Full wwPDB EM Validation Report (i)

Sep 16, 2026 – 02:19 AM EDT

PDB ID	:	8EKC / pdb_00008ekc
EMDB ID	:	EMD-28197
Title	:	Escherichia coli 70S ribosome bound to thermorubin, deacylated P-site tRNAfMet and aminoacylated A-site Phe-tRNA
Authors	:	Rybak, M.Y.; Gagnon, M.G.
Deposited on	:	2022-09-20
Resolution	:	2.70 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 (i) symbol.

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

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

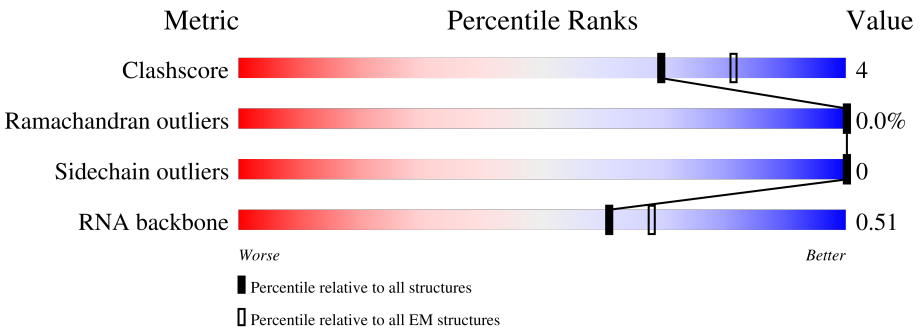
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

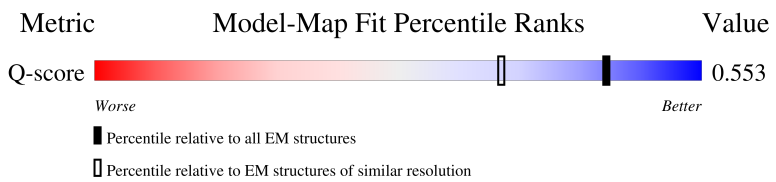
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	69% 27% • •
2	b	241	59% 78% 15% 7%
3	c	233	• 77% 12% 12%

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Mol	Chain	Length	Quality of chain
4	d	206	74% 25%
5	e	167	78% 15% 7%
6	f	131	63% 16% 21%
7	g	156	80% 17%
8	h	130	87% 12%
9	i	130	80% 18%
10	j	103	10% 74% 21% 5%
11	k	129	78% 12% 9%
12	l	124	87% 10%
13	m	118	88% 9%
14	n	101	84% 15%
15	o	89	93% 6%
16	p	82	88% 11%
17	q	84	86% 8% 6%
18	r	75	60% 12% 28%
19	s	92	79% 11% 10%
20	t	87	77% 22%
21	u	71	8% 69% 8% 23%
22	w	76	59% 32% 7%
23	x	77	82% 13%
24	v	24	42% 8% 50%
25	A	2904	76% 19%
26	B	120	78% 18%
27	C	273	92% 8%
28	D	209	93% 7%

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Mol	Chain	Length	Quality of chain
29	E	201	91% 9%
30	F	179	79% 20%
31	G	177	90% 10%
32	H	149	17% 22% 5% 72%
33	L	142	91% 9%
34	M	123	88% 12%
35	N	144	92% 8%
36	O	136	95%
37	P	127	86% 7% 7%
38	Q	117	93% 6%
39	R	115	90% 9%
40	S	118	95%
41	T	103	98%
42	U	110	96%
43	V	100	93% 7%
44	W	104	79% 19%
45	X	94	91% 9%
46	Y	85	92% 7%
47	Z	78	92% 6%
48	1	63	92% 5%
49	2	59	85% 14%
50	3	70	73% 13% 14%
51	4	57	88% 9%
52	5	55	89% 7%
53	6	46	98%

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Mol	Chain	Length	Quality of chain
54	7	65	94% 5% •
55	8	38	84% 16%

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 144543 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
			Total	C	N	O	S		
7	g	152	1191	741	230	216	4	0	0

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S		
12	l	121	942	582	193	162	5	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	u	55	460	287	95	77	1	0	0

- Molecule 22 is a RNA chain called A-site phenylalanine tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
22	w	74	1591	713	285	517	74	2	0	0

- Molecule 23 is a RNA chain called P-site initiator tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
23	x	76	1625	725	294	529	76	1	0	0

- Molecule 24 is a RNA chain called M-F-Stop mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
24	v	12	255	115	46	82	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
25	A	2845	61097	27261	11245	19746	2845	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	H	41	303	194	54	54	1	0	0

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S Ribosomal Protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called Ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	Y	84	634	391	129	113	1	0	0

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	1	61	495	305	97	92	1	0	0

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	2	58	449	281	87	79	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	3	60	468	290	87	85	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	4	55	434	263	92	78	1	0	0

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	5	51	417	269	76	72	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	6	46	377	228	90	57	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	7	64	504	323	105	74	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	8	38	302	185	65	48	4	0	0

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
56	a	132	132	132	0
56	l	1	1	1	0
56	n	1	1	1	0
56	w	1	1	1	0
56	x	2	2	2	0
56	v	2	2	2	0
56	A	555	555	555	0
56	B	10	10	10	0
56	C	3	3	3	0
56	D	1	1	1	0
56	N	1	1	1	0
56	P	1	1	1	0
56	S	1	1	1	0
56	V	1	1	1	0
56	4	1	1	1	0

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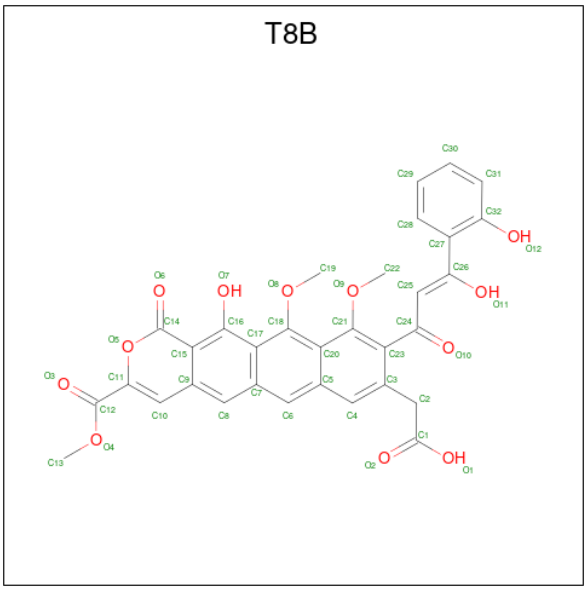
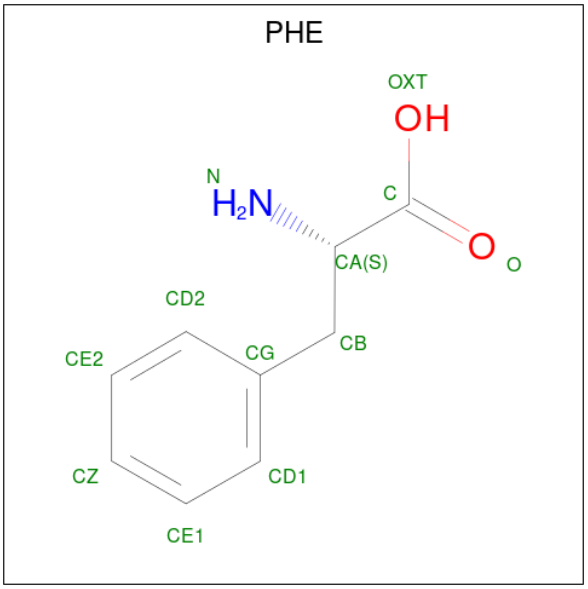
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
56	7	1	1	1	0

