	f	423	G
38	f	424	G
38	f	428	G
38	f	429	U
38	f	436	C
38	f	437	U
38	f	452	A
38	f	465	A
38	f	466	A
38	f	467	U
38	f	468	A
38	f	469	C
38	f	478	A
38	f	479	U
38	f	482	A
38	f	484	G
38	f	485	U
38	f	486	U
38	f	495	A
38	f	496	A
38	f	497	G
38	f	505	G
38	f	511	C
38	f	513	C
38	f	518	C
38	f	521	G
38	f	527	G
38	f	530	G
38	f	531	U
38	f	532	A
38	f	538	G
38	f	545	C
38	f	547	A
38	f	559	A
38	f	572	A
38	f	573	A
38	f	575	G
38	f	576	C
38	f	577	G
38	f	596	A
38	f	619	U

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Mol	Chain	Res	Type
38	f	627	G
38	f	633	G
38	f	650	G
38	f	653	U
38	f	665	A
38	f	687	A
38	f	695	A
38	f	703	G
38	f	721	G
38	f	723	U
38	f	724	G
38	f	731	G
38	f	734	G
38	f	755	G
38	f	758	C
38	f	760	G
38	f	777	A
38	f	793	U
38	f	794	A
38	f	810	C
38	f	813	U
38	f	815	A
38	f	817	C
38	f	819	A
38	f	821	G
38	f	828	U
38	f	829	G
38	f	832	G
38	f	841	C
38	f	843	U
38	f	844	G
38	f	846	G
38	f	876	C
38	f	885	G
38	f	914	A
38	f	922	G
38	f	926	G
38	f	934	C
38	f	935	A
38	f	960	U
38	f	966	G
38	f	969	A

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Mol	Chain	Res	Type
38	f	971	G
38	f	975	A
38	f	976	G
38	f	977	A
38	f	983	A
38	f	992	U
38	f	993	G
38	f	1004	A
38	f	1005	A
38	f	1018	G
38	f	1020	G
38	f	1026	G
38	f	1030	U
38	f	1031	C
38	f	1032	G
38	f	1033	G
38	f	1036	A
38	f	1043	G
38	f	1044	A
38	f	1054	C
38	f	1065	U
38	f	1086	U
38	f	1089	G
38	f	1094	G
38	f	1095	U
38	f	1101	A
38	f	1108	G
38	f	1132	C
38	f	1133	G
38	f	1136	C
38	f	1137	C
38	f	1139	G
38	f	1140	C
38	f	1141	C
38	f	1142	G
38	f	1143	G
38	f	1159	U
38	f	1160	G
38	f	1161	C
38	f	1167	A
38	f	1171	A
38	f	1184	G

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Mol	Chain	Res	Type
38	f	1196	A
38	f	1197	A
38	f	1200	C
38	f	1201	A
38	f	1202	U
38	f	1212	U
38	f	1213	A
38	f	1214	C
38	f	1227	A
38	f	1238	A
38	f	1256	A
38	f	1257	A
38	f	1258	G
38	f	1275	A
38	f	1280	A
38	f	1285	A
38	f	1287	A
38	f	1290	G
38	f	1293	C
38	f	1299	A
38	f	1305	G
38	f	1317	C
38	f	1320	C
38	f	1322	C
38	f	1337	G
38	f	1340	A
38	f	1346	A
38	f	1353	G
38	f	1363	A
38	f	1364	U
38	f	1368	A
38	f	1370	G
38	f	1378	C
38	f	1379	G
38	f	1419	G
38	f	1429	A
38	f	1441	A
38	f	1446	A
38	f	1452	C
38	f	1454	G
38	f	1487	G
38	f	1492	A

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Mol	Chain	Res	Type
38	f	1493	A
38	f	1494	G
38	f	1497	G
38	f	1503	A
38	f	1505	G
38	f	1506	U
38	f	1517	G
38	f	1519	A
38	f	1526	G
38	f	1529	G
38	f	1530	G
38	f	1534	A
38	f	1535	C
38	f	1536	C
38	f	1540	U

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	2	58	A
5	4	13	C
7	A	271	G
7	A	404	A
7	A	479	A
7	A	885	C
7	A	1913	A
7	A	2146	C
7	A	2428	G

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

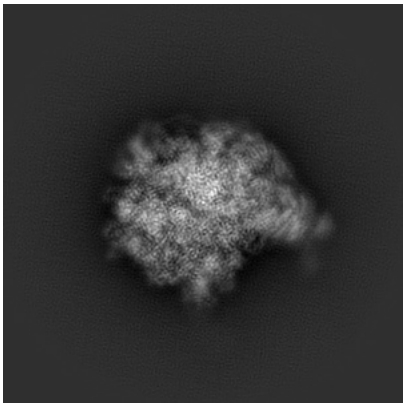
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30598. These allow visual inspection of the internal detail of the map and identification of artifacts.

