Full wwPDB EM Validation Report ⓘ

Sep 16, 2026 – 07:27 AM EDT

PDB ID	:	8FZH / pdb_00008fzh
EMDB ID	:	EMD-29628
Title	:	Cryo-EM structure of an E. coli non-rotated ribosome termination complex bound with RF1, P- and E-site tRNAPhe (State II-D)
Authors	:	Rybak, M.Y.; Li, L.; Lin, J.; Gagnon, M.G.
Deposited on	:	2023-01-28
Resolution	:	2.90 Å(reported)
Based on initial model	:	7K00

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

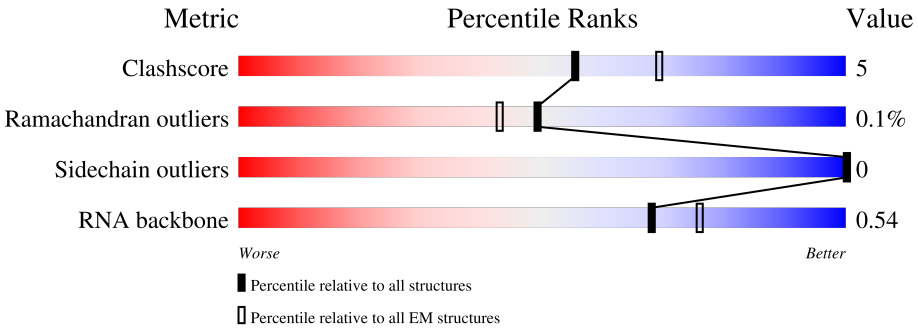
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

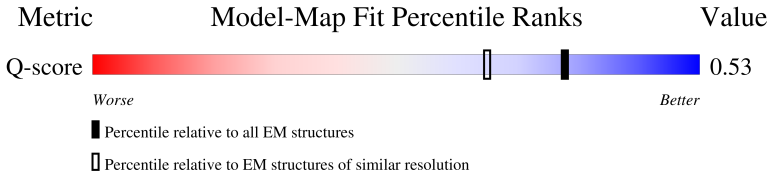
1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	a	1542	72% 24%
2	b	241	68% 25% 7%
3	c	233	74% 14% 12%

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Mol	Chain	Length	Quality of chain
4	d	206	85% 14%
5	e	167	81% 12% 7%
6	f	131	56% 23% 21%
7	g	156	81% 17%
8	h	130	82% 18%
9	i	130	70% 28%
10	j	103	73% 22% 5%
11	k	129	76% 14% 9%
12	l	124	85% 12%
13	m	118	82% 15%
14	n	101	89% 10%
15	o	89	85% 13%
16	p	82	89% 10%
17	q	84	89% 5% 6%
18	r	75	56% 16% 28%
19	s	92	74% 16% 10%
20	t	87	90% 9%
21	u	71	83% 15%
22	x	76	66% 29% 5%
22	y	76	38% 36% 21%
23	z	21	33% 5% 14% 48%
24	w	360	16% 73% 24%
25	A	2904	73% 23%
26	B	120	72% 27%
27	C	273	89% 11%

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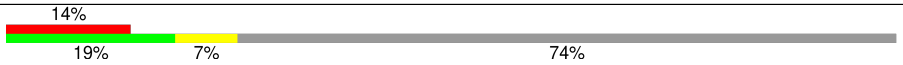
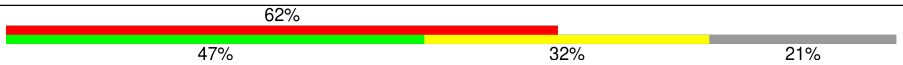
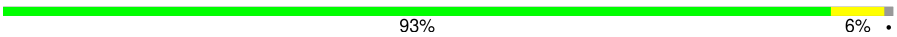
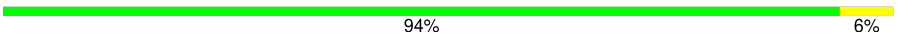
Mol	Chain	Length	Quality of chain
28	D	209	
29	E	201	
30	F	179	
31	G	177	
32	H	149	
33	I	165	
34	J	142	
35	L	142	
36	M	123	
37	N	144	
38	O	136	
39	P	127	
40	Q	117	
41	R	115	
42	S	118	
43	T	103	
44	U	110	
45	V	100	
46	W	104	
47	X	94	
48	Y	85	
49	Z	78	
50	1	63	
51	2	59	
52	3	70	

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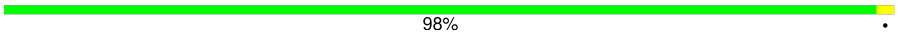
Mol	Chain	Length	Quality of chain
53	4	57	
54	5	55	
55	6	46	
56	7	65	
57	8	38	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 150294 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1528	32803	14637	6019	10619	1528	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	224	1754	1110	315	321	8	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	156	1152	717	217	212	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	103	839	530	151	151	7	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	152	Total	C	N	O	S	0	0
			1191	741	230	216	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	119	IAS	ASN	conflict	UNP A0A0H3PWX2

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	121	Total	C	N	O	S	0	0
			942	582	193	162	5		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	54	Total	C	N	O	0	0
			446	283	85	78		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 22 is a RNA chain called P-site phenylalanyl-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	x	76	Total	C	N	O	P	S	0	0
			1632	731	290	533	76	2		
22	y	74	Total	C	N	O	P	S	0	0
			1584	707	285	517	74	1		

- Molecule 23 is a RNA chain called F-UAA mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	z	11	Total	C	N	O	P	0	0
			232	105	41	75	11		

- Molecule 24 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	w	349	Total	C	N	O	S	0	0
			2750	1679	513	545	13		

- Molecule 25 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A	2899	Total	C	N	O	P	0	0
			62252	27778	11456	20119	2899		

- Molecule 26 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	120	Total	C	N	O	P	0	0
			2572	1145	470	837	120		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	D	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	H	39	Total	C	N	O	S	0	0
			287	184	51	51	1		

- Molecule 33 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	I	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 34 is a protein called 50S ribosomal protein L11.

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

- Molecule 35 is a protein called 50S ribosomal protein L13.

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

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	M	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	N	144	Total	C	N	O	S	0	0
			1052	653	207	190	2		

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	O	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	82	MS6	MET	conflict	UNP E6BI61

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	P	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 40 is a protein called 50S ribosomal protein L18.

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

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

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

- Molecule 43 is a protein called Ribosomal protein L21.

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

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	V	93	Total 738	C 466	N 139	O 131	S 2	0	0

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called 50S ribosomal protein L25.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Y	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 49 is a protein called 50S ribosomal protein L28.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	1	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	2	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	3	60	Total	C	N	O	S	0	0
			468	290	87	85	6		

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	4	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 54 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	5	51	Total 417	C 269	N 76	O 72	0	0

- Molecule 55 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	6	46	Total 377	C 228	N 90	O 57	S 2	0	0

- Molecule 56 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	7	64	Total 504	C 323	N 105	O 74	S 2	0	0

- Molecule 57 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	8	38	Total 302	C 185	N 65	O 48	S 4	0	0

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

Mol	Chain	Residues	Atoms		AltConf
58	a	125	Total 125	Mg 125	0
58	e	1	Total 1	Mg 1	0
58	n	1	Total 1	Mg 1	0
58	x	2	Total 2	Mg 2	0
58	y	1	Total 1	Mg 1	0
58	z	1	Total 1	Mg 1	0
58	A	439	Total 439	Mg 439	0
58	B	11	Total 11	Mg 11	0
58	C	3	Total 3	Mg 3	0

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Mol	Chain	Residues	Atoms	AltConf
58	O	3	Total Mg 3 3	0
58	P	2	Total Mg 2 2	0
58	S	1	Total Mg 1 1	0
58	V	1	Total Mg 1 1	0
58	X	1	Total Mg 1 1	0
58	4	1	Total Mg 1 1	0
58	6	1	Total Mg 1 1	0
58	7	1	Total Mg 1 1	0

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
59	3	1	Total Zn 1 1	0
59	8	1	Total Zn 1 1	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	AltConf
60	a	32	Total O 32 32	0
60	k	1	Total O 1 1	0
60	y	1	Total O 1 1	0
60	A	215	Total O 215 215	0
60	B	6	Total O 6 6	0
60	E	1	Total O 1 1	0
60	N	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
60	P	1	Total O 1 1	0
60	S	1	Total O 1 1	0
60	Z	1	Total O 1 1	0
60	7	1	Total O 1 1	0
60	8	1	Total O 1 1	0

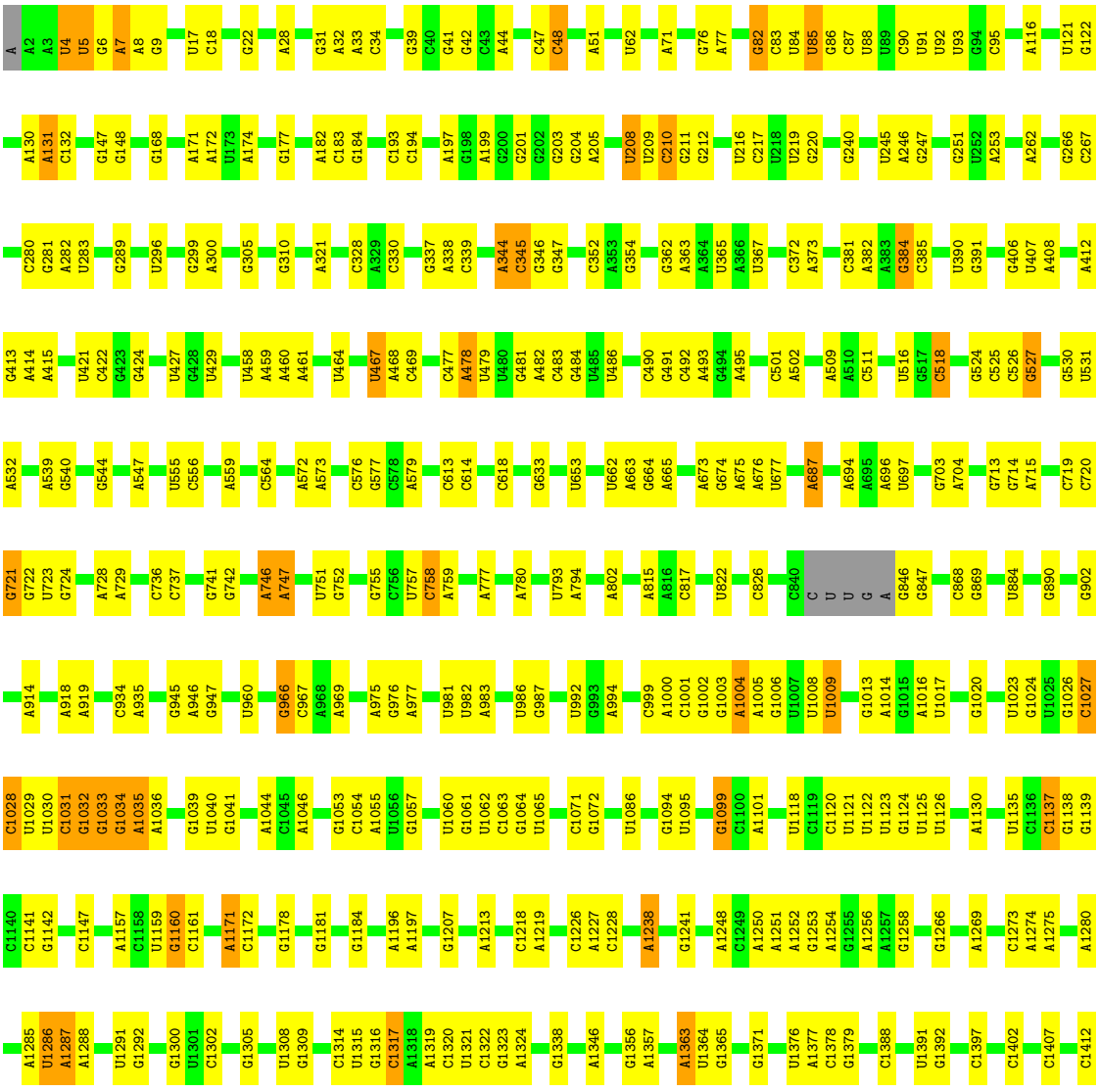
3 Residue-property plots (i)

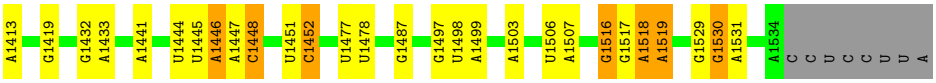
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S Ribosomal RNA

Chain a:



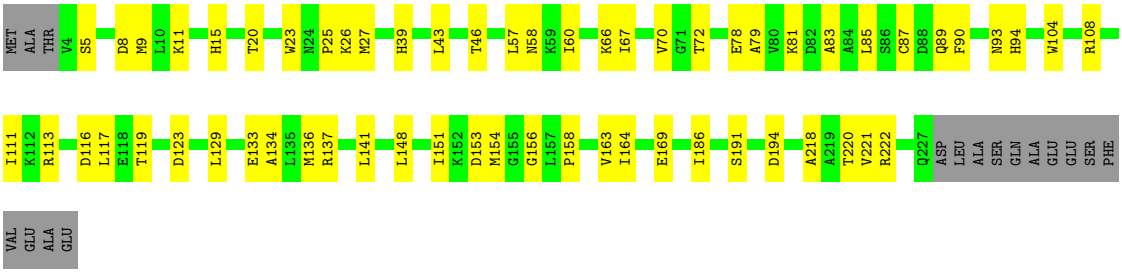




• Molecule 2: 30S ribosomal protein S2

Chain b:

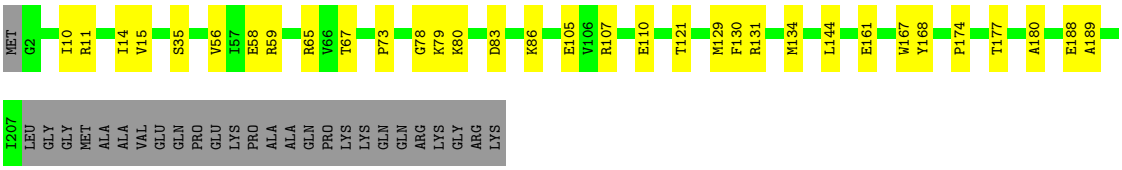




• Molecule 3: 30S ribosomal protein S3

Chain c:





• Molecule 4: 30S ribosomal protein S4

Chain d:





• Molecule 5: 30S ribosomal protein S5

Chain e:

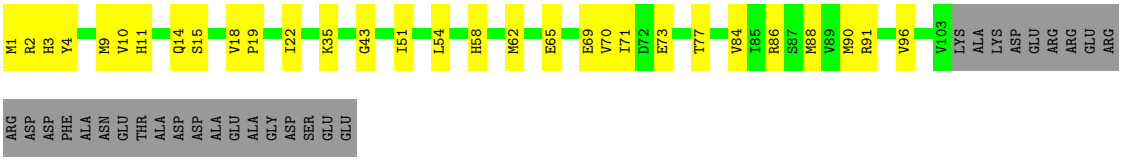




• Molecule 6: 30S ribosomal protein S6

Chain f:

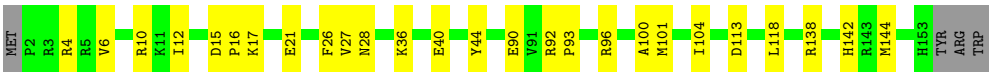




• Molecule 7: 30S ribosomal protein S7

Chain g:

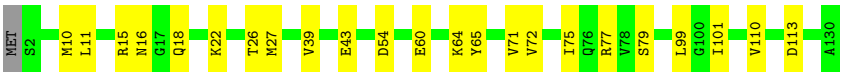




• Molecule 8: 30S ribosomal protein S8

Chain h:

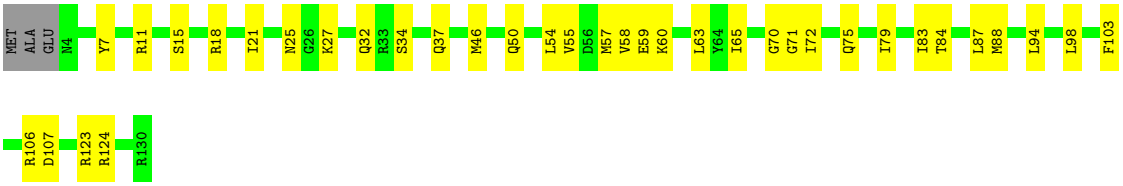




• Molecule 9: 30S ribosomal protein S9

Chain i:

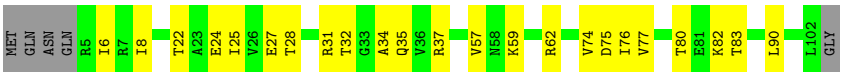




• Molecule 10: 30S ribosomal protein S10

Chain j:





• Molecule 11: 30S ribosomal protein S11

Chain k:

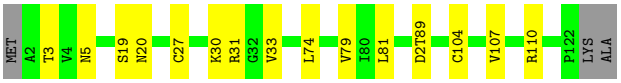




• Molecule 12: 30S ribosomal protein S12

Chain l:

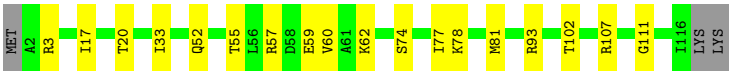




• Molecule 13: 30S ribosomal protein S13

Chain m:





• Molecule 14: 30S ribosomal protein S14

Chain n:

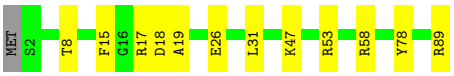




• Molecule 15: 30S ribosomal protein S15

Chain o:

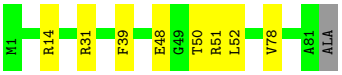




• Molecule 16: 30S ribosomal protein S16

Chain p:





• Molecule 17: 30S ribosomal protein S17

Chain q:

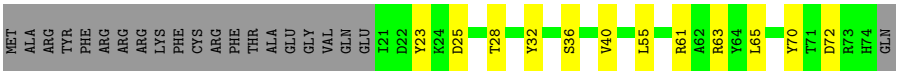




• Molecule 18: 30S ribosomal protein S18

Chain r:

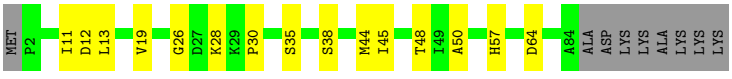




• Molecule 19: 30S ribosomal protein S19

Chain s:





• Molecule 20: 30S ribosomal protein S20

Chain t:





• Molecule 21: 30S ribosomal protein S21

Chain u:

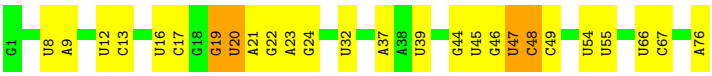




• Molecule 22: P-site phenylalanyl-tRNA

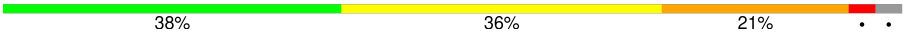
Chain x:

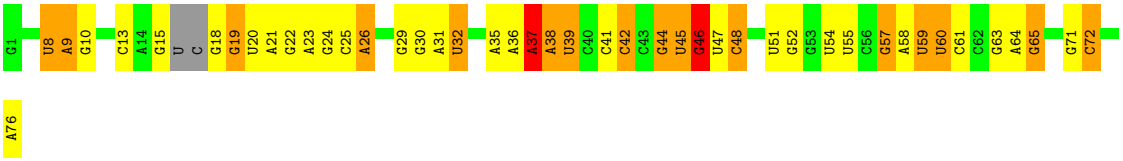




• Molecule 22: P-site phenylalanyl-tRNA

Chain y:





• Molecule 23: F-UAA mRNA

Chain z:

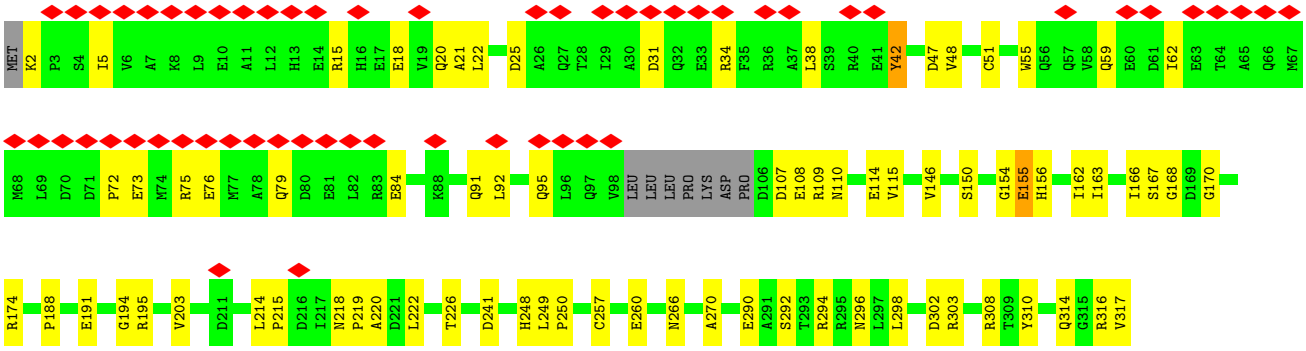




• Molecule 24: Peptide chain release factor 1

Chain w:



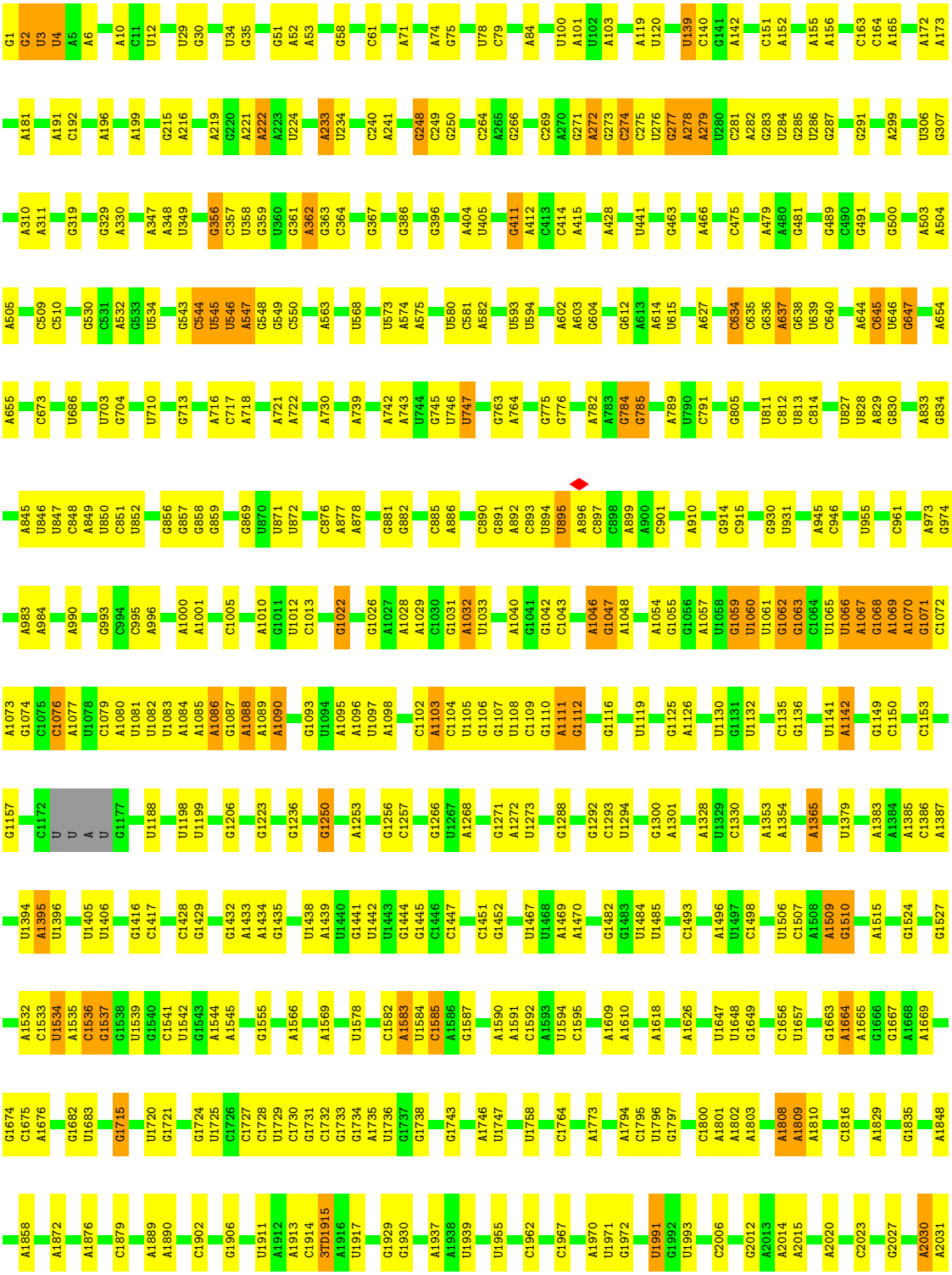


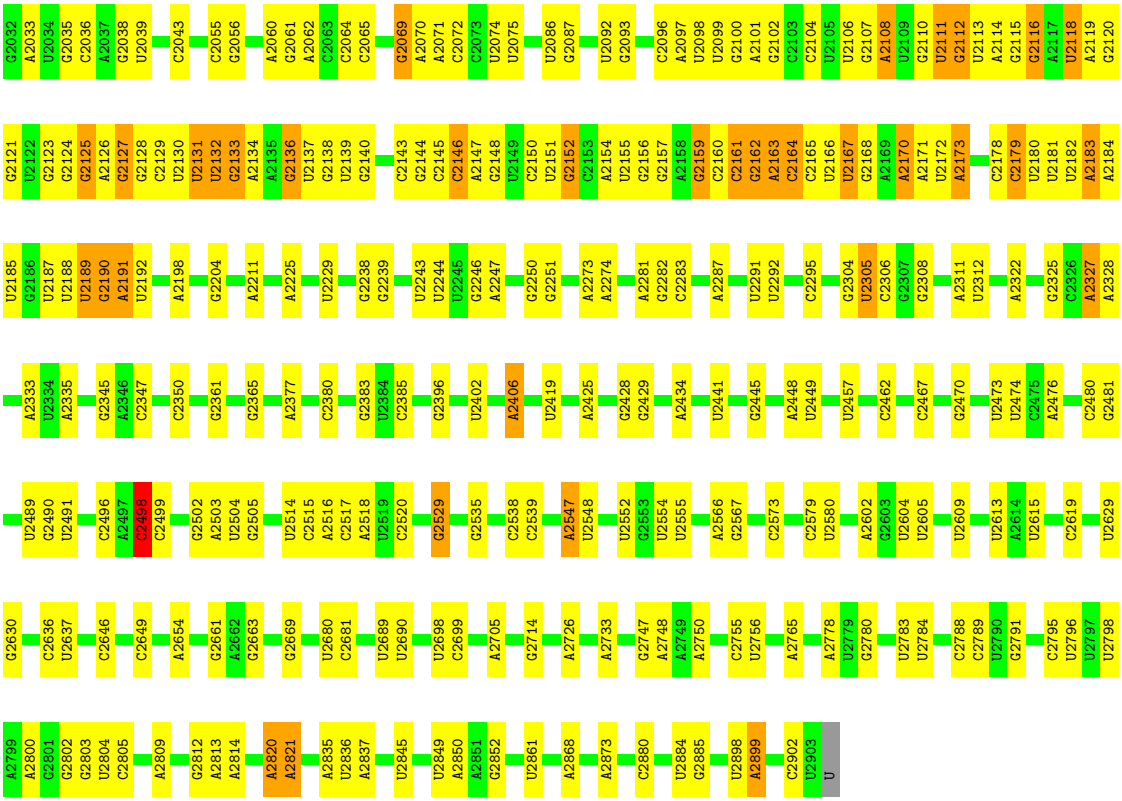


• Molecule 25: 23S Ribosomal RNA

Chain A:



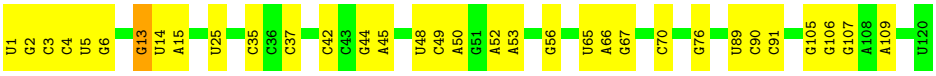




• Molecule 26: 5S Ribosomal RNA

Chain B:





• Molecule 27: 50S ribosomal protein L2

Chain C:

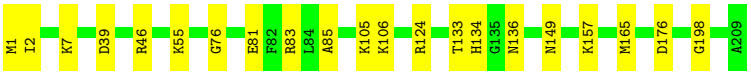




• Molecule 28: 50S ribosomal protein L3

Chain D:





• Molecule 29: 50S ribosomal protein L4

Chain E:

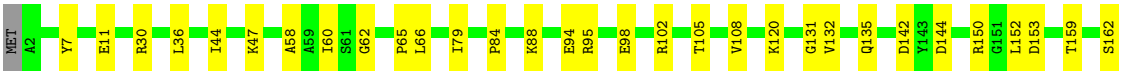


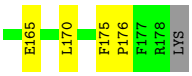


• Molecule 30: 50S ribosomal protein L5

Chain F:



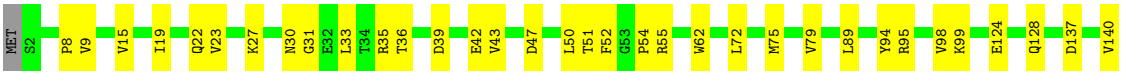




• Molecule 31: 50S ribosomal protein L6

Chain G:



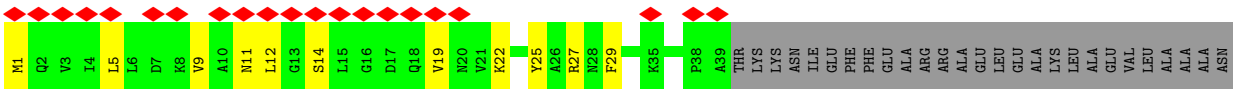




• Molecule 32: 50S ribosomal protein L9

Chain H:





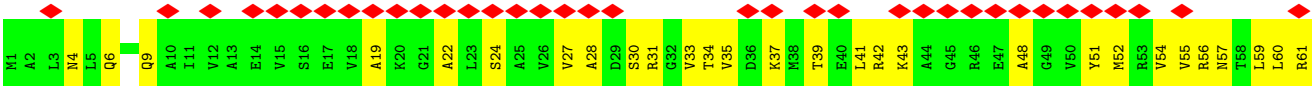


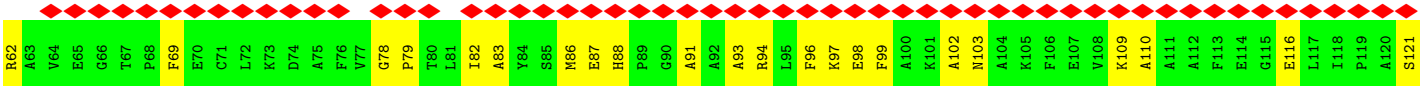


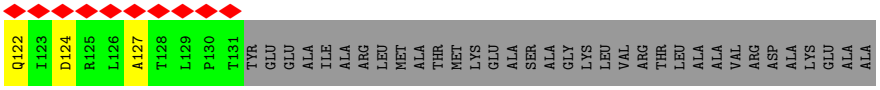
• Molecule 33: 50S ribosomal protein L10

Chain I:



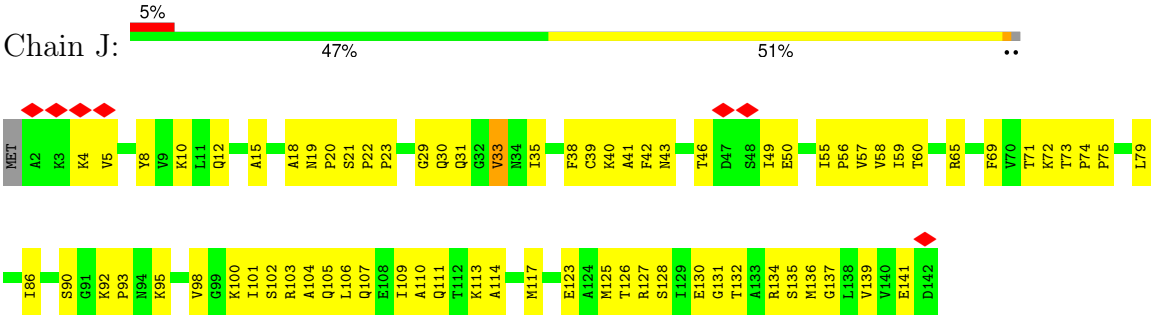






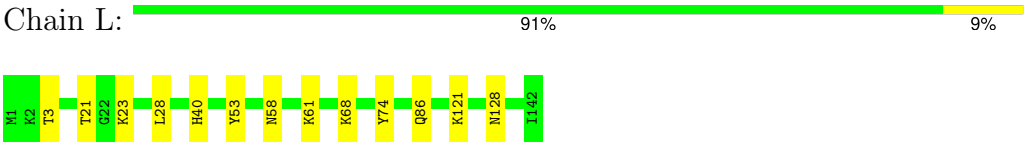
• Molecule 34: 50S ribosomal protein L11

Chain J:



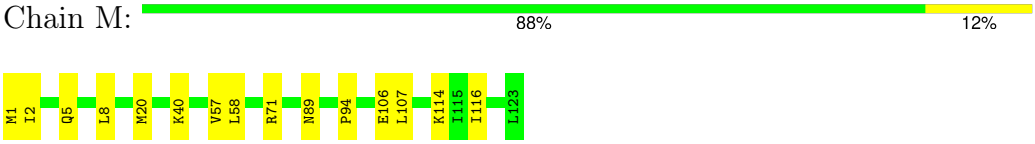
• Molecule 35: 50S ribosomal protein L13

Chain L:



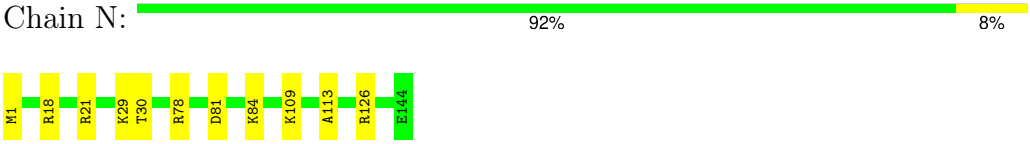
• Molecule 36: 50S ribosomal protein L14

Chain M:



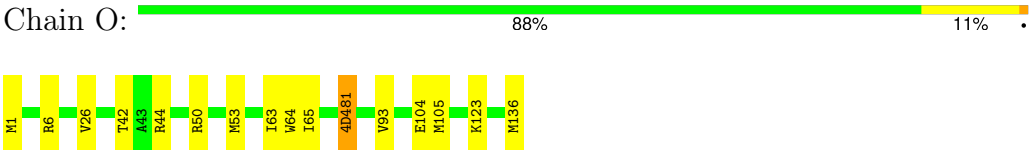
• Molecule 37: 50S ribosomal protein L15

Chain N:



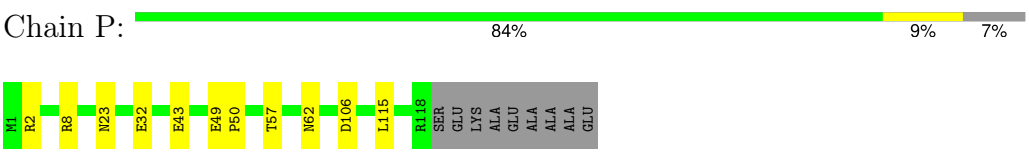
• Molecule 38: 50S ribosomal protein L16

Chain O:



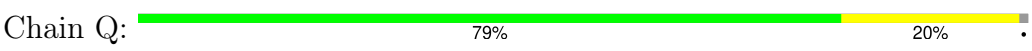
• Molecule 39: 50S ribosomal protein L17

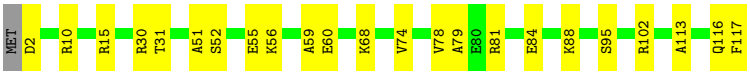
Chain P:



• Molecule 40: 50S ribosomal protein L18

Chain Q:





• Molecule 41: 50S ribosomal protein L19

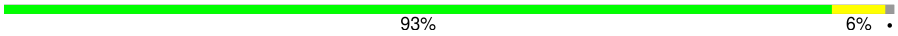
Chain R:

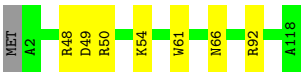




• Molecule 42: 50S ribosomal protein L20

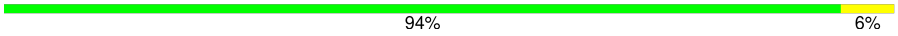
Chain S:





• Molecule 43: Ribosomal protein L21

Chain T:





• Molecule 44: 50S ribosomal protein L22

Chain U:

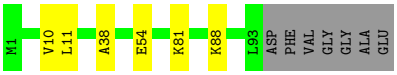




• Molecule 45: 50S ribosomal protein L23

Chain V:

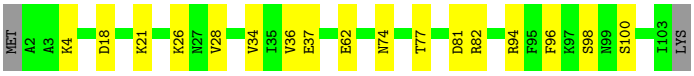




• Molecule 46: 50S ribosomal protein L24

Chain W:

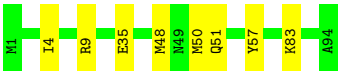




• Molecule 47: 50S ribosomal protein L25

Chain X:

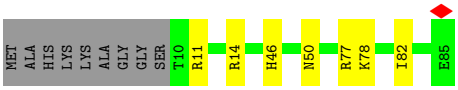




• Molecule 48: 50S ribosomal protein L27

Chain Y:

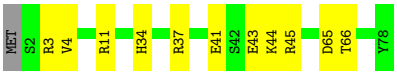




• Molecule 49: 50S ribosomal protein L28

Chain Z:

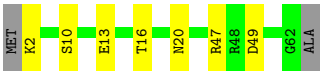




• Molecule 50: 50S ribosomal protein L29

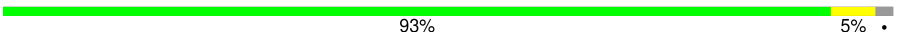
Chain 1:

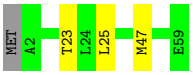




• Molecule 51: 50S ribosomal protein L30

Chain 2:





• Molecule 52: 50S ribosomal protein L31

Chain 3:





• Molecule 53: 50S ribosomal protein L32

Chain 4:

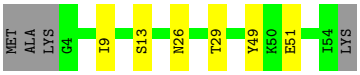




• Molecule 54: 50S ribosomal protein L33

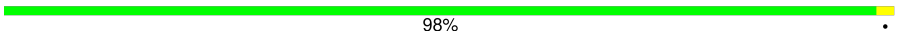
Chain 5:





• Molecule 55: 50S ribosomal protein L34

Chain 6:

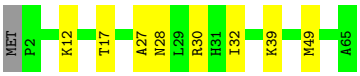




• Molecule 56: 50S ribosomal protein L35

Chain 7:

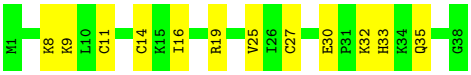




• Molecule 57: 50S ribosomal protein L36

Chain 8:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	146778	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.44	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.673	Depositor
Minimum map value	-0.545	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MEQ, 5MU, 2MA, IAS, 7MG, H2U, 1MG, G7M, 4OC, D2T, 5MC, MS6, MA6, OMC, 6MZ, PSU, 4SU, UR3, ZN, OMG, 2MG, OMU, MIA, 3TD, MG, 4D4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	a	0.27	0/36450	0.31	0/56856
2	b	0.18	0/1785	0.40	0/2404
3	c	0.20	0/1651	0.32	0/2225
4	d	0.22	0/1665	0.35	0/2227
5	e	0.25	0/1165	0.38	0/1568
6	f	0.24	0/858	0.48	0/1160
7	g	0.18	0/1206	0.33	0/1617
8	h	0.25	0/989	0.36	0/1326
9	i	0.21	0/1034	0.39	0/1375
10	j	0.22	0/796	0.39	0/1077
11	k	0.21	0/884	0.30	0/1191
12	l	0.26	0/945	0.40	0/1268
13	m	0.21	0/900	0.34	0/1204
14	n	0.22	0/817	0.33	0/1088
15	o	0.25	0/722	0.39	0/964
16	p	0.24	0/653	0.35	0/877
17	q	0.23	0/650	0.39	0/871
18	r	0.25	0/453	0.33	0/609
19	s	0.20	0/680	0.32	0/915
20	t	0.25	0/676	0.36	0/895
21	u	0.18	0/597	0.31	0/792
22	x	0.26	0/1651	0.29	0/2569
22	y	0.19	0/1605	0.32	0/2497
23	z	0.29	0/259	0.40	0/400
24	w	0.22	0/2788	0.41	0/3753
25	A	0.32	0/69147	0.34	0/107869
26	B	0.27	0/2876	0.33	0/4483
27	C	0.30	0/2121	0.37	0/2852
28	D	0.31	0/1576	0.37	0/2119
29	E	0.27	0/1571	0.35	0/2113
30	F	0.21	0/1434	0.31	0/1926

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	G	0.20	0/1343	0.34	0/1816
32	H	0.12	0/290	0.33	0/392
33	I	0.14	0/1001	0.39	0/1350
34	J	0.14	0/1046	0.41	0/1410
35	L	0.29	0/1152	0.34	0/1551
36	M	0.29	0/955	0.39	0/1279
37	N	0.27	0/1061	0.33	0/1412
38	O	0.27	0/1073	0.38	0/1433
39	P	0.31	0/958	0.40	0/1281
40	Q	0.24	0/902	0.35	0/1209
41	R	0.28	0/929	0.33	0/1242
42	S	0.32	0/960	0.30	0/1278
43	T	0.29	0/829	0.38	0/1107
44	U	0.28	0/864	0.34	0/1156
45	V	0.25	0/744	0.32	0/994
46	W	0.26	0/787	0.46	0/1051
47	X	0.25	0/766	0.34	0/1025
48	Y	0.27	0/589	0.43	0/779
49	Z	0.27	0/635	0.33	0/848
50	1	0.23	0/496	0.32	0/660
51	2	0.29	0/453	0.29	0/605
52	3	0.16	0/475	0.31	0/633
53	4	0.30	0/440	0.34	0/588
54	5	0.25	0/424	0.33	0/565
55	6	0.32	0/380	0.28	0/498
56	7	0.29	0/513	0.33	0/676
57	8	0.28	0/303	0.38	0/397
All	All	0.28	0/160972	0.34	0/240325

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
38	O	0	1
56	7	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
56	7	30	ARG	Peptide
38	O	81	4D4	Mainchain

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	a	32803	0	16528	180	0
2	b	1754	0	1782	43	0
3	c	1624	0	1696	19	0
4	d	1643	0	1707	18	0
5	e	1152	0	1196	11	0
6	f	839	0	833	25	0
7	g	1191	0	1245	18	0
8	h	979	0	1031	14	0
9	i	1022	0	1070	28	0
10	j	786	0	828	17	0
11	k	877	0	883	12	0
12	l	942	0	999	8	0
13	m	891	0	952	10	0
14	n	805	0	844	7	0
15	o	714	0	734	8	0
16	p	643	0	661	5	0
17	q	641	0	682	2	0
18	r	446	0	472	8	0
19	s	663	0	688	9	0
20	t	670	0	719	6	0
21	u	589	0	629	9	0
22	x	1632	0	839	4	0
22	y	1584	0	804	38	0
23	z	232	0	118	5	0
24	w	2750	0	2677	61	0
25	A	62252	0	31334	387	0
26	B	2572	0	1301	10	0
27	C	2082	0	2153	15	0
28	D	1566	0	1618	16	0
29	E	1552	0	1619	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	F	1410	0	1444	22	0
31	G	1323	0	1371	20	0
32	H	287	0	307	10	0
33	I	988	0	1025	42	0
34	J	1032	0	1085	55	0
35	L	1129	0	1162	9	0
36	M	946	0	1023	12	0
37	N	1052	0	1127	9	0
38	O	1075	0	1145	10	0
39	P	945	0	989	7	0
40	Q	892	0	923	16	0
41	R	917	0	962	9	0
42	S	947	0	1019	6	0
43	T	816	0	839	5	0
44	U	857	0	922	10	0
45	V	738	0	807	3	0
46	W	779	0	831	10	0
47	X	753	0	780	6	0
48	Y	582	0	599	4	0
49	Z	625	0	652	8	0
50	1	495	0	526	4	0
51	2	449	0	488	2	0
52	3	468	0	460	10	0
53	4	434	0	445	4	0
54	5	417	0	451	3	0
55	6	377	0	418	1	0
56	7	504	0	572	4	0
57	8	302	0	340	10	0
58	4	1	0	0	0	0
58	6	1	0	0	0	0
58	7	1	0	0	0	0
58	A	439	0	0	0	0
58	B	11	0	0	0	0
58	C	3	0	0	0	0
58	O	3	0	0	0	0
58	P	2	0	0	0	0
58	S	1	0	0	0	0
58	V	1	0	0	0	0
58	X	1	0	0	0	0
58	a	125	0	0	0	0
58	e	1	0	0	0	0
58	n	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	x	2	0	0	0	0
58	y	1	0	0	0	0
58	z	1	0	0	0	0
59	3	1	0	0	0	0
59	8	1	0	0	0	0
60	7	1	0	0	0	0
60	8	1	0	0	0	0
60	A	215	0	0	1	0
60	B	6	0	0	0	0
60	E	1	0	0	0	0
60	N	1	0	0	1	0
60	P	1	0	0	0	0
60	S	1	0	0	0	0
60	Z	1	0	0	1	0
60	a	32	0	0	2	0
60	k	1	0	0	0	0
60	y	1	0	0	0	0
All	All	150294	0	101354	1205	0