- Molecule 57 is Thermorubin (CCD ID: T8B) (formula: $C_{32}H_{24}O_{12}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
57	a	1	44	32	12	0

- Molecule 58 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
58	w	1	11	9	1	1	0

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
60	a	37	37	37	0
60	n	1	1	1	0
60	A	247	247	247	0
60	B	4	4	4	0
60	C	1	1	1	0
60	D	1	1	1	0
60	E	1	1	1	0
60	N	1	1	1	0
60	P	1	1	1	0
60	R	1	1	1	0
60	T	1	1	1	0
60	V	1	1	1	0
60	Z	1	1	1	0
60	4	1	1	1	0

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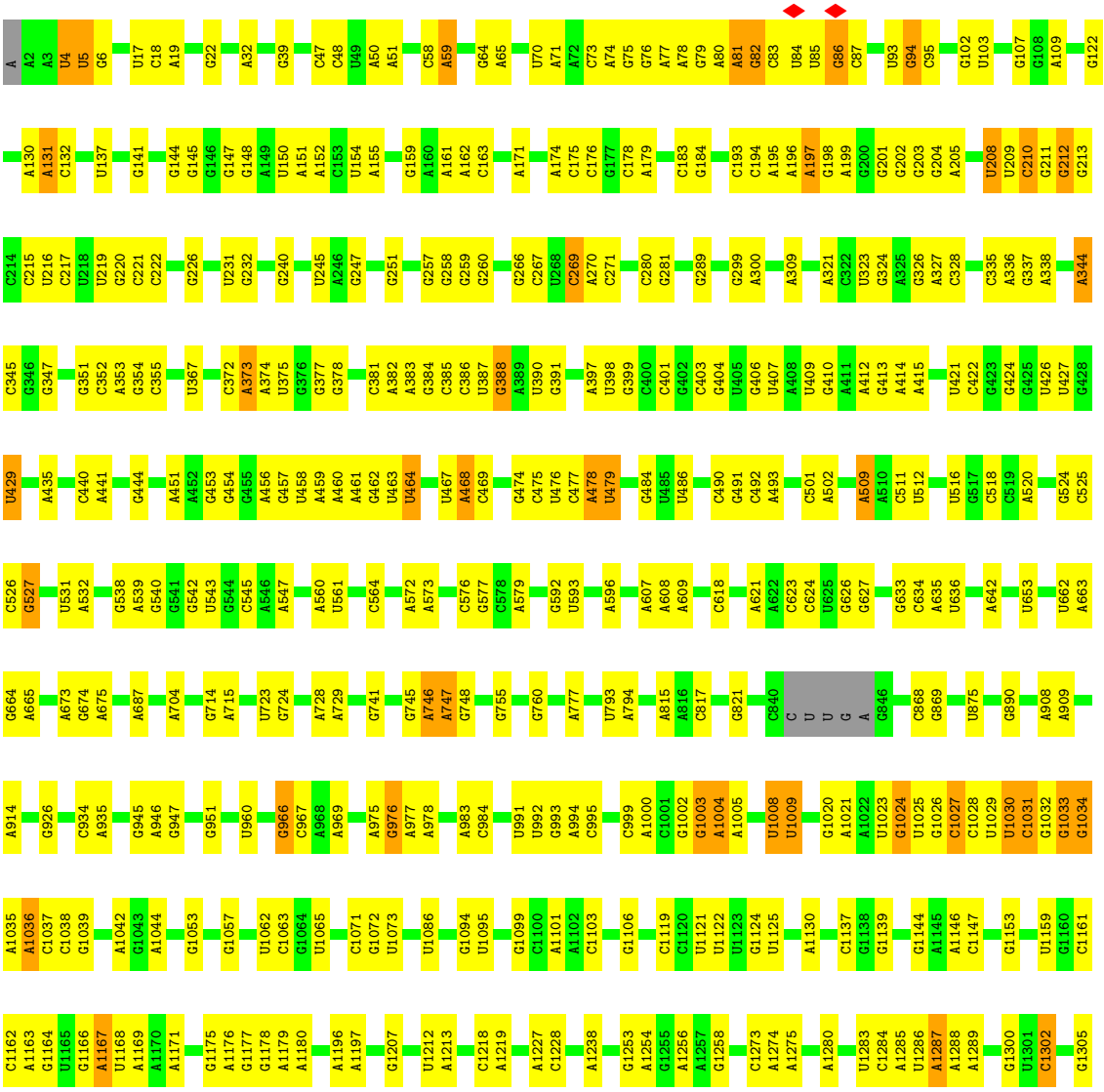
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
60	8	1	1	1	0

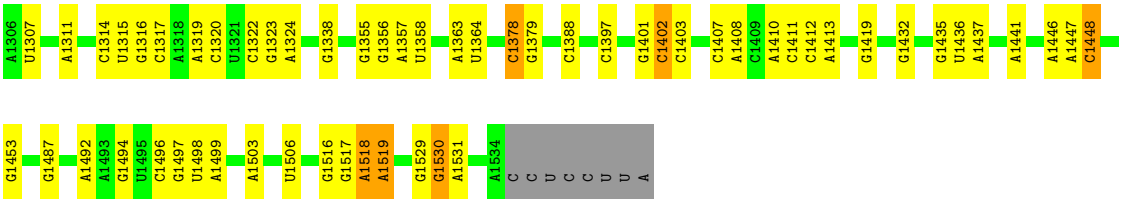
3 Residue-property plots (i)