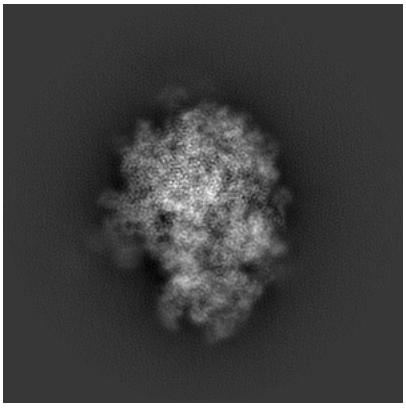
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

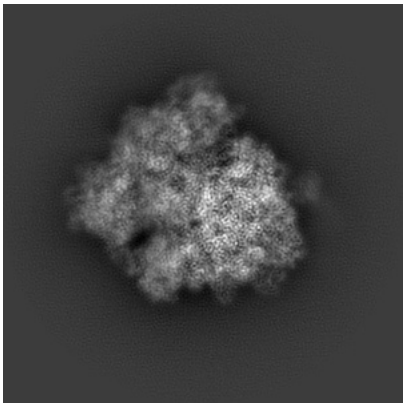
6.1.1 Primary map



X



Y

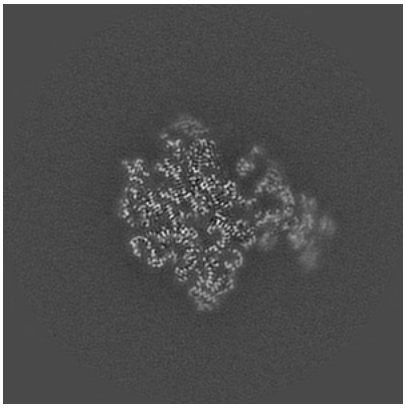


Z

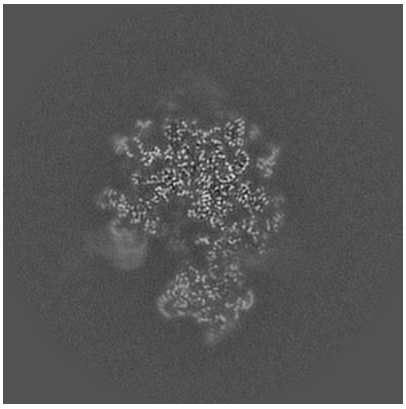
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

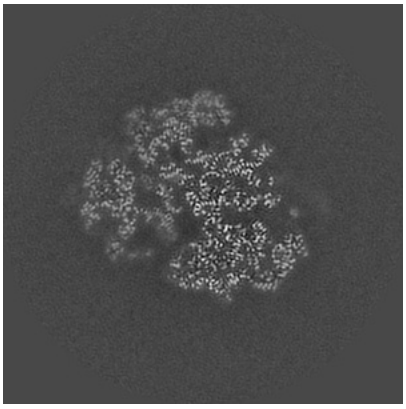
6.2.1 Primary map



X Index: 160



Y Index: 160

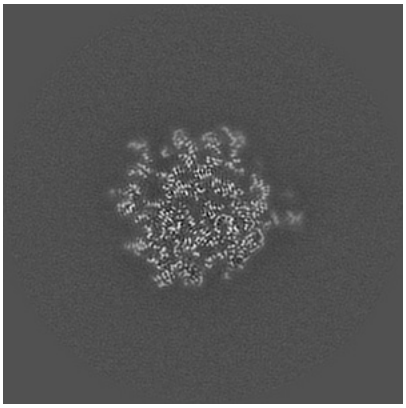


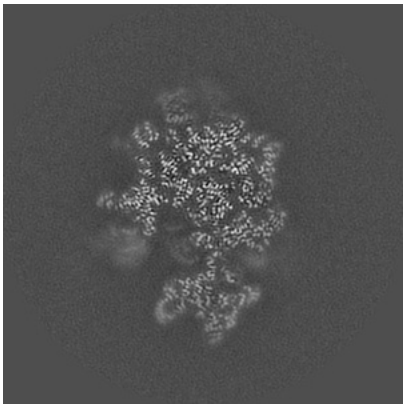
Z Index: 160

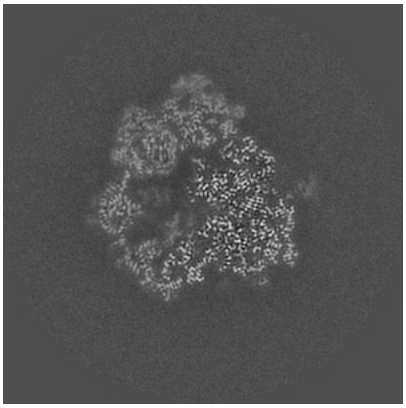
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 186