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

All (1205) 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)
6:f:2:ARG:HD3	6:f:91:ARG:HH12	1.17	1.08
22:y:15:G:N2	22:y:48:C:H42	1.56	1.02
22:y:15:G:H22	22:y:48:C:N4	1.61	0.98
22:y:51:U:H3	22:y:63:G:H1	1.12	0.97
25:A:713:G:H21	25:A:718:A:H62	1.13	0.96
1:a:76:G:H1	1:a:93:U:H3	1.02	0.95
2:b:119:THR:O	2:b:123:ASP:HB2	1.68	0.94
25:A:1724:G:H1	25:A:1736:U:H3	1.00	0.93
25:A:2100:G:H1	25:A:2189:U:H3	1.20	0.86
22:y:15:G:N2	22:y:48:C:N4	2.18	0.85
1:a:1009:U:H3	1:a:1020:G:H1	0.87	0.85
25:A:2127:G:N2	25:A:2161:C:O2'	2.10	0.83
24:w:226:THR:HG22	24:w:241:ASP:HB3	1.63	0.79
25:A:2114:A:H1'	25:A:2167:U:H5'	1.65	0.79
9:i:106:ARG:NH1	9:i:107:ASP:O	2.16	0.78
22:y:15:G:N1	22:y:48:C:N3	2.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:742:G:OP1	15:o:58:ARG:NH2	2.17	0.77
25:A:1065:U:O2	25:A:1074:G:O6	2.02	0.76
6:f:19:PRO:O	6:f:22:ILE:HB	1.86	0.76
34:J:90:SER:HB3	34:J:136:MET:HA	1.68	0.76
25:A:2102:G:H1	25:A:2187:U:H3	1.34	0.76
24:w:248:HIS:CD2	24:w:250:PRO:HD2	2.21	0.75
1:a:673:A:H2'	1:a:674:G:C8	2.22	0.75
25:A:881:G:N1	25:A:895:U:N3	2.34	0.75
1:a:201:G:HO2'	1:a:469:C:HO2'	1.34	0.75
31:G:31:GLY:HA3	31:G:79:VAL:HG22	1.69	0.75
41:R:89:ARG:NH1	41:R:115:ASN:O	2.20	0.75
34:J:92:LYS:HB2	34:J:95:LYS:HB2	1.68	0.74
9:i:25:ASN:OD1	9:i:27:LYS:NZ	2.15	0.74
25:A:2104:C:N4	25:A:2185:U:O4	2.20	0.74
8:h:18:GLN:HE21	8:h:72:VAL:HG22	1.51	0.74
24:w:51:CYS:SG	24:w:91:GLN:NE2	2.62	0.73
25:A:713:G:N2	25:A:718:A:H62	1.85	0.73
26:B:1:U:H2'	26:B:2:G:H8	1.53	0.73
5:e:160:SER:OG	5:e:163:GLU:OE1	2.05	0.73
27:C:165:VAL:HG21	27:C:181:MET:HE1	1.69	0.73
22:y:36:A:C6	22:y:37:MIA:H8	2.24	0.72
41:R:14:LYS:HE2	41:R:77:HIS:HA	1.71	0.72
31:G:89:LEU:HD12	31:G:94:TYR:HB3	1.71	0.72
1:a:1137:C:O2	1:a:1138:G:N2	2.23	0.71
24:w:15:ARG:HA	24:w:18:GLU:HB3	1.72	0.71
25:A:1093:G:H21	25:A:1098:A:H62	1.36	0.71
9:i:58:VAL:HG13	9:i:59:GLU:OE2	1.91	0.71
34:J:10:LYS:HE3	34:J:58:VAL:HG22	1.72	0.71
1:a:1226:C:H2'	13:m:102:THR:HG22	1.74	0.70
24:w:314:GLN:OE1	24:w:316:ARG:NH1	2.24	0.70
25:A:881:G:H1	25:A:895:U:H3	1.39	0.70
25:A:2139:U:O2	25:A:2152:G:O6	2.09	0.70
25:A:2189:U:H2'	25:A:2190:G:H8	1.56	0.70
29:E:122:GLU:HG2	29:E:123:LYS:HG2	1.73	0.70
37:N:18:ARG:NH1	60:N:201:HOH:O	2.24	0.70
22:y:60:U:H5'	22:y:61:C:H5	1.56	0.70
3:c:35:SER:OG	3:c:59:ARG:NH2	2.25	0.70
1:a:76:G:N2	1:a:93:U:O2	2.22	0.69
35:L:3:THR:HG21	42:S:61:TRP:HE1	1.56	0.69
21:u:62:ARG:O	21:u:66:ARG:NH1	2.26	0.69
25:A:1068:G:O2'	25:A:1069:A:O5'	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:36:LEU:HD22	5:e:134:ILE:HD13	1.75	0.69
33:I:31:ARG:H	33:I:109:LYS:HD2	1.58	0.69
34:J:56:PRO:HG2	34:J:72:LYS:HD3	1.75	0.69
52:3:9:TYR:O	52:3:25:ARG:NH2	2.26	0.69
16:p:39:PHE:HD1	16:p:50:THR:HG22	1.58	0.69
25:A:2134:A:H61	25:A:2156:G:H2'	1.58	0.69
25:A:2144:G:O2'	25:A:2147:A:N1	2.25	0.69
25:A:713:G:H21	25:A:718:A:N6	1.89	0.68
11:k:13:ARG:N	11:k:76:GLU:OE2	2.26	0.68
25:A:2125:G:H21	25:A:2173:A:H62	1.42	0.68
34:J:33:VAL:H	34:J:65:ARG:HE	1.41	0.68
3:c:14:ILE:HG22	3:c:15:VAL:HG13	1.75	0.68
25:A:881:G:O6	25:A:895:U:O4	2.12	0.68
28:D:46:ARG:NH1	28:D:85:ALA:O	2.27	0.68
25:A:1802:A:H2'	25:A:1803:A:C8	2.29	0.68
1:a:1054:C:N4	24:w:194:GLY:O	2.27	0.68
38:O:64:TRP:HB2	38:O:104:GLU:HB2	1.76	0.67
1:a:1356:G:H2'	1:a:1357:A:C8	2.30	0.67
23:z:20:U:OP2	24:w:195:ARG:NH1	2.26	0.67
30:F:30:ARG:H	30:F:159:THR:HG22	1.60	0.67
9:i:15:SER:HB3	9:i:70:GLY:HA3	1.75	0.67
20:t:44:LYS:HD2	20:t:87:ALA:HA	1.75	0.67
24:w:154:GLY:O	24:w:156:HIS:N	2.27	0.67
6:f:9:MET:SD	6:f:86:ARG:HB3	2.35	0.67
24:w:62:ILE:HG21	24:w:84:GLU:HB2	1.75	0.67
22:y:9:A:H1'	22:y:45:U:H2'	1.75	0.67
26:B:1:U:H2'	26:B:2:G:C8	2.30	0.67
1:a:1031:C:O2'	1:a:1032:G:N2	2.28	0.67
5:e:13:GLU:HG3	5:e:39:VAL:HG12	1.77	0.67
2:b:67:ILE:HG12	2:b:89:GLN:HE21	1.60	0.67
10:j:35:GLN:NE2	10:j:77:VAL:HB	2.10	0.66
24:w:260:GLU:H	24:w:266:ASN:HD21	1.41	0.66
25:A:1534:U:O2'	25:A:1537:G:N1	2.28	0.66
25:A:1715:G:O2'	25:A:1743:G:O6	2.09	0.66
34:J:57:VAL:HG12	34:J:71:THR:HA	1.77	0.66
25:A:2136:G:H1	25:A:2156:G:H21	1.44	0.65
36:M:40:LYS:NZ	36:M:89:ASN:OD1	2.29	0.65
1:a:407:U:O2'	4:d:113:GLU:OE2	2.11	0.65
25:A:1046:A:H62	33:I:4:ASN:HD21	1.44	0.65
13:m:77:ILE:HG22	13:m:81:MET:HE3	1.77	0.65
56:7:17:THR:HG21	56:7:49:MET:HE1	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2159:G:H2'	25:A:2160:C:C6	2.30	0.65
11:k:93:ARG:NH2	11:k:112:ASP:OD2	2.29	0.65
24:w:15:ARG:HH12	24:w:22:LEU:HD12	1.59	0.65
2:b:83:ALA:O	2:b:87:CYS:HB2	1.97	0.65
25:A:1724:G:N2	25:A:1736:U:O2	2.20	0.65
25:A:1509:A:O2'	25:A:1510:G:O5'	2.15	0.65
25:A:1649:G:O2'	39:P:106:ASP:OD2	2.10	0.65
1:a:1086:U:H3	1:a:1099:G:H22	1.46	0.64
7:g:90:GLU:OE2	7:g:96:ARG:NH2	2.30	0.64
25:A:139:U:H5"	25:A:140:C:H5	1.61	0.64
25:A:2189:U:H2'	25:A:2190:G:C8	2.32	0.64
19:s:11:ILE:HD12	19:s:38:SER:HB3	1.78	0.64
1:a:1009:U:O2	1:a:1020:G:N2	2.23	0.64
25:A:1250:G:N7	37:N:18:ARG:NH2	2.45	0.64
13:m:107:ARG:NH1	13:m:111:GLY:O	2.31	0.64
25:A:1119:U:OP1	47:X:83:LYS:NZ	2.31	0.64
24:w:174:ARG:NH2	24:w:342:GLU:OE2	2.29	0.64
25:A:1065:U:O2	25:A:1074:G:C6	2.50	0.64
2:b:58:ASN:HB3	2:b:220:THR:HG22	1.79	0.64
46:W:74:ASN:HD22	46:W:77:THR:HG22	1.62	0.64
1:a:147:G:H2'	1:a:148:G:C8	2.33	0.63
1:a:337:G:H2'	1:a:338:A:C8	2.33	0.63
40:Q:51:ALA:HB3	40:Q:78:VAL:HG22	1.79	0.63
24:w:115:VAL:HG12	24:w:203:VAL:HG22	1.80	0.63
1:a:1123:U:O3'	10:j:37:ARG:NH2	2.32	0.63
34:J:49:ILE:HG13	34:J:50:GLU:H	1.63	0.63
18:r:63:ARG:HD3	18:r:70:TYR:HA	1.80	0.63
1:a:544:G:OP1	4:d:56:ARG:NH2	2.31	0.63
34:J:12:GLN:HE22	34:J:57:VAL:HG13	1.61	0.63
3:c:129:MET:HE3	3:c:131:ARG:HG3	1.80	0.63
1:a:1397:C:H42	23:z:20:U:H2'	1.64	0.63
1:a:1026:G:O6	1:a:1035:A:N1	2.32	0.62
24:w:108:GLU:HB3	24:w:170:GLY:HA2	1.80	0.62
5:e:105:ILE:HD12	5:e:123:VAL:HG12	1.81	0.62
2:b:111:ILE:HD13	2:b:148:LEU:HD13	1.81	0.62
13:m:17:ILE:O	13:m:20:THR:OG1	2.17	0.62
35:L:58:ASN:ND2	35:L:128:ASN:OD1	2.31	0.62
24:w:42:TYR:OH	25:A:1067:A:OP1	2.17	0.62
25:A:2146:C:H4'	25:A:2147:A:C4	2.35	0.62
46:W:28:VAL:HG12	46:W:34:VAL:HG12	1.81	0.62
32:H:9:VAL:HG22	32:H:11:ASN:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2146:C:O2'	25:A:2147:A:N7	2.33	0.62
24:w:188:PRO:HG2	24:w:191:GLU:HB2	1.82	0.61
11:k:13:ARG:NH1	11:k:77:TYR:OH	2.34	0.61
25:A:2190:G:H2'	25:A:2191:A:C8	2.34	0.61
25:A:858:G:OP1	48:Y:78:LYS:NZ	2.33	0.61
25:A:1093:G:N2	25:A:1098:A:H62	1.98	0.61
25:A:2127:G:H21	25:A:2173:A:H1'	1.66	0.61
34:J:20:PRO:HG3	34:J:39:CYS:HB3	1.83	0.61
34:J:74:PRO:O	34:J:113:LYS:NZ	2.34	0.61
1:a:427:U:OP1	4:d:13:ARG:NH2	2.33	0.61
49:Z:37:ARG:NH1	60:Z:101:HOH:O	2.34	0.61
1:a:1147:C:O2'	9:i:7:TYR:OH	2.13	0.61
22:y:29:G:H2'	22:y:30:G:C8	2.36	0.61
29:E:168:ASP:OD2	29:E:170:ARG:NH1	2.33	0.61
32:H:11:ASN:ND2	32:H:25:TYR:OH	2.30	0.61
45:V:38:ALA:O	45:V:81:LYS:NZ	2.33	0.61
14:n:69:ARG:NH1	14:n:71:HIS:O	2.34	0.61
50:1:16:THR:O	50:1:20:ASN:ND2	2.34	0.61
1:a:1516:2MG:N2	1:a:1519:MA6:OP2	2.31	0.60
5:e:34:THR:HG22	5:e:52:LYS:HG3	1.82	0.60
28:D:133:THR:HG22	28:D:134:HIS:H	1.66	0.60
1:a:946:A:H2'	1:a:947:G:C8	2.37	0.60
9:i:21:ILE:HG22	9:i:63:LEU:HG	1.83	0.60
14:n:46:LEU:HD12	19:s:13:LEU:HD12	1.84	0.60
1:a:458:U:H2'	1:a:459:A:H8	1.66	0.60
34:J:111:GLN:HA	34:J:114:ALA:HB3	1.83	0.60
9:i:75:GLN:O	9:i:79:ILE:HG12	2.01	0.60
19:s:50:ALA:HB1	19:s:57:HIS:HB3	1.82	0.60
27:C:107:PRO:HD2	27:C:110:LEU:HD22	1.82	0.60
44:U:4:ILE:HG12	44:U:106:VAL:HG22	1.83	0.60
34:J:114:ALA:HA	34:J:117:MET:HB3	1.84	0.60
24:w:214:LEU:HD12	24:w:215:PRO:HD2	1.83	0.60
33:I:94:ARG:O	33:I:98:GLU:N	2.32	0.60
1:a:1006:G:O6	1:a:1023:U:O2	2.20	0.60
44:U:59:GLU:HG3	44:U:66:ILE:HD11	1.83	0.60
25:A:1111:A:O2'	25:A:1112:G:OP1	2.20	0.59
4:d:87:GLY:HA3	4:d:197:GLU:HG3	1.83	0.59
22:y:9:A:O4'	22:y:46:7MG:N2	2.34	0.59
22:y:58:A:O2'	22:y:59:U:OP1	2.19	0.59
5:e:153:VAL:HG21	8:h:99:LEU:HD22	1.85	0.59
22:y:51:U:H2'	22:y:52:G:C8	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1065:U:H2'	25:A:1066:U:C6	2.37	0.59
30:F:60:ILE:O	30:F:102:ARG:NH2	2.35	0.59
1:a:1009:U:O4	1:a:1020:G:O6	2.20	0.59
32:H:12:LEU:HD13	32:H:19:VAL:HG11	1.83	0.59
13:m:3:ARG:O	13:m:57:ARG:NH1	2.35	0.59
31:G:95:ARG:HG3	31:G:128:GLN:HG3	1.84	0.59
25:A:284:U:H3	25:A:356:G:H1	1.50	0.59
33:I:87:GLU:OE1	33:I:93:ALA:N	2.33	0.59
34:J:102:SER:HA	34:J:141:GLU:HB3	1.85	0.59
4:d:44:ARG:HE	4:d:46:PRO:HB3	1.67	0.59
1:a:618:C:H1'	16:p:14:ARG:HH12	1.68	0.59
1:a:1130:A:OP1	9:i:18:ARG:NH2	2.35	0.59
23:z:12:A:H3'	23:z:13:A:H8	1.66	0.59
29:E:141:MET:HE2	29:E:143:LEU:HD11	1.84	0.59
1:a:344:A:H5"	1:a:345:C:H5	1.66	0.58
25:A:930:G:H1'	51:2:25:LEU:HD21	1.85	0.58
25:A:1153:C:OP1	42:S:92:ARG:NH2	2.37	0.58
46:W:18:ASP:HB2	46:W:21:LYS:HD2	1.85	0.58
27:C:29:PRO:HG2	27:C:34:LEU:HD11	1.85	0.58
33:I:51:TYR:HE2	33:I:88:HIS:HB2	1.69	0.58
50:1:10:SER:OG	50:1:13:GLU:OE1	2.12	0.58
11:k:29:ASN:OD1	11:k:30:THR:N	2.36	0.58
11:k:67:ALA:HB2	11:k:96:THR:HG23	1.84	0.58
26:B:76:G:OP1	47:X:9:ARG:NH1	2.35	0.58
25:A:636:G:N7	37:N:109:LYS:HE2	2.18	0.58
25:A:856:G:H2'	25:A:857:G:C8	2.38	0.58
9:i:123:ARG:NH1	9:i:124:ARG:O	2.37	0.58
25:A:61:C:OP2	50:1:47:ARG:NH2	2.32	0.58
25:A:1083:U:H4'	33:I:41:LEU:HD13	1.86	0.58
25:A:2126:A:N6	25:A:2163:A:O2'	2.37	0.58
10:j:59:LYS:HE2	10:j:62:ARG:NH2	2.19	0.58
2:b:66:LYS:HA	2:b:89:GLN:HE22	1.68	0.57
22:x:23:A:H2'	22:x:24:G:C8	2.39	0.57
25:A:1590:A:H2'	25:A:1591:A:H8	1.68	0.57
25:A:2291:U:OP1	25:A:2380:C:O2'	2.22	0.57
52:3:28:VAL:HG21	52:3:32:LEU:HD11	1.86	0.57
21:u:29:LEU:HA	21:u:32:VAL:HG12	1.85	0.57
25:A:1081:U:OP1	34:J:127:ARG:NH2	2.34	0.57
25:A:2190:G:H2'	25:A:2191:A:H8	1.66	0.57
25:A:276:U:H2'	25:A:277:G:C8	2.38	0.57
25:A:2160:C:OP2	25:A:2161:C:N4	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:y:36:A:C5	22:y:37:MIA:H8	2.39	0.57
25:A:2377:A:O2'	40:Q:117:PHE:O	2.22	0.57
1:a:757:U:OP1	1:a:822:U:O2'	2.20	0.57
1:a:1034:G:H2'	1:a:1035:A:H5'	1.86	0.57
34:J:123:GLU:O	34:J:126:THR:OG1	2.18	0.57
2:b:43:LEU:HA	2:b:46:THR:HG22	1.87	0.57
8:h:22:LYS:O	8:h:65:TYR:OH	2.20	0.57
25:A:475:C:O2	25:A:479:A:N6	2.37	0.57
25:A:881:G:N2	25:A:895:U:O2	2.37	0.57
25:A:1048:A:OP2	25:A:1110:G:N2	2.37	0.57
24:w:15:ARG:HH11	24:w:18:GLU:HG3	1.68	0.57
25:A:1054:A:O2'	33:I:30:SER:O	2.19	0.57
1:a:1013:G:N2	1:a:1016:A:OP2	2.26	0.56
2:b:67:ILE:H	2:b:89:GLN:NE2	2.03	0.56
13:m:33:ILE:HD13	13:m:60:VAL:HG22	1.87	0.56
1:a:1530:G:O6	21:u:46:LYS:NZ	2.35	0.56
19:s:35:SER:OG	19:s:38:SER:OG	2.23	0.56
25:A:1086:A:O2'	25:A:1087:G:N7	2.37	0.56
36:M:94:PRO:HG2	36:M:114:LYS:HD2	1.87	0.56
1:a:1035:A:O2'	1:a:1036:A:H5"	2.05	0.56
1:a:1057:G:O2'	3:c:188:GLU:OE2	2.19	0.56
4:d:13:ARG:NH1	4:d:36:GLN:O	2.38	0.56
25:A:278:A:N6	25:A:362:A:N7	2.53	0.56
25:A:2159:G:H2'	25:A:2160:C:H6	1.71	0.56
39:P:57:THR:OG1	39:P:62:ASN:ND2	2.38	0.56
1:a:492:C:H2'	1:a:493:A:C8	2.40	0.56
8:h:15:ARG:NH1	8:h:75:ILE:O	2.38	0.56
22:y:60:U:H5'	22:y:61:C:C5	2.38	0.56
1:a:219:U:H2'	1:a:220:G:H8	1.70	0.56
2:b:70:VAL:HB	2:b:163:VAL:HG22	1.87	0.56
18:r:25:ASP:OD2	18:r:28:THR:OG1	2.17	0.56
15:o:17:ARG:HG3	15:o:17:ARG:HH11	1.71	0.56
22:y:44:G:HO2'	22:y:45:U:P	2.28	0.56
24:w:302:ASP:O	24:w:303:ARG:HG2	2.05	0.56
24:w:55:TRP:CD1	24:w:91:GLN:HG3	2.39	0.56
6:f:43:GLY:HA2	6:f:58:HIS:CE1	2.40	0.56
7:g:4:ARG:HB3	7:g:6:VAL:HG23	1.88	0.56
25:A:1433:A:H2'	25:A:1434:A:C8	2.40	0.56
25:A:2154:A:H2'	25:A:2155:U:C6	2.40	0.56
52:3:13:THR:OG1	52:3:23:LYS:NZ	2.38	0.56
25:A:1665:A:H1'	36:M:1:MET:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1004:A:H2'	1:a:1005:A:C8	2.41	0.55
2:b:129:LEU:HB2	2:b:134:ALA:HB2	1.88	0.55
10:j:35:GLN:HE21	10:j:77:VAL:HB	1.68	0.55
25:A:2183:A:H2'	25:A:2184:A:C8	2.41	0.55
1:a:1287:A:H2'	1:a:1288:A:C8	2.42	0.55
8:h:26:THR:OG1	8:h:60:GLU:OE1	2.19	0.55
25:A:1469:A:H2'	25:A:1470:A:C8	2.41	0.55
25:A:2123:G:N2	25:A:2124:G:O6	2.39	0.55
6:f:10:VAL:HG12	6:f:84:VAL:HA	1.89	0.55
13:m:52:GLN:O	13:m:55:THR:OG1	2.20	0.55
25:A:2155:U:H3'	25:A:2156:G:H8	1.71	0.55
27:C:68:LYS:NZ	27:C:150:LYS:O	2.39	0.55
51:2:23:THR:HG23	51:2:47:MET:HB2	1.87	0.55
2:b:133:GLU:HA	2:b:136:MET:HG2	1.87	0.55
25:A:2064:C:H2'	25:A:2065:C:C6	2.42	0.55
33:I:48:ALA:HB3	33:I:51:TYR:CE1	2.42	0.55
34:J:41:ALA:HB1	34:J:69:PHE:CZ	2.40	0.55
7:g:26:PHE:HD1	7:g:101:MET:HG2	1.71	0.55
11:k:46:THR:HG23	11:k:49:GLY:H	1.70	0.55
24:w:292:SER:O	24:w:296:ASN:ND2	2.40	0.55
24:w:349:GLN:HA	24:w:352:GLN:HG2	1.88	0.55
34:J:5:VAL:HA	34:J:8:TYR:CZ	2.42	0.55
41:R:63:LYS:HE3	41:R:65:SER:HB3	1.89	0.55
1:a:1062:U:H2'	1:a:1063:C:C6	2.42	0.55
6:f:15:SER:HA	6:f:18:VAL:HG23	1.88	0.55
24:w:290:GLU:OE2	24:w:294:ARG:NH2	2.40	0.55
25:A:545:U:H2'	25:A:548:G:H22	1.72	0.55
25:A:2106:U:H2'	25:A:2107:G:C8	2.42	0.55
25:A:2116:G:N2	25:A:2171:A:H61	2.05	0.55
34:J:12:GLN:NE2	34:J:55:ILE:O	2.39	0.55
25:A:2154:A:H2'	25:A:2155:U:H6	1.72	0.55
4:d:99:ASP:OD1	4:d:100:ASN:N	2.40	0.54
11:k:72:ASP:O	11:k:75:LYS:NZ	2.35	0.54
36:M:5:GLN:HG2	36:M:20:MET:HE3	1.88	0.54
22:y:23:A:H2'	22:y:24:G:C8	2.41	0.54
25:A:291:G:O6	25:A:349:U:O2	2.26	0.54
25:A:593:U:H2'	25:A:594:U:C6	2.42	0.54
26:B:14:U:OP2	26:B:70:C:O2'	2.25	0.54
30:F:162:SER:OG	30:F:165:GLU:OE1	2.23	0.54
1:a:83:C:H2'	1:a:85:U:H5"	1.88	0.54
25:A:2554:U:H2'	25:A:2555:U:C6	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:458:U:H2'	1:a:459:A:C8	2.42	0.54
3:c:58:GLU:OE1	3:c:65:ARG:NH1	2.41	0.54
25:A:549:G:H2'	25:A:550:C:C6	2.43	0.54
25:A:1028:A:H2'	25:A:1029:A:C8	2.43	0.54
25:A:2150:C:H2'	25:A:2151:U:C6	2.43	0.54
33:I:87:GLU:OE2	33:I:96:PHE:N	2.41	0.54
34:J:19:ASN:O	34:J:21:SER:N	2.40	0.54
44:U:29:VAL:HB	44:U:55:ILE:HD11	1.90	0.54
7:g:144:MET:HE1	22:y:31:A:H1'	1.90	0.54
25:A:1047:G:HO2'	25:A:1048:A:H8	1.56	0.54
25:A:2498:OMC:HM22	25:A:2499:C:H5'	1.89	0.54
1:a:1071:C:H2'	1:a:1072:G:H8	1.73	0.54
14:n:53:ARG:HB3	14:n:59:ARG:NH1	2.23	0.54
25:A:1063:G:C4	34:J:136:MET:HE1	2.43	0.54
25:A:1353:A:H2'	25:A:1354:A:C8	2.43	0.54
29:E:122:GLU:OE1	29:E:122:GLU:N	2.38	0.54
31:G:98:VAL:HG11	31:G:124:GLU:HA	1.90	0.54
1:a:714:G:H2'	1:a:715:A:C8	2.43	0.53
3:c:78:GLY:HA3	3:c:83:ASP:OD1	2.09	0.53
24:w:219:PRO:HA	24:w:222:LEU:HD12	1.89	0.53
25:A:1669:A:H5'	36:M:5:GLN:HE22	1.73	0.53
25:A:2579:C:O2'	28:D:136:ASN:OD1	2.26	0.53
34:J:29:GLY:HA3	34:J:35:ILE:HD11	1.90	0.53
57:8:14:CYS:HA	57:8:27:CYS:HB3	1.89	0.53
22:y:22:G:H2'	22:y:23:A:H8	1.73	0.53
25:A:721:A:H2'	25:A:722:A:C8	2.43	0.53
34:J:18:ALA:HA	34:J:42:PHE:CD2	2.43	0.53
25:A:1084:A:C8	33:I:56:ARG:HD3	2.43	0.53
25:A:1590:A:H2'	25:A:1591:A:C8	2.43	0.53
1:a:1323:G:H2'	1:a:1324:A:C8	2.43	0.53
6:f:51:ILE:O	6:f:54:LEU:HG	2.08	0.53
25:A:1532:A:H2'	25:A:1533:C:C6	2.44	0.53
30:F:176:PRO:HB3	52:3:44:PHE:CE1	2.44	0.53
34:J:132:THR:O	34:J:135:SER:OG	2.23	0.53
1:a:17:U:H2'	1:a:18:C:C6	2.44	0.53
1:a:1273:C:H2'	1:a:1274:A:O4'	2.08	0.53
1:a:1433:A:N7	60:a:3203:HOH:O	2.34	0.53
22:y:19:G:O2'	25:A:2112:G:N3	2.40	0.53
2:b:83:ALA:O	2:b:87:CYS:CB	2.57	0.53
25:A:52:A:H2'	25:A:53:A:C8	2.43	0.53
25:A:1141:U:H4'	25:A:1142:A:O4'	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:I:97:LYS:HD3	33:I:127:ALA:HA	1.89	0.53
25:A:1434:A:H2'	25:A:1435:G:C8	2.43	0.53
25:A:849:A:H2'	25:A:850:U:H6	1.73	0.53
25:A:1060:U:H1'	25:A:1062:G:H21	1.72	0.53
53:4:53:LYS:NZ	53:4:55:ILE:O	2.40	0.53
2:b:164:ILE:HD13	2:b:186:ILE:HD13	1.90	0.53
20:t:9:LYS:O	20:t:13:GLN:HG2	2.09	0.53
25:A:1417:C:O2'	25:A:1587:G:O2'	2.24	0.53
13:m:74:SER:O	13:m:78:LYS:HG2	2.09	0.53
22:y:51:U:O2	22:y:63:G:N2	2.30	0.53
25:A:849:A:H2'	25:A:850:U:C6	2.45	0.53
25:A:2116:G:H1	25:A:2164:C:N4	2.06	0.53
28:D:1:MET:HG2	28:D:2:ILE:H	1.74	0.53
1:a:1377:A:OP1	7:g:92:ARG:NH2	2.42	0.52
10:j:6:ILE:HB	10:j:76:ILE:HB	1.90	0.52
22:y:60:U:OP2	22:y:61:C:N4	2.41	0.52
25:A:1077:A:H2	25:A:1088:A:N7	2.07	0.52
25:A:1734:G:H2'	25:A:1735:A:H8	1.74	0.52
25:A:2111:U:H3	25:A:2147:A:H1'	1.74	0.52
25:A:2547:A:H2'	25:A:2548:U:C6	2.44	0.52
30:F:132:VAL:HG22	30:F:152:LEU:HB3	1.91	0.52
1:a:477:C:H2'	1:a:478:A:C8	2.44	0.52
1:a:728:A:H2'	1:a:729:A:C8	2.44	0.52
24:w:110:ASN:ND2	24:w:168:GLY:H	2.07	0.52
24:w:155:GLU:HG2	24:w:156:HIS:H	1.73	0.52
25:A:1102:C:C2	25:A:1103:A:C8	2.97	0.52
25:A:2636:C:O5'	28:D:81:GLU:HG3	2.09	0.52
32:H:5:LEU:HD11	32:H:12:LEU:HD11	1.90	0.52
34:J:56:PRO:HD3	34:J:75:PRO:HD3	1.90	0.52
12:l:33:VAL:HG22	12:l:79:VAL:HG12	1.92	0.52
25:A:1125:G:OP2	25:A:1126:A:O2'	2.23	0.52
46:W:98:SER:OG	46:W:98:SER:O	2.26	0.52
22:y:23:A:H2'	22:y:24:G:H8	1.74	0.52
25:A:549:G:H2'	25:A:550:C:H6	1.74	0.52
25:A:2102:G:N2	25:A:2187:U:O2	2.31	0.52
25:A:2467:C:O2	38:O:123:LYS:NZ	2.42	0.52
25:A:2680:U:O2'	25:A:2681:C:H5'	2.08	0.52
40:Q:2:ASP:N	40:Q:2:ASP:OD1	2.39	0.52
1:a:346:G:OP1	41:R:39:ARG:NH2	2.37	0.52
25:A:1084:A:H5'	33:I:55:VAL:HA	1.90	0.52
26:B:13:G:O2'	26:B:15:A:OP2	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:J:113:LYS:HB3	34:J:125:MET:HE1	1.90	0.52
40:Q:84:GLU:OE1	40:Q:84:GLU:N	2.43	0.52
2:b:15:HIS:HB3	2:b:43:LEU:HD21	1.90	0.52
2:b:20:THR:O	2:b:23:TRP:HD1	1.92	0.52
9:i:54:LEU:HD22	9:i:103:PHE:HE1	1.75	0.52
19:s:19:VAL:HG11	19:s:44:MET:HG2	1.92	0.52
25:A:833:A:H2'	25:A:834:G:C8	2.44	0.52
25:A:1434:A:H2'	25:A:1435:G:H8	1.74	0.52
25:A:2304:G:H22	25:A:2312:U:H3	1.57	0.52
17:q:17:MET:HG3	17:q:20:SER:HB2	1.92	0.52
25:A:644:A:H2'	25:A:645:C:O4'	2.09	0.52
25:A:2637:U:OP1	28:D:83:ARG:NH1	2.43	0.52
19:s:45:ILE:HD12	19:s:64:ASP:HA	1.90	0.52
27:C:5:LYS:NZ	27:C:14:ARG:O	2.38	0.52
30:F:131:GLY:HA2	30:F:153:ASP:HA	1.89	0.52
25:A:545:U:O2'	25:A:546:U:OP1	2.25	0.52
25:A:1720:U:H2'	25:A:1721:G:O4'	2.10	0.52
34:J:8:TYR:CD2	34:J:60:THR:HA	2.44	0.52
1:a:1248:A:H2	9:i:72:ILE:HD11	1.75	0.52
2:b:90:PHE:CG	2:b:154:MET:HE1	2.45	0.52
7:g:113:ASP:HB3	7:g:118:LEU:HD23	1.90	0.52
1:a:171:A:H2'	1:a:172:A:C8	2.45	0.51
6:f:90:MET:SD	18:r:61:ARG:HD3	2.50	0.51
7:g:100:ALA:O	7:g:104:ILE:HG13	2.09	0.51
9:i:79:ILE:O	9:i:83:ILE:HG12	2.10	0.51
22:y:44:G:O2'	22:y:45:U:OP1	2.20	0.51
25:A:441:U:O2'	29:E:41:GLN:NE2	2.43	0.51
6:f:2:ARG:HD3	6:f:91:ARG:NH1	2.03	0.51
25:A:2114:A:C5	25:A:2115:G:H1'	2.45	0.51
31:G:47:ASP:N	31:G:47:ASP:OD1	2.43	0.51
40:Q:55:GLU:OE2	40:Q:81:ARG:NH2	2.42	0.51
1:a:674:G:H2'	1:a:675:A:H8	1.75	0.51
24:w:110:ASN:HD22	24:w:167:SER:HA	1.76	0.51
25:A:191:A:H2'	25:A:192:C:H6	1.75	0.51
25:A:272:A:H2'	25:A:273:G:H8	1.75	0.51
27:C:71:LYS:HG2	27:C:102:ARG:NH1	2.26	0.51
38:O:50:ARG:HD3	38:O:65:ILE:HD11	1.92	0.51
25:A:1667:G:O2'	25:A:1991:U:O4	2.26	0.51
1:a:1040:U:H2'	1:a:1041:G:C8	2.46	0.51
2:b:104:TRP:HE1	2:b:108:ARG:HH21	1.59	0.51
3:c:121:THR:HG23	3:c:189:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2130:U:H1'	25:A:2159:G:C6	2.46	0.51
33:I:78:GLY:N	33:I:79:PRO:HD2	2.26	0.51
10:j:24:GLU:OE1	10:j:90:LEU:HD21	2.11	0.51
25:A:1292:G:H2'	25:A:1293:C:C6	2.46	0.51
27:C:79:GLU:OE1	27:C:101:ARG:NH1	2.43	0.51
33:I:27:VAL:HG23	33:I:110:ALA:HA	1.93	0.51
40:Q:52:SER:O	40:Q:55:GLU:HG2	2.10	0.51
9:i:34:SER:OG	9:i:37:GLN:HG3	2.11	0.51
11:k:97:ILE:HG22	21:u:12:PHE:HZ	1.76	0.51
25:A:1054:A:H5"	33:I:31:ARG:NH1	2.26	0.51
25:A:1073:A:H2'	25:A:1074:G:C8	2.46	0.51
46:W:81:ASP:OD1	46:W:82:ARG:N	2.42	0.51
1:a:8:A:N6	4:d:202:GLU:O	2.44	0.51
1:a:208:U:H2'	1:a:210:C:H1'	1.93	0.51
25:A:1105:U:H2'	25:A:1106:G:H8	1.76	0.51
25:A:1385:A:O2'	25:A:1396:U:O2	2.28	0.51
25:A:2243:U:H2'	25:A:2244:U:C6	2.46	0.51
30:F:176:PRO:HB3	52:3:44:PHE:HE1	1.76	0.51
2:b:93:ASN:O	2:b:94:HIS:ND1	2.44	0.51
25:A:240:C:OP2	25:A:241:A:O2'	2.20	0.51
25:A:2111:U:N3	25:A:2147:A:N3	2.58	0.51
25:A:2295:C:OP1	40:Q:10:ARG:NH1	2.44	0.51
34:J:15:ALA:O	34:J:46:THR:HG21	2.11	0.51
1:a:662:U:H2'	1:a:663:A:C8	2.46	0.50
7:g:138:ARG:HD2	7:g:142:HIS:CD2	2.46	0.50
25:A:2134:A:N6	25:A:2156:G:N3	2.59	0.50
37:N:81:ASP:HA	37:N:84:LYS:HD3	1.92	0.50
43:T:14:VAL:HG12	43:T:20:VAL:HG21	1.92	0.50
48:Y:46:HIS:CE1	48:Y:77:ARG:HD3	2.46	0.50
1:a:1397:C:H41	23:z:21:A:H2'	1.76	0.50
6:f:9:MET:HE1	18:r:65:LEU:HD22	1.93	0.50
25:A:1084:A:N3	25:A:1105:U:O2'	2.34	0.50
25:A:1365:A:O2'	49:Z:11:ARG:NH2	2.34	0.50
25:A:1447:C:O2'	25:A:1544:A:N3	2.43	0.50
31:G:15:VAL:HG23	31:G:27:LYS:O	2.11	0.50
31:G:19:ILE:HD11	31:G:43:VAL:HG23	1.92	0.50
31:G:42:GLU:OE1	31:G:55:ARG:NE	2.34	0.50
34:J:18:ALA:HA	34:J:42:PHE:HD2	1.75	0.50
1:a:918:A:H2'	1:a:919:A:C8	2.46	0.50
25:A:299:A:N3	25:A:319:G:O2'	2.41	0.50
34:J:4:LYS:O	34:J:8:TYR:OH	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:U:72:THR:HG21	44:U:108:SER:HB3	1.94	0.50
24:w:155:GLU:HG2	24:w:156:HIS:N	2.26	0.50
30:F:94:GLU:O	30:F:98:GLU:HG3	2.11	0.50
34:J:103:ARG:O	34:J:106:LEU:HG	2.12	0.50
1:a:846:G:H2'	1:a:847:G:C8	2.47	0.50
24:w:110:ASN:ND2	24:w:167:SER:HA	2.26	0.50
24:w:294:ARG:O	24:w:298:LEU:HB2	2.12	0.50
25:A:2189:U:O2'	25:A:2190:G:OP1	2.27	0.50
41:R:31:TRP:CE3	41:R:38:LYS:HG2	2.46	0.50
49:Z:65:ASP:OD1	49:Z:66:THR:N	2.45	0.50
1:a:1314:C:H2'	1:a:1315:U:C6	2.46	0.50
11:k:49:GLY:O	11:k:69:ARG:NH2	2.44	0.50
28:D:39:ASP:OD2	28:D:39:ASP:N	2.44	0.50
33:I:28:ALA:HA	33:I:82:ILE:HA	1.93	0.50
1:a:524:G:H2'	1:a:525:C:C6	2.47	0.50
1:a:1530:G:H2'	1:a:1531:A:H8	1.77	0.50
4:d:157:ALA:O	4:d:160:GLU:HG2	2.12	0.50
12:l:3:THR:HG22	12:l:5:ASN:H	1.77	0.50
22:y:9:A:H5'	22:y:46:7MG:HN22	1.76	0.50
25:A:1536:C:H4'	25:A:1537:G:H5"	1.93	0.50
25:A:2071:A:H2'	25:A:2072:C:C6	2.46	0.50
1:a:1376:U:O4	7:g:10:ARG:NH1	2.34	0.50
25:A:279:A:N6	25:A:361:G:H1'	2.26	0.50
1:a:1266:G:N2	1:a:1269:A:OP2	2.38	0.50
25:A:2120:G:H2'	25:A:2121:G:C8	2.47	0.50
25:A:2529:G:H4'	31:G:175:LYS:HD3	1.94	0.50
30:F:47:LYS:HZ1	30:F:84:PRO:HD2	1.77	0.50
1:a:780:A:N7	60:a:3204:HOH:O	2.35	0.49
25:A:1082:U:O3'	33:I:42:ARG:NH2	2.41	0.49
25:A:1432:G:H2'	25:A:1433:A:C8	2.47	0.49
1:a:696:A:H2'	1:a:697:U:H6	1.77	0.49
25:A:279:A:OP2	25:A:361:G:N2	2.44	0.49
25:A:851:C:H2'	25:A:852:U:C6	2.47	0.49
25:A:2107:G:O6	25:A:2183:A:N6	2.45	0.49
2:b:153:ASP:N	2:b:153:ASP:OD1	2.45	0.49
8:h:43:GLU:HG3	8:h:101:ILE:HD13	1.94	0.49
25:A:357:C:H2'	25:A:358:U:C6	2.48	0.49
38:O:53:MET:HE2	38:O:63:ILE:HD13	1.93	0.49
1:a:719:C:OP2	1:a:720:C:N4	2.38	0.49
1:a:746:A:H2'	1:a:747:A:C8	2.47	0.49
25:A:78:U:H2'	25:A:79:C:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:155:A:H2'	25:A:156:A:C8	2.48	0.49
25:A:742:A:H2'	25:A:743:A:C8	2.47	0.49
25:A:1071:G:N3	25:A:1089:A:O2'	2.38	0.49
25:A:1727:C:H2'	25:A:1728:C:O4'	2.13	0.49
34:J:79:LEU:HD21	34:J:109:ILE:HD12	1.94	0.49
40:Q:74:VAL:O	40:Q:78:VAL:HG23	2.12	0.49
1:a:751:U:H2'	1:a:752:G:O4'	2.13	0.49
15:o:17:ARG:HG3	15:o:17:ARG:NH1	2.26	0.49
25:A:2795:C:H2'	25:A:2796:U:H6	1.77	0.49
1:a:390:U:H2'	1:a:391:G:C8	2.48	0.49
1:a:1122:U:H2'	1:a:1123:U:C6	2.48	0.49
4:d:174:ASP:OD2	4:d:177:LYS:HG2	2.12	0.49
6:f:88:MET:HE2	6:f:90:MET:SD	2.51	0.49
6:f:90:MET:HE1	18:r:23:TYR:CZ	2.48	0.49
25:A:2246:G:H2'	25:A:2247:A:C8	2.47	0.49
28:D:7:LYS:HE2	28:D:198:GLY:HA2	1.95	0.49
1:a:82:G:H2'	1:a:83:C:C6	2.47	0.49
25:A:703:U:H2'	25:A:704:G:O4'	2.12	0.49
25:A:1069:A:H5'	25:A:1070:A:H8	1.77	0.49
25:A:2187:U:H2'	25:A:2188:U:C6	2.48	0.49
33:I:57:ASN:HB2	33:I:62:ARG:HG2	1.94	0.49
33:I:99:PHE:O	33:I:103:ASN:N	2.45	0.49
38:O:136:MET:HE2	47:X:57:TYR:CD1	2.48	0.49
2:b:87:CYS:SG	2:b:221:VAL:HG11	2.53	0.49
25:A:191:A:H2'	25:A:192:C:C6	2.48	0.49
25:A:1532:A:H2'	25:A:1533:C:H6	1.76	0.49
25:A:1794:A:H2'	25:A:1795:C:C6	2.48	0.49
30:F:62:GLY:O	30:F:95:ARG:NH1	2.45	0.49
32:H:25:TYR:HE1	32:H:29:PHE:HD2	1.59	0.49
47:X:48:MET:SD	47:X:51:GLN:NE2	2.86	0.49
1:a:216:U:H2'	1:a:217:C:C6	2.47	0.49
1:a:1218:C:H2'	1:a:1219:A:C8	2.47	0.49
24:w:92:LEU:HD21	24:w:349:GLN:OE1	2.13	0.49
25:A:973:A:H5'	25:A:1188:U:H1'	1.94	0.49
25:A:1000:A:H2'	25:A:1001:A:C8	2.48	0.49
25:A:1386:C:H2'	25:A:1387:A:C8	2.47	0.49
31:G:30:ASN:HB3	31:G:79:VAL:O	2.13	0.49
39:P:32:GLU:OE1	39:P:115:LEU:HD12	2.13	0.49
1:a:82:G:H1'	1:a:87:C:H41	1.78	0.48
1:a:204:G:H2'	1:a:205:A:H8	1.78	0.48
1:a:539:A:H2'	1:a:540:G:C8	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:35:LYS:HG2	6:f:65:GLU:HB3	1.94	0.48
25:A:869:G:O3'	38:O:6:ARG:NH2	2.46	0.48
25:A:1353:A:H2'	25:A:1354:A:H8	1.77	0.48
34:J:100:LYS:HD2	34:J:139:VAL:HB	1.95	0.48
1:a:219:U:H2'	1:a:220:G:C8	2.48	0.48
1:a:1171:A:H2'	1:a:1172:C:C6	2.47	0.48
15:o:47:LYS:O	15:o:53:ARG:NH2	2.46	0.48
25:A:639:U:H2'	25:A:640:C:C6	2.47	0.48
8:h:64:LYS:HG3	8:h:71:VAL:HG21	1.96	0.48
22:y:15:G:O6	22:y:48:C:O2	2.32	0.48
25:A:151:C:H2'	25:A:152:A:H8	1.78	0.48
25:A:894:U:H2'	25:A:895:U:O4'	2.13	0.48
25:A:1108:U:H2'	25:A:1109:C:C6	2.48	0.48
25:A:1328:A:H2'	25:A:1330:C:C5	2.49	0.48
25:A:2462:C:H1'	25:A:2491:U:O4	2.14	0.48
25:A:2898:U:H2'	25:A:2899:A:H8	1.78	0.48
29:E:171:ASP:OD1	29:E:171:ASP:N	2.47	0.48
1:a:28:A:O2'	1:a:296:U:OP1	2.26	0.48
1:a:148:G:O2'	1:a:1446:A:H8	1.96	0.48
1:a:999:C:H2'	1:a:1000:A:C8	2.48	0.48
7:g:93:PRO:HA	7:g:96:ARG:HD2	1.95	0.48
22:y:36:A:H2'	22:y:37:MIA:H4'	1.95	0.48
25:A:463:G:N2	25:A:466:A:OP2	2.37	0.48
25:A:881:G:O6	25:A:895:U:C4	2.66	0.48
25:A:2170:A:C2	25:A:2171:A:H1'	2.49	0.48
25:A:2812:G:H2'	25:A:2813:A:C8	2.49	0.48
47:X:4:ILE:HG12	47:X:50:MET:HE1	1.95	0.48
2:b:117:LEU:CD2	2:b:141:LEU:HB2	2.43	0.48
5:e:76:LEU:HD23	5:e:76:LEU:H	1.77	0.48
7:g:15:ASP:OD1	7:g:15:ASP:N	2.43	0.48
25:A:155:A:H2'	25:A:156:A:H8	1.78	0.48
3:c:130:PHE:O	3:c:134:MET:HG3	2.12	0.48
24:w:338:ASP:HA	24:w:341:ILE:HG12	1.96	0.48
25:A:272:A:H2'	25:A:273:G:C8	2.48	0.48
44:U:82:MET:HB2	44:U:98:LYS:HB2	1.96	0.48
1:a:1250:A:H2'	1:a:1251:A:C8	2.47	0.48
25:A:645:C:H2'	25:A:647:G:N7	2.28	0.48
25:A:1438:U:H2'	25:A:1439:A:H8	1.77	0.48
25:A:2281:A:O2'	25:A:2282:G:H5'	2.13	0.48
30:F:58:ALA:HB2	30:F:65:PRO:HD3	1.96	0.48
1:a:1317:C:OP1	14:n:56:SER:OG	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1106:G:H5'	33:I:62:ARG:HH22	1.79	0.48
28:D:105:LYS:HD3	28:D:105:LYS:HA	1.75	0.48
31:G:8:PRO:HB3	31:G:51:THR:HG22	1.95	0.48
1:a:846:G:H2'	1:a:847:G:H8	1.79	0.48
3:c:73:PRO:HG3	3:c:105:GLU:HB3	1.95	0.48
9:i:84:THR:HG22	9:i:88:MET:HE2	1.95	0.48
25:A:1093:G:H21	25:A:1098:A:N6	2.08	0.48
25:A:2795:C:H2'	25:A:2796:U:C6	2.49	0.48
33:I:59:LEU:HB3	33:I:62:ARG:HB2	1.95	0.48
1:a:501:C:H2'	1:a:502:A:C8	2.49	0.47
2:b:133:GLU:O	2:b:137:ARG:HG2	2.14	0.47
3:c:79:LYS:O	3:c:80:LYS:HG2	2.14	0.47
22:y:51:U:H2'	22:y:52:G:H8	1.79	0.47
24:w:72:PRO:HB2	24:w:75:ARG:NH1	2.29	0.47
25:A:282:A:H2'	25:A:283:G:C8	2.49	0.47
1:a:1530:G:H2'	1:a:1531:A:C8	2.49	0.47
4:d:104:ARG:HG3	4:d:168:PRO:HG2	1.95	0.47
7:g:12:ILE:HG23	7:g:21:GLU:HG2	1.96	0.47
9:i:55:VAL:HG21	9:i:87:LEU:HD21	1.95	0.47
22:y:31:A:H3'	22:y:32:PSU:H6	1.79	0.47
25:A:876:C:H2'	25:A:877:A:O4'	2.14	0.47
25:A:1796:U:H2'	25:A:1797:G:H8	1.79	0.47
27:C:145:GLU:HB2	27:C:188:CYS:HB3	1.95	0.47
36:M:106:GLU:OE1	36:M:106:GLU:N	2.47	0.47
7:g:138:ARG:HD2	7:g:142:HIS:HD2	1.78	0.47
16:p:48:GLU:OE1	16:p:51:ARG:NH2	2.28	0.47
21:u:10:GLU:N	21:u:10:GLU:OE1	2.48	0.47
25:A:546:U:H3'	25:A:547:A:H8	1.80	0.47
25:A:1070:A:N7	25:A:1096:A:O2'	2.37	0.47
25:A:1902:C:H4'	27:C:242:LYS:O	2.13	0.47
25:A:2139:U:O2	25:A:2152:G:C6	2.66	0.47
38:O:53:MET:HE3	38:O:105:MET:HE3	1.95	0.47
40:Q:56:LYS:NZ	40:Q:60:GLU:HB3	2.29	0.47
57:8:11:CYS:HB3	57:8:33:HIS:HE1	1.79	0.47
1:a:826:C:O2	8:h:16:ASN:ND2	2.47	0.47
19:s:12:ASP:OD2	19:s:35:SER:OG	2.30	0.47
25:A:1506:U:H2'	25:A:1507:C:C6	2.50	0.47
34:J:104:ALA:HA	34:J:107:GLN:NE2	2.29	0.47
1:a:1120:C:H2'	1:a:1121:U:H6	1.78	0.47
1:a:1447:A:H5"	1:a:1448:C:H5	1.80	0.47
9:i:65:ILE:HG21	9:i:79:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:59:GLU:O	13:m:62:LYS:HG2	2.14	0.47