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

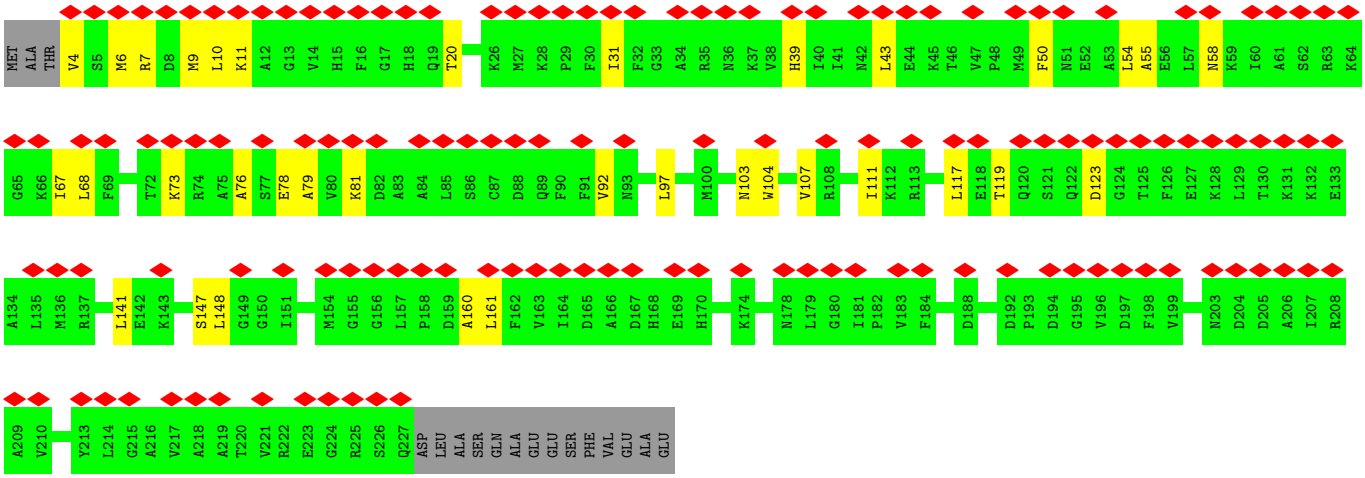
Chain a: 69% 27%





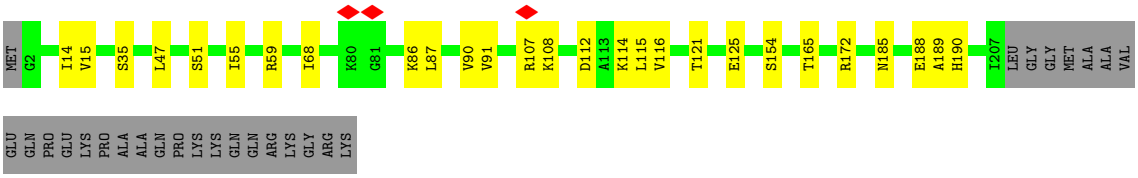
- Molecule 2: 30S ribosomal protein S2

Chain b:



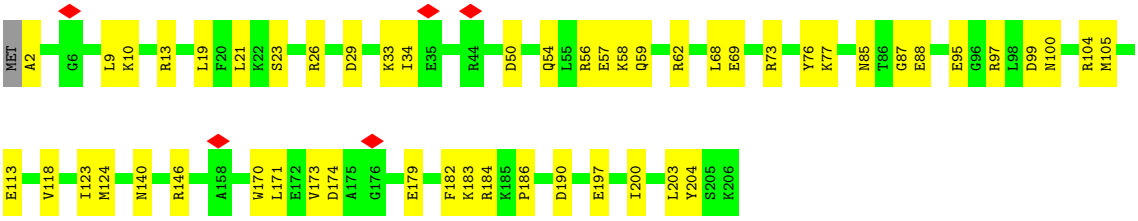
- Molecule 3: 30S ribosomal protein S3

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

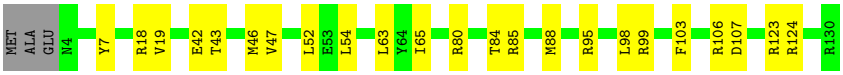
Chain g:

• Molecule 8: 30S ribosomal protein S8

Chain h:

• Molecule 9: 30S ribosomal protein S9

Chain i:

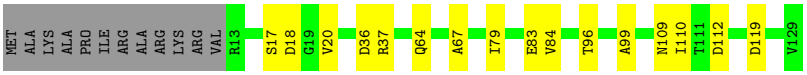


• Molecule 10: 30S ribosomal protein S10

Chain j:

• Molecule 11: 30S ribosomal protein S11

Chain k:

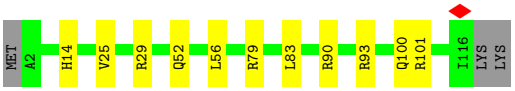


• Molecule 12: 30S ribosomal protein S12

Chain l: 87% 10%

• Molecule 13: 30S ribosomal protein S13

Chain m: 88% 9%

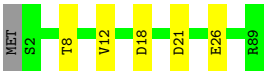


• Molecule 14: 30S ribosomal protein S14

Chain n: 84% 15%

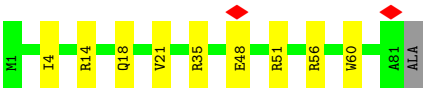
• Molecule 15: 30S ribosomal protein S15

Chain o: 93% 6%



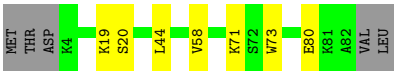
• Molecule 16: 30S ribosomal protein S16

Chain p: 88% 11%



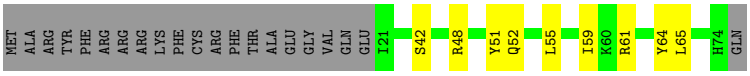
• Molecule 17: 30S ribosomal protein S17

Chain q: 86% 8% 6%



• Molecule 18: 30S ribosomal protein S18

Chain r: 60% 12% 28%

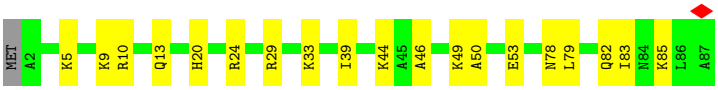


• Molecule 19: 30S ribosomal protein S19

Chain s:

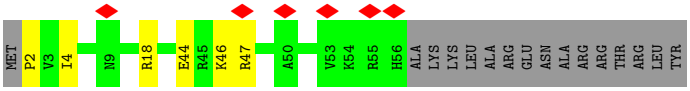
• Molecule 20: 30S ribosomal protein S20

Chain t:



• Molecule 21: 30S ribosomal protein S21

Chain u:



• Molecule 22: A-site phenylalanine tRNA

Chain w:

• Molecule 23: P-site initiator tRNA

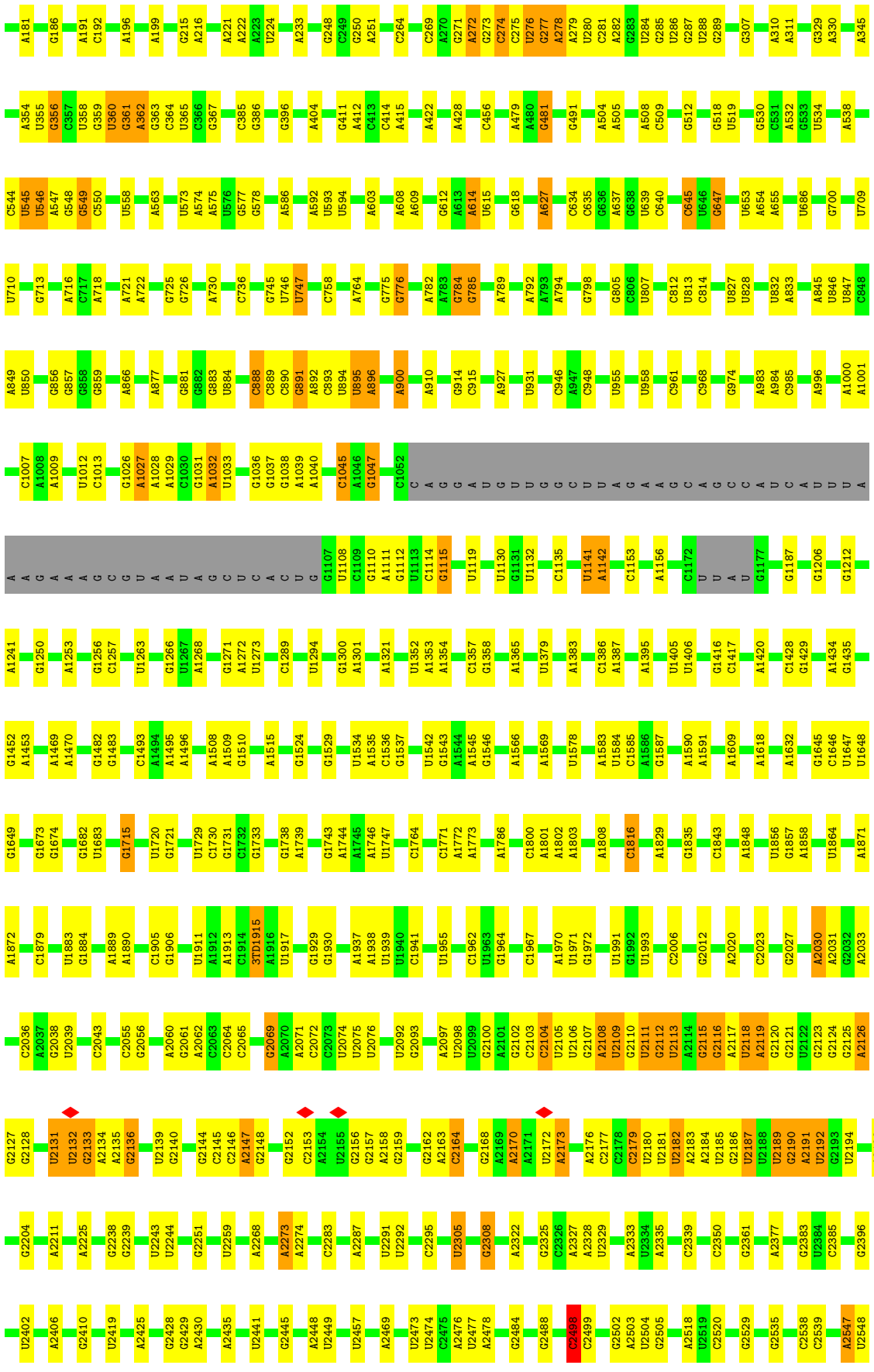
Chain x:

• Molecule 24: M-F-Stop mRNA

Chain v:

• Molecule 25: 23S Ribosomal RNA

Chain A: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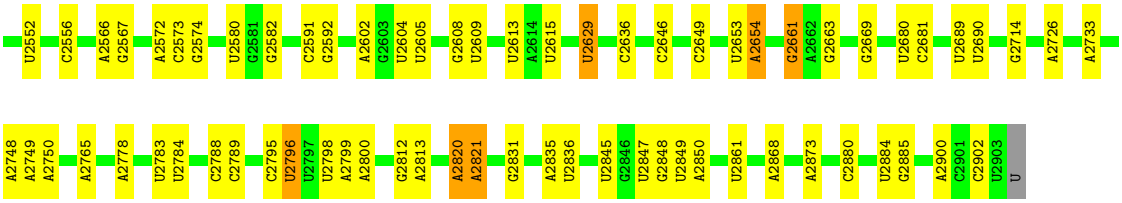
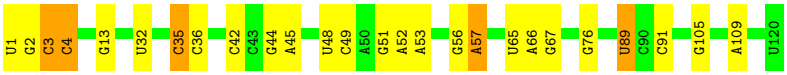
A354 U355 G356 C357 U358 G359 U360 G361 A362 G363 C364 U365 C366 G367 C385 G386 G396 A404 G411 A412 C413 C414 A415 A422 A428 C456 A479 A480 G481 G491 A504 A505 A508 C509 G512 G518 U519 G530 C531 A532 G533 U534 A538
C544 U545 U546 A547 G548 G549 C550 U558 A563 U573 A574 A575 U576 G577 G578 A586 A592 U593 U594 A603 A608 A609 G612 A613 A614 U615 G618 A627 C634 C635 G636 A637 G638 U639 C640 C645 U646 G647 U653 A654 A655 U686 G700 U709
U710 G713 A716 C717 A718 A721 A722 G725 G726 A730 C736 G745 U746 U747 C758 A764 G775 G776 A782 A783 G784 G785 A789 A792 A793 A794 G798 G805 C806 U807 C812 U813 C814 U827 U828 U832 A833 A845 U846 U847 C848
A849 U850 G856 G857 G858 G859 A866 A877 G881 G882 G883 U884 C888 C889 C890 G891 A892 C893 U894 U895 A896 A900 A910 G914 C915 A927 U931 C946 A947 C948 U955 U958 C961 C968 G974 A983 A984 C985 A996 A1000 A1001
C1007 A1008 A1009 U1012 C1013 G1026 A1027 A1028 A1029 C1030 G1031 A1032 U1033 G1036 G1037 G1038 A1039 A1040 C1045 A1046 G1047 C1052 C A G G A U G U U G G C U U A G A A G C C A U A G U U A A U G1107 U1108 C1109 G1110 A1111 G1112 U1113 C1114 G1115 U1119 U1130 C1131 U1132 C1135 U1141 A1142 C1153 A1156 C1172 U U A U G1177 G1187 G1206 G1212
A1241 G1250 A1253 G1256 C1257 U1263 G1266 U1267 A1268 G1271 A1272 U1273 C1289 U1294 G1300 A1301 A1321 U1352 A1353 A1354 C1357 G1358 A1365 U1379 A1383 C1386 A1387 A1395 U1405 U1406 G1416 C1417 A1420 C1428 G1429 A1434 G1435
G1452 A1453 A1469 A1470 G1482 G1483 C1493 A1494 A1495 A1496 A1508 A1509 G1510 A1515 G1524 G1529 U1534 A1535 C1536 G1537 U1542 G1543 A1544 A1545 G1546 A1566 A1569 U1578 A1583 U1584 C1585 A1586 G1587 A1590 A1591 A1609 A1618 A1632 G1645 C1646 U1647 U1648
G1649 G1673 G1674 G1682 U1683 G1715 U1720 G1721 U1729 C1730 G1731 C1732 G1733 G1738 A1739 G1743 A1744 A1745 A1746 U1747 C1764 C1771 A1772 A1773 A1786 C1800 A1801 A1802 A1803 A1808 C1816 A1829 G1835 C1843 A1848 U1856 G1857 A1858 U1864 A1871
A1872 C1879 U1883 G1884 A1889 A1890 C1905 G1906 U1911 A1912 A1913 C1914 3TD1915 A1916 U1917 G1929 G1930 A1937 A1938 U1939 U1940 C1941 U1955 C1962 U1963 G1964 C1967 A1970 U1971 G1972 U1991 G1992 U1993 C2006 G2012 A2020 C2023 G2027 A2030 A2031 G2032 A2033
C2036 A2037 G2038 U2039 C2043 C2055 G2056 A2060 G2061 A2062 C2063 C2064 C2065 G2069 A2070 A2071 C2072 G2073 U2074 U2075 U2076 U2092 G2093 A2097 U2098 U2099 G2100 A2101 G2102 C2103 C2104 U2105 U2106 G2107 A2108 U2109 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126
G2127 G2128 U2131 U2132 G2133 A2134 A2135 G2136 U2139 G2140 G2144 C2145 C2146 A2147 G2148 G2152 C2153 A2154 U2155 G2156 G2157 A2158 G2159 G2162 A2163 C2164 G2168 A2169 A2170 A2171 U2172 A2173 A2176 C2177 C2178 C2179 U2180 U2181 U2182 A2183 A2184 U2185 G2186 U2187 U2188 U2189 G2190 A2191 U2192 G2193 U2194 A2198
G2204 A2211 A2225 G2238 G2239 U2243 U2244 G2251 U2259 A2268 A2273 A2274 C2283 A2287 U2291 U2292 C2295 U2305 G2308 A2322 G2325 C2326 A2327 A2328 U2329 A2333 U2334 A2335 C2339 C2350 G2361 A2377 G2383 U2384 C2385 G2396
U2402 A2406 G2410 U2419 A2425 G2428 G2429 A2430 A2435 U2441 G2445 A2448 U2449 U2457 A2469 U2473 U2474 C2475 A2476 U2477 A2478 G2484 G2488 C2498 C2499 G2502 A2503 U2504 G2505 A2518 U2519 C2520 G2529 G2535 C2538 C2539 A2547 U2548