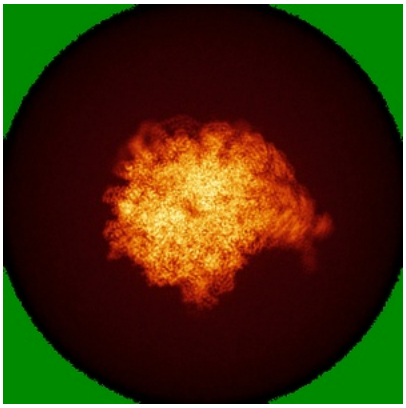

Y Index: 165

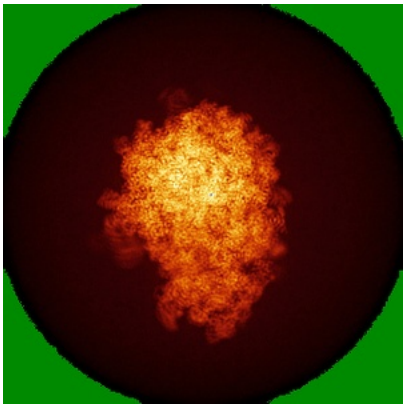

Z Index: 146

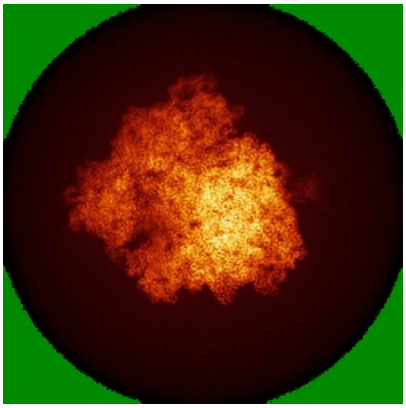
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

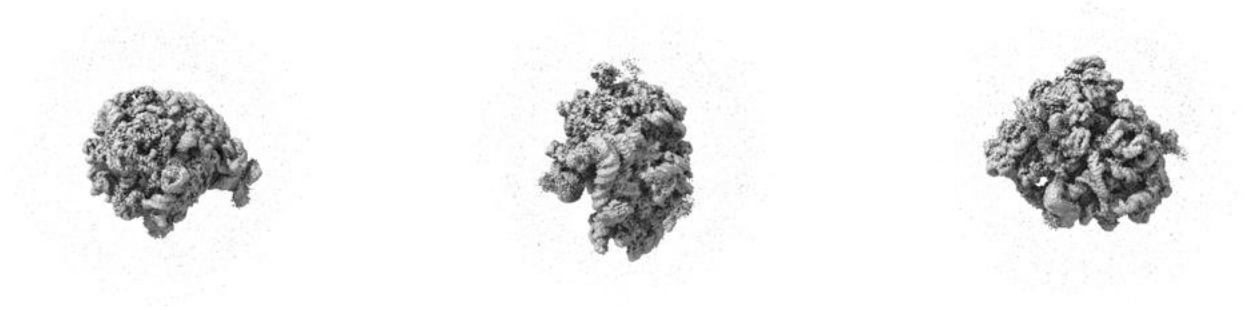

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

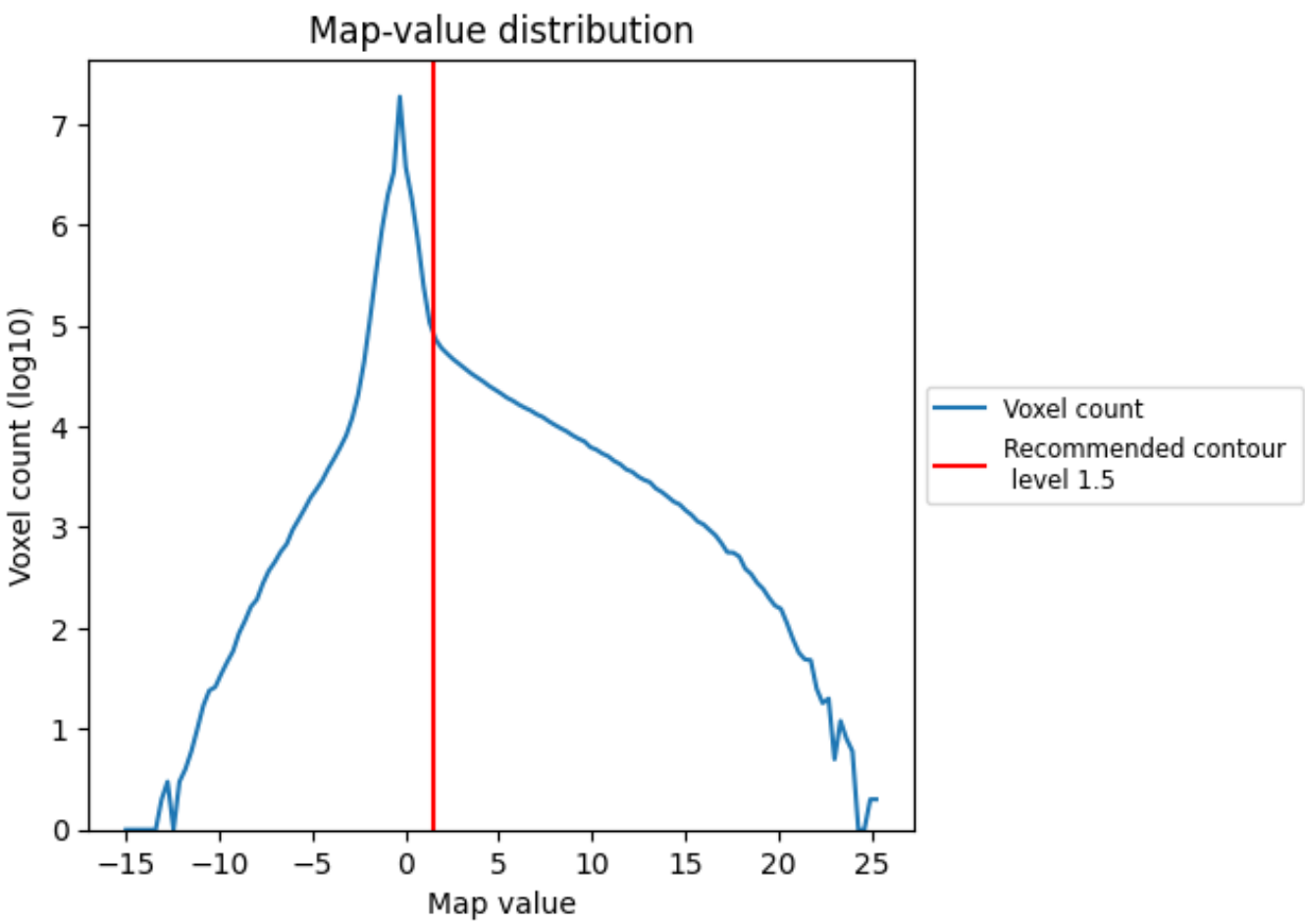
6.6 Mask visualisation (i)