25:A:1071:G:H2'	25:A:1072:C:C6	2.50	0.47
34:J:130:GLU:CD	34:J:134:ARG:HE	2.22	0.47
24:w:72:PRO:HB2	24:w:75:ARG:HH12	1.79	0.47
25:A:307:G:N1	25:A:310:A:OP2	2.40	0.47
25:A:1889:A:H2'	25:A:1890:A:C8	2.49	0.47
25:A:2136:G:O2'	25:A:2137:U:O4'	2.20	0.47
29:E:176:ASP:N	29:E:176:ASP:OD1	2.47	0.47
33:I:57:ASN:HA	33:I:62:ARG:HE	1.79	0.47
34:J:86:ILE:HD13	34:J:98:VAL:HG22	1.95	0.47
39:P:8:ARG:HD2	39:P:43:GLU:HG2	1.96	0.47
1:a:131:A:O2'	1:a:262:A:N3	2.48	0.47
4:d:160:GLU:HA	4:d:163:GLU:OE1	2.15	0.47
25:A:1022:G:O6	35:L:68:LYS:NZ	2.39	0.47
25:A:1063:G:N7	34:J:90:SER:OG	2.48	0.47
25:A:1915:3TD:H6	25:A:1915:3TD:O5'	2.15	0.47
25:A:2162:G:H2'	25:A:2162:G:N3	2.30	0.47
34:J:30:GLN:HE21	34:J:31:GLN:HE21	1.62	0.47
49:Z:41:GLU:OE2	49:Z:44:LYS:NZ	2.34	0.47
52:3:26:SER:OG	52:3:27:THR:N	2.44	0.47
1:a:62:U:OP1	1:a:385:C:O2'	2.33	0.47
1:a:82:G:H1'	1:a:87:C:N4	2.29	0.47
1:a:337:G:H2'	1:a:338:A:H8	1.77	0.47
3:c:110:GLU:HB2	3:c:144:LEU:HD22	1.97	0.47
25:A:602:A:O2'	25:A:604:G:O2'	2.21	0.47
25:A:1010:A:OP1	42:S:66:ASN:ND2	2.32	0.47
26:B:48:U:OP1	40:Q:30:ARG:NH2	2.48	0.47
31:G:23:VAL:HG22	31:G:36:THR:HG22	1.97	0.47
24:w:55:TRP:CE2	24:w:59:GLN:HG3	2.50	0.47
25:A:784:G:H5'	25:A:785:G:OP1	2.15	0.47
25:A:1076:C:O2'	34:J:93:PRO:HD2	2.15	0.47
1:a:90:C:H2'	1:a:91:U:C6	2.49	0.47
1:a:1118:U:OP1	9:i:11:ARG:NH1	2.48	0.47
25:A:3:U:H2'	25:A:4:U:C6	2.50	0.47
25:A:1386:C:H2'	25:A:1387:A:H8	1.78	0.47
25:A:2099:U:H2'	25:A:2100:G:C8	2.50	0.47
33:I:6:GLN:N	33:I:6:GLN:OE1	2.48	0.47
34:J:58:VAL:HG12	34:J:60:THR:H	1.80	0.47
41:R:88:ARG:HH21	41:R:112:GLU:HB2	1.80	0.47
46:W:96:PHE:O	46:W:100:SER:HA	2.15	0.47
2:b:67:ILE:H	2:b:89:GLN:HE21	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:32:GLN:OE1	9:i:32:GLN:N	2.48	0.46
11:k:119:IAS:OXT	21:u:35:ARG:NH2	2.29	0.46
18:r:32:TYR:CG	18:r:55:LEU:HD21	2.50	0.46
22:y:57:G:OP2	22:y:57:G:H8	1.97	0.46
25:A:881:G:H2'	25:A:882:G:H8	1.80	0.46
53:4:11:SER:O	53:4:15:MET:HG3	2.16	0.46
1:a:310:G:H5"	16:p:31:ARG:HB2	1.97	0.46
10:j:24:GLU:O	10:j:27:GLU:HG3	2.15	0.46
25:A:1808:A:H3'	25:A:1809:A:C8	2.48	0.46
25:A:2756:U:OP2	57:8:19:ARG:NE	2.35	0.46
2:b:8:ASP:HA	2:b:11:LYS:HE3	1.97	0.46
2:b:66:LYS:HG3	2:b:158:PRO:HA	1.98	0.46
10:j:25:ILE:HA	10:j:28:THR:HG22	1.98	0.46
25:A:347:A:H2'	25:A:348:A:C8	2.51	0.46
25:A:1664:A:H2	36:M:1:MET:HE2	1.81	0.46
25:A:2138:G:H2'	25:A:2139:U:O4'	2.16	0.46
42:S:48:ARG:NE	42:S:49:ASP:OD1	2.45	0.46
52:3:12:ILE:HD12	52:3:32:LEU:HD13	1.96	0.46
1:a:390:U:H2'	1:a:391:G:H8	1.81	0.46
6:f:4:TYR:CE1	6:f:71:ILE:HG13	2.50	0.46
8:h:39:VAL:HG21	8:h:110:VAL:HG12	1.97	0.46
25:A:219:A:N3	25:A:234:U:O2'	2.40	0.46
25:A:277:G:H4'	25:A:278:A:O5'	2.14	0.46
25:A:414:C:H2'	25:A:415:A:C8	2.51	0.46
25:A:414:C:H2'	25:A:415:A:H8	1.81	0.46
18:r:36:SER:HA	18:r:72:ASP:HB2	1.97	0.46
25:A:2246:G:H2'	25:A:2247:A:H8	1.80	0.46
35:L:23:LYS:HD3	35:L:28:LEU:HD13	1.96	0.46
49:Z:4:VAL:HG22	49:Z:11:ARG:HG2	1.97	0.46
1:a:459:A:H2'	1:a:460:A:C8	2.50	0.46
1:a:945:G:C2	1:a:946:A:C8	3.04	0.46
1:a:1060:U:H2'	1:a:1061:G:H8	1.80	0.46
2:b:23:TRP:CD1	2:b:39:HIS:HE1	2.33	0.46
40:Q:15:ARG:NH2	40:Q:95:SER:OG	2.49	0.46
4:d:177:LYS:HG3	4:d:179:GLU:HG3	1.96	0.46
5:e:83:HIS:HE1	5:e:148:ASN:H	1.64	0.46
6:f:9:MET:HA	6:f:58:HIS:O	2.15	0.46
25:A:1066:U:O4	25:A:1069:A:N7	2.49	0.46
25:A:1724:G:H2'	25:A:1725:U:C6	2.50	0.46
25:A:1746:A:H2'	25:A:1747:U:C6	2.50	0.46
33:I:99:PHE:HA	33:I:102:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:57:MET:HG3	9:i:60:LYS:HB2	1.98	0.46
24:w:95:GLN:HE21	24:w:356:LEU:HD11	1.79	0.46
25:A:1328:A:H2'	25:A:1330:C:C4	2.50	0.46
32:H:5:LEU:HD12	32:H:14:SER:O	2.16	0.46
57:8:8:LYS:O	57:8:35:GLN:NE2	2.48	0.46
25:A:574:A:OP2	60:A:3501:HOH:O	2.21	0.46
25:A:1111:A:HO2'	25:A:1112:G:P	2.37	0.46
57:8:27:CYS:SG	57:8:33:HIS:HB2	2.56	0.46
1:a:1014:A:C2	1:a:1219:A:H1'	2.50	0.45
25:A:139:U:H5"	25:A:140:C:C5	2.47	0.45
38:O:26:VAL:HG13	38:O:104:GLU:OE1	2.16	0.45
46:W:4:LYS:O	46:W:94:ARG:NH1	2.46	0.45
1:a:674:G:H2'	1:a:675:A:C8	2.51	0.45
10:j:80:THR:HG22	10:j:82:LYS:H	1.82	0.45
15:o:8:THR:OG1	15:o:31:LEU:HD11	2.16	0.45
30:F:108:VAL:HG11	30:F:176:PRO:HG3	1.98	0.45
30:F:144:ASP:OD1	30:F:144:ASP:N	2.48	0.45
37:N:109:LYS:HG2	37:N:126:ARG:HB2	1.97	0.45
1:a:1033:G:C8	1:a:1034:G:C8	3.04	0.45
15:o:78:TYR:OH	15:o:89:ARG:O	2.28	0.45
22:y:37:MIA:H2'	22:y:37:MIA:N3	2.31	0.45
25:A:881:G:H2'	25:A:882:G:C8	2.51	0.45
25:A:1032:A:OP1	57:8:8:LYS:HG2	2.16	0.45
25:A:2128:G:H2'	25:A:2129:C:C6	2.51	0.45
25:A:2836:U:H2'	25:A:2837:A:C8	2.51	0.45
44:U:37:THR:HG23	44:U:38:TYR:CD2	2.52	0.45
1:a:687:A:C2	1:a:704:A:C5	3.04	0.45
1:a:999:C:H2'	1:a:1000:A:H8	1.80	0.45
1:a:1316:G:N1	1:a:1319:A:OP2	2.49	0.45
21:u:63:GLU:HA	21:u:66:ARG:HH12	1.82	0.45
24:w:73:GLU:HA	24:w:76:GLU:OE2	2.16	0.45
25:A:279:A:H61	25:A:361:G:H1'	1.81	0.45
25:A:1484:U:H2'	25:A:1485:U:H6	1.80	0.45
25:A:2698:U:H2'	25:A:2699:C:C6	2.51	0.45
34:J:8:TYR:HB2	34:J:59:ILE:HG13	1.99	0.45
34:J:98:VAL:HG12	34:J:137:GLY:C	2.42	0.45
57:8:11:CYS:HB3	57:8:33:HIS:CE1	2.52	0.45
9:i:27:LYS:HD3	9:i:27:LYS:N	2.31	0.45
24:w:55:TRP:HD1	24:w:91:GLN:HG3	1.81	0.45
24:w:347:GLU:O	24:w:350:ALA:HB3	2.17	0.45
25:A:1:G:H2'	25:A:2:G:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:222:A:C2	25:A:233:A:H5”	2.51	0.45
25:A:2086:U:H2’	25:A:2087:G:C8	2.52	0.45
25:A:2788:C:H2’	25:A:2789:C:C6	2.51	0.45
28:D:124:ARG:HG3	28:D:165:MET:HG3	1.97	0.45
29:E:108:ILE:HG23	37:N:1:MET:HE1	1.97	0.45
31:G:22:GLN:HE21	31:G:39:ASP:HA	1.80	0.45
3:c:83:ASP:O	3:c:86:LYS:HG2	2.16	0.45
9:i:54:LEU:HD22	9:i:103:PHE:CE1	2.52	0.45
22:y:25:C:O2’	22:y:26:A:O5’	2.30	0.45
31:G:137:ASP:HB3	31:G:140:VAL:HB	1.98	0.45
1:a:694:A:H4’	22:y:37:MIA:C6	2.47	0.45
2:b:78:GLU:HG2	2:b:79:ALA:N	2.32	0.45
22:y:37:MIA:H5’	22:y:38:A:N7	2.32	0.45
24:w:107:ASP:OD1	24:w:109:ARG:NH1	2.50	0.45
25:A:813:U:H2’	25:A:814:C:C6	2.52	0.45
25:A:1073:A:H2’	25:A:1074:G:H8	1.82	0.45
40:Q:68:LYS:HG2	40:Q:102:ARG:HB3	1.98	0.45
44:U:73:LYS:HB2	44:U:106:VAL:HB	1.97	0.45
49:Z:43:GLU:HG3	49:Z:45:ARG:HG2	1.98	0.45
1:a:1356:G:H2’	1:a:1357:A:H8	1.79	0.45
9:i:55:VAL:HG11	9:i:94:LEU:HD23	1.98	0.45
9:i:57:MET:O	9:i:57:MET:HG2	2.16	0.45
24:w:55:TRP:HB2	24:w:91:GLN:HG3	1.98	0.45
25:A:172:A:H2’	25:A:173:A:C8	2.52	0.45
25:A:673:C:OP1	29:E:49:ARG:NH1	2.45	0.45
25:A:1594:U:H2’	25:A:1595:C:C6	2.51	0.45
25:A:2802:G:H2’	25:A:2803:G:H8	1.81	0.45
25:A:2820:A:OP2	39:P:2:ARG:NH2	2.49	0.45
27:C:203:ARG:NH1	27:C:214:ARG:HH21	2.15	0.45
30:F:66:LEU:HD23	30:F:88:LYS:HD3	1.99	0.45
34:J:110:ALA:O	34:J:114:ALA:N	2.50	0.45
36:M:107:LEU:HB2	36:M:116:ILE:HD11	1.99	0.45
1:a:1171:A:H2’	1:a:1172:C:H6	1.81	0.45
2:b:81:LYS:NZ	2:b:85:LEU:HD11	2.32	0.45
9:i:46:MET:O	9:i:50:GLN:HG3	2.17	0.45
22:y:41:C:H2’	22:y:42:C:C6	2.52	0.45
24:w:317:VAL:HG11	24:w:332:VAL:HG21	1.99	0.45
25:A:851:C:H2’	25:A:852:U:H6	1.80	0.45
25:A:1294:U:O2’	39:P:23:ASN:ND2	2.50	0.45
25:A:1484:U:H2’	25:A:1485:U:C6	2.52	0.45
40:Q:88:LYS:HE2	40:Q:116:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1308:U:H2'	1:a:1309:G:H8	1.82	0.45
3:c:174:PRO:HB2	3:c:177:THR:HG22	1.98	0.45
25:A:248:G:H5'	25:A:250:G:N7	2.32	0.45
25:A:581:C:H2'	25:A:582:A:C8	2.52	0.45
25:A:2845:U:H5"	41:R:52:ASN:O	2.17	0.45
25:A:993:G:H1'	43:T:91:GLN:HE21	1.82	0.44
25:A:1066:U:H2'	25:A:1067:A:H5"	1.99	0.44
25:A:1198:U:H2'	25:A:1199:U:C6	2.53	0.44
25:A:2291:U:H2'	25:A:2292:U:C6	2.52	0.44
35:L:40:HIS:H	35:L:40:HIS:CD2	2.36	0.44
42:S:50:ARG:O	42:S:54:LYS:NZ	2.46	0.44
52:3:30:HIS:ND1	52:3:31:ASP:O	2.47	0.44
1:a:41:G:H2'	1:a:42:G:H8	1.81	0.44
1:a:481:G:O2'	1:a:483:C:N4	2.49	0.44
1:a:736:C:H2'	1:a:737:C:H6	1.82	0.44
1:a:1178:G:N2	1:a:1181:G:OP2	2.49	0.44
2:b:81:LYS:HZ2	2:b:85:LEU:HD11	1.83	0.44
2:b:151:ILE:HA	2:b:154:MET:HE3	1.99	0.44
10:j:27:GLU:O	10:j:31:ARG:HG2	2.17	0.44
22:y:9:A:H4'	22:y:46:7MG:OP2	2.17	0.44
25:A:282:A:N6	25:A:359:G:O6	2.50	0.44
25:A:2147:A:H2'	25:A:2148:G:O4'	2.17	0.44
33:I:54:VAL:O	33:I:56:ARG:NH1	2.50	0.44
33:I:59:LEU:HD23	33:I:61:ARG:H	1.81	0.44
8:h:113:ASP:OD1	8:h:113:ASP:N	2.49	0.44
10:j:34:ALA:HB2	10:j:80:THR:H	1.83	0.44
1:a:246:A:C2	1:a:282:A:C5	3.06	0.44
1:a:362:G:N2	1:a:365:U:OP2	2.50	0.44
1:a:1040:U:H2'	1:a:1041:G:H8	1.82	0.44
6:f:62:MET:HE3	6:f:62:MET:HB2	1.87	0.44
24:w:308:ARG:HD2	24:w:310:TYR:OH	2.17	0.44
25:A:2131:U:O5'	25:A:2133:G:H4'	2.17	0.44
25:A:2143:C:H2'	25:A:2144:G:C8	2.52	0.44
30:F:170:LEU:O	30:F:175:PHE:HB2	2.17	0.44
33:I:27:VAL:O	33:I:83:ALA:N	2.51	0.44
46:W:26:LYS:HZ3	46:W:37:GLU:HB2	1.82	0.44
1:a:981:U:OP1	14:n:9:ARG:NH1	2.48	0.44
25:A:306:U:H2'	25:A:307:G:O4'	2.17	0.44
25:A:2101:A:H2'	25:A:2102:G:H8	1.82	0.44
25:A:2128:G:H2'	25:A:2129:C:H6	1.83	0.44
25:A:2820:A:N3	25:A:2820:A:H2'	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:21:ASN:HB3	27:C:24:LEU:HG	2.00	0.44
44:U:11:ARG:NH2	44:U:99:ARG:O	2.51	0.44
1:a:31:G:O2'	1:a:48:C:N4	2.50	0.44
4:d:19:LEU:HD22	4:d:64:ILE:HG13	2.00	0.44
25:A:363:G:H2'	25:A:364:C:C6	2.53	0.44
25:A:885:C:H2'	25:A:886:A:H8	1.82	0.44
26:B:49:C:H2'	26:B:50:A:C8	2.53	0.44
1:a:4:U:H2'	1:a:5:U:H5"	1.99	0.44
1:a:131:A:H2'	1:a:132:C:C6	2.53	0.44
1:a:946:A:H2'	1:a:947:G:H8	1.81	0.44
1:a:1477:U:H2'	1:a:1478:U:C6	2.53	0.44
20:t:79:LEU:HD23	20:t:79:LEU:HA	1.85	0.44
24:w:257:CYS:HB2	24:w:270:ALA:HB2	1.98	0.44
25:A:1068:G:H2'	25:A:1069:A:C5	2.52	0.44
25:A:1080:A:H1'	34:J:128:SER:HA	1.99	0.44
25:A:1682:G:H2'	25:A:1683:U:C6	2.53	0.44
33:I:122:GLN:NE2	33:I:124:ASP:OD2	2.51	0.44
1:a:1371:G:O3'	9:i:71:GLY:HA3	2.18	0.44
6:f:73:GLU:O	6:f:77:THR:HG23	2.18	0.44
25:A:568:U:H1'	25:A:2030:6MZ:H9C1	2.00	0.44
25:A:1223:G:OP1	43:T:68:ARG:NH1	2.50	0.44
25:A:2160:C:H2'	25:A:2161:C:O4'	2.17	0.44
33:I:22:ALA:HB1	33:I:91:ALA:HA	1.99	0.44
57:8:9:LYS:HE3	57:8:16:ILE:HG12	2.00	0.44
1:a:76:G:H2'	1:a:77:A:C8	2.52	0.44
1:a:1238:A:H2	1:a:1241:G:N3	2.16	0.44
2:b:26:LYS:NZ	2:b:194:ASP:OD2	2.44	0.44
3:c:105:GLU:OE2	3:c:107:ARG:NH1	2.51	0.44
7:g:27:VAL:HG11	7:g:40:GLU:HG2	2.00	0.44
25:A:645:C:H2'	25:A:647:G:C8	2.53	0.44
25:A:848:C:H2'	25:A:849:A:H8	1.83	0.44
25:A:2038:G:H2'	25:A:2039:U:O4'	2.18	0.44
29:E:17:THR:O	29:E:21:ARG:HG3	2.18	0.44
33:I:121:SER:OG	33:I:122:GLN:N	2.50	0.44
1:a:757:U:H2'	1:a:758:C:O4'	2.18	0.43
21:u:17:ARG:O	21:u:21:ARG:HG2	2.18	0.43
22:x:66:U:H2'	22:x:67:C:C6	2.53	0.43
25:A:1266:G:O2'	25:A:2012:G:O6	2.33	0.43
27:C:75:PRO:HG2	27:C:97:LYS:HD2	2.00	0.43
34:J:21:SER:CB	34:J:23:PRO:HD2	2.48	0.43
34:J:72:LYS:NZ	34:J:73:THR:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:O:1:MET:SD	38:O:44:ARG:HG3	2.57	0.43
6:f:3:HIS:CD2	6:f:65:GLU:OE1	2.72	0.43
12:l:74:LEU:HD21	12:l:104:CYS:HB3	2.00	0.43
34:J:18:ALA:HB1	34:J:38:PHE:O	2.18	0.43
45:V:54:GLU:HB3	45:V:88:LYS:HD2	1.99	0.43
2:b:57:LEU:O	2:b:60:ILE:HG22	2.19	0.43
12:l:19:SER:OG	12:l:20:ASN:N	2.51	0.43
24:w:21:ALA:O	24:w:25:ASP:HB3	2.18	0.43
25:A:274:C:H2'	25:A:275:C:O4'	2.18	0.43
25:A:1090:A:C2	25:A:1102:C:H1'	2.53	0.43
26:B:5:U:H2'	26:B:6:G:H8	1.83	0.43
27:C:125:LYS:HB2	27:C:126:PRO:HD2	2.00	0.43
31:G:33:LEU:HB3	31:G:75:MET:HE3	1.99	0.43
57:8:30:GLU:HG3	57:8:32:LYS:HB2	2.01	0.43
1:a:1141:C:H2'	1:a:1142:G:H8	1.84	0.43
1:a:1251:A:H2'	1:a:1252:A:C8	2.53	0.43
2:b:72:THR:OG1	2:b:169:GLU:OE2	2.33	0.43
7:g:28:ASN:OD1	7:g:36:LYS:NZ	2.52	0.43
23:z:12:A:H3'	23:z:13:A:C8	2.51	0.43
30:F:135:GLN:OE1	30:F:150:ARG:N	2.45	0.43
31:G:9:VAL:HG23	31:G:50:LEU:HB3	1.99	0.43
33:I:19:ALA:HA	33:I:69:PHE:HE2	1.82	0.43
33:I:34:THR:HA	33:I:37:LYS:HB2	2.00	0.43
34:J:101:ILE:O	34:J:141:GLU:N	2.26	0.43
1:a:459:A:H2'	1:a:460:A:H8	1.82	0.43
2:b:90:PHE:CB	2:b:154:MET:HE1	2.49	0.43
25:A:1541:C:H2'	25:A:1542:U:C6	2.54	0.43
26:B:49:C:H2'	26:B:50:A:H8	1.84	0.43
28:D:124:ARG:HA	28:D:165:MET:HE3	2.00	0.43
32:H:25:TYR:CE1	32:H:29:PHE:HD2	2.37	0.43
36:M:2:ILE:HD12	36:M:8:LEU:HD21	2.00	0.43
1:a:460:A:H2'	1:a:461:A:H8	1.83	0.43
1:a:664:G:H22	1:a:741:G:H1	1.67	0.43
3:c:167:TRP:O	3:c:168:TYR:HD1	2.01	0.43
4:d:116:GLN:HE21	4:d:120:HIS:CE1	2.36	0.43
6:f:69:GLU:HG2	6:f:70:VAL:N	2.34	0.43
8:h:11:LEU:HG	8:h:75:ILE:HG12	1.99	0.43
19:s:30:PRO:HA	19:s:48:THR:HG23	2.00	0.43
22:x:19:G:H4'	22:x:20:U:OP2	2.19	0.43
24:w:62:ILE:HD13	24:w:84:GLU:HA	2.01	0.43
24:w:76:GLU:O	24:w:79:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:29:U:H2'	25:A:30:G:C8	2.54	0.43
25:A:411:G:OP2	25:A:2406:A:O2'	2.35	0.43
25:A:2118:U:O4	25:A:2148:G:N2	2.45	0.43
25:A:2327:A:H2'	25:A:2328:A:C8	2.53	0.43
45:V:10:VAL:HG23	45:V:11:LEU:HD13	1.99	0.43
1:a:1120:C:H2'	1:a:1121:U:C6	2.54	0.43
1:a:1160:G:C2	1:a:1161:C:C6	3.07	0.43
1:a:1391:U:H2'	1:a:1392:G:C8	2.53	0.43
6:f:69:GLU:O	6:f:73:GLU:OE1	2.37	0.43
7:g:17:LYS:HE3	7:g:44:TYR:CE1	2.54	0.43
25:A:500:G:N1	25:A:503:A:OP2	2.47	0.43
25:A:1079:C:O2	34:J:131:GLY:HA3	2.19	0.43
25:A:1441:G:H2'	25:A:1442:U:C6	2.53	0.43
25:A:2188:U:H2'	25:A:2189:U:O4'	2.19	0.43
27:C:16:VAL:HG22	27:C:206:GLY:HA3	2.01	0.43
28:D:106:LYS:NZ	28:D:176:ASP:OD1	2.52	0.43
31:G:99:LYS:HG3	31:G:99:LYS:O	2.19	0.43
53:4:28:LEU:HD13	53:4:37:LYS:HG2	2.01	0.43
1:a:736:C:H2'	1:a:737:C:C6	2.53	0.43
5:e:104:GLY:O	5:e:122:ASN:HA	2.19	0.43
25:A:612:G:O2'	25:A:614:A:N7	2.44	0.43
25:A:2014:A:H2'	25:A:2015:A:C8	2.54	0.43
25:A:2120:G:H2'	25:A:2121:G:H8	1.83	0.43
39:P:49:GLU:HB2	39:P:50:PRO:HD3	2.01	0.43
1:a:1120:C:C2	1:a:1121:U:C5	3.07	0.43
1:a:1444:U:H2'	1:a:1445:U:C6	2.54	0.43
24:w:2:LYS:HE3	24:w:5:ILE:HG21	2.00	0.43
25:A:548:G:H2'	25:A:549:G:O4'	2.19	0.43
25:A:1068:G:O2'	25:A:1069:A:O4'	2.36	0.43
25:A:2273:A:H2'	25:A:2274:A:C8	2.54	0.43
2:b:113:ARG:NH1	2:b:117:LEU:HD12	2.33	0.43
3:c:56:VAL:HB	3:c:67:THR:HG22	2.01	0.43
8:h:10:MET:HG3	8:h:27:MET:SD	2.59	0.43
25:A:1:G:H2'	25:A:2:G:C8	2.54	0.43
25:A:282:A:H2'	25:A:283:G:H8	1.84	0.43
25:A:2020:A:H5'	53:4:9:THR:CG2	2.49	0.43
25:A:2189:U:HO2'	25:A:2190:G:P	2.42	0.43
25:A:2305:U:H2'	25:A:2306:C:C6	2.54	0.43
36:M:71:ARG:HA	36:M:71:ARG:HD3	1.89	0.43
43:T:28:ALA:HB3	43:T:31:GLU:OE1	2.19	0.43
25:A:249:C:O2	56:7:12:LYS:NZ	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1054:A:H2'	25:A:1055:G:C8	2.54	0.42
33:I:52:MET:HG3	33:I:86:MET:SD	2.58	0.42
48:Y:50:ASN:HB2	48:Y:82:ILE:HB	2.01	0.42
54:5:9:ILE:HD12	54:5:51:GLU:HG3	2.00	0.42
2:b:5:SER:HB3	2:b:8:ASP:CG	2.44	0.42
10:j:31:ARG:HA	10:j:31:ARG:NE	2.34	0.42
10:j:75:ASP:OD1	10:j:76:ILE:N	2.52	0.42
11:k:25:ALA:O	11:k:88:GLY:HA3	2.19	0.42
15:o:18:ASP:OD1	15:o:19:ALA:N	2.52	0.42
24:w:345:ILE:O	24:w:349:GLN:HG2	2.19	0.42
25:A:546:U:H5"	25:A:547:A:N7	2.34	0.42
25:A:2788:C:O2'	25:A:2809:A:N3	2.44	0.42
31:G:35:ARG:HA	31:G:35:ARG:HD3	1.89	0.42
57:8:16:ILE:HD13	57:8:25:VAL:HG22	2.00	0.42
1:a:676:A:H2'	1:a:677:U:H6	1.85	0.42
1:a:1027:C:C4	1:a:1028:C:N4	2.88	0.42
5:e:164:ILE:HG13	5:e:165:LEU:HD22	2.00	0.42
8:h:77:ARG:NH2	8:h:79:SER:O	2.52	0.42
24:w:31:ASP:OD1	24:w:31:ASP:N	2.52	0.42
25:A:151:C:H2'	25:A:152:A:C8	2.54	0.42
25:A:273:G:H2'	25:A:274:C:C6	2.54	0.42
25:A:878:A:N7	25:A:899:A:H2	2.17	0.42
25:A:1656:C:H2'	25:A:1657:U:H6	1.84	0.42
25:A:1675:C:O2	28:D:133:THR:HG22	2.19	0.42
25:A:2070:A:H2'	25:A:2071:A:C8	2.54	0.42
25:A:2516:A:O2'	25:A:2517:C:H5'	2.19	0.42
25:A:2849:U:H4'	25:A:2868:A:C2	2.54	0.42
34:J:8:TYR:CB	34:J:59:ILE:HG13	2.50	0.42
35:L:21:THR:HG23	35:L:61:LYS:HD2	2.02	0.42
54:5:13:SER:HB3	54:5:49:TYR:CZ	2.55	0.42
1:a:1321:U:OP2	1:a:1322:C:O2'	2.34	0.42
3:c:10:ILE:HG23	3:c:11:ARG:HG3	2.01	0.42
14:n:26:GLU:OE2	14:n:27:LEU:HD12	2.20	0.42
15:o:15:PHE:CE2	15:o:26:GLU:HB3	2.54	0.42
22:y:64:A:H2'	22:y:65:G:C8	2.54	0.42
24:w:47:ASP:OD1	24:w:48:VAL:N	2.53	0.42
25:A:1095:A:H2'	25:A:1096:A:C8	2.54	0.42
25:A:1469:A:H2'	25:A:1470:A:H8	1.85	0.42
25:A:1527:G:N1	25:A:1544:A:OP2	2.46	0.42
25:A:2166:U:H5"	25:A:2167:U:H5	1.84	0.42
25:A:2184:A:H2'	25:A:2185:U:C6	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:106:G:H2'	26:B:107:G:O4'	2.19	0.42
37:N:78:ARG:HB3	37:N:113:ALA:O	2.19	0.42
1:a:1001:C:H2'	1:a:1002:G:H8	1.83	0.42
12:l:107:VAL:HG23	12:l:110:ARG:HB2	2.02	0.42
25:A:811:U:H2'	37:N:21:ARG:HA	2.01	0.42
25:A:2093:G:OP2	32:H:22:LYS:HD3	2.20	0.42
25:A:2146:C:H4'	25:A:2147:A:C5	2.54	0.42
48:Y:11:ARG:O	48:Y:14:ARG:NH1	2.49	0.42
50:1:2:LYS:NZ	50:1:49:ASP:OD1	2.27	0.42
1:a:6:G:O2'	1:a:7:A:H8	2.03	0.42
1:a:384:G:H2'	1:a:385:C:C6	2.54	0.42
1:a:696:A:H2'	1:a:697:U:C6	2.54	0.42
1:a:713:G:H2'	1:a:714:G:C8	2.55	0.42
6:f:96:VAL:HG12	6:f:96:VAL:O	2.20	0.42
20:t:49:LYS:HB2	20:t:49:LYS:HE2	1.85	0.42
25:A:1046:A:O2'	33:I:61:ARG:HB3	2.19	0.42
25:A:1068:G:HO2'	25:A:1069:A:P	2.41	0.42
25:A:2108:A:H8	25:A:2108:A:OP2	2.02	0.42
25:A:2480:C:H2'	25:A:2481:G:H5'	2.02	0.42
25:A:2898:U:H2'	25:A:2899:A:C8	2.54	0.42
1:a:721:G:H4'	1:a:722:G:O4'	2.19	0.42
1:a:868:C:H2'	1:a:869:G:O4'	2.20	0.42
1:a:1363:A:O2'	1:a:1365:G:N7	2.45	0.42
25:A:361:G:H8	25:A:361:G:OP2	2.02	0.42
25:A:1042:G:H2'	25:A:1043:C:C6	2.54	0.42
25:A:1365:A:OP1	49:Z:3:ARG:NH1	2.53	0.42
25:A:2074:U:H2'	25:A:2075:U:C6	2.55	0.42
25:A:2125:G:N2	25:A:2173:A:H62	2.14	0.42
25:A:2804:U:H2'	25:A:2805:C:H6	1.84	0.42
25:A:2813:A:H2'	25:A:2814:A:C8	2.54	0.42
29:E:164:LEU:HB2	29:E:167:VAL:HG22	2.02	0.42
33:I:24:SER:HB2	33:I:116:GLU:HG2	2.00	0.42
41:R:5:ILE:O	41:R:9:GLU:HG3	2.20	0.42
46:W:26:LYS:NZ	46:W:37:GLU:HB2	2.34	0.42
54:5:26:ASN:ND2	54:5:29:THR:OG1	2.53	0.42
2:b:23:TRP:CZ3	2:b:25:PRO:HA	2.55	0.42
5:e:14:LYS:HE3	5:e:116:GLU:CD	2.45	0.42
7:g:4:ARG:HD3	7:g:4:ARG:HA	1.87	0.42
7:g:16:PRO:HA	9:i:46:MET:SD	2.60	0.42
10:j:32:THR:HG21	10:j:83:THR:HA	2.01	0.42
19:s:26:GLY:O	19:s:28:LYS:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1103:A:N3	25:A:1103:A:H2'	2.35	0.42
25:A:2139:U:H2'	25:A:2140:G:C8	2.55	0.42
25:A:2144:G:H1'	25:A:2147:A:H61	1.84	0.42
37:N:29:LYS:HB3	37:N:30:THR:H	1.70	0.42
1:a:555:U:H2'	1:a:556:C:C6	2.54	0.42
4:d:69:GLU:OE2	4:d:204:TYR:OH	2.28	0.42
25:A:995:C:O2	35:L:3:THR:HG23	2.19	0.42
25:A:2804:U:H2'	25:A:2805:C:C6	2.55	0.42
33:I:39:THR:O	33:I:43:LYS:N	2.53	0.42
34:J:39:CYS:SG	34:J:40:LYS:N	2.93	0.42
40:Q:79:ALA:HB3	40:Q:113:ALA:HB3	2.02	0.42
24:w:95:GLN:NE2	24:w:356:LEU:HD11	2.35	0.42
24:w:218:ASN:HD21	24:w:220:ALA:HB3	1.85	0.42
25:A:544:C:H5'	25:A:545:U:OP2	2.20	0.42
25:A:1107:G:H2'	25:A:1108:U:C6	2.55	0.42
25:A:1444:G:H2'	25:A:1445:G:H8	1.85	0.42
25:A:2180:U:H2'	25:A:2181:U:O4'	2.20	0.42
25:A:2229:U:O2	49:Z:34:HIS:HE1	2.03	0.42
25:A:2783:U:H2'	25:A:2784:U:C6	2.55	0.42
30:F:142:ASP:OD1	30:F:142:ASP:N	2.51	0.42
1:a:1518:MA6:H92	1:a:1519:MA6:N6	2.35	0.41
2:b:23:TRP:CG	2:b:39:HIS:HE1	2.38	0.41
2:b:27:MET:HE3	2:b:191:SER:O	2.20	0.41
20:t:35:VAL:HG11	20:t:79:LEU:HD13	2.02	0.41
24:w:146:VAL:HG12	24:w:166:ILE:HG12	2.01	0.41
25:A:1405:U:H2'	25:A:1406:U:C6	2.55	0.41
25:A:2705:A:O2'	25:A:2852:G:OP1	2.36	0.41
1:a:1291:U:H2'	1:a:1292:G:H8	1.85	0.41
2:b:154:MET:HB3	2:b:156:GLY:O	2.20	0.41
11:k:100:LEU:HD23	11:k:100:LEU:HA	1.86	0.41
13:m:93:ARG:HA	13:m:93:ARG:HD3	1.84	0.41
1:a:33:A:H2'	1:a:34:C:C6	2.55	0.41
1:a:41:G:H2'	1:a:42:G:C8	2.54	0.41
1:a:464:U:N3	1:a:467:U:OP2	2.48	0.41
4:d:152:GLN:O	4:d:155:VAL:HG22	2.19	0.41
16:p:52:LEU:HD12	16:p:78:VAL:HG21	2.02	0.41
24:w:249:LEU:HB2	24:w:250:PRO:HD3	2.01	0.41
25:A:634:C:H2'	25:A:635:C:C6	2.55	0.41
25:A:742:A:H2'	25:A:743:A:H8	1.85	0.41
25:A:1059:G:C8	34:J:117:MET:HE1	2.55	0.41
25:A:1582:C:H2'	25:A:1583:A:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1724:G:H2'	25:A:1725:U:H6	1.84	0.41
25:A:2128:G:H1'	25:A:2173:A:O2'	2.20	0.41
25:A:2365:G:N7	56:7:39:LYS:NZ	2.68	0.41
33:I:51:TYR:CE2	33:I:88:HIS:HB2	2.50	0.41
35:L:74:TYR:O	35:L:86:GLN:HA	2.21	0.41
1:a:1125:U:HO2'	1:a:1126:U:P	2.43	0.41
9:i:84:THR:HG23	9:i:98:LEU:HD13	2.02	0.41
12:l:30:LYS:O	12:l:81:LEU:HD12	2.21	0.41
21:u:21:ARG:HA	21:u:21:ARG:HD2	1.90	0.41
22:y:18:G:H5"	22:y:60:U:H2'	2.03	0.41
25:A:1149:G:H2'	25:A:1150:C:C6	2.55	0.41
25:A:1496:A:H2'	25:A:1498:C:C5	2.56	0.41
25:A:2116:G:H22	25:A:2171:A:H61	1.67	0.41
25:A:2250:G:O2'	25:A:2496:C:OP1	2.26	0.41
40:Q:56:LYS:O	40:Q:59:ALA:N	2.45	0.41
6:f:1:MET:HE3	6:f:65:GLU:HG3	2.03	0.41
10:j:8:ILE:HB	10:j:74:VAL:HG23	2.02	0.41
20:t:85:LYS:HE3	20:t:85:LYS:HB3	1.88	0.41
25:A:993:G:H1'	43:T:91:GLN:NE2	2.35	0.41
25:A:1809:A:H2'	25:A:1810:A:C8	2.56	0.41
30:F:44:ILE:HD11	30:F:79:ILE:HG22	2.01	0.41
34:J:105:GLN:O	34:J:109:ILE:HG12	2.20	0.41
44:U:70:LYS:HE2	44:U:70:LYS:HB2	1.92	0.41
1:a:1451:U:H5"	1:a:1452:C:C5	2.55	0.41
25:A:1110:G:H5"	25:A:1111:A:OP1	2.20	0.41
30:F:36:LEU:HB3	30:F:152:LEU:HD11	2.02	0.41
32:H:1:MET:HE3	32:H:1:MET:HB2	1.95	0.41
36:M:58:LEU:HA	36:M:89:ASN:HD21	1.85	0.41
47:X:35:GLU:OE2	47:X:35:GLU:N	2.48	0.41
1:a:193:C:H2'	1:a:194:C:C6	2.56	0.41
1:a:1253:G:H2'	1:a:1254:A:C8	2.56	0.41
3:c:177:THR:HG23	3:c:180:ALA:HB2	2.02	0.41
25:A:286:U:C2	25:A:287:G:C8	3.08	0.41
25:A:2489:U:H2'	25:A:2490:G:O4'	2.20	0.41
27:C:270:ARG:HG3	27:C:271:ARG:N	2.35	0.41
36:M:40:LYS:HE3	36:M:57:VAL:HG12	2.03	0.41
38:O:42:THR:HG22	38:O:93:VAL:HG12	2.01	0.41
1:a:299:G:H2'	1:a:300:A:C8	2.56	0.41
1:a:1000:A:H2'	1:a:1001:C:C6	2.55	0.41
1:a:1412:C:H2'	1:a:1413:A:C8	2.55	0.41
4:d:182:PHE:O	4:d:183:LYS:HE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:8:ILE:HB	10:j:74:VAL:CG2	2.51	0.41
24:w:150:SER:O	24:w:162:ILE:HD12	2.20	0.41
25:A:581:C:H2'	25:A:582:A:H8	1.84	0.41
25:A:2140:G:H22	25:A:2151:U:H1'	1.85	0.41
25:A:2514:U:H2'	25:A:2515:C:C6	2.55	0.41
33:I:6:GLN:HA	33:I:9:GLN:HG3	2.02	0.41
56:7:27:ALA:O	56:7:28:ASN:HB2	2.21	0.41
1:a:1055:A:O2'	3:c:161:GLU:O	2.35	0.41
1:a:1253:G:H2'	1:a:1254:A:H8	1.85	0.41
2:b:116:ASP:O	2:b:119:THR:OG1	2.33	0.41
18:r:32:TYR:O	18:r:40:VAL:HG22	2.21	0.41
24:w:18:GLU:OE1	34:J:22:PRO:HB3	2.21	0.41
24:w:115:VAL:HG22	24:w:162:ILE:CG2	2.51	0.41
25:A:871:U:H2'	25:A:872:U:C6	2.55	0.41
25:A:1054:A:H2'	25:A:1055:G:H8	1.85	0.41
25:A:1582:C:O2'	25:A:1585:C:N3	2.50	0.41
25:A:1591:A:H2'	25:A:1592:C:C6	2.56	0.41
25:A:2187:U:H2'	25:A:2188:U:H6	1.85	0.41
25:A:2619:C:H5"	28:D:157:LYS:HG2	2.03	0.41
25:A:2820:A:HO2'	25:A:2821:A:P	2.43	0.41
30:F:7:TYR:CE1	30:F:11:GLU:HG3	2.55	0.41
30:F:120:LYS:HE2	30:F:120:LYS:HB3	1.86	0.41
33:I:33:VAL:HG12	33:I:35:VAL:HG22	2.01	0.41
40:Q:31:THR:O	40:Q:102:ARG:NH2	2.45	0.41
41:R:88:ARG:NH2	41:R:112:GLU:HB2	2.36	0.41
52:3:58:ASP:OD2	52:3:58:ASP:C	2.64	0.41
22:x:47:U:O2'	22:x:48:C:OP1	2.30	0.41
24:w:20:GLN:NE2	25:A:1095:A:N1	2.63	0.41
25:A:2179:C:H2'	25:A:2180:U:C5	2.56	0.41
25:A:2180:U:H2'	25:A:2181:U:C6	2.55	0.41
28:D:157:LYS:HE3	28:D:157:LYS:HB3	1.93	0.41
1:a:363:A:N6	12:l:27:CYS:SG	2.94	0.40
6:f:11:HIS:HB3	6:f:14:GLN:NE2	2.36	0.40
6:f:18:VAL:HG11	6:f:58:HIS:CE1	2.56	0.40
9:i:98:LEU:HD23	9:i:98:LEU:HA	1.89	0.40
12:l:31:ARG:HE	12:l:31:ARG:HB3	1.72	0.40
25:A:2099:U:H2'	25:A:2100:G:H8	1.86	0.40
28:D:55:LYS:HB2	28:D:76:GLY:O	2.21	0.40
46:W:36:VAL:O	46:W:62:GLU:HG2	2.20	0.40
1:a:986:U:H2'	1:a:987:G:O4'	2.21	0.40
6:f:4:TYR:CD1	6:f:71:ILE:HG13	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:22:THR:O	10:j:25:ILE:HG22	2.21	0.40
24:w:114:GLU:HG2	24:w:163:ILE:HG23	2.04	0.40
25:A:1394:U:H2'	25:A:1395:A:O4'	2.21	0.40
25:A:2092:U:OP2	32:H:27:ARG:NH1	2.54	0.40
34:J:21:SER:HB3	34:J:22:PRO:HD2	2.03	0.40
1:a:381:C:H2'	1:a:382:A:O4'	2.21	0.40
1:a:518:C:O2'	1:a:530:G:N2	2.55	0.40
1:a:1026:G:C6	1:a:1027:C:C4	3.10	0.40
1:a:1286:U:H2'	1:a:1287:A:H5'	2.04	0.40
25:A:1106:G:H5'	33:I:62:ARG:NH2	2.36	0.40
25:A:1534:U:HO2'	25:A:1537:G:H1	1.66	0.40
25:A:2096:C:H2'	25:A:2097:A:C8	2.57	0.40
25:A:2131:U:H5'	25:A:2132:U:H5'	2.03	0.40
29:E:63:LYS:HB3	29:E:63:LYS:HE3	1.93	0.40
29:E:67:ARG:HE	29:E:67:ARG:HB3	1.69	0.40
30:F:105:THR:HA	52:3:38:SER:HB2	2.02	0.40
44:U:48:LYS:O	44:U:52:GLU:HG2	2.22	0.40
55:6:1:MET:HE2	55:6:1:MET:HB3	1.89	0.40
1:a:490:C:H2'	1:a:491:G:H8	1.85	0.40
1:a:613:C:H2'	1:a:614:C:C6	2.57	0.40
1:a:982:U:H4'	1:a:983:A:O4'	2.21	0.40
1:a:1124:G:N2	1:a:1125:U:O4	2.45	0.40
2:b:5:SER:O	2:b:9:MET:HG2	2.21	0.40
2:b:218:ALA:O	2:b:222:ARG:HG3	2.22	0.40
14:n:83:LYS:HD3	14:n:83:LYS:HA	1.87	0.40
24:w:34:ARG:HH21	24:w:38:LEU:HD11	1.87	0.40
25:A:534:U:O2'	42:S:49:ASP:OD2	2.31	0.40
25:A:637:A:H4'	25:A:638:G:O5'	2.22	0.40
34:J:43:ASN:HA	34:J:46:THR:HB	2.02	0.40
1:a:1157:A:C2	1:a:1181:G:C4	3.10	0.40
8:h:54:ASP:OD1	8:h:54:ASP:N	2.54	0.40
17:q:57:ASP:OD1	17:q:82:ALA:N	2.36	0.40
22:y:71:G:H2'	22:y:72:C:O4'	2.22	0.40
25:A:885:C:N4	25:A:892:A:H61	2.20	0.40
25:A:984:A:N3	25:A:984:A:H2'	2.36	0.40
25:A:2747:G:O6	25:A:2755:C:H5"	2.22	0.40
31:G:52:PHE:CE2	31:G:72:LEU:HD12	2.56	0.40
31:G:54:PRO:HD3	31:G:62:TRP:CZ3	2.56	0.40
33:I:57:ASN:CA	33:I:62:ARG:HE	2.34	0.40
33:I:59:LEU:HD23	33:I:60:LEU:N	2.36	0.40
35:L:53:TYR:CE2	35:L:121:LYS:HG2	2.57	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	
2	b	222/241 (92%)	209 (94%)	13 (6%)	0	100	100
3	c	204/233 (88%)	189 (93%)	15 (7%)	0	100	100
4	d	203/206 (98%)	196 (97%)	7 (3%)	0	100	100
5	e	154/167 (92%)	148 (96%)	6 (4%)	0	100	100
6	f	101/131 (77%)	96 (95%)	5 (5%)	0	100	100
7	g	150/156 (96%)	139 (93%)	11 (7%)	0	100	100
8	h	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
9	i	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
10	j	96/103 (93%)	92 (96%)	3 (3%)	1 (1%)	12	39
11	k	113/129 (88%)	108 (96%)	5 (4%)	0	100	100
12	l	118/124 (95%)	113 (96%)	5 (4%)	0	100	100
13	m	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
14	n	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
15	o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	p	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
17	q	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
18	r	52/75 (69%)	50 (96%)	2 (4%)	0	100	100
19	s	81/92 (88%)	76 (94%)	5 (6%)	0	100	100
20	t	84/87 (97%)	84 (100%)	0	0	100	100
21	u	68/71 (96%)	65 (96%)	3 (4%)	0	100	100
24	w	345/360 (96%)	316 (92%)	27 (8%)	2 (1%)	21	51
27	C	269/273 (98%)	261 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
28	D	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	24 54
29	E	199/201 (99%)	192 (96%)	7 (4%)	0	100 100
30	F	175/179 (98%)	166 (95%)	9 (5%)	0	100 100
31	G	174/177 (98%)	164 (94%)	10 (6%)	0	100 100
32	H	37/149 (25%)	34 (92%)	3 (8%)	0	100 100
33	I	129/165 (78%)	107 (83%)	22 (17%)	0	100 100
34	J	139/142 (98%)	118 (85%)	20 (14%)	1 (1%)	18 48
35	L	140/142 (99%)	139 (99%)	1 (1%)	0	100 100
36	M	121/123 (98%)	116 (96%)	5 (4%)	0	100 100
37	N	142/144 (99%)	137 (96%)	5 (4%)	0	100 100
38	O	132/136 (97%)	128 (97%)	4 (3%)	0	100 100
39	P	116/127 (91%)	112 (97%)	4 (3%)	0	100 100
40	Q	114/117 (97%)	108 (95%)	6 (5%)	0	100 100
41	R	112/115 (97%)	107 (96%)	5 (4%)	0	100 100
42	S	115/118 (98%)	115 (100%)	0	0	100 100
43	T	101/103 (98%)	98 (97%)	3 (3%)	0	100 100
44	U	108/110 (98%)	106 (98%)	2 (2%)	0	100 100
45	V	91/100 (91%)	84 (92%)	7 (8%)	0	100 100
46	W	100/104 (96%)	95 (95%)	5 (5%)	0	100 100
47	X	92/94 (98%)	91 (99%)	1 (1%)	0	100 100
48	Y	74/85 (87%)	74 (100%)	0	0	100 100
49	Z	75/78 (96%)	74 (99%)	1 (1%)	0	100 100
50	1	59/63 (94%)	57 (97%)	2 (3%)	0	100 100
51	2	56/59 (95%)	55 (98%)	1 (2%)	0	100 100
52	3	56/70 (80%)	55 (98%)	1 (2%)	0	100 100
53	4	53/57 (93%)	51 (96%)	2 (4%)	0	100 100
54	5	49/55 (89%)	48 (98%)	1 (2%)	0	100 100
55	6	44/46 (96%)	43 (98%)	1 (2%)	0	100 100
56	7	62/65 (95%)	56 (90%)	5 (8%)	1 (2%)	7 27
57	8	36/38 (95%)	35 (97%)	1 (3%)	0	100 100
All	All	6072/6553 (93%)	5781 (95%)	285 (5%)	6 (0%)	49 77