• Molecule 26: 5S Ribosomal RNA

Chain B:

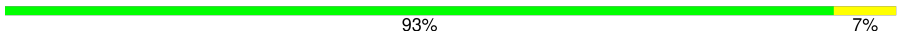


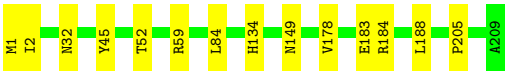
• Molecule 27: 50S ribosomal protein L2

Chain C:

• Molecule 28: 50S ribosomal protein L3

Chain D:





• Molecule 29: 50S ribosomal protein L4

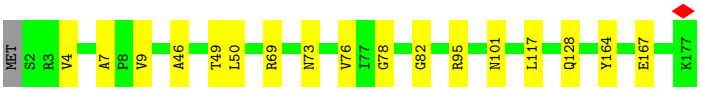
Chain E:

• Molecule 30: 50S ribosomal protein L5

Chain F:

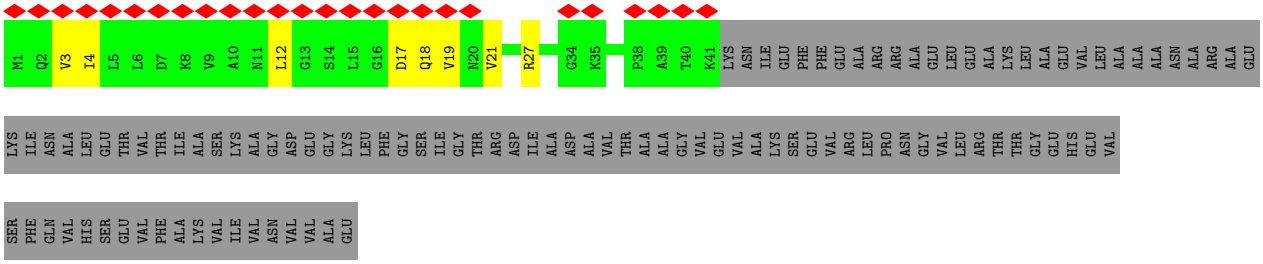
• Molecule 31: 50S ribosomal protein L6

Chain G:



- Molecule 32: 50S ribosomal protein L9

Chain H:

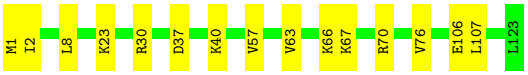


- Molecule 33: 50S ribosomal protein L13

Chain L:

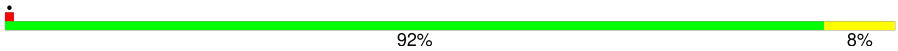
- Molecule 34: 50S ribosomal protein L14

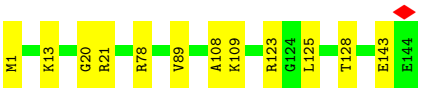
Chain M:



- Molecule 35: 50S Ribosomal Protein L15

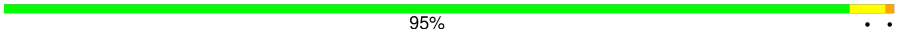
Chain N:

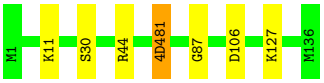




- Molecule 36: 50S ribosomal protein L16

Chain O:





- Molecule 37: 50S ribosomal protein L17

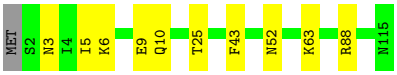
Chain P:

• Molecule 38: 50S ribosomal protein L18

Chain Q:

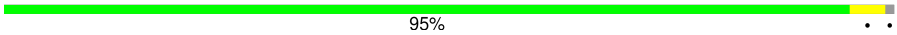
• Molecule 39: 50S ribosomal protein L19

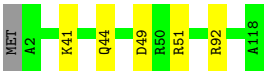
Chain R:



• Molecule 40: 50S ribosomal protein L20

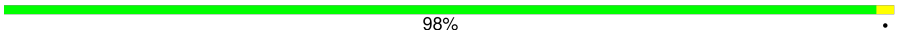
Chain S:

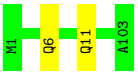




• Molecule 41: Ribosomal protein L21

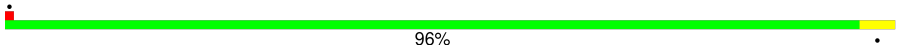
Chain T:

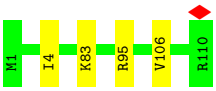




• Molecule 42: 50S ribosomal protein L22

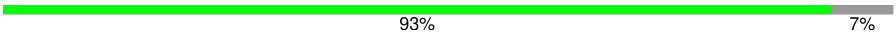
Chain U:





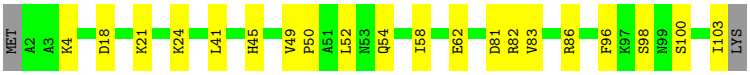
• Molecule 43: 50S ribosomal protein L23

Chain V:



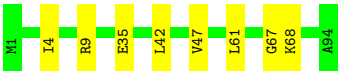
• Molecule 44: 50S ribosomal protein L24

Chain W:



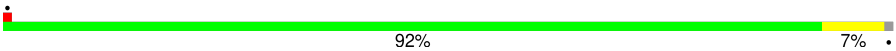
• Molecule 45: 50S ribosomal protein L25

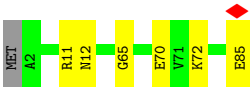
Chain X:



• Molecule 46: 50S ribosomal protein L27

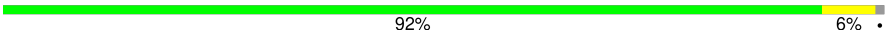
Chain Y:





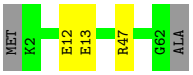
• Molecule 47: 50S ribosomal protein L28

Chain Z:



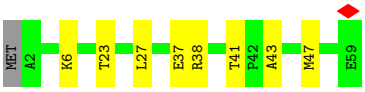
• Molecule 48: 50S ribosomal protein L29

Chain 1:



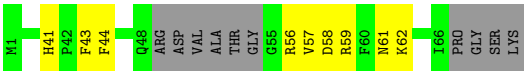
• Molecule 49: 50S ribosomal protein L30

Chain 2:



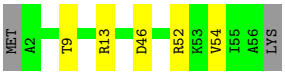
• Molecule 50: 50S ribosomal protein L31

Chain 3:



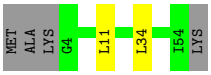
• Molecule 51: 50S ribosomal protein L32

Chain 4:



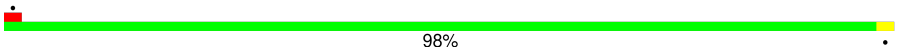
- Molecule 52: 50S ribosomal protein L33

Chain 5:



- Molecule 53: 50S ribosomal protein L34

Chain 6:

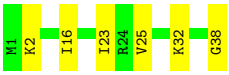


- Molecule 54: 50S ribosomal protein L35

Chain 7:

- Molecule 55: 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	310702	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	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.941	Depositor
Minimum map value	-0.713	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	440.32, 440.32, 440.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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: T8B, 2MG, UR3, G7M, MG, 4SU, 5MC, IAS, 1MG, H2U, MIA, D2T, 4OC, MEQ, 4D4, OMU, OMG, ZN, 5MU, OMC, PSU, 2MA, MS6, 6MZ, MA6, 3TD

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	0.26	0/36450	0.32	0/56856
2	b	0.14	0/1785	0.35	0/2404
3	c	0.18	0/1651	0.36	0/2225
4	d	0.18	0/1665	0.39	0/2227
5	e	0.24	0/1165	0.39	0/1568
6	f	0.23	0/858	0.44	0/1160
7	g	0.18	0/1206	0.40	0/1617
8	h	0.23	0/989	0.36	0/1326
9	i	0.18	0/1034	0.33	0/1375
10	j	0.17	0/796	0.42	0/1077
11	k	0.22	0/884	0.35	0/1191
12	l	0.23	0/945	0.43	0/1268
13	m	0.19	0/900	0.31	0/1204
14	n	0.17	0/817	0.29	0/1088
15	o	0.24	0/722	0.36	0/964
16	p	0.17	0/653	0.39	0/877
17	q	0.21	0/650	0.39	0/871
18	r	0.23	0/453	0.34	0/609
19	s	0.17	0/680	0.31	0/915
20	t	0.24	0/676	0.49	0/895
21	u	0.15	0/467	0.25	0/620
22	w	0.33	0/1605	0.39	0/2494
23	x	0.27	0/1725	0.31	0/2689
24	v	0.27	0/285	0.25	0/441
25	A	0.39	0/67852	0.40	1/105848 (0.0%)
26	B	0.30	0/2876	0.35	0/4483
27	C	0.32	0/2121	0.41	0/2852
28	D	0.34	0/1576	0.44	0/2119
29	E	0.29	0/1571	0.37	0/2113
30	F	0.22	0/1434	0.34	0/1926
31	G	0.23	0/1343	0.39	0/1816

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	H	0.15	0/306	0.44	0/413
33	L	0.32	0/1152	0.37	0/1551
34	M	0.32	0/955	0.41	0/1279
35	N	0.31	0/1061	0.38	0/1412
36	O	0.31	0/1073	0.42	0/1433
37	P	0.35	0/958	0.45	0/1281
38	Q	0.25	0/902	0.36	0/1209
39	R	0.32	0/929	0.36	0/1242
40	S	0.36	0/960	0.36	0/1278
41	T	0.31	0/829	0.38	0/1107
42	U	0.31	0/864	0.32	0/1156
43	V	0.29	0/744	0.38	0/994
44	W	0.27	0/787	0.43	0/1051
45	X	0.27	0/766	0.35	0/1025
46	Y	0.31	0/642	0.44	0/848
47	Z	0.29	0/635	0.36	0/848
48	1	0.25	0/496	0.29	0/660
49	2	0.30	0/453	0.37	0/605
50	3	0.14	0/475	0.28	0/633
51	4	0.34	0/440	0.38	0/588
52	5	0.25	0/424	0.41	0/565
53	6	0.36	0/380	0.37	0/498
54	7	0.33	0/513	0.37	0/676
55	8	0.30	0/303	0.37	0/397
All	All	0.33	0/154881	0.37	1/231867 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
36	O	0	1
54	7	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	512	G	O4'-C1'-N9	5.47	116.41	108.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
54	7	30	ARG	Peptide
36	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	242	0
2	b	1754	0	1782	28	0
3	c	1624	0	1696	17	0
4	d	1643	0	1707	40	0
5	e	1152	0	1196	17	0
6	f	839	0	833	16	0
7	g	1191	0	1245	15	0
8	h	979	0	1031	11	0
9	i	1022	0	1070	19	0
10	j	786	0	828	13	0
11	k	877	0	884	9	0
12	l	942	0	999	8	0
13	m	891	0	952	9	0
14	n	805	0	844	9	0
15	o	714	0	734	3	0
16	p	643	0	661	7	0
17	q	641	0	682	4	0
18	r	446	0	472	6	0
19	s	663	0	688	8	0
20	t	670	0	719	15	0
21	u	460	0	486	5	0
22	w	1591	0	817	8	0
23	x	1625	0	829	2	0
24	v	255	0	129	0	0
25	A	61097	0	30752	210	0
26	B	2572	0	1301	11	0
27	C	2082	0	2154	14	0
28	D	1566	0	1618	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	E	1552	0	1619	11	0
30	F	1410	0	1444	28	0
31	G	1323	0	1371	9	0
32	H	303	0	327	5	0
33	L	1129	0	1162	9	0
34	M	946	0	1023	9	0
35	N	1052	0	1127	8	0
36	O	1075	0	1146	4	0
37	P	945	0	989	6	0
38	Q	892	0	923	5	0
39	R	917	0	962	6	0
40	S	947	0	1019	4	0
41	T	816	0	839	1	0
42	U	857	0	922	2	0
43	V	738	0	807	0	0
44	W	779	0	831	11	0
45	X	753	0	780	5	0
46	Y	634	0	653	3	0
47	Z	625	0	652	3	0
48	1	495	0	526	2	0
49	2	449	0	488	4	0
50	3	468	0	460	6	0
51	4	434	0	445	4	0
52	5	417	0	451	1	0
53	6	377	0	418	1	0
54	7	504	0	572	1	0
55	8	302	0	340	4	0
56	4	1	0	0	0	0
56	7	1	0	0	0	0
56	A	555	0	0	0	0
56	B	10	0	0	0	0
56	C	3	0	0	0	0
56	D	1	0	0	0	0
56	N	1	0	0	0	0
56	P	1	0	0	0	0
56	S	1	0	0	0	0
56	V	1	0	0	0	0
56	a	132	0	0	0	0
56	l	1	0	0	0	0
56	n	1	0	0	0	0
56	v	2	0	0	0	0
56	w	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	x	2	0	0	0	0
57	a	44	0	20	3	0
58	w	11	0	8	0	0
59	3	1	0	0	0	0
59	8	1	0	0	0	0
60	4	1	0	0	0	0
60	8	1	0	0	1	0
60	A	247	0	0	2	0
60	B	4	0	0	0	0
60	C	1	0	0	0	0
60	D	1	0	0	0	0
60	E	1	0	0	1	0
60	N	1	0	0	0	0
60	P	1	0	0	0	0
60	R	1	0	0	0	0
60	T	1	0	0	0	0
60	V	1	0	0	0	0
60	Z	1	0	0	1	0
60	a	37	0	0	0	0
60	n	1	0	0	0	0
All	All	144543	0	95961	826	0