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

7 Map analysis (i)

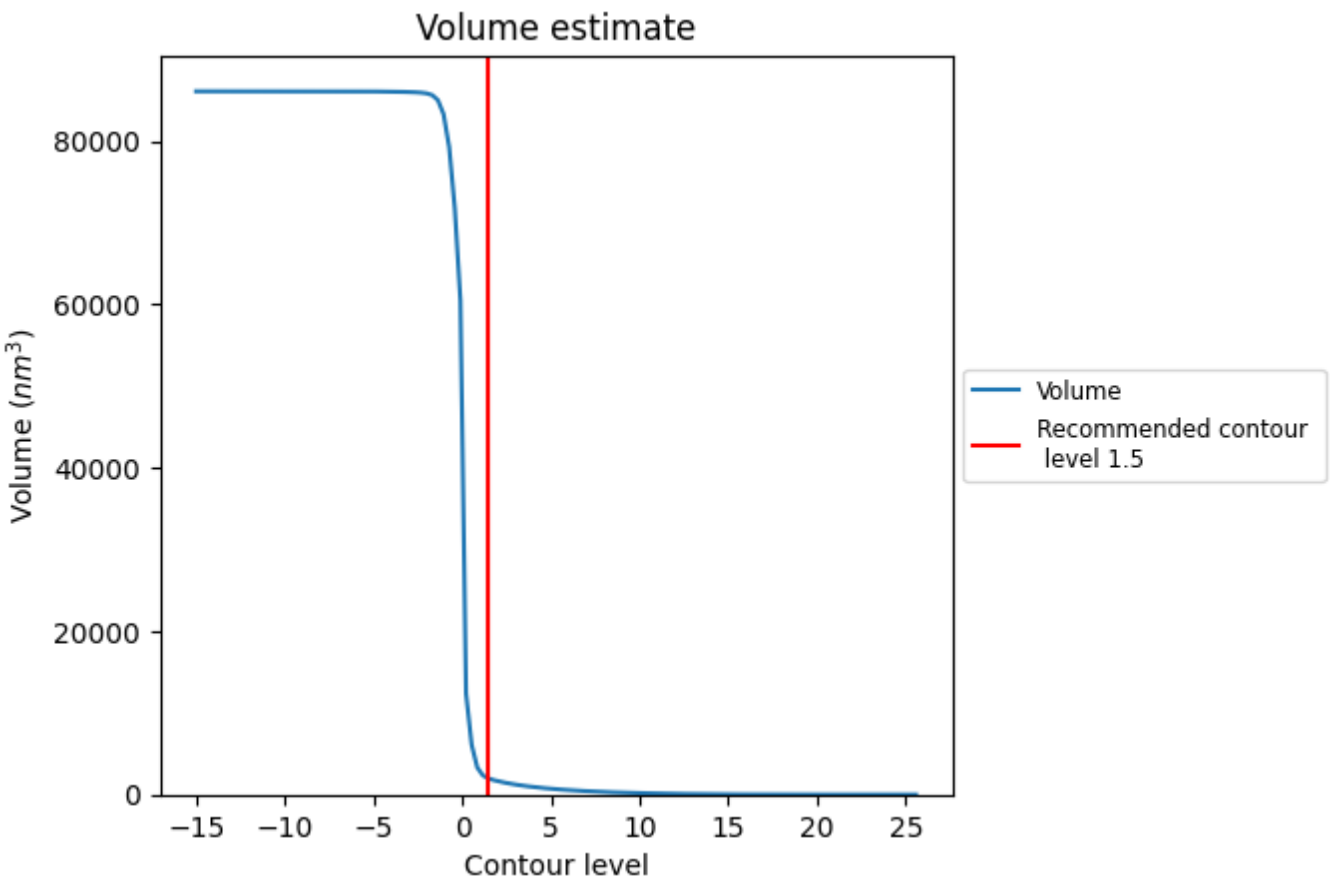
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