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	w	42	TYR
24	w	155	GLU
28	D	149	ASN
10	j	57	VAL
34	J	33	VAL
56	7	32	ILE

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	
2	b	186/199 (94%)	186 (100%)	0	100	100
3	c	170/190 (90%)	170 (100%)	0	100	100
4	d	172/173 (99%)	172 (100%)	0	100	100
5	e	119/126 (94%)	119 (100%)	0	100	100
6	f	90/112 (80%)	90 (100%)	0	100	100
7	g	125/129 (97%)	125 (100%)	0	100	100
8	h	104/105 (99%)	104 (100%)	0	100	100
9	i	105/107 (98%)	105 (100%)	0	100	100
10	j	86/90 (96%)	86 (100%)	0	100	100
11	k	89/98 (91%)	89 (100%)	0	100	100
12	l	101/103 (98%)	101 (100%)	0	100	100
13	m	93/96 (97%)	93 (100%)	0	100	100
14	n	83/84 (99%)	83 (100%)	0	100	100
15	o	76/77 (99%)	76 (100%)	0	100	100
16	p	65/65 (100%)	65 (100%)	0	100	100
17	q	73/78 (94%)	73 (100%)	0	100	100
18	r	47/65 (72%)	47 (100%)	0	100	100
19	s	72/79 (91%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	t	65/66 (98%)	65 (100%)	0	100	100
21	u	60/61 (98%)	60 (100%)	0	100	100
24	w	289/300 (96%)	289 (100%)	0	100	100
27	C	216/218 (99%)	216 (100%)	0	100	100
28	D	163/163 (100%)	163 (100%)	0	100	100
29	E	165/165 (100%)	165 (100%)	0	100	100
30	F	148/150 (99%)	148 (100%)	0	100	100
31	G	137/138 (99%)	137 (100%)	0	100	100
32	H	30/114 (26%)	30 (100%)	0	100	100
33	I	100/123 (81%)	100 (100%)	0	100	100
34	J	109/110 (99%)	109 (100%)	0	100	100
35	L	116/116 (100%)	116 (100%)	0	100	100
36	M	104/104 (100%)	104 (100%)	0	100	100
37	N	103/103 (100%)	103 (100%)	0	100	100
38	O	107/107 (100%)	107 (100%)	0	100	100
39	P	98/103 (95%)	98 (100%)	0	100	100
40	Q	86/87 (99%)	86 (100%)	0	100	100
41	R	99/100 (99%)	99 (100%)	0	100	100
42	S	89/90 (99%)	89 (100%)	0	100	100
43	T	84/84 (100%)	84 (100%)	0	100	100
44	U	93/93 (100%)	93 (100%)	0	100	100
45	V	80/84 (95%)	80 (100%)	0	100	100
46	W	83/85 (98%)	83 (100%)	0	100	100
47	X	78/78 (100%)	78 (100%)	0	100	100
48	Y	58/63 (92%)	58 (100%)	0	100	100
49	Z	67/68 (98%)	67 (100%)	0	100	100
50	1	54/55 (98%)	54 (100%)	0	100	100
51	2	48/49 (98%)	48 (100%)	0	100	100
52	3	53/62 (86%)	53 (100%)	0	100	100
53	4	46/48 (96%)	46 (100%)	0	100	100
54	5	46/49 (94%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	6	38/38 (100%)	38 (100%)	0	100	100
56	7	51/52 (98%)	51 (100%)	0	100	100
57	8	34/34 (100%)	34 (100%)	0	100	100
All	All	5053/5336 (95%)	5053 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	18	HIS
2	b	39	HIS
2	b	51	ASN
2	b	89	GLN
2	b	190	ASN
3	c	3	GLN
4	d	41	HIS
4	d	74	ASN
4	d	116	GLN
4	d	136	GLN
4	d	152	GLN
4	d	196	ASN
5	e	19	ASN
5	e	83	HIS
5	e	122	ASN
6	f	14	GLN
6	f	37	HIS
6	f	52	ASN
6	f	58	HIS
6	f	94	HIS
7	g	142	HIS
8	h	18	GLN
8	h	118	GLN
9	i	81	HIS
9	i	110	GLN
9	i	126	GLN
10	j	15	HIS
10	j	58	ASN
11	k	24	HIS
11	k	28	ASN
11	k	81	ASN

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Mol	Chain	Res	Type
11	k	109	ASN
12	l	46	ASN
12	l	77	HIS
12	l	96	HIS
13	m	14	HIS
13	m	105	ASN
14	n	66	GLN
15	o	40	GLN
15	o	50	HIS
16	p	26	ASN
16	p	29	ASN
17	q	45	HIS
18	r	31	ASN
18	r	52	GLN
18	r	74	HIS
19	s	14	HIS
19	s	52	HIS
19	s	83	HIS
20	t	70	ASN
20	t	84	ASN
24	w	16	HIS
24	w	91	GLN
24	w	94	GLN
24	w	95	GLN
24	w	97	GLN
24	w	110	ASN
24	w	238	ASN
24	w	266	ASN
24	w	320	HIS
27	C	25	HIS
27	C	46	ASN
27	C	70	ASN
27	C	90	ASN
27	C	128	ASN
27	C	143	ASN
28	D	49	GLN
28	D	134	HIS
28	D	173	GLN
29	E	41	GLN
29	E	90	GLN
29	E	97	ASN
29	E	115	GLN

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Mol	Chain	Res	Type
31	G	20	ASN
31	G	22	GLN
31	G	48	ASN
31	G	115	HIS
32	H	11	ASN
33	I	4	ASN
33	I	103	ASN
34	J	6	GLN
34	J	31	GLN
35	L	40	HIS
35	L	47	HIS
35	L	76	HIS
35	L	80	HIS
36	M	5	GLN
37	N	54	GLN
38	O	45	GLN
39	P	23	ASN
39	P	62	ASN
40	Q	38	GLN
40	Q	61	GLN
42	S	20	GLN
42	S	81	ASN
43	T	66	HIS
43	T	86	GLN
43	T	89	HIS
43	T	91	GLN
44	U	7	HIS
44	U	9	HIS
44	U	40	ASN
44	U	57	ASN
46	W	54	GLN
46	W	74	ASN
47	X	12	GLN
47	X	49	ASN
48	Y	46	HIS
48	Y	50	ASN
49	Z	16	ASN
49	Z	36	HIS
50	1	31	GLN
51	2	49	ASN
52	3	61	ASN
55	6	6	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1526/1542 (98%)	201 (13%)	0
22	x	75/76 (98%)	15 (20%)	0
22	y	72/76 (94%)	24 (33%)	0
23	z	10/21 (47%)	3 (30%)	0
25	A	2897/2904 (99%)	387 (13%)	12 (0%)
26	B	119/120 (99%)	18 (15%)	2 (1%)
All	All	4699/4739 (99%)	648 (13%)	14 (0%)

All (648) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	U
1	a	5	U
1	a	7	A
1	a	9	G
1	a	22	G
1	a	32	A
1	a	39	G
1	a	44	A
1	a	47	C
1	a	48	C
1	a	51	A
1	a	71	A
1	a	82	G
1	a	84	U
1	a	85	U
1	a	86	G
1	a	88	U
1	a	92	U
1	a	95	C
1	a	116	A
1	a	121	U
1	a	122	G
1	a	130	A
1	a	131	A
1	a	168	G
1	a	174	A
1	a	177	G
1	a	182	A
1	a	183	C
1	a	184	G

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Mol	Chain	Res	Type
1	a	197	A
1	a	199	A
1	a	203	G
1	a	208	U
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	240	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	253	A
1	a	266	G
1	a	267	C
1	a	280	C
1	a	281	G
1	a	283	U
1	a	289	G
1	a	305	G
1	a	321	A
1	a	328	C
1	a	330	C
1	a	339	C
1	a	344	A
1	a	345	C
1	a	347	G
1	a	352	C
1	a	354	G
1	a	367	U
1	a	372	C
1	a	373	A
1	a	384	G
1	a	406	G
1	a	408	A
1	a	412	A
1	a	413	G
1	a	414	A
1	a	415	A
1	a	421	U
1	a	422	C
1	a	424	G

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Mol	Chain	Res	Type
1	a	429	U
1	a	467	U
1	a	468	A
1	a	478	A
1	a	479	U
1	a	482	A
1	a	484	G
1	a	486	U
1	a	495	A
1	a	509	A
1	a	511	C
1	a	518	C
1	a	526	C
1	a	527	G7M
1	a	531	U
1	a	532	A
1	a	547	A
1	a	559	A
1	a	564	C
1	a	572	A
1	a	573	A
1	a	576	C
1	a	577	G
1	a	579	A
1	a	633	G
1	a	653	U
1	a	665	A
1	a	687	A
1	a	703	G
1	a	721	G
1	a	723	U
1	a	724	G
1	a	746	A
1	a	747	A
1	a	755	G
1	a	758	C
1	a	759	A
1	a	777	A
1	a	793	U
1	a	794	A
1	a	802	A
1	a	815	A

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Mol	Chain	Res	Type
1	a	817	C
1	a	884	U
1	a	890	G
1	a	902	G
1	a	914	A
1	a	934	C
1	a	935	A
1	a	960	U
1	a	966	2MG
1	a	969	A
1	a	975	A
1	a	976	G
1	a	977	A
1	a	992	U
1	a	994	A
1	a	1003	G
1	a	1004	A
1	a	1008	U
1	a	1009	U
1	a	1017	U
1	a	1024	G
1	a	1027	C
1	a	1028	C
1	a	1029	U
1	a	1030	U
1	a	1031	C
1	a	1032	G
1	a	1033	G
1	a	1034	G
1	a	1035	A
1	a	1039	G
1	a	1044	A
1	a	1046	A
1	a	1053	G
1	a	1064	G
1	a	1065	U
1	a	1094	G
1	a	1095	U
1	a	1099	G
1	a	1101	A
1	a	1135	U
1	a	1137	C

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Mol	Chain	Res	Type
1	a	1139	G
1	a	1159	U
1	a	1160	G
1	a	1171	A
1	a	1184	G
1	a	1196	A
1	a	1197	A
1	a	1213	A
1	a	1227	A
1	a	1228	C
1	a	1238	A
1	a	1256	A
1	a	1258	G
1	a	1275	A
1	a	1280	A
1	a	1285	A
1	a	1286	U
1	a	1287	A
1	a	1300	G
1	a	1302	C
1	a	1305	G
1	a	1317	C
1	a	1320	C
1	a	1338	G
1	a	1346	A
1	a	1363	A
1	a	1364	U
1	a	1378	C
1	a	1379	G
1	a	1388	C
1	a	1419	G
1	a	1432	G
1	a	1441	A
1	a	1446	A
1	a	1448	C
1	a	1452	C
1	a	1487	G
1	a	1497	G
1	a	1499	A
1	a	1503	A
1	a	1506	U
1	a	1507	A

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Mol	Chain	Res	Type
1	a	1517	G
1	a	1529	G
1	a	1530	G
22	x	9	A
22	x	12	U
22	x	13	C
22	x	16	U
22	x	17	C
22	x	19	G
22	x	20	U
22	x	21	A
22	x	22	G
22	x	44	G
22	x	45	U
22	x	47	U
22	x	48	C
22	x	49	C
22	x	76	A
22	y	8	4SU
22	y	9	A
22	y	10	G
22	y	13	C
22	y	19	G
22	y	20	U
22	y	21	A
22	y	26	A
22	y	35	A
22	y	37	MIA
22	y	38	A
22	y	39	PSU
22	y	42	C
22	y	44	G
22	y	45	U
22	y	46	7MG
22	y	47	U
22	y	48	C
22	y	57	G
22	y	59	U
22	y	60	U
22	y	65	G
22	y	72	C
22	y	76	A

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Mol	Chain	Res	Type
23	z	12	A
23	z	20	U
23	z	21	A
25	A	2	G
25	A	4	U
25	A	6	A
25	A	10	A
25	A	12	U
25	A	34	U
25	A	35	G
25	A	51	G
25	A	58	G
25	A	71	A
25	A	74	A
25	A	75	G
25	A	84	A
25	A	100	U
25	A	101	A
25	A	103	A
25	A	119	A
25	A	120	U
25	A	139	U
25	A	142	A
25	A	163	C
25	A	164	C
25	A	165	A
25	A	181	A
25	A	196	A
25	A	199	A
25	A	215	G
25	A	216	A
25	A	221	A
25	A	222	A
25	A	224	U
25	A	233	A
25	A	248	G
25	A	264	C
25	A	266	G
25	A	269	C
25	A	271	G
25	A	272	A
25	A	274	C

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Mol	Chain	Res	Type
25	A	277	G
25	A	278	A
25	A	279	A
25	A	281	C
25	A	285	G
25	A	311	A
25	A	329	G
25	A	330	A
25	A	356	G
25	A	362	A
25	A	367	G
25	A	386	G
25	A	396	G
25	A	404	A
25	A	405	U
25	A	411	G
25	A	412	A
25	A	428	A
25	A	481	G
25	A	489	G
25	A	491	G
25	A	504	A
25	A	505	A
25	A	509	C
25	A	510	C
25	A	530	G
25	A	532	A
25	A	543	G
25	A	544	C
25	A	545	U
25	A	546	U
25	A	547	A
25	A	563	A
25	A	573	U
25	A	575	A
25	A	580	U
25	A	603	A
25	A	615	U
25	A	627	A
25	A	634	C
25	A	637	A
25	A	645	C

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Mol	Chain	Res	Type
25	A	646	U
25	A	647	G
25	A	654	A
25	A	655	A
25	A	686	U
25	A	710	U
25	A	716	A
25	A	717	C
25	A	730	A
25	A	739	A
25	A	747	5MU
25	A	763	G
25	A	764	A
25	A	775	G
25	A	776	G
25	A	782	A
25	A	784	G
25	A	785	G
25	A	789	A
25	A	791	C
25	A	805	G
25	A	812	C
25	A	827	U
25	A	828	U
25	A	829	A
25	A	830	G
25	A	845	A
25	A	846	U
25	A	847	U
25	A	859	G
25	A	890	C
25	A	891	G
25	A	893	C
25	A	895	U
25	A	896	A
25	A	897	C
25	A	901	C
25	A	910	A
25	A	914	G
25	A	915	C
25	A	931	U
25	A	945	A