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

All (826) 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)
1:a:1009:U:H3	1:a:1020:G:H1	0.98	0.96
25:A:544:C:O2	25:A:549:G:N2	2.01	0.94
25:A:284:U:H3	25:A:356:G:H1	1.18	0.90
1:a:137:U:H3	1:a:226:G:H1	1.19	0.87
4:d:58:LYS:NZ	4:d:69:GLU:OE2	2.09	0.85
25:A:544:C:N3	25:A:549:G:N1	2.25	0.85
25:A:280:U:O4	25:A:361:G:N2	2.12	0.82
2:b:119:THR:O	2:b:123:ASP:HB2	1.79	0.81
25:A:713:G:H21	25:A:718:A:H62	1.29	0.80
9:i:47:VAL:HG13	9:i:80:ARG:HD2	1.63	0.80
33:L:58:ASN:HD21	33:L:128:ASN:HD22	1.30	0.79
25:A:2107:G:N2	25:A:2182:U:O2	2.17	0.77
25:A:2831:G:OP2	28:D:59:ARG:NH2	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:W:4:LYS:HD2	44:W:83:VAL:HB	1.67	0.76
1:a:1026:G:O6	1:a:1035:A:N1	2.19	0.76
9:i:88:MET:HE3	9:i:98:LEU:HD12	1.67	0.75
1:a:1027:C:N4	1:a:1033:G:O6	2.18	0.75
1:a:458:U:H3	1:a:474:G:H1	1.32	0.75
1:a:1009:U:O2	1:a:1020:G:N2	2.19	0.75
1:a:427:U:OP1	4:d:13:ARG:NH2	2.19	0.74
5:e:153:VAL:HG21	8:h:99:LEU:HD22	1.71	0.72
25:A:2120:G:N1	25:A:2179:C:N4	2.37	0.72
1:a:1166:G:N1	1:a:1169:A:OP2	2.20	0.72
25:A:275:C:O2	25:A:362:A:N6	2.23	0.72
25:A:2116:G:H1	25:A:2164:C:H42	1.37	0.72
25:A:2136:G:H22	25:A:2156:G:H1'	1.55	0.71
25:A:2189:U:H2'	25:A:2190:G:H8	1.56	0.70
9:i:123:ARG:NH1	9:i:124:ARG:O	2.24	0.70
25:A:881:G:H1	25:A:895:U:H3	1.37	0.70
4:d:19:LEU:HB2	4:d:21:LEU:HD22	1.75	0.69
28:D:2:ILE:HD11	28:D:84:LEU:HD12	1.74	0.69
4:d:124:MET:HG3	4:d:146:ARG:HG3	1.73	0.69
1:a:460:A:H2'	1:a:461:A:C8	2.28	0.68
45:X:42:LEU:HD13	45:X:47:VAL:HG21	1.75	0.68
3:c:14:ILE:HG22	3:c:15:VAL:HG23	1.74	0.68
1:a:673:A:H2'	1:a:674:G:C8	2.28	0.68
25:A:1649:G:O2'	37:P:106:ASP:OD2	2.11	0.68
21:u:44:GLU:OE1	21:u:47:ARG:NH2	2.27	0.68
22:w:19:G:O2'	25:A:896:A:N1	2.23	0.68
1:a:1179:A:OP2	9:i:95:ARG:NH2	2.28	0.67
49:2:27:LEU:O	49:2:38:ARG:NH1	2.26	0.67
7:g:68:ASN:HD22	7:g:130:ASN:HD21	1.42	0.67
25:A:2115:G:N2	25:A:2118:U:OP2	2.28	0.67
6:f:45:ARG:NH2	6:f:102:MET:SD	2.68	0.67
10:j:8:ILE:HG12	10:j:100:ILE:HG12	1.76	0.67
30:F:162:SER:OG	30:F:165:GLU:OE1	2.13	0.67
46:Y:70:GLU:HG3	46:Y:72:LYS:HE2	1.75	0.67
54:7:17:THR:HG21	54:7:49:MET:HE1	1.77	0.67
1:a:1147:C:HO2'	9:i:7:TYR:HH	1.41	0.67
39:R:3:ASN:HA	39:R:6:LYS:HE3	1.77	0.67
7:g:28:ASN:OD1	7:g:36:LYS:NZ	2.28	0.67
25:A:2105:U:H2'	25:A:2106:U:C6	2.30	0.66
25:A:2128:G:N3	25:A:2173:A:O2'	2.28	0.66
1:a:4:U:H2'	1:a:5:U:H5"	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:2:6:LYS:NZ	49:2:37:GLU:OE1	2.29	0.66
1:a:459:A:H2'	1:a:460:A:C8	2.31	0.66
6:f:15:SER:HA	6:f:18:VAL:HG23	1.78	0.65
6:f:90:MET:HE1	18:r:61:ARG:HD3	1.79	0.65
1:a:1057:G:O2'	3:c:188:GLU:OE1	2.14	0.65
10:j:84:VAL:HG12	10:j:88:MET:HE1	1.78	0.65
25:A:881:G:O6	25:A:895:U:O4	2.14	0.65
37:P:30:ARG:NH1	37:P:74:GLU:OE2	2.29	0.65
11:k:67:ALA:HB2	11:k:96:THR:HG23	1.78	0.65
9:i:106:ARG:NH1	9:i:107:ASP:O	2.30	0.65
25:A:2144:G:H1'	25:A:2147:A:H61	1.62	0.65
1:a:137:U:O2	1:a:226:G:N2	2.26	0.65
1:a:426:U:OP1	4:d:33:LYS:NZ	2.28	0.65
25:A:2134:A:H61	25:A:2156:G:H2'	1.62	0.64
20:t:39:ILE:HD11	20:t:83:ILE:HG13	1.78	0.64
25:A:2120:G:C6	25:A:2179:C:N4	2.66	0.64
19:s:11:ILE:HD11	19:s:15:LEU:HD22	1.79	0.64
47:Z:74:ARG:NH2	47:Z:76:GLU:OE2	2.31	0.64
16:p:4:ILE:HG12	16:p:21:VAL:HG22	1.80	0.63
1:a:1314:C:OP1	19:s:6:LYS:NZ	2.25	0.63
1:a:195:A:H2'	1:a:196:A:C8	2.33	0.63
1:a:1447:A:H5"	1:a:1448:C:H5	1.63	0.63
44:W:18:ASP:HB2	44:W:21:LYS:HD2	1.80	0.63
2:b:20:THR:HA	2:b:39:HIS:CE1	2.34	0.63
4:d:87:GLY:HA3	4:d:197:GLU:HG3	1.79	0.63
11:k:17:SER:HA	11:k:79:ILE:HA	1.79	0.63
25:A:2134:A:O2'	25:A:2159:G:N3	2.32	0.63