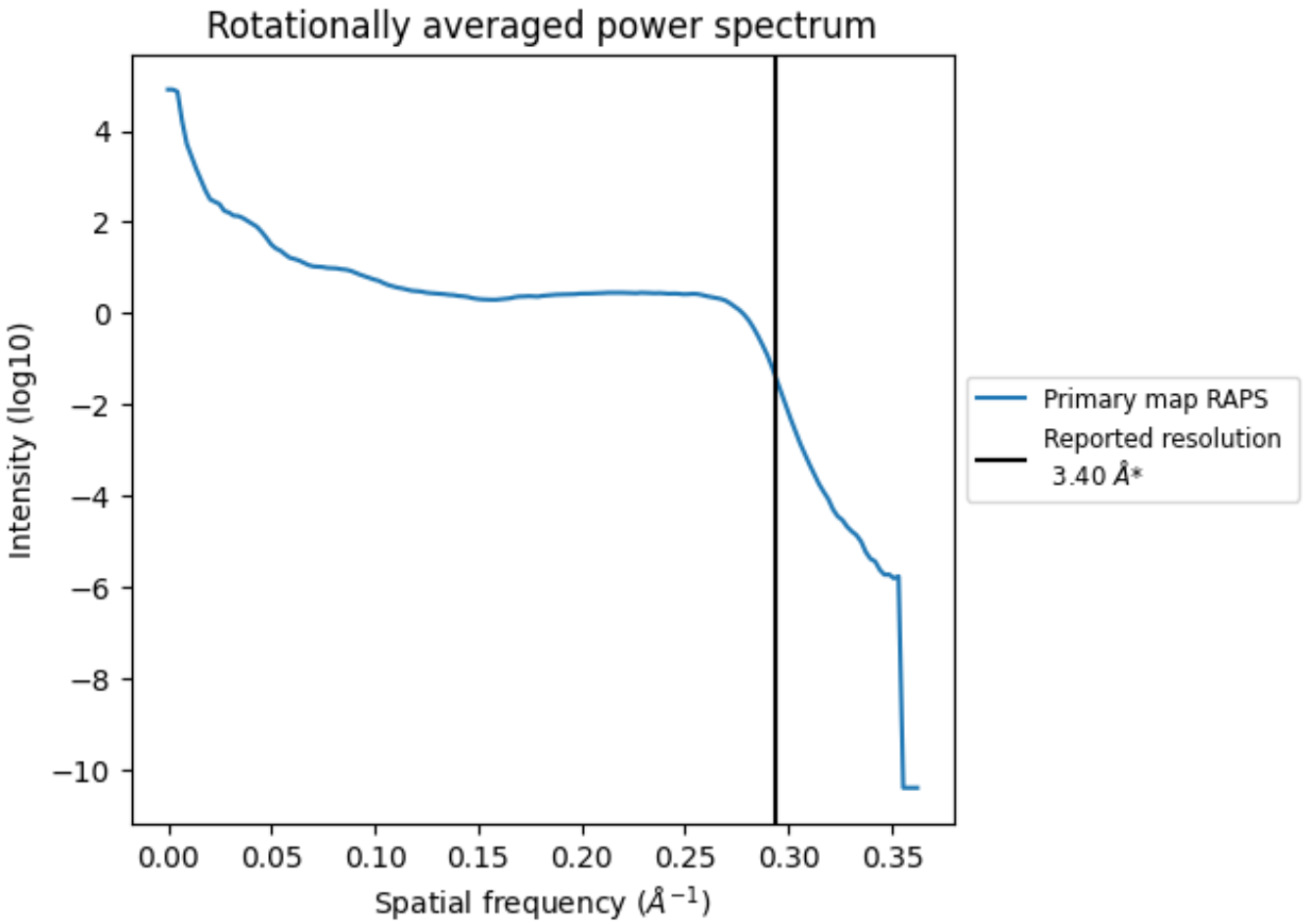
7.2 Volume estimate (i)



The volume at the recommended contour level is 1962 nm^3; this corresponds to an approximate mass of 1772 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 (i)