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Mol	Chain	Res	Type
25	A	946	C
25	A	961	C
25	A	974	G
25	A	983	A
25	A	990	A
25	A	996	A
25	A	1005	C
25	A	1012	U
25	A	1013	C
25	A	1022	G
25	A	1026	G
25	A	1032	A
25	A	1033	U
25	A	1040	A
25	A	1046	A
25	A	1047	G
25	A	1057	A
25	A	1059	G
25	A	1060	U
25	A	1061	U
25	A	1062	G
25	A	1063	G
25	A	1066	U
25	A	1067	A
25	A	1068	G
25	A	1069	A
25	A	1070	A
25	A	1071	G
25	A	1076	C
25	A	1085	A
25	A	1086	A
25	A	1088	A
25	A	1090	A
25	A	1097	U
25	A	1103	A
25	A	1104	C
25	A	1111	A
25	A	1112	G
25	A	1116	G
25	A	1130	U
25	A	1132	U
25	A	1135	C

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Mol	Chain	Res	Type
25	A	1136	G
25	A	1142	A
25	A	1157	G
25	A	1206	G
25	A	1236	G
25	A	1250	G
25	A	1253	A
25	A	1256	G
25	A	1257	C
25	A	1268	A
25	A	1271	G
25	A	1272	A
25	A	1273	U
25	A	1288	G
25	A	1300	G
25	A	1301	A
25	A	1365	A
25	A	1379	U
25	A	1383	A
25	A	1395	A
25	A	1416	G
25	A	1428	C
25	A	1429	G
25	A	1451	C
25	A	1452	G
25	A	1467	U
25	A	1482	G
25	A	1493	C
25	A	1509	A
25	A	1510	G
25	A	1515	A
25	A	1524	G
25	A	1534	U
25	A	1535	A
25	A	1536	C
25	A	1537	G
25	A	1539	U
25	A	1545	A
25	A	1555	G
25	A	1566	A
25	A	1569	A
25	A	1578	U

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Mol	Chain	Res	Type
25	A	1583	A
25	A	1584	U
25	A	1585	C
25	A	1609	A
25	A	1610	A
25	A	1626	A
25	A	1647	U
25	A	1648	U
25	A	1663	G
25	A	1664	A
25	A	1674	G
25	A	1676	A
25	A	1715	G
25	A	1729	U
25	A	1730	C
25	A	1731	G
25	A	1732	C
25	A	1733	G
25	A	1738	G
25	A	1758	U
25	A	1764	C
25	A	1773	A
25	A	1800	C
25	A	1801	A
25	A	1808	A
25	A	1809	A
25	A	1816	C
25	A	1829	A
25	A	1848	A
25	A	1858	A
25	A	1872	A
25	A	1876	A
25	A	1879	C
25	A	1906	G
25	A	1913	A
25	A	1914	C
25	A	1929	G
25	A	1930	G
25	A	1937	A
25	A	1955	U
25	A	1967	C
25	A	1970	A

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Mol	Chain	Res	Type
25	A	1971	U
25	A	1972	G
25	A	1991	U
25	A	1993	U
25	A	2006	C
25	A	2023	C
25	A	2027	G
25	A	2031	A
25	A	2033	A
25	A	2035	G
25	A	2036	C
25	A	2043	C
25	A	2055	C
25	A	2056	G
25	A	2060	A
25	A	2061	G
25	A	2062	A
25	A	2069	G7M
25	A	2098	U
25	A	2108	A
25	A	2110	G
25	A	2111	U
25	A	2112	G
25	A	2113	U
25	A	2116	G
25	A	2118	U
25	A	2119	A
25	A	2125	G
25	A	2127	G
25	A	2131	U
25	A	2132	U
25	A	2133	G
25	A	2136	G
25	A	2145	C
25	A	2146	C
25	A	2152	G
25	A	2157	G
25	A	2159	G
25	A	2161	C
25	A	2162	G
25	A	2163	A
25	A	2164	C

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Mol	Chain	Res	Type
25	A	2165	C
25	A	2167	U
25	A	2168	G
25	A	2170	A
25	A	2172	U
25	A	2173	A
25	A	2178	C
25	A	2179	C
25	A	2182	U
25	A	2183	A
25	A	2189	U
25	A	2190	G
25	A	2192	U
25	A	2198	A
25	A	2204	G
25	A	2211	A
25	A	2225	A
25	A	2238	G
25	A	2239	G
25	A	2283	C
25	A	2287	A
25	A	2305	U
25	A	2308	G
25	A	2311	A
25	A	2322	A
25	A	2325	G
25	A	2327	A
25	A	2333	A
25	A	2335	A
25	A	2345	G
25	A	2347	C
25	A	2350	C
25	A	2361	G
25	A	2383	G
25	A	2385	C
25	A	2396	G
25	A	2402	U
25	A	2406	A
25	A	2419	U
25	A	2425	A
25	A	2428	G
25	A	2429	G

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Mol	Chain	Res	Type
25	A	2434	A
25	A	2441	U
25	A	2448	A
25	A	2470	G
25	A	2474	U
25	A	2476	A
25	A	2498	OMC
25	A	2502	G
25	A	2505	G
25	A	2518	A
25	A	2520	C
25	A	2529	G
25	A	2535	G
25	A	2539	C
25	A	2547	A
25	A	2566	A
25	A	2567	G
25	A	2573	C
25	A	2602	A
25	A	2609	U
25	A	2613	U
25	A	2615	U
25	A	2629	U
25	A	2630	G
25	A	2646	C
25	A	2649	C
25	A	2654	A
25	A	2661	G
25	A	2663	G
25	A	2669	G
25	A	2689	U
25	A	2690	U
25	A	2714	G
25	A	2726	A
25	A	2733	A
25	A	2748	A
25	A	2750	A
25	A	2765	A
25	A	2778	A
25	A	2780	G
25	A	2791	G
25	A	2798	U

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Mol	Chain	Res	Type
25	A	2800	A
25	A	2820	A
25	A	2821	A
25	A	2835	A
25	A	2850	A
25	A	2861	U
25	A	2873	A
25	A	2880	C
25	A	2884	U
25	A	2885	G
25	A	2899	A
25	A	2902	C
26	B	4	C
26	B	13	G
26	B	25	U
26	B	35	C
26	B	37	C
26	B	42	C
26	B	44	G
26	B	45	A
26	B	52	A
26	B	53	A
26	B	56	G
26	B	65	U
26	B	67	G
26	B	89	U
26	B	90	C
26	B	91	C
26	B	105	G
26	B	109	A

All (14) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	3	U
25	A	271	G
25	A	277	G
25	A	545	U
25	A	784	G
25	A	1031	G
25	A	1068	G
25	A	1111	A

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Mol	Chain	Res	Type
25	A	2189	U
25	A	2191	A
25	A	2473	U
25	A	2538	C
26	B	3	C
26	B	66	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	4SU	x	8	22	18,21,22	2.02	4 (22%)	25,30,33	1.92	5 (20%)
25	H2U	A	2449	25	18,21,22	1.28	3 (16%)	19,30,33	0.83	0
1	PSU	a	516	1	18,21,22	1.46	5 (27%)	21,30,33	2.11	4 (19%)
12	D2T	l	89	12	8,9,10	2.48	1 (12%)	6,11,13	2.53	3 (50%)
25	PSU	A	2605	25	18,21,22	1.45	4 (22%)	21,30,33	2.13	4 (19%)
25	PSU	A	2457	25	18,21,22	1.51	5 (27%)	21,30,33	2.17	5 (23%)
38	MS6	O	82	38	5,7,8	0.53	0	2,7,9	1.11	0
1	2MG	a	1516	1	23,26,27	1.27	4 (17%)	33,38,41	2.21	7 (21%)
25	PSU	A	746	25,58	18,21,22	1.46	4 (22%)	21,30,33	1.93	3 (14%)
25	OMC	A	2498	25,58	19,22,23	0.84	1 (5%)	25,31,34	0.98	1 (4%)
22	5MU	y	54	22	19,22,23	1.41	6 (31%)	27,32,35	2.06	8 (29%)
22	PSU	x	39	22	18,21,22	1.42	4 (22%)	21,30,33	2.12	4 (19%)
1	2MG	a	966	1	23,26,27	1.30	4 (17%)	33,38,41	2.30	9 (27%)
22	PSU	x	32	22	18,21,22	1.44	4 (22%)	21,30,33	2.02	3 (14%)
38	4D4	O	81	38	9,11,12	2.48	3 (33%)	7,13,15	1.22	1 (14%)
22	5MU	x	54	22	19,22,23	1.40	5 (26%)	27,32,35	2.08	6 (22%)
1	2MG	a	1207	1	23,26,27	1.26	3 (13%)	33,38,41	2.29	9 (27%)
22	MIA	y	37	22	21,24,32	1.60	4 (19%)	30,35,47	2.30	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MA6	a	1519	1	23,26,27	1.48	6 (26%)	33,38,41	2.46	13 (39%)
22	PSU	y	39	22	18,21,22	1.34	2 (11%)	21,30,33	2.11	4 (19%)
22	PSU	y	55	22	18,21,22	1.36	2 (11%)	21,30,33	2.05	4 (19%)
25	PSU	A	955	25	18,21,22	1.46	3 (16%)	21,30,33	2.11	5 (23%)
22	PSU	y	32	22	18,21,22	1.36	2 (11%)	21,30,33	2.05	5 (23%)
25	5MU	A	1939	25	19,22,23	1.38	4 (21%)	27,32,35	2.22	6 (22%)
25	2MG	A	2445	25	23,26,27	1.29	4 (17%)	33,38,41	2.27	10 (30%)
25	PSU	A	2504	25	18,21,22	1.45	4 (22%)	21,30,33	2.05	3 (14%)
1	G7M	a	527	1	23,26,27	1.57	3 (13%)	34,39,42	1.76	5 (14%)
1	5MC	a	1407	1	19,22,23	1.43	3 (15%)	26,32,35	1.16	3 (11%)
25	6MZ	A	1618	25	22,25,26	1.42	4 (18%)	29,36,39	2.26	10 (34%)
1	4OC	a	1402	58,1	20,23,24	0.74	0	25,32,35	0.98	2 (8%)
22	7MG	x	46	22	23,26,27	1.35	3 (13%)	27,39,42	2.61	6 (22%)
25	1MG	A	745	25	23,26,27	1.11	3 (13%)	33,39,42	1.75	5 (15%)
25	PSU	A	1917	25	18,21,22	1.48	4 (22%)	21,30,33	2.05	3 (14%)
25	6MZ	A	2030	25	22,25,26	1.44	6 (27%)	29,36,39	2.22	11 (37%)
25	3TD	A	1915	25,58	19,22,23	4.09	7 (36%)	23,32,35	1.82	3 (13%)
25	5MC	A	1962	25	19,22,23	1.39	3 (15%)	26,32,35	1.14	2 (7%)
25	PSU	A	2580	25	18,21,22	1.49	5 (27%)	21,30,33	2.16	4 (19%)
22	7MG	y	46	22	23,26,27	1.33	3 (13%)	27,39,42	2.60	6 (22%)
25	5MU	A	747	25	19,22,23	1.40	4 (21%)	27,32,35	2.14	6 (22%)
25	OMG	A	2251	25,22,58	23,26,27	1.23	3 (13%)	32,38,41	2.03	6 (18%)
25	G7M	A	2069	25	23,26,27	1.58	4 (17%)	34,39,42	1.75	5 (14%)
25	2MG	A	1835	25	23,26,27	1.28	3 (13%)	33,38,41	2.22	6 (18%)
11	IAS	k	119	11	6,7,8	0.97	0	3,8,10	1.47	1 (33%)
25	2MA	A	2503	25,58	22,25,26	1.44	5 (22%)	32,37,40	2.30	9 (28%)
22	PSU	x	55	22	18,21,22	1.38	3 (16%)	21,30,33	2.12	3 (14%)
25	PSU	A	1911	25	18,21,22	1.44	4 (22%)	21,30,33	2.13	5 (23%)
25	PSU	A	2604	25	18,21,22	1.45	4 (22%)	21,30,33	2.14	4 (19%)
1	UR3	a	1498	1	19,22,23	0.95	2 (10%)	26,32,35	1.80	3 (11%)
28	MEQ	D	150	28	8,9,10	0.49	0	5,10,12	0.22	0
25	OMU	A	2552	25	19,22,23	1.32	4 (21%)	25,31,34	1.91	5 (20%)
22	4SU	y	8	22	18,21,22	1.88	4 (22%)	25,30,33	2.16	4 (16%)
1	5MC	a	967	1	19,22,23	1.46	3 (15%)	26,32,35	1.13	3 (11%)
22	MIA	x	37	22	28,31,32	2.37	7 (25%)	38,44,47	2.75	16 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MA6	a	1518	1	23,26,27	1.48	5 (21%)	33,38,41	2.38	12 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	4SU	x	8	22	-	0/7/25/26	0/2/2/2
25	H2U	A	2449	25	-	0/7/38/39	0/2/2/2
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
12	D2T	l	89	12	-	2/7/12/14	-
25	PSU	A	2605	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2457	25	-	0/7/25/26	0/2/2/2
38	MS6	O	82	38	-	2/4/6/8	-
1	2MG	a	1516	1	-	0/9/27/28	0/3/3/3
25	PSU	A	746	25,58	-	4/7/25/26	0/2/2/2
25	OMC	A	2498	25,58	-	2/9/27/28	0/2/2/2
22	5MU	y	54	22	-	3/7/25/26	0/2/2/2
22	PSU	x	39	22	-	0/7/25/26	0/2/2/2
1	2MG	a	966	1	-	2/9/27/28	0/3/3/3
22	PSU	x	32	22	-	0/7/25/26	0/2/2/2
38	4D4	O	81	38	-	4/11/12/14	-
22	5MU	x	54	22	-	0/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	2/9/27/28	0/3/3/3
22	MIA	y	37	22	-	4/7/25/34	0/3/3/3
1	MA6	a	1519	1	-	4/11/29/30	0/3/3/3
22	PSU	y	39	22	-	6/7/25/26	0/2/2/2
22	PSU	y	55	22	-	0/7/25/26	0/2/2/2
25	PSU	A	955	25	-	0/7/25/26	0/2/2/2
22	PSU	y	32	22	-	0/7/25/26	0/2/2/2
25	5MU	A	1939	25	-	0/7/25/26	0/2/2/2
25	2MG	A	2445	25	-	0/9/27/28	0/3/3/3
25	PSU	A	2504	25	-	1/7/25/26	0/2/2/2
1	G7M	a	527	1	-	2/7/25/26	0/3/3/3
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
25	6MZ	A	1618	25	-	0/9/27/28	0/3/3/3
1	4OC	a	1402	58,1	-	2/9/29/30	0/2/2/2
22	7MG	x	46	22	-	0/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	1MG	A	745	25	-	0/7/25/26	0/3/3/3
25	PSU	A	1917	25	-	2/7/25/26	0/2/2/2
25	6MZ	A	2030	25	-	2/9/27/28	0/3/3/3
25	3TD	A	1915	25,58	-	0/7/25/26	0/2/2/2
25	5MC	A	1962	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2580	25	-	1/7/25/26	0/2/2/2
22	7MG	y	46	22	-	5/7/37/38	0/3/3/3
25	5MU	A	747	25	-	0/7/25/26	0/2/2/2
25	OMG	A	2251	25,22,58	-	0/9/27/28	0/3/3/3
25	G7M	A	2069	25	-	0/7/25/26	0/3/3/3
25	2MG	A	1835	25	-	0/9/27/28	0/3/3/3
11	IAS	k	119	11	-	0/7/7/8	-
25	2MA	A	2503	25,58	-	1/7/25/26	0/3/3/3
22	PSU	x	55	22	-	0/7/25/26	0/2/2/2
25	PSU	A	1911	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2604	25	-	0/7/25/26	0/2/2/2
1	UR3	a	1498	1	-	0/7/25/26	0/2/2/2
28	MEQ	D	150	28	-	3/8/9/11	-
25	OMU	A	2552	25	-	0/9/27/28	0/2/2/2
22	4SU	y	8	22	-	0/7/25/26	0/2/2/2
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
22	MIA	x	37	22	-	4/15/33/34	0/3/3/3
1	MA6	a	1518	1	-	1/11/29/30	0/3/3/3

All (190) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1915	3TD	C6-C5	12.22	1.48	1.35
25	A	1915	3TD	C2-N1	9.36	1.48	1.37
22	x	37	MIA	C2-S10	-7.81	1.69	1.75
22	x	37	MIA	C13-C14	6.97	1.53	1.32
12	l	89	D2T	CB-CA	-6.39	1.52	1.54
38	O	81	4D4	CZ-NE	5.87	1.44	1.33
25	A	1915	3TD	C6-N1	5.48	1.45	1.36
25	A	2069	G7M	C5-N7	-5.32	1.33	1.39
1	a	527	G7M	C5-N7	-5.26	1.33	1.39
22	x	8	4SU	C4-S4	-5.10	1.59	1.68
22	y	8	4SU	C4-S4	-5.02	1.59	1.68
22	y	37	MIA	C5-C4	4.95	1.47	1.39
1	a	967	5MC	C5-C4	4.94	1.47	1.44
1	a	1407	5MC	C5-C4	4.85	1.47	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1915	3TD	C2-N3	4.80	1.48	1.38
25	A	1962	5MC	C5-C4	4.67	1.47	1.44
22	x	8	4SU	C4-N3	-4.28	1.33	1.37
1	a	1519	MA6	C5-C4	4.24	1.46	1.39
1	a	1518	MA6	C5-C4	4.23	1.46	1.39
25	A	2503	2MA	C5-C4	4.10	1.46	1.39
25	A	1618	6MZ	C5-C4	4.04	1.46	1.39
25	A	2030	6MZ	C5-C4	3.99	1.46	1.39
22	x	37	MIA	C5-C4	3.86	1.46	1.39
22	x	46	7MG	C4-N9	-3.82	1.33	1.37
22	y	8	4SU	C4-N3	-3.63	1.33	1.37
22	y	55	PSU	C6-C5	3.29	1.38	1.35
22	y	32	PSU	C6-C5	3.29	1.38	1.35
25	A	2457	PSU	C4-N3	-3.26	1.32	1.38
25	A	2449	H2U	C2-N3	-3.24	1.32	1.38
22	y	46	7MG	C5-C4	3.24	1.47	1.37
25	A	2605	PSU	C4-N3	-3.23	1.32	1.38
22	y	39	PSU	C6-C5	3.22	1.38	1.35
22	x	8	4SU	C5-C4	-3.21	1.38	1.42
25	A	2504	PSU	C4-N3	-3.17	1.32	1.38
25	A	2604	PSU	C4-N3	-3.17	1.32	1.38
25	A	2552	OMU	C4-N3	-3.15	1.33	1.38
25	A	1917	PSU	C6-C5	3.10	1.38	1.35
25	A	955	PSU	C4-N3	-3.09	1.33	1.38
1	a	516	PSU	C4-N3	-3.06	1.33	1.38
25	A	1911	PSU	C4-N3	-3.06	1.33	1.38
25	A	2580	PSU	C4-N3	-3.05	1.33	1.38
25	A	747	5MU	C4-N3	-3.03	1.33	1.38
38	O	81	4D4	CZ-NH1	3.03	1.45	1.34
22	y	37	MIA	C5-C6	3.01	1.49	1.41
22	x	32	PSU	C4-N3	-3.00	1.33	1.38
25	A	746	PSU	C4-N3	-3.00	1.33	1.38
1	a	1519	MA6	C5-C6	3.00	1.49	1.41
25	A	1835	2MG	C6-N1	-2.99	1.33	1.38
25	A	2449	H2U	C4-N3	-2.98	1.32	1.37
1	a	527	G7M	C5-C4	2.98	1.45	1.38
22	x	46	7MG	C5-C4	2.97	1.46	1.37
22	x	39	PSU	C4-N3	-2.97	1.33	1.38
1	a	1207	2MG	C5-C4	2.94	1.46	1.38
25	A	1939	5MU	C4-N3	-2.94	1.33	1.38
22	y	46	7MG	C4-N9	-2.92	1.34	1.37
25	A	1915	3TD	O2-C2	-2.92	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	745	1MG	C5-C4	2.91	1.46	1.38
25	A	2445	2MG	C6-N1	-2.91	1.33	1.38
22	x	54	5MU	C4-N3	-2.91	1.33	1.38
22	x	55	PSU	C6-C5	2.91	1.38	1.35
25	A	1917	PSU	C4-N3	-2.90	1.33	1.38
1	a	1518	MA6	C5-C6	2.87	1.48	1.41
1	a	966	2MG	C6-N1	-2.87	1.33	1.38
25	A	2069	G7M	C5-C4	2.86	1.45	1.38
25	A	2251	OMG	C6-N1	-2.86	1.33	1.38
1	a	966	2MG	C5-C4	2.86	1.46	1.38
25	A	1911	PSU	C6-C5	2.85	1.38	1.35
1	a	1516	2MG	C5-C4	2.82	1.46	1.38
1	a	1207	2MG	C6-N1	-2.82	1.33	1.38
25	A	2069	G7M	C6-N1	-2.81	1.33	1.38
22	x	55	PSU	C4-N3	-2.81	1.33	1.38
1	a	527	G7M	C6-N1	-2.80	1.33	1.38
22	y	8	4SU	C5-C4	-2.79	1.39	1.42
25	A	1962	5MC	C6-N1	-2.78	1.33	1.38
25	A	1835	2MG	C5-C4	2.78	1.46	1.38
25	A	2552	OMU	C2-N3	-2.76	1.33	1.38
1	a	1516	2MG	C6-N1	-2.75	1.33	1.38
22	x	39	PSU	C6-C5	2.74	1.38	1.35
22	y	39	PSU	C4-N3	-2.71	1.33	1.38
25	A	2251	OMG	C5-C4	2.70	1.46	1.38
25	A	955	PSU	C6-C5	2.68	1.38	1.35
25	A	1618	6MZ	C5-C6	2.68	1.48	1.41
22	y	54	5MU	C6-C5	2.67	1.39	1.34
25	A	1939	5MU	C6-N1	-2.67	1.33	1.38
25	A	2030	6MZ	C5-N7	-2.67	1.34	1.39
25	A	747	5MU	C6-N1	-2.67	1.33	1.38
22	x	8	4SU	C2-N3	-2.66	1.33	1.38
22	y	55	PSU	C4-N3	-2.66	1.33	1.38
25	A	2504	PSU	C6-C5	2.64	1.38	1.35
22	x	32	PSU	C6-C5	2.63	1.38	1.35
22	y	54	5MU	C4-N3	-2.63	1.33	1.38
22	y	46	7MG	C6-N1	-2.62	1.34	1.38
22	y	32	PSU	C4-N3	-2.61	1.34	1.38
25	A	2503	2MA	C5-N7	-2.60	1.34	1.39
1	a	1518	MA6	C5-N7	-2.60	1.34	1.39
25	A	1939	5MU	C2-N3	-2.60	1.33	1.38
25	A	2604	PSU	C6-C5	2.59	1.38	1.35
25	A	955	PSU	C2-N3	-2.58	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	2445	2MG	C5-C4	2.58	1.45	1.38
22	x	54	5MU	C6-C5	2.58	1.38	1.34
25	A	2605	PSU	C6-C5	2.58	1.38	1.35
25	A	2457	PSU	C6-C5	2.56	1.38	1.35
1	a	516	PSU	C6-C5	2.56	1.38	1.35
25	A	747	5MU	C2-N3	-2.55	1.33	1.38
25	A	2605	PSU	C2-N3	-2.55	1.33	1.37
1	a	967	5MC	C6-C5	2.55	1.38	1.34
25	A	746	PSU	C6-C5	2.55	1.38	1.35
25	A	2251	OMG	C5-N7	-2.54	1.34	1.39
25	A	2445	2MG	C5-N7	-2.54	1.34	1.39
25	A	2449	H2U	C2-N1	-2.54	1.32	1.35
25	A	2030	6MZ	C5-C6	2.53	1.48	1.41
25	A	2580	PSU	C2-N1	-2.53	1.33	1.36
25	A	2504	PSU	C2-N3	-2.52	1.33	1.37
22	x	54	5MU	C6-N1	-2.52	1.33	1.38
25	A	2552	OMU	C5-C4	-2.50	1.38	1.43
22	x	46	7MG	C6-N1	-2.50	1.34	1.38
1	a	966	2MG	C5-N7	-2.49	1.34	1.39
22	x	37	MIA	C5-N7	-2.48	1.34	1.39
25	A	2604	PSU	C2-N3	-2.48	1.33	1.37
1	a	1407	5MC	C6-N1	-2.47	1.33	1.38
25	A	2030	6MZ	C4-N9	-2.47	1.32	1.37
1	a	967	5MC	C6-N1	-2.46	1.33	1.38
22	x	32	PSU	C2-N3	-2.45	1.33	1.37
25	A	2503	2MA	C5-C6	2.45	1.47	1.41
22	x	37	MIA	C5-C6	2.44	1.47	1.41
25	A	1618	6MZ	C5-N7	-2.44	1.34	1.39
25	A	2580	PSU	C2-N3	-2.43	1.33	1.37
22	x	54	5MU	C2-N3	-2.43	1.33	1.38
25	A	2580	PSU	C6-C5	2.43	1.38	1.35
1	a	1407	5MC	C6-C5	2.42	1.38	1.34
25	A	2457	PSU	C2-N3	-2.42	1.33	1.37
25	A	746	PSU	C2-N3	-2.42	1.33	1.37
25	A	1915	3TD	O4-C4	-2.41	1.18	1.23
22	y	54	5MU	C2-N1	2.41	1.42	1.38
1	a	516	PSU	C2-N3	-2.41	1.33	1.37
25	A	1917	PSU	C2-N1	-2.41	1.33	1.36
22	x	39	PSU	C2-N3	-2.40	1.33	1.37
25	A	747	5MU	C6-C5	2.39	1.38	1.34
25	A	2457	PSU	C2-N1	-2.39	1.33	1.36
22	y	8	4SU	C2-N3	-2.38	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1915	3TD	C4-N3	2.35	1.45	1.40
25	A	1911	PSU	C2-N3	-2.35	1.33	1.37
25	A	1618	6MZ	C4-N9	-2.34	1.32	1.37
25	A	1939	5MU	C6-C5	2.33	1.38	1.34
25	A	1835	2MG	C5-N7	-2.33	1.34	1.39
25	A	2580	PSU	O4'-C1'	-2.32	1.40	1.43
22	x	37	MIA	C4-N9	-2.32	1.32	1.37
22	y	37	MIA	C5-N7	-2.29	1.34	1.39
22	y	54	5MU	C4-C5	2.28	1.48	1.44
1	a	1516	2MG	C5-N7	-2.28	1.34	1.39
1	a	1519	MA6	C5-N7	-2.26	1.34	1.39
25	A	2605	PSU	C2-N1	-2.25	1.33	1.36
22	y	37	MIA	C8-N7	2.24	1.36	1.31
1	a	1518	MA6	C8-N9	-2.24	1.33	1.37
25	A	746	PSU	C2-N1	-2.24	1.33	1.36
25	A	745	1MG	C5-N7	-2.23	1.34	1.39
25	A	1917	PSU	C2-N3	-2.22	1.33	1.37
22	x	55	PSU	C2-N3	-2.19	1.33	1.37
22	y	54	5MU	C6-N1	-2.18	1.34	1.38
25	A	2503	2MA	C8-N7	2.17	1.35	1.31
1	a	1519	MA6	C4-N9	-2.17	1.33	1.37
25	A	2552	OMU	C6-N1	-2.17	1.32	1.38
25	A	2504	PSU	C2-N1	-2.16	1.33	1.36
25	A	1962	5MC	C6-C5	2.15	1.38	1.34
22	y	54	5MU	C2-N3	-2.15	1.34	1.38
1	a	516	PSU	C2-N1	-2.14	1.33	1.36
25	A	2503	2MA	C4-N9	-2.14	1.33	1.37
1	a	1207	2MG	C5-N7	-2.14	1.34	1.39
1	a	966	2MG	C2-N3	2.13	1.36	1.32
22	x	32	PSU	C2-N1	-2.13	1.33	1.36
1	a	1516	2MG	C4-N9	-2.12	1.32	1.38
1	a	516	PSU	O4'-C1'	-2.12	1.40	1.43
22	x	39	PSU	C2-N1	-2.12	1.33	1.36
1	a	1519	MA6	C8-N7	2.10	1.35	1.31
25	A	2604	PSU	C2-N1	-2.08	1.33	1.36
1	a	1518	MA6	C4-N9	-2.06	1.33	1.37
1	a	1498	UR3	C6-N1	-2.05	1.33	1.38
25	A	2445	2MG	C4-N9	-2.05	1.32	1.38
1	a	1519	MA6	C8-N9	-2.05	1.34	1.37
25	A	745	1MG	C4-N9	-2.04	1.32	1.38
22	x	54	5MU	C4-C5	2.04	1.48	1.44
25	A	2457	PSU	O4'-C1'	-2.03	1.41	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1498	UR3	C5-C4	-2.02	1.38	1.43
25	A	2030	6MZ	C8-N7	2.02	1.35	1.31
25	A	1911	PSU	O4'-C1'	-2.02	1.41	1.43
22	x	37	MIA	C8-N7	2.01	1.35	1.31
25	A	2030	6MZ	C8-N9	-2.01	1.34	1.37
25	A	2069	G7M	C4-N9	-2.01	1.33	1.38
25	A	2498	OMC	C6-N1	-2.01	1.33	1.38
38	O	81	4D4	CZ-NH2	-2.00	1.25	1.32