25:A:273:G:O6	25:A:274:C:N4	2.32	0.62
20:t:5:LYS:O	20:t:5:LYS:HD3	1.98	0.62
25:A:1802:A:H2'	25:A:1803:A:C8	2.33	0.62
25:A:10:A:H2	25:A:2629:U:H3	1.47	0.62
1:a:542:G:OP1	4:d:10:LYS:NZ	2.33	0.62
3:c:35:SER:OG	3:c:59:ARG:NH2	2.32	0.62
1:a:1180:A:OP2	9:i:99:ARG:NH2	2.33	0.62
6:f:21:MET:HA	6:f:24:ARG:HD3	1.82	0.62
1:a:634:C:H2'	1:a:635:A:H8	1.63	0.62
11:k:36:ASP:OD1	11:k:37:ARG:N	2.32	0.62
19:s:50:ALA:HB1	19:s:57:HIS:HB3	1.82	0.62
1:a:208:U:H2'	1:a:210:C:H1'	1.80	0.61
8:h:18:GLN:HE21	8:h:70:ALA:HB1	1.64	0.61
25:A:2131:U:H5'	25:A:2132:U:H5"	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:35:GLU:HG3	27:C:64:ILE:HD11	1.81	0.61
30:F:116:GLY:HA3	30:F:178:ARG:HB3	1.83	0.61
42:U:4:ILE:HG12	42:U:106:VAL:HG22	1.81	0.61
1:a:1397:C:OP2	5:e:29:ARG:NH2	2.34	0.61
7:g:57:SER:OG	7:g:60:GLU:OE1	2.19	0.61
29:E:176:ASP:OD1	29:E:179:SER:OG	2.18	0.61
1:a:946:A:H2'	1:a:947:G:C8	2.36	0.61
35:N:89:VAL:HG11	35:N:123:ARG:HH21	1.66	0.60
1:a:1124:G:OP1	10:j:37:ARG:NH1	2.34	0.60
7:g:16:PRO:HG3	9:i:43:THR:HG22	1.83	0.60
26:B:1:U:H2'	26:B:2:G:H8	1.66	0.60
1:a:1323:G:H2'	1:a:1324:A:C8	2.36	0.60
33:L:45:THR:HB	33:L:48:VAL:HG12	1.83	0.60
1:a:1356:G:H2'	1:a:1357:A:C8	2.37	0.60
31:G:46:ALA:HB3	31:G:49:THR:HB	1.83	0.60
9:i:42:GLU:HG3	9:i:46:MET:HE1	1.84	0.60
25:A:276:U:H2'	25:A:277:G:C8	2.37	0.60
1:a:257:G:H2'	1:a:258:G:H8	1.66	0.60
1:a:154:U:H2'	1:a:155:A:H8	1.66	0.60
25:A:856:G:H2'	25:A:857:G:C8	2.37	0.60
33:L:19:ASP:O	33:L:23:LYS:NZ	2.35	0.60
2:b:68:LEU:HD11	2:b:92:VAL:HG23	1.84	0.59
12:l:33:VAL:HG22	12:l:79:VAL:HG12	1.85	0.59
17:q:58:VAL:HG22	17:q:80:GLU:HB2	1.84	0.59
44:W:86:ARG:NH2	44:W:100:SER:OG	2.34	0.59
25:A:534:U:O2'	40:S:49:ASP:OD2	2.15	0.59
1:a:492:C:H2'	1:a:493:A:C8	2.37	0.59
28:D:178:VAL:HB	28:D:188:LEU:HD12	1.85	0.59
1:a:1218:C:H2'	1:a:1219:A:C8	2.38	0.59
25:A:1434:A:H2'	25:A:1435:G:C8	2.37	0.59
25:A:1434:A:H2'	25:A:1435:G:H8	1.68	0.58
1:a:1086:U:H3	1:a:1099:G:H22	1.52	0.58
3:c:55:ILE:HG23	3:c:68:ILE:HG22	1.85	0.58
22:w:23:A:H2'	22:w:24:G:C8	2.38	0.58
25:A:1417:C:HO2'	25:A:1587:G:HO2'	1.49	0.58
19:s:11:ILE:HD12	19:s:38:SER:HB3	1.83	0.58
1:a:404:G:O6	4:d:2:ALA:N	2.36	0.58
6:f:37:HIS:HB3	6:f:97:THR:HG22	1.85	0.58
51:4:52:ARG:HH21	51:4:54:VAL:HG12	1.68	0.58
22:w:20:U:N3	22:w:59:U:OP1	2.36	0.58
1:a:201:G:H21	1:a:469:C:H1'	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1026:G:O2'	1:a:1027:C:OP1	2.21	0.58
25:A:1843:C:H4'	27:C:251:GLN:HE22	1.68	0.58
27:C:165:VAL:HG21	27:C:181:MET:HE1	1.85	0.58
1:a:490:C:H2'	1:a:491:G:H8	1.68	0.58
16:p:18:GLN:OE1	16:p:35:ARG:NE	2.28	0.58
1:a:410:G:OP1	4:d:26:ARG:NH2	2.36	0.58
1:a:1023:U:H2'	1:a:1024:G:C8	2.39	0.58
27:C:2:ALA:N	27:C:20:VAL:O	2.37	0.57
1:a:324:G:N1	1:a:327:A:OP2	2.36	0.57
1:a:407:U:O2'	4:d:113:GLU:OE2	2.20	0.57
1:a:746:A:H2'	1:a:747:A:C8	2.40	0.57
1:a:355:C:O2'	1:a:388:G:N2	2.37	0.57
1:a:178:C:H2'	1:a:179:A:H8	1.69	0.57
29:E:108:ILE:HG23	35:N:1:MET:HE1	1.87	0.57
3:c:125:GLU:OE2	3:c:190:HIS:N	2.38	0.57
44:W:81:ASP:OD2	44:W:82:ARG:N	2.38	0.57
1:a:323:U:H2'	1:a:324:G:O4'	2.04	0.57
5:e:15:LEU:HD12	5:e:37:THR:HG22	1.86	0.57
25:A:126:A:OP1	53:6:45:SER:OG	2.19	0.57
25:A:2184:A:H2'	25:A:2185:U:C6	2.41	0.56
27:C:100:GLU:OE2	27:C:102:ARG:HD2	2.05	0.56
1:a:490:C:H2'	1:a:491:G:C8	2.41	0.56
14:n:34:VAL:O	14:n:41:ARG:NH2	2.37	0.56
1:a:335:C:H2'	1:a:336:A:H8	1.71	0.56
1:a:456:A:H2'	1:a:457:G:C8	2.41	0.56
50:3:58:ASP:OD1	50:3:62:LYS:NZ	2.34	0.56
1:a:175:C:H2'	1:a:176:C:C6	2.41	0.56
7:g:9:GLN:NE2	7:g:10:ARG:O	2.39	0.56
8:h:43:GLU:HG3	8:h:101:ILE:HD13	1.87	0.56
25:A:888:C:H2'	25:A:889:