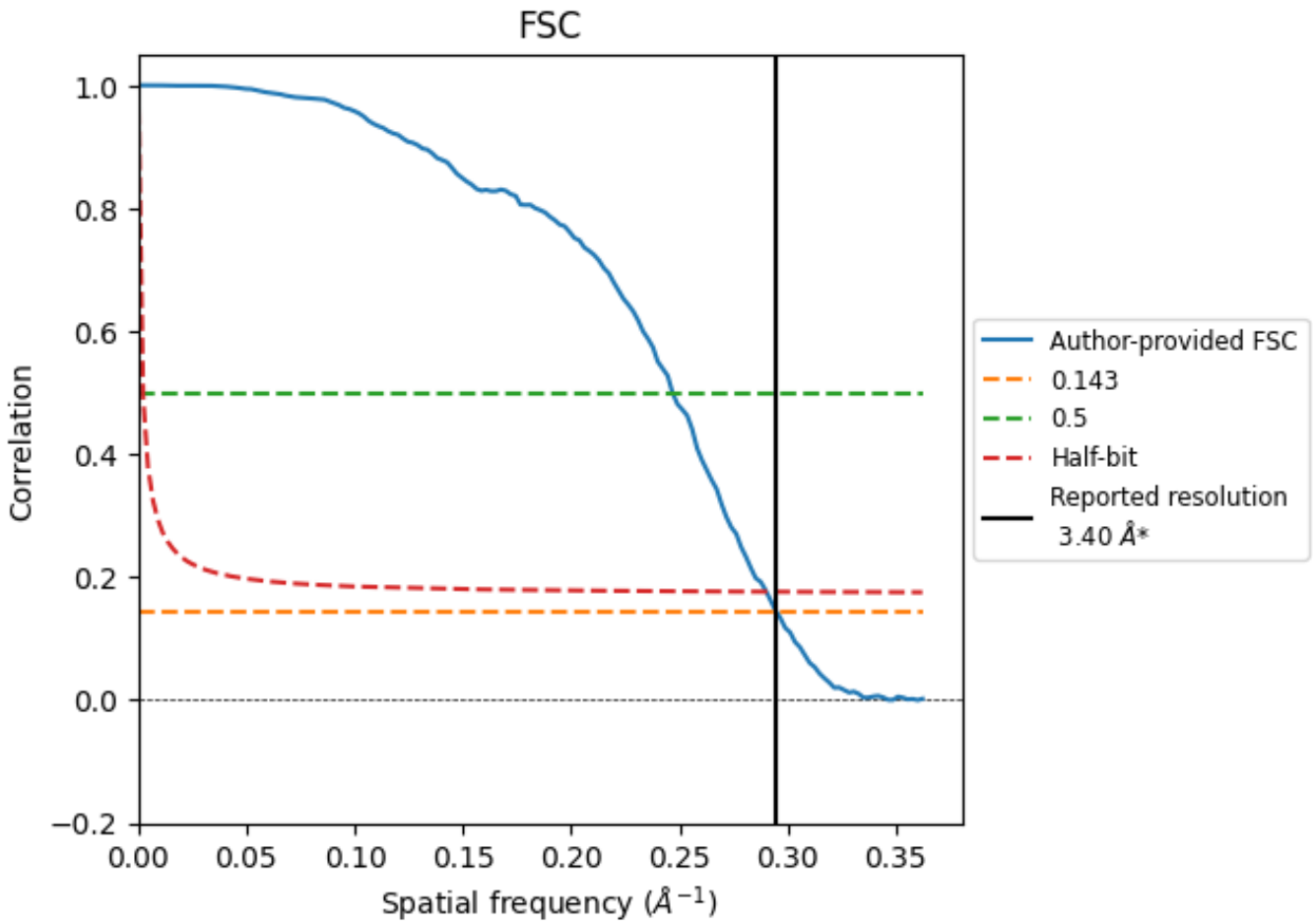


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

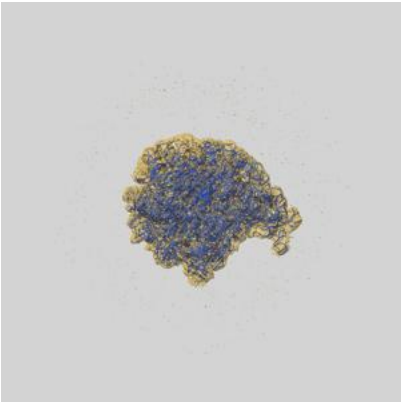
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	4.05	3.45
Unmasked-calculated*	-	-	-

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

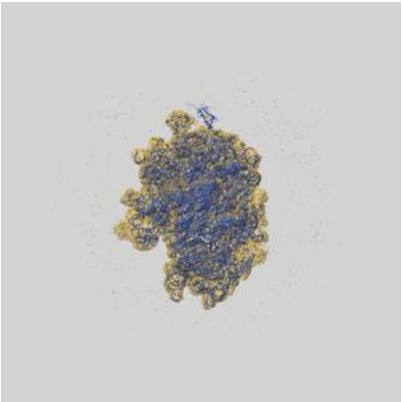
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30598 and PDB model 7D6Z. Per-residue inclusion information can be found in section 3 on page 15.