All (277) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	y	46	7MG	N9-C4-N3	8.88	138.47	125.46
22	x	46	7MG	N9-C4-N3	8.43	137.81	125.46
25	A	2503	2MA	C5-C4-N3	-8.16	118.59	127.18
22	x	37	MIA	C5-C4-N3	-7.96	118.79	127.18
25	A	1835	2MG	C2-N3-C4	7.43	121.30	112.00
25	A	2445	2MG	C2-N3-C4	7.40	121.25	112.00
1	a	1207	2MG	C2-N3-C4	7.39	121.24	112.00
1	a	966	2MG	C2-N3-C4	7.37	121.22	112.00
22	y	37	MIA	C5-C4-N3	-7.11	116.93	126.72
1	a	1516	2MG	C2-N3-C4	7.07	120.85	112.00
1	a	1498	UR3	C4-N3-C2	-7.06	118.90	124.58
22	x	37	MIA	C12-C13-C14	-7.04	114.37	127.01
25	A	2457	PSU	N1-C2-N3	6.89	122.43	115.17
25	A	2604	PSU	N1-C2-N3	6.74	122.28	115.17
25	A	2580	PSU	N1-C2-N3	6.70	122.24	115.17
25	A	955	PSU	N1-C2-N3	6.68	122.21	115.17
1	a	966	2MG	C5-C4-N3	-6.67	117.77	128.39
25	A	1911	PSU	N1-C2-N3	6.67	122.21	115.17
1	a	516	PSU	N1-C2-N3	6.66	122.19	115.17
22	x	39	PSU	N1-C2-N3	6.54	122.07	115.17
25	A	2605	PSU	N1-C2-N3	6.51	122.04	115.17
25	A	1917	PSU	N1-C2-N3	6.51	122.04	115.17
22	x	55	PSU	N1-C2-N3	6.49	122.02	115.17
22	y	39	PSU	N1-C2-N3	6.48	122.00	115.17
22	x	32	PSU	N1-C2-N3	6.47	121.99	115.17
22	y	55	PSU	N1-C2-N3	6.46	121.98	115.17
22	y	8	4SU	C4-N3-C2	-6.45	121.13	127.31
25	A	2251	OMG	C5-C4-N3	-6.38	118.24	128.39
22	y	32	PSU	N1-C2-N3	6.35	121.87	115.17
22	x	37	MIA	N3-C4-N9	6.32	135.01	126.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	2504	PSU	N1-C2-N3	6.32	121.83	115.17
25	A	1835	2MG	C5-C4-N3	-6.28	118.39	128.39
25	A	2503	2MA	N3-C4-N9	6.23	134.89	126.99
1	a	1207	2MG	C5-C4-N3	-6.18	118.55	128.39
25	A	2445	2MG	C5-C4-N3	-6.17	118.56	128.39
25	A	746	PSU	N1-C2-N3	6.12	121.63	115.17
1	a	1518	MA6	C5-C4-N3	-6.05	118.38	126.72
25	A	1618	6MZ	C5-C4-N3	-5.88	118.61	126.72
1	a	1516	2MG	C5-C4-N3	-5.86	119.07	128.39
22	y	8	4SU	C5-C4-N3	5.82	120.16	114.75
25	A	1915	3TD	N1-C2-N3	5.79	120.34	116.13
1	a	527	G7M	N9-C4-N3	5.74	137.44	125.95
1	a	1519	MA6	C5-C4-N3	-5.69	118.88	126.72
22	x	46	7MG	N9-C8-N7	-5.67	95.35	103.37
1	a	527	G7M	C5-C4-N3	-5.60	117.57	128.15
25	A	1939	5MU	C4-N3-C2	-5.47	120.17	127.34
22	y	46	7MG	C5-C4-N3	-5.42	117.95	128.13
22	y	37	MIA	N3-C4-N9	5.42	136.39	127.17
25	A	2069	G7M	C5-C4-N3	-5.40	117.95	128.15
25	A	2069	G7M	N9-C4-N3	5.40	136.74	125.95
25	A	745	1MG	C5-C4-N3	-5.39	119.81	128.39
25	A	1939	5MU	N3-C2-N1	5.37	121.89	114.89
22	x	8	4SU	C4-N3-C2	-5.36	122.17	127.31
25	A	2030	6MZ	C5-C4-N3	-5.36	119.33	126.72
22	x	46	7MG	C5-C4-N3	-5.34	118.10	128.13
25	A	747	5MU	C4-N3-C2	-5.28	120.42	127.34
25	A	2251	OMG	C2-N3-C4	5.27	121.38	112.30
22	y	46	7MG	N9-C8-N7	-5.23	95.96	103.37
25	A	747	5MU	N3-C2-N1	5.21	121.67	114.89
22	x	54	5MU	C4-N3-C2	-5.11	120.64	127.34
25	A	2552	OMU	C4-N3-C2	-5.09	120.30	126.61
22	x	8	4SU	C5-C4-N3	5.08	119.48	114.75
1	a	966	2MG	N9-C4-N3	5.03	136.01	125.95
22	x	54	5MU	N3-C2-N1	5.03	121.44	114.89
25	A	2069	G7M	C2-N3-C4	4.93	120.80	112.30
1	a	1519	MA6	C10-N6-C6	-4.91	108.04	120.52
1	a	527	G7M	C2-N3-C4	4.75	120.47	112.30
22	y	54	5MU	N3-C2-N1	4.70	121.01	114.89
25	A	1835	2MG	N9-C4-N3	4.68	135.30	125.95
22	y	54	5MU	C4-N3-C2	-4.66	121.23	127.34
1	a	1519	MA6	C4-C5-N7	-4.64	105.28	110.58
25	A	2251	OMG	N9-C4-N3	4.61	135.16	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1518	MA6	C10-N6-C6	-4.58	108.86	120.52
25	A	2445	2MG	N9-C4-N3	4.58	135.10	125.95
25	A	1939	5MU	C5-C4-N3	4.56	119.29	115.32
25	A	747	5MU	C5-C4-N3	4.48	119.22	115.32
25	A	2605	PSU	C4-N3-C2	-4.47	120.22	126.37
25	A	1618	6MZ	N3-C4-N9	4.45	134.74	127.17
1	a	1518	MA6	N3-C4-N9	4.45	134.73	127.17
22	x	39	PSU	C4-N3-C2	-4.44	120.25	126.37
1	a	1519	MA6	C2-N1-C6	4.44	122.67	111.83
25	A	745	1MG	C2-N3-C4	4.43	121.93	111.98
22	x	54	5MU	C5-C4-N3	4.38	119.13	115.32
22	y	39	PSU	C4-N3-C2	-4.37	120.35	126.37
25	A	1911	PSU	C4-N3-C2	-4.37	120.35	126.37
25	A	2604	PSU	C4-N3-C2	-4.36	120.37	126.37
25	A	2552	OMU	N3-C2-N1	4.35	120.55	114.89
22	x	46	7MG	C2-N3-C4	4.33	119.77	112.30
25	A	1939	5MU	O4-C4-C5	-4.33	119.96	124.92
22	y	46	7MG	C2-N3-C4	4.32	119.74	112.30
22	y	37	MIA	C2-N3-C4	4.31	122.35	111.83
22	x	55	PSU	C4-N3-C2	-4.31	120.44	126.37
25	A	955	PSU	C4-N3-C2	-4.29	120.45	126.37
25	A	2457	PSU	C4-N3-C2	-4.28	120.47	126.37
1	a	1207	2MG	N9-C4-N3	4.25	134.46	125.95
25	A	1915	3TD	C4-N3-C2	-4.25	120.11	124.61
1	a	1518	MA6	C2-N1-C6	4.20	122.10	111.83
22	y	54	5MU	C5-C4-N3	4.20	118.98	115.32
25	A	2580	PSU	C4-N3-C2	-4.17	120.62	126.37
25	A	2552	OMU	C5-C4-N3	4.16	120.63	114.80
22	x	37	MIA	C16-C14-C13	-4.16	110.16	122.66
12	l	89	D2T	CB1-SB-CB	4.16	109.85	102.36
25	A	2504	PSU	C4-N3-C2	-4.15	120.65	126.37
22	y	32	PSU	C4-N3-C2	-4.15	120.66	126.37
1	a	1516	2MG	N9-C4-N3	4.14	134.22	125.95
22	y	55	PSU	C4-N3-C2	-4.13	120.68	126.37
25	A	747	5MU	O4-C4-C5	-4.12	120.21	124.92
1	a	516	PSU	C4-N3-C2	-4.09	120.74	126.37
22	x	37	MIA	N6-C6-N1	4.04	123.75	118.33
25	A	2030	6MZ	N3-C4-N9	4.04	134.03	127.17
25	A	746	PSU	C4-N3-C2	-4.03	120.81	126.37
1	a	1518	MA6	C4-C5-N7	-4.03	105.98	110.58
25	A	2030	6MZ	C6-C5-N7	4.03	136.82	132.43
1	a	1519	MA6	C2-N3-C4	4.02	121.64	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	y	54	5MU	O4-C4-C5	-4.01	120.33	124.92
25	A	745	1MG	N9-C4-N3	4.01	133.97	125.95
22	x	32	PSU	C4-N3-C2	-3.99	120.87	126.37
25	A	1618	6MZ	C6-C5-N7	3.90	136.69	132.43
25	A	2580	PSU	O2-C2-N1	-3.90	118.77	122.79
22	y	8	4SU	N3-C2-N1	3.88	119.95	114.89
1	a	1518	MA6	C2-N3-C4	3.88	121.30	111.83
22	x	55	PSU	O2-C2-N1	-3.88	118.79	122.79
1	a	1519	MA6	N3-C4-N9	3.83	133.67	127.17
1	a	1519	MA6	N1-C2-N3	-3.78	122.85	128.58
25	A	1917	PSU	C4-N3-C2	-3.77	121.17	126.37
25	A	2457	PSU	O2-C2-N1	-3.77	118.90	122.79
25	A	2030	6MZ	C4-C5-N7	-3.76	106.28	110.58
25	A	1618	6MZ	C2-N3-C4	3.76	121.01	111.83
22	x	54	5MU	C5-C6-N1	-3.76	119.23	123.31
25	A	1939	5MU	C5-C6-N1	-3.75	119.24	123.31
22	x	54	5MU	O4-C4-C5	-3.75	120.63	124.92
25	A	2030	6MZ	C9-N6-C6	-3.73	119.39	122.85
25	A	1618	6MZ	C4-C5-N7	-3.72	106.33	110.58
25	A	747	5MU	C5-C6-N1	-3.71	119.28	123.31
25	A	1618	6MZ	C9-N6-C6	-3.70	119.42	122.85
22	y	8	4SU	C5-C4-S4	-3.70	120.08	124.31
25	A	1917	PSU	O2-C2-N1	-3.68	119.00	122.79
22	x	37	MIA	C2-N3-C4	3.67	121.91	112.29
22	x	39	PSU	O2-C2-N1	-3.67	119.01	122.79
22	y	37	MIA	C4-C5-N7	-3.65	106.40	110.58
1	a	516	PSU	O2-C2-N1	-3.59	119.09	122.79
1	a	1516	2MG	C6-C5-N7	3.59	136.81	130.29
1	a	1207	2MG	C6-C5-N7	3.57	136.79	130.29
22	y	39	PSU	O2-C2-N1	-3.57	119.11	122.79
22	y	32	PSU	O2-C2-N1	-3.56	119.11	122.79
22	y	55	PSU	O2-C2-N1	-3.56	119.11	122.79
25	A	2030	6MZ	C2-N3-C4	3.54	120.48	111.83
25	A	2604	PSU	O2-C2-N1	-3.52	119.16	122.79
22	x	8	4SU	N3-C2-N1	3.50	119.44	114.89
22	y	37	MIA	N3-C2-N1	-3.48	123.32	128.58
25	A	2503	2MA	C4-C5-N7	-3.45	106.64	110.58
22	x	37	MIA	C6-C5-N7	3.39	136.13	132.43
1	a	1498	UR3	C5-C4-N3	3.39	119.51	115.04
25	A	746	PSU	O2-C2-N1	-3.38	119.30	122.79
25	A	1911	PSU	O2-C2-N1	-3.37	119.31	122.79
25	A	2552	OMU	O4-C4-C5	-3.34	119.40	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	l	89	D2T	OD2-CG-CB	3.34	120.36	113.15
25	A	2605	PSU	O2-C2-N1	-3.33	119.35	122.79
22	x	32	PSU	O2-C2-N1	-3.31	119.37	122.79
1	a	1518	MA6	N1-C2-N3	-3.30	123.59	128.58
1	a	1519	MA6	C9-N6-C6	-3.30	112.13	120.52
25	A	2445	2MG	C6-C5-N7	3.30	136.29	130.29
25	A	2504	PSU	O2-C2-N1	-3.29	119.40	122.79
25	A	2251	OMG	C6-C5-N7	3.26	136.22	130.29
22	x	37	MIA	C4-C5-N7	-3.24	106.88	110.58
1	a	1518	MA6	C9-N6-C6	-3.23	112.30	120.52
25	A	2030	6MZ	N1-C2-N3	-3.19	123.76	128.58
22	x	8	4SU	C5-C4-S4	-3.17	120.68	124.31
25	A	1835	2MG	C6-C5-N7	3.13	135.98	130.29
25	A	1618	6MZ	N1-C2-N3	-3.13	123.85	128.58
22	x	37	MIA	C15-C14-C13	-3.12	113.30	122.66
25	A	955	PSU	O2-C2-N1	-3.06	119.63	122.79
1	a	1519	MA6	C5-N7-C8	3.04	108.23	103.45
22	x	37	MIA	C11-S10-C2	-3.03	99.97	102.25
25	A	1962	5MC	C5-C4-N3	-3.03	118.64	121.75
22	y	54	5MU	C5-C6-N1	-3.01	120.04	123.31
22	x	37	MIA	C4-N9-C8	3.01	108.89	105.74
1	a	1519	MA6	C6-C5-N7	2.99	138.21	133.43
1	a	1207	2MG	N1-C2-N2	2.96	119.58	116.56
1	a	1407	5MC	C5-C4-N3	-2.94	118.75	121.75
25	A	745	1MG	C6-C5-N7	2.93	135.88	129.36
25	A	2503	2MA	N6-C6-N1	2.90	120.94	117.03
1	a	967	5MC	C5-C6-N1	-2.90	120.17	123.31
25	A	1939	5MU	O2-C2-N1	-2.88	119.04	122.80
25	A	1962	5MC	C5-C6-N1	-2.88	120.19	123.31
22	x	46	7MG	C5-C6-N1	2.85	115.96	110.94
25	A	2030	6MZ	C4-N9-C8	2.85	108.73	105.74
1	a	1519	MA6	C10-N6-C9	-2.80	107.17	116.18
1	a	1207	2MG	C4-C5-N7	-2.78	106.26	110.67
22	y	46	7MG	C5-C6-N1	2.78	115.83	110.94
22	x	54	5MU	O2-C2-N1	-2.77	119.19	122.80
22	y	54	5MU	C1'-N1-C2	2.74	122.52	117.59
1	a	966	2MG	C6-C5-N7	2.74	135.27	130.29
1	a	1407	5MC	O2-C2-N3	-2.73	118.03	122.33
25	A	2030	6MZ	C5-N7-C8	2.71	107.70	103.45
25	A	745	1MG	C4-C5-N7	-2.70	106.39	110.67
25	A	1915	3TD	C1'-C5-C4	2.70	121.70	117.61
1	a	1516	2MG	C4-C5-N7	-2.70	106.40	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1618	6MZ	C4-N9-C8	2.68	108.56	105.74
1	a	967	5MC	C5-C4-N3	-2.68	119.01	121.75
38	O	81	4D4	O-C-CA	-2.65	117.95	124.77
1	a	1518	MA6	C5-N7-C8	2.65	107.61	103.45
1	a	1407	5MC	C5-C6-N1	-2.62	120.46	123.31
25	A	2251	OMG	C4-C5-N7	-2.62	106.52	110.67
1	a	1207	2MG	CM2-N2-C2	-2.60	118.07	123.65
25	A	2503	2MA	C2-N1-C6	2.59	122.08	118.10
25	A	1618	6MZ	C5-N7-C8	2.58	107.51	103.45
25	A	2503	2MA	C4-N9-C8	2.57	108.44	105.74
22	x	37	MIA	N3-C2-N1	-2.55	122.34	127.00
25	A	2445	2MG	N1-C2-N2	2.53	119.15	116.56
25	A	2503	2MA	C5-N7-C8	2.52	107.42	103.45
25	A	2445	2MG	C4-C5-N7	-2.52	106.67	110.67
22	y	37	MIA	O4'-C1'-N9	2.51	112.92	108.09
22	y	54	5MU	C1'-N1-C6	-2.49	117.05	121.15
1	a	966	2MG	C2-N1-C6	-2.49	121.54	124.55
25	A	747	5MU	O2-C2-N1	-2.48	119.57	122.80
25	A	2498	OMC	O2-C2-N3	-2.47	118.43	122.33
1	a	1518	MA6	N1-C6-N6	2.47	119.86	116.86
11	k	119	IAS	OD1-CG-CB	-2.45	118.24	125.38
25	A	2580	PSU	O4'-C1'-C2'	2.44	108.53	105.15
22	y	37	MIA	C5-N7-C8	2.43	107.27	103.45
22	x	37	MIA	C5-N7-C8	2.43	107.26	103.45
1	a	1516	2MG	N1-C2-N2	2.41	119.02	116.56
25	A	1835	2MG	C4-C5-N7	-2.41	106.86	110.67
1	a	1207	2MG	N2-C2-N3	-2.38	117.48	120.51
25	A	2069	G7M	O6-C6-C5	-2.38	122.70	128.01
1	a	1518	MA6	C10-N6-C9	-2.37	108.56	116.18
1	a	966	2MG	CM2-N2-C2	-2.36	118.59	123.65
1	a	966	2MG	C4-C5-N7	-2.35	106.95	110.67
22	x	37	MIA	C5-C6-N6	-2.33	117.53	122.03
25	A	1911	PSU	C5-C6-N1	-2.33	118.91	122.14
1	a	527	G7M	O6-C6-C5	-2.32	122.83	128.01
1	a	1402	4OC	C6-C5-C4	2.32	119.79	117.00
25	A	2030	6MZ	N9-C8-N7	-2.31	110.66	113.94
1	a	1519	MA6	C4-N9-C8	2.30	108.16	105.74
1	a	966	2MG	O6-C6-C5	-2.30	120.46	126.53
1	a	516	PSU	O4'-C1'-C2'	2.30	108.33	105.15
25	A	2604	PSU	C5-C6-N1	-2.29	118.96	122.14
25	A	2445	2MG	O6-C6-C5	-2.29	120.49	126.53
25	A	2457	PSU	C5-C6-N1	-2.28	118.98	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	2503	2MA	C6-C5-N7	2.26	136.45	132.09
25	A	2605	PSU	C5-C6-N1	-2.24	119.03	122.14
22	x	37	MIA	N9-C8-N7	-2.23	110.77	113.94
22	y	55	PSU	C5-C6-N1	-2.23	119.05	122.14
1	a	967	5MC	O2-C2-N3	-2.21	118.85	122.33
25	A	2069	G7M	C5-C6-N1	2.20	116.38	111.84
22	x	46	7MG	O6-C6-C5	-2.19	122.24	127.62
22	y	46	7MG	C5-C4-N9	-2.16	103.56	106.33
25	A	2251	OMG	O6-C6-C5	-2.16	120.83	126.53
22	x	37	MIA	C16-C14-C15	-2.15	109.63	114.59
25	A	2552	OMU	O2-C2-N1	-2.15	120.00	122.80
1	a	1519	MA6	N9-C8-N7	-2.15	110.89	113.94
25	A	2457	PSU	O4'-C1'-C2'	2.12	108.08	105.15
25	A	1618	6MZ	N9-C8-N7	-2.10	110.96	113.94
22	y	32	PSU	C5-C6-N1	-2.09	119.24	122.14
1	a	1516	2MG	O6-C6-C5	-2.09	121.01	126.53
22	x	8	4SU	C1'-N1-C2	2.09	121.35	117.59
1	a	527	G7M	C5-C6-N1	2.09	116.16	111.84
25	A	955	PSU	C5-C6-N1	-2.09	119.24	122.14
1	a	1402	4OC	O2-C2-N3	-2.09	119.04	122.33
25	A	955	PSU	O2-C2-N3	-2.08	118.16	121.86
22	y	39	PSU	C5-C6-N1	-2.08	119.25	122.14
25	A	2445	2MG	CM2-N2-C2	-2.08	119.18	123.65
25	A	2445	2MG	C2-N1-C6	-2.08	122.04	124.55
25	A	2503	2MA	N9-C8-N7	-2.08	110.99	113.94
12	l	89	D2T	OD2-CG-OD1	-2.07	119.37	124.08
25	A	1835	2MG	O6-C6-C5	-2.04	121.14	126.53
22	x	39	PSU	C5-C6-N1	-2.04	119.30	122.14
25	A	2445	2MG	C5-C6-N1	2.04	118.45	113.25
22	y	32	PSU	O4'-C1'-C2'	2.04	107.97	105.15
25	A	2030	6MZ	C2-N1-C6	2.04	122.00	115.24
1	a	966	2MG	C5-C6-N1	2.03	118.43	113.25
1	a	1518	MA6	C4-N9-C8	2.03	107.87	105.74
22	y	54	5MU	C5M-C5-C4	2.02	120.94	118.78
1	a	1498	UR3	C1'-N1-C2	2.02	120.34	117.04
25	A	1911	PSU	O4'-C1'-C2'	2.01	107.94	105.15
1	a	1207	2MG	C2-N1-C6	-2.01	122.12	124.55

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	527	G7M	O4'-C4'-C5'-O5'
1	a	1207	2MG	N1-C2-N2-CM2
1	a	1207	2MG	N3-C2-N2-CM2
12	l	89	D2T	CA-CB-SB-CB1
12	l	89	D2T	CG-CB-SB-CB1
22	x	37	MIA	C12-C13-C14-C15
22	y	37	MIA	C2'-C1'-N9-C4
22	y	39	PSU	O4'-C1'-C5-C6
22	y	46	7MG	C4'-C5'-O5'-P
28	D	150	MEQ	O-C-CA-CB
38	O	81	4D4	C-CA-CB-OB
38	O	81	4D4	C-CA-CB-CG
38	O	81	4D4	N-CA-CB-CG
25	A	746	PSU	C2'-C1'-C5-C4
25	A	746	PSU	O4'-C1'-C5-C6
1	a	527	G7M	C3'-C4'-C5'-O5'
22	y	37	MIA	C2'-C1'-N9-C8
38	O	82	MS6	CA-CB-CG-SD
28	D	150	MEQ	NE2-CD-CG-CB
1	a	1402	4OC	O4'-C4'-C5'-O5'
28	D	150	MEQ	OE1-CD-CG-CB
1	a	966	2MG	C3'-C4'-C5'-O5'
1	a	1519	MA6	C5-C6-N6-C9
1	a	1519	MA6	C5-C6-N6-C10
25	A	1917	PSU	C3'-C4'-C5'-O5'
22	y	54	5MU	C3'-C4'-C5'-O5'
38	O	82	MS6	CB-CG-SD-CE
22	y	46	7MG	O4'-C1'-N9-C4
25	A	2030	6MZ	O4'-C4'-C5'-O5'
22	y	46	7MG	C3'-C4'-C5'-O5'
22	x	37	MIA	C5-C6-N6-C12
22	y	46	7MG	C2'-C1'-N9-C8
22	y	39	PSU	C3'-C4'-C5'-O5'
1	a	1519	MA6	N1-C6-N6-C10
1	a	966	2MG	O4'-C4'-C5'-O5'
25	A	1917	PSU	O4'-C4'-C5'-O5'
25	A	2498	OMC	O4'-C4'-C5'-O5'
22	y	54	5MU	O4'-C4'-C5'-O5'
25	A	2498	OMC	C3'-C2'-O2'-CM2
22	y	39	PSU	C4'-C5'-O5'-P
22	y	39	PSU	O4'-C1'-C5-C4
25	A	746	PSU	O4'-C1'-C5-C4
22	x	37	MIA	N6-C12-C13-C14

Continued on next page...

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Mol	Chain	Res	Type	Atoms
22	x	37	MIA	N1-C6-N6-C12
1	a	1518	MA6	C5-C6-N6-C9
22	y	39	PSU	O4'-C4'-C5'-O5'
22	y	46	7MG	O4'-C1'-N9-C8
25	A	2030	6MZ	C3'-C4'-C5'-O5'
22	y	37	MIA	C4'-C5'-O5'-P
25	A	2504	PSU	O4'-C4'-C5'-O5'
1	a	1519	MA6	O4'-C4'-C5'-O5'
22	y	39	PSU	C2'-C1'-C5-C6
38	O	81	4D4	N-CA-CB-OB
25	A	746	PSU	C2'-C1'-C5-C6
1	a	1402	4OC	C3'-C4'-C5'-O5'
22	y	37	MIA	O4'-C4'-C5'-O5'
25	A	2580	PSU	O4'-C4'-C5'-O5'
22	y	54	5MU	C2'-C1'-N1-C2
25	A	2503	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	a	1516	2MG	1	0
25	A	2498	OMC	1	0
22	y	37	MIA	6	0
1	a	1519	MA6	2	0
22	y	32	PSU	1	0
25	A	2030	6MZ	1	0
25	A	1915	3TD	1	0
22	y	46	7MG	3	0
11	k	119	IAS	1	0
1	a	1518	MA6	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 597 ligands modelled in this entry, 597 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

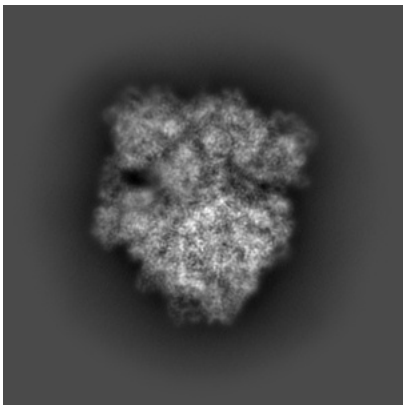
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29628. These allow visual inspection of the internal detail of the map and identification of artifacts.

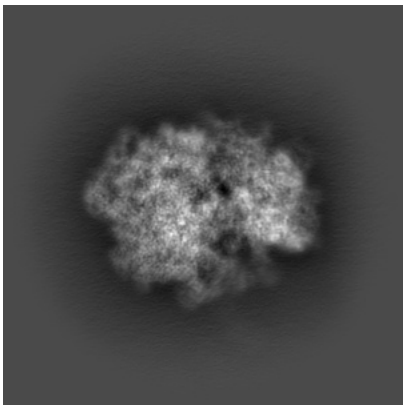
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

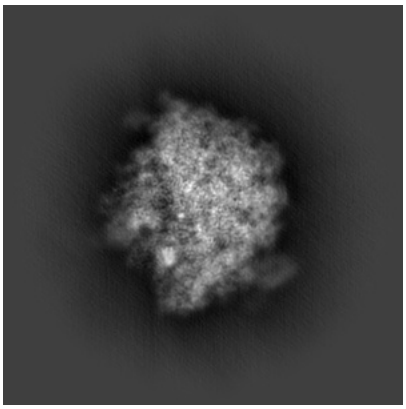
6.1.1 Primary map



X

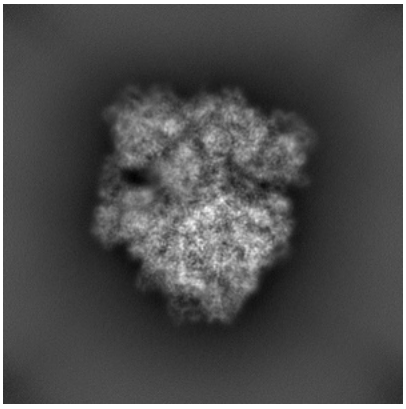


Y

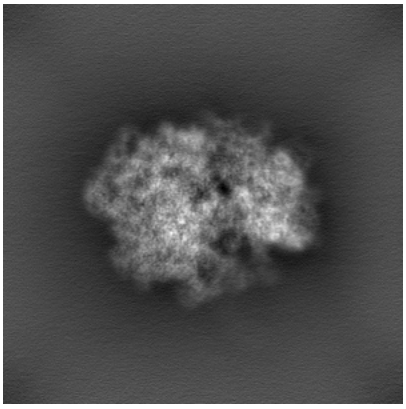


Z

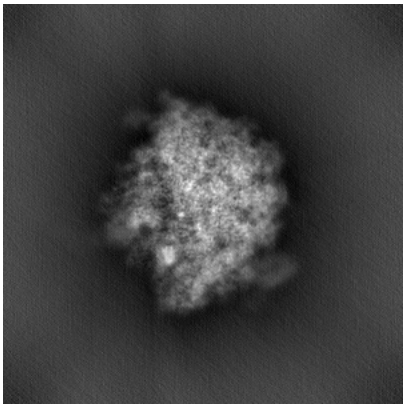
6.1.2 Raw map



X



Y

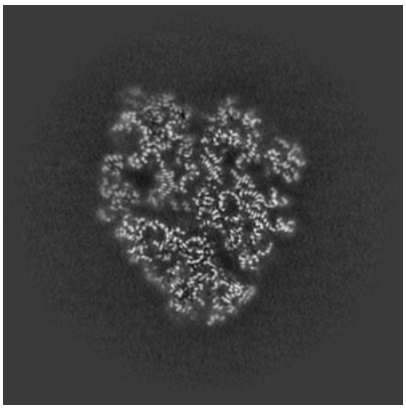


Z

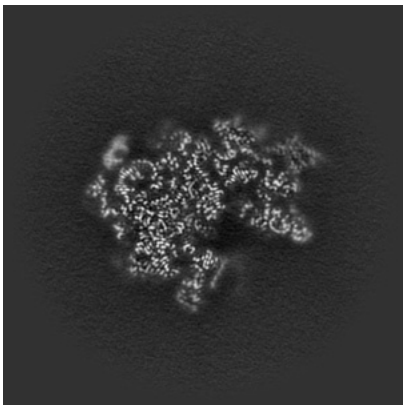
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

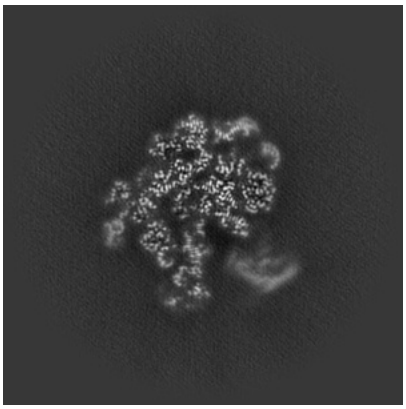
6.2.1 Primary map



X Index: 256

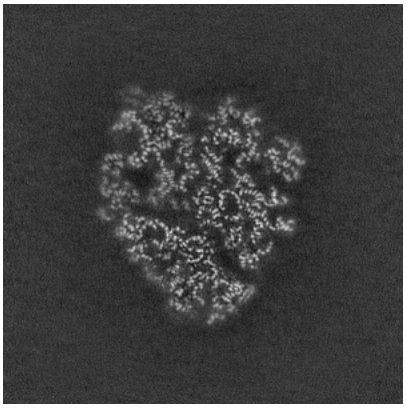


Y Index: 256

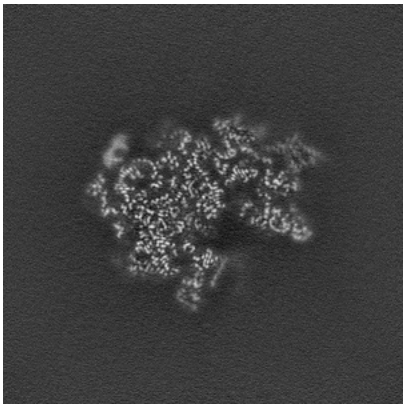


Z Index: 256

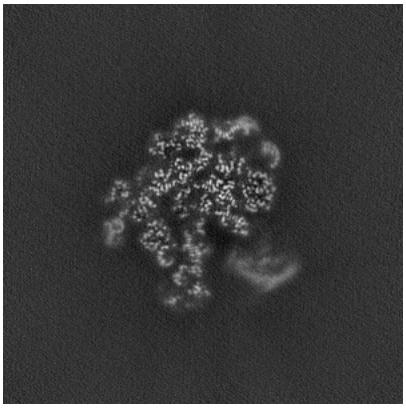
6.2.2 Raw map



X Index: 256



Y Index: 256

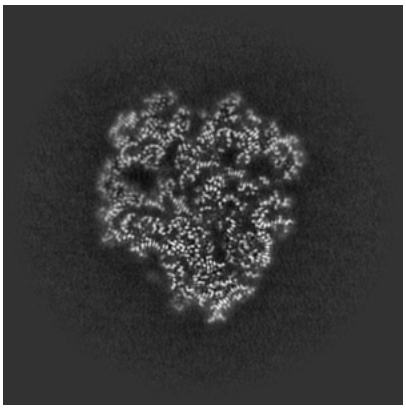


Z Index: 256

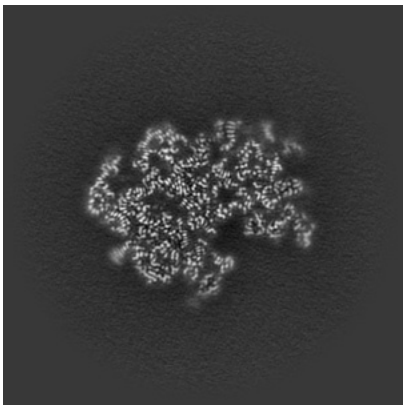
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

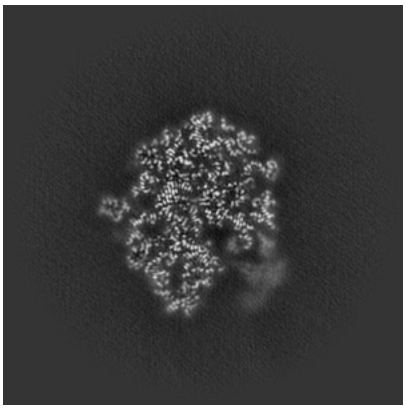
6.3.1 Primary map



X Index: 249

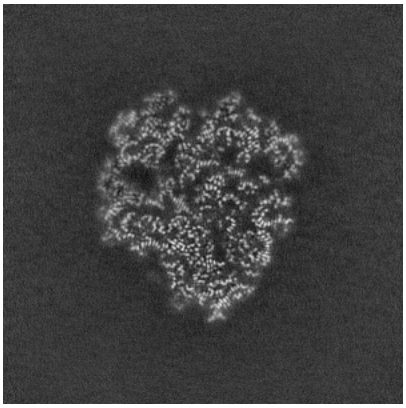


Y Index: 271

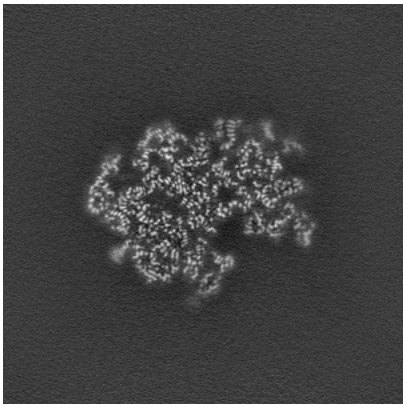


Z Index: 232

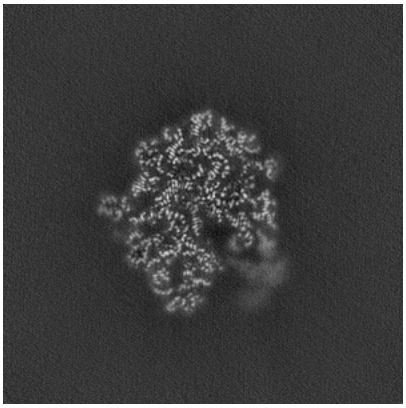
6.3.2 Raw map



X Index: 249



Y Index: 271

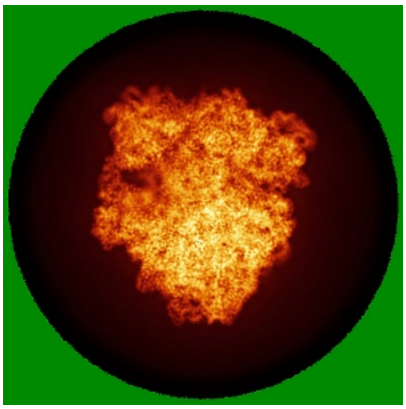


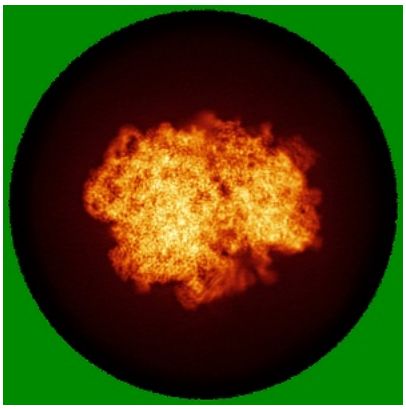
Z Index: 234

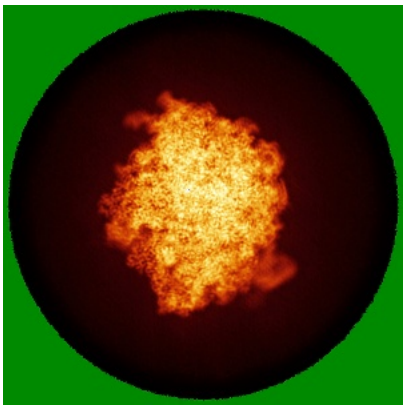
The images above show the largest variance slices of the map in three orthogonal directions.