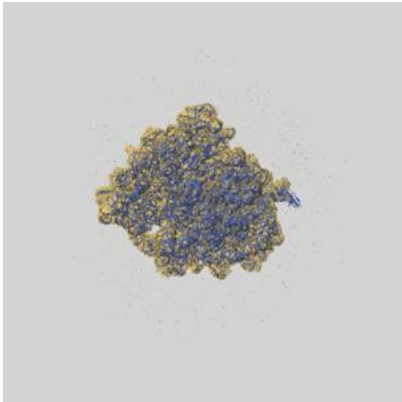
9.1 Map-model overlay (i)



X



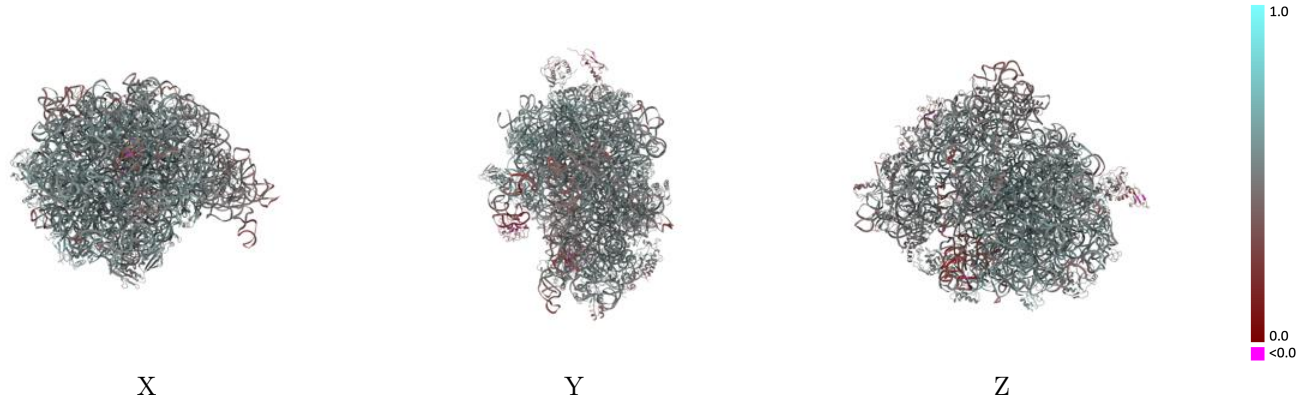
Y



Z

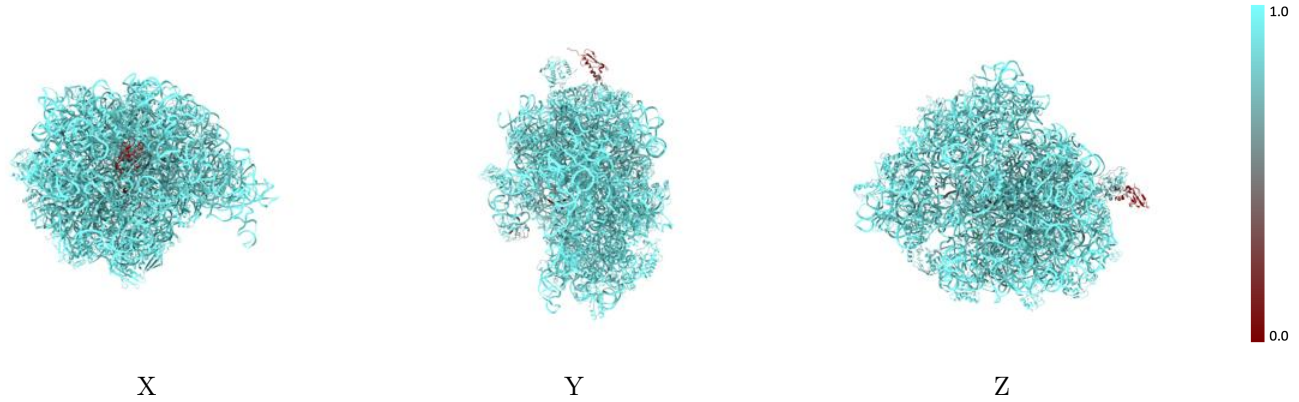
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



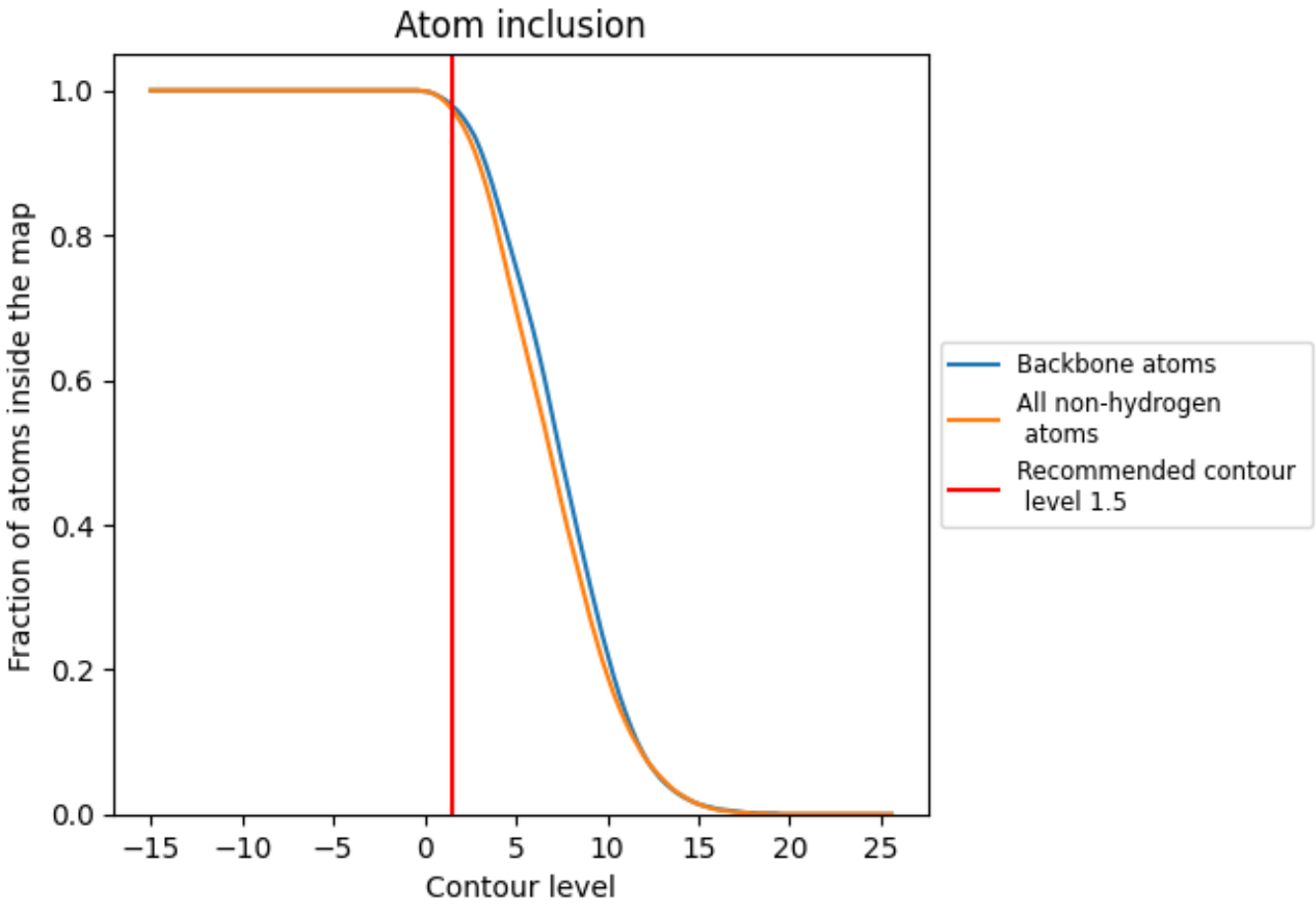
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.5).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9740	0.5050
0	0.9680	0.4600
1	0.8500	0.4020
2	0.9540	0.3200
3	0.9630	0.4720
4	0.3710	0.3900
6	0.7260	0.4510
A	0.9960	0.5210
B	0.9980	0.5200
C	0.9820	0.5700
D	0.9810	0.5600
E	0.9880	0.5520
F	0.9760	0.4950
G	0.9820	0.5180
H	0.9690	0.5040
I	0.7500	0.2130
J	0.9840	0.5670
K	0.9760	0.5520
L	0.9790	0.5560
M	0.9840	0.5660
N	0.9910	0.5640
O	0.9910	0.5330
P	0.9730	0.5540
Q	0.9920	0.5660
R	0.9750	0.5520
S	0.9640	0.5570
T	0.9790	0.5520
U	0.9820	0.5290
V	0.9840	0.5490
W	0.9820	0.5760
X	0.9850	0.5640
Y	0.9560	0.5140
Z	0.9610	0.5170
a	0.9670	0.5610
b	0.9100	0.5480

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Chain	Atom inclusion	Q-score
c	0.9750	0.5740
d	0.9820	0.5840
e	0.9900	0.5670
f	0.9970	0.4880
g	0.8380	0.4190
h	0.2200	0.3370
i	0.9670	0.4670
j	0.9730	0.5140
k	0.9420	0.3810
l	0.9730	0.5250
m	0.9640	0.4830
n	0.9730	0.4870
o	0.9720	0.5260
p	0.9700	0.4720
q	0.9760	0.4610
r	0.9770	0.5160
s	0.9450	0.4750
t	0.9790	0.4810
u	0.9740	0.4900
v	0.9750	0.5080
w	0.9410	0.4790
x	0.9590	0.4680
y	0.9860	0.5290
z	0.9740	0.5000