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

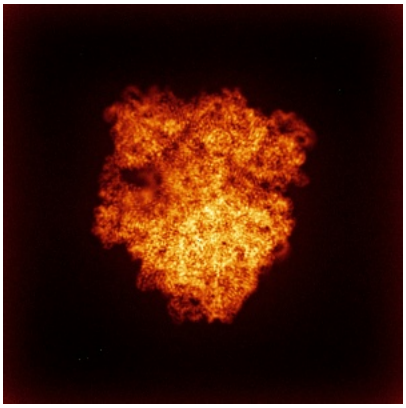
6.4.1 Primary map

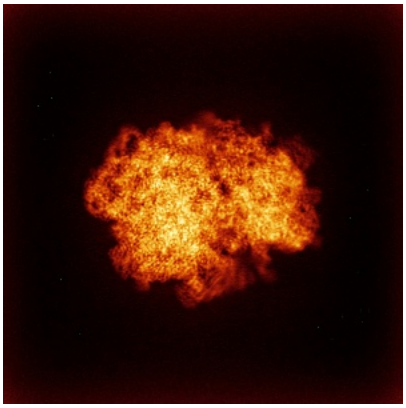

X

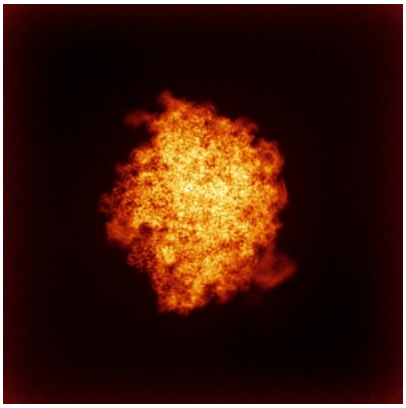

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

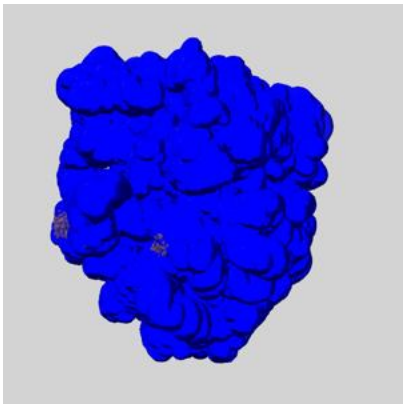
6.6 Mask visualisation

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

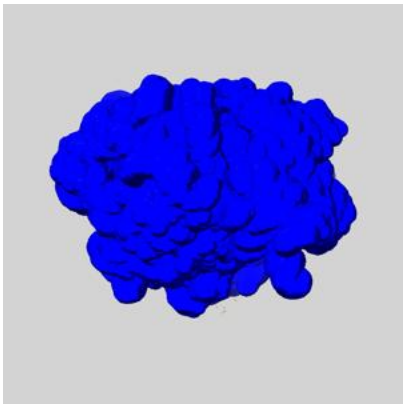
A mask typically either:

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

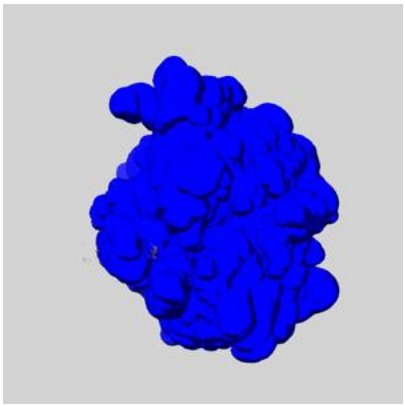
6.6.1 emd_29628_msk_1.map



X



Y

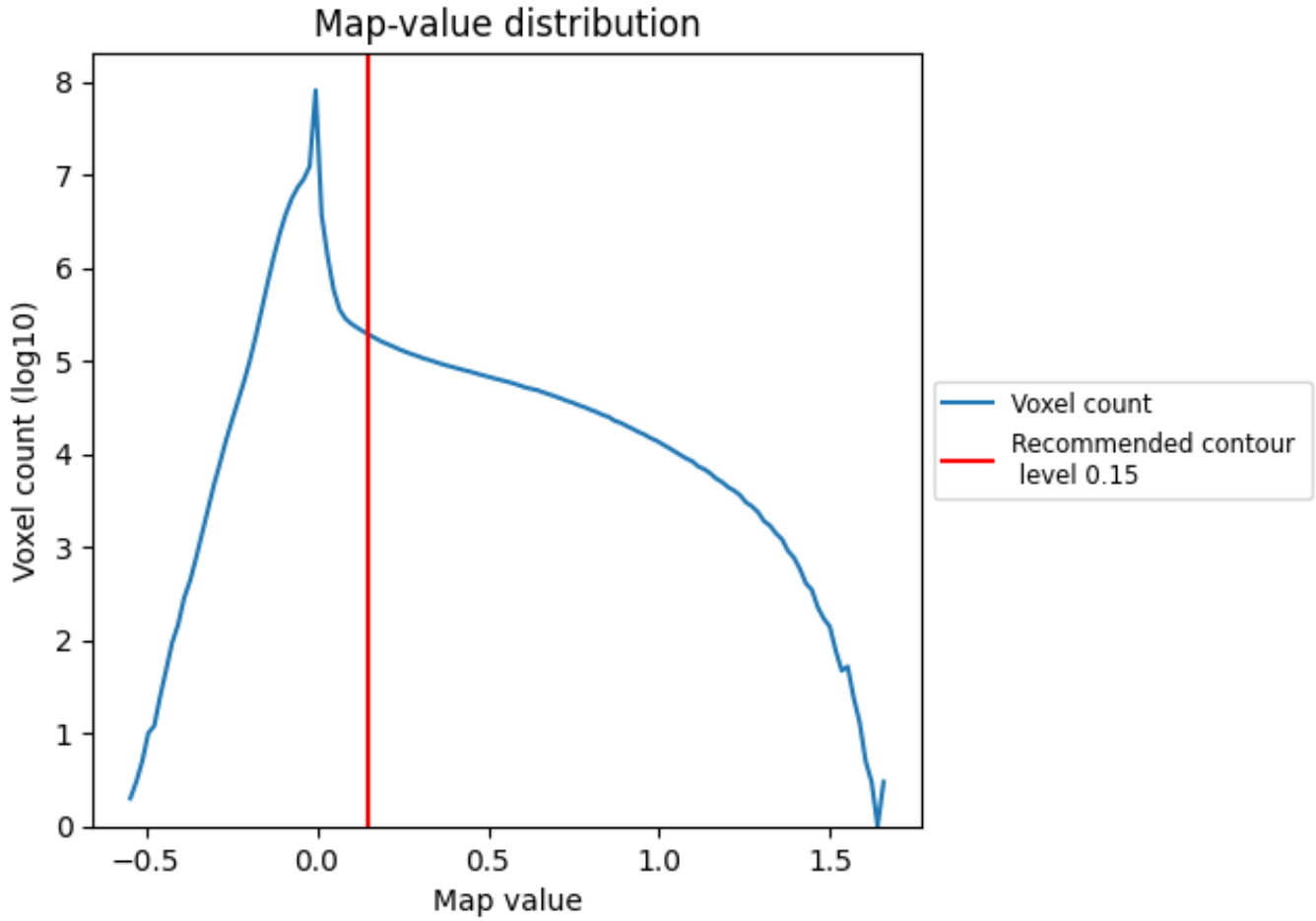


Z

7 Map analysis

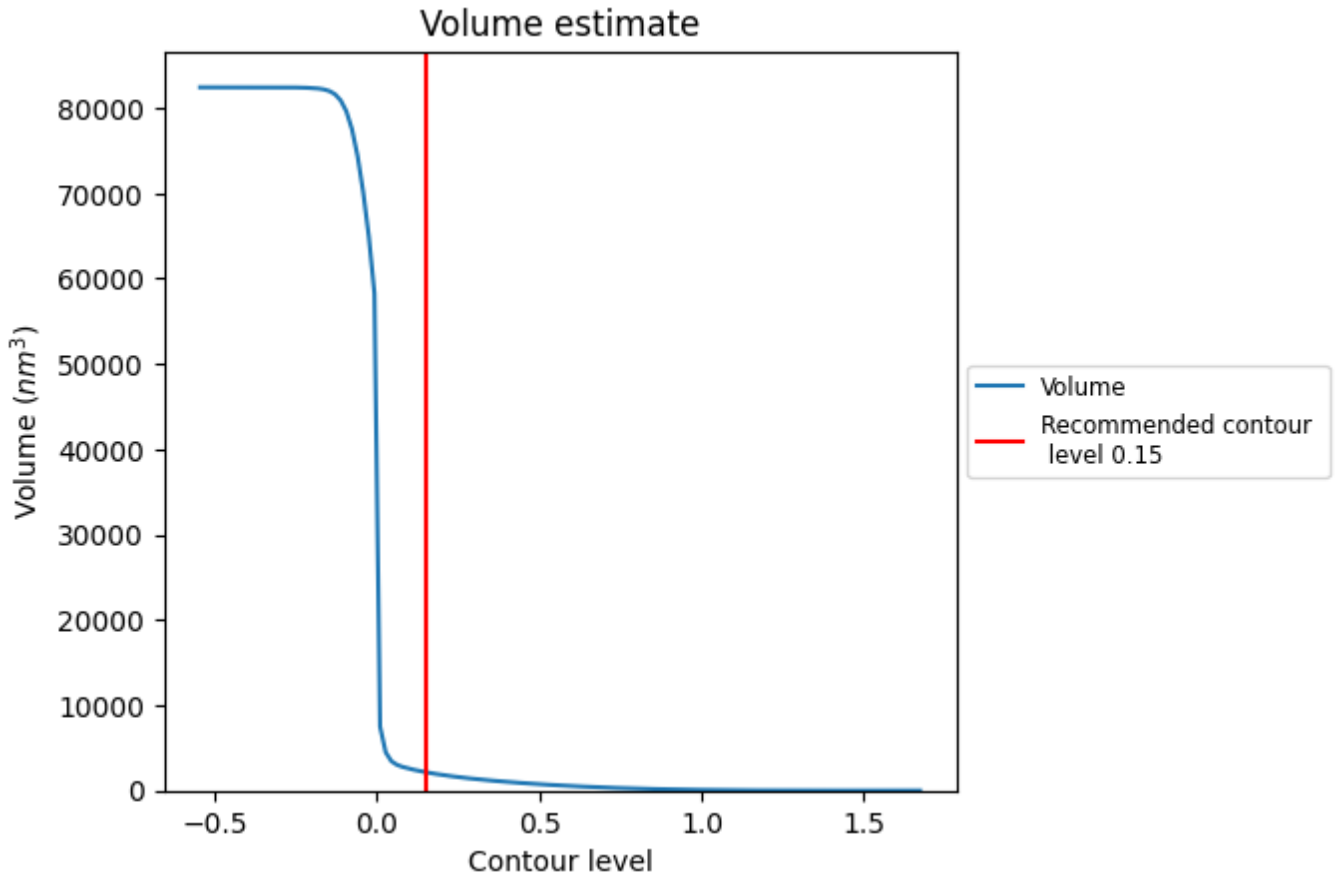
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

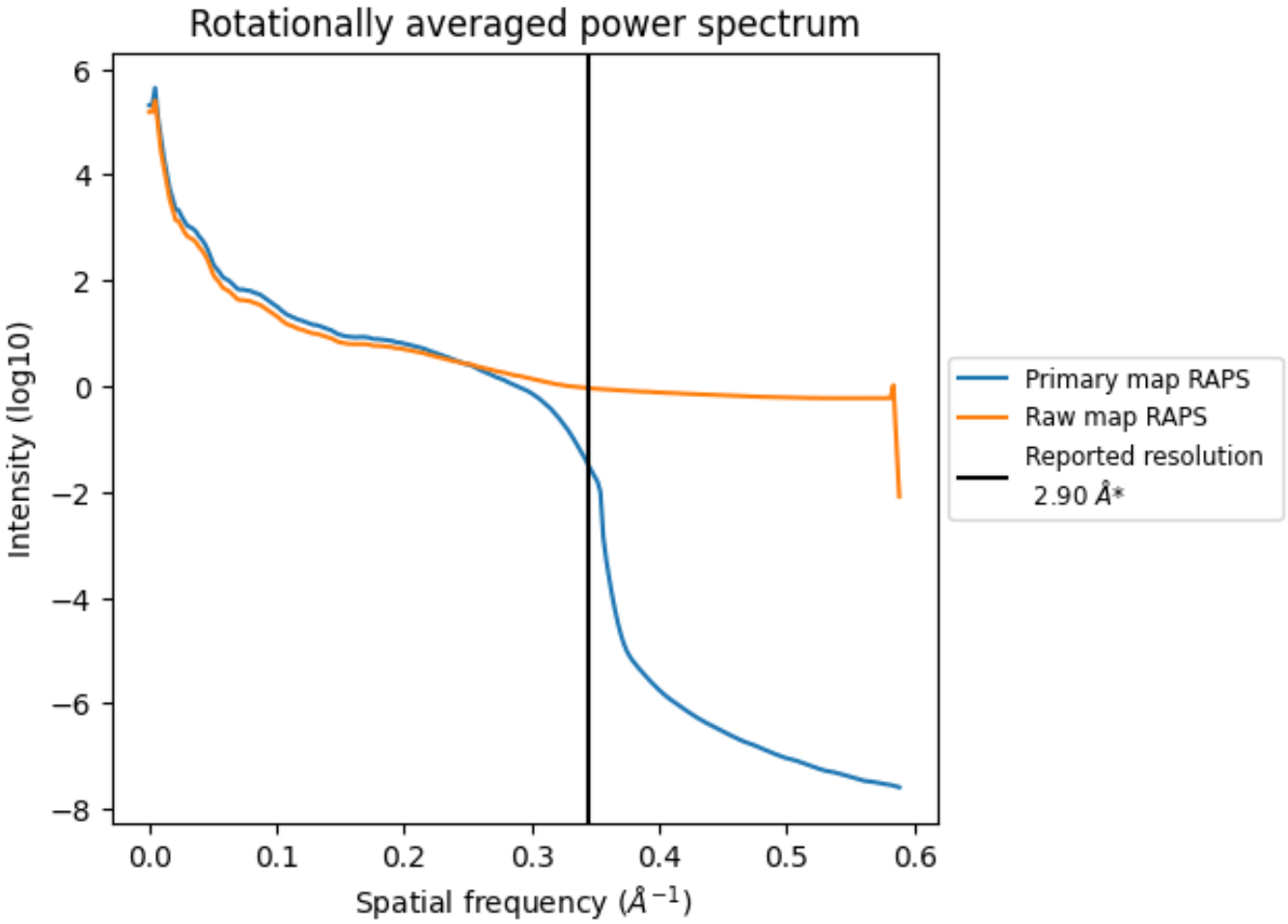
7.2 Volume estimate



The volume at the recommended contour level is 2153 nm^3; this corresponds to an approximate mass of 1945 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)

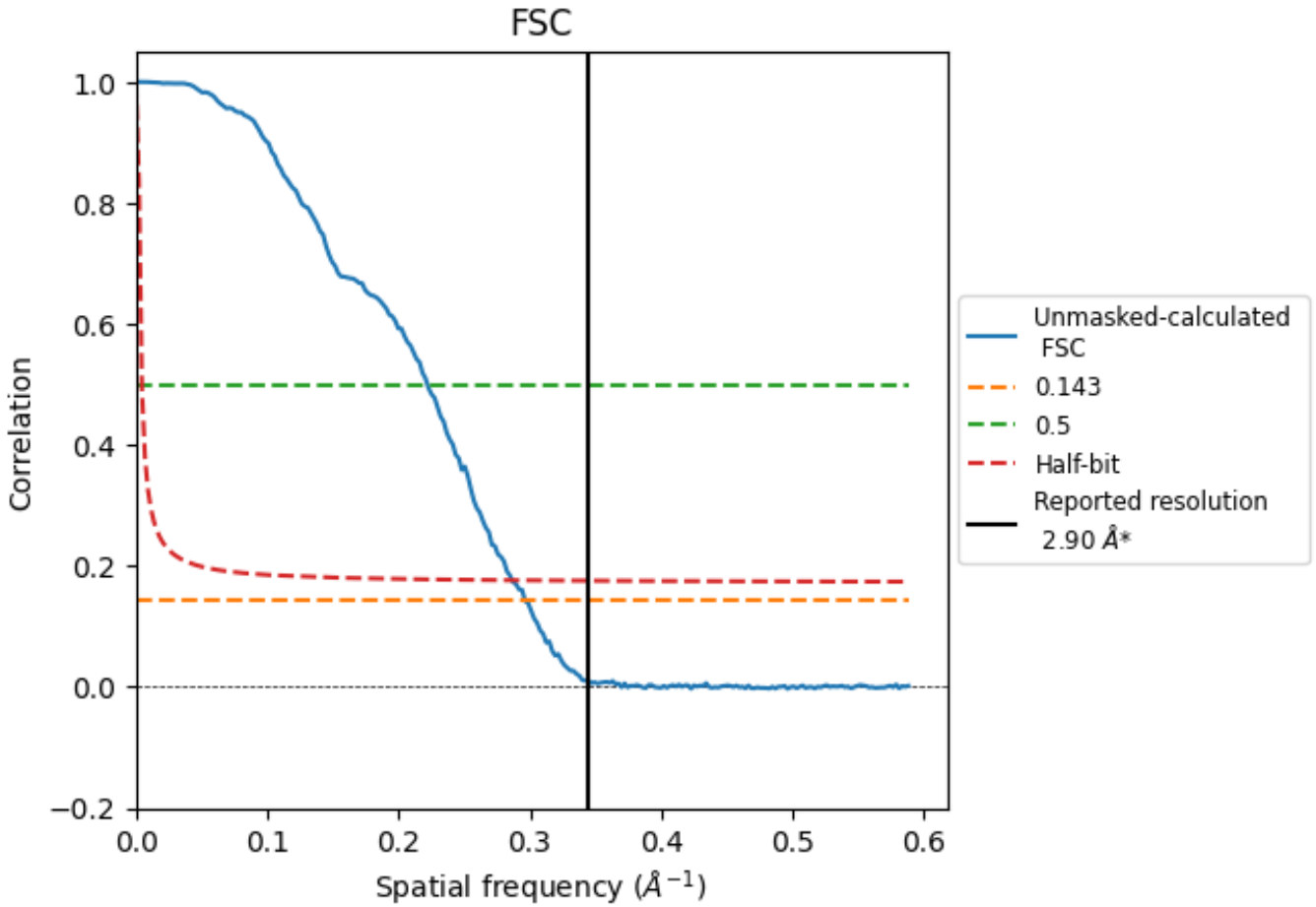


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

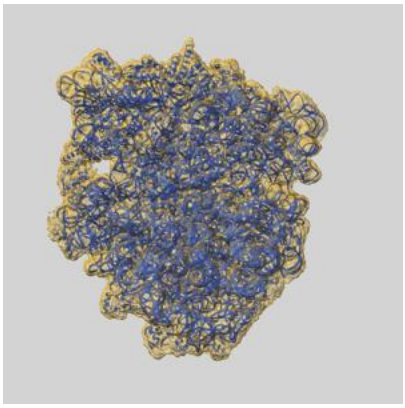
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.37	4.50	3.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.37 differs from the reported value 2.9 by more than 10 %

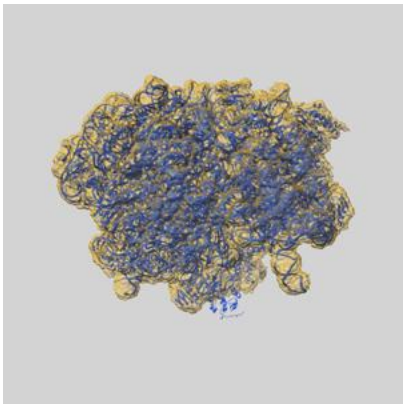
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29628 and PDB model 8FZH. Per-residue inclusion information can be found in section 3 on page 17.

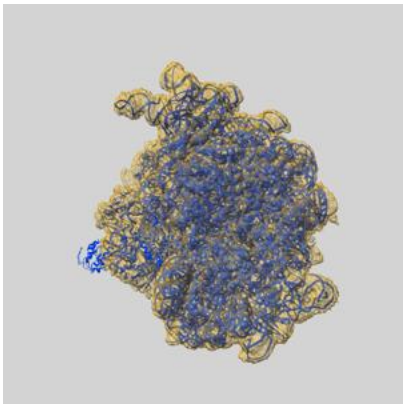
9.1 Map-model overlay



X



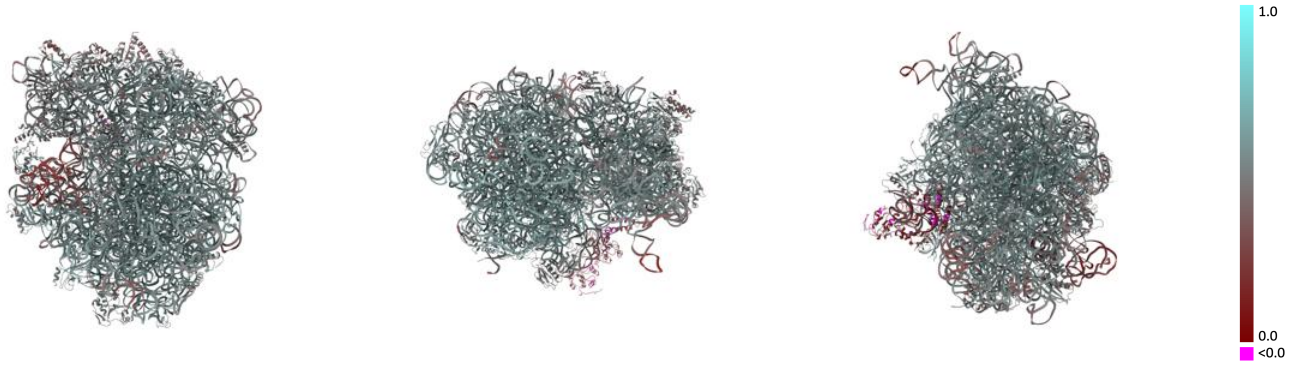
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

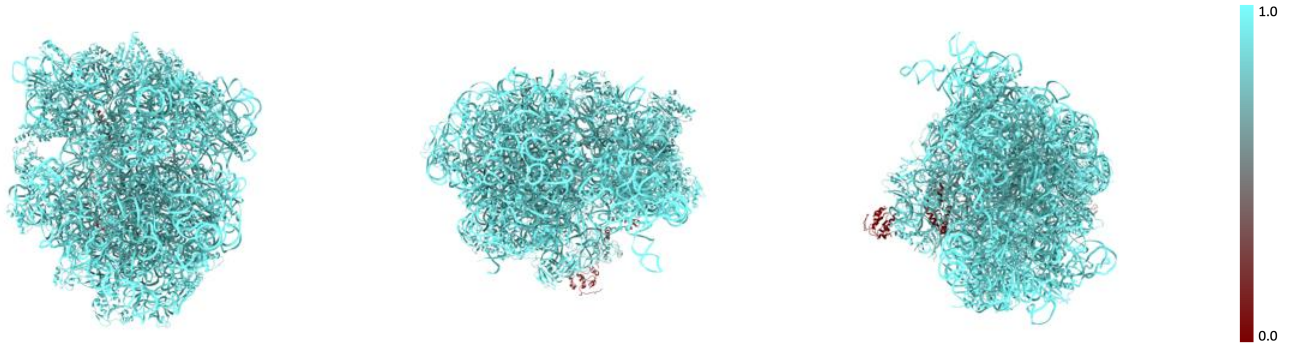
9.2 Q-score mapped to coordinate model



X Y Z

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.

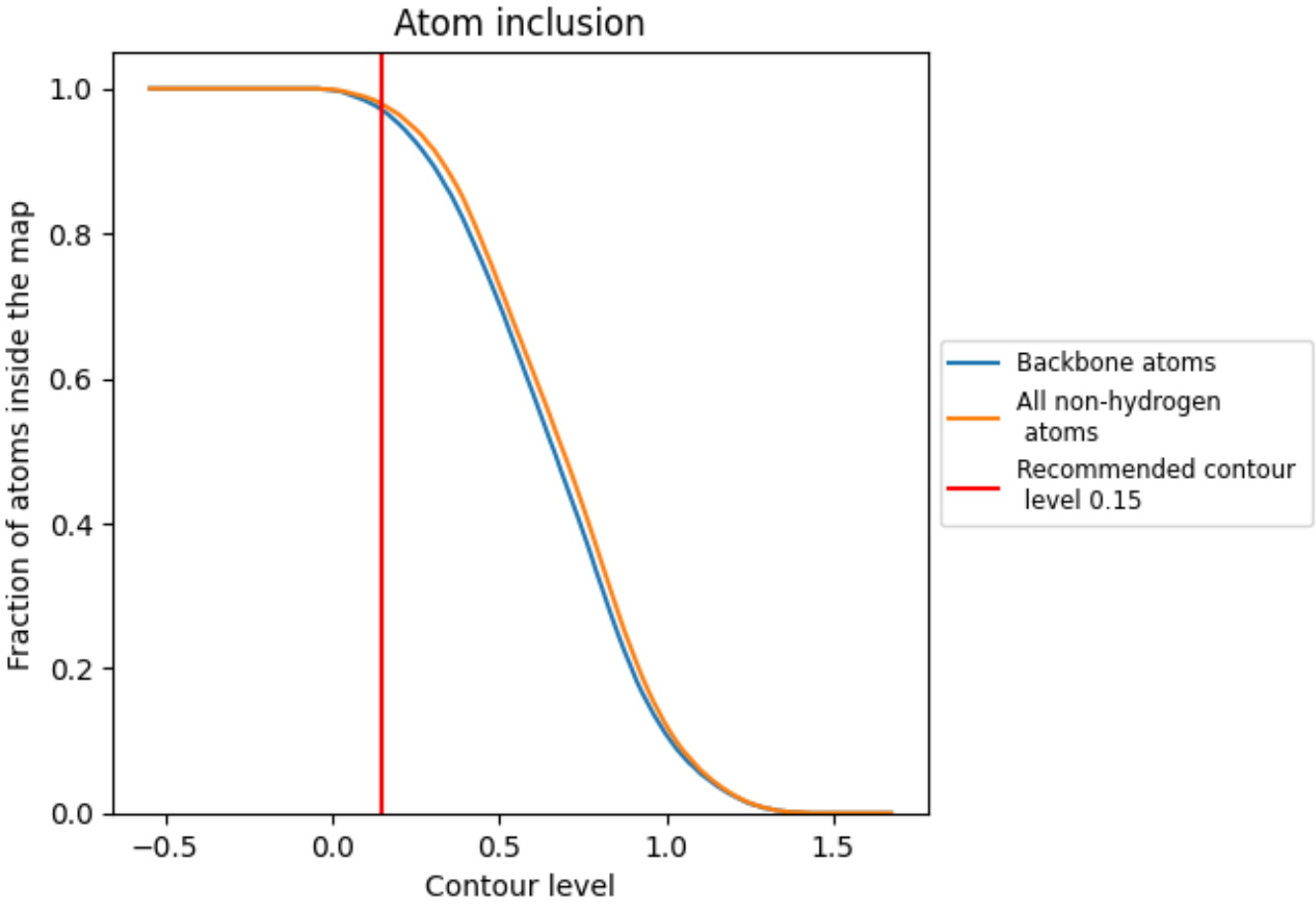
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion (i)



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

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9780	0.5300
1	0.9810	0.5070
2	0.9770	0.5600
3	0.9740	0.4790
4	0.9880	0.5820
5	0.9680	0.5490
6	0.9750	0.5890
7	0.9840	0.5910
8	0.9690	0.5630
A	0.9980	0.5490
B	0.9990	0.5350
C	0.9750	0.5800
D	0.9810	0.5740
E	0.9850	0.5460
F	0.9680	0.5040
G	0.9730	0.4890
H	0.4890	0.4270
I	0.1910	0.1780
J	0.8880	0.1890
L	0.9770	0.5700
M	0.9660	0.5700
N	0.9800	0.5680
O	0.9720	0.5710
P	0.9850	0.5790
Q	0.9860	0.5270
R	0.9620	0.5670
S	0.9920	0.5770
T	0.9770	0.5620
U	0.9740	0.5630
V	0.9650	0.5500
W	0.9870	0.5320
X	0.9810	0.5450
Y	0.9720	0.5750
Z	0.9800	0.5570
a	0.9990	0.5330



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Chain	Atom inclusion	Q-score
b	0.9000	0.4490
c	0.9610	0.5130
d	0.9820	0.5080
e	0.9750	0.5370
f	0.9680	0.4850
g	0.9520	0.4650
h	0.9760	0.5350
i	0.9890	0.4950
j	0.9700	0.4660
k	0.9770	0.5220
l	0.9660	0.5650
m	0.9780	0.5040
n	0.9870	0.5120
o	0.9580	0.5000
p	0.9790	0.5320
q	0.9730	0.5360
r	0.9740	0.5130
s	0.9850	0.5080
t	0.9560	0.5110
u	0.9120	0.4710
w	0.7730	0.4110
x	0.9890	0.5440
y	0.9160	0.3190
z	0.9870	0.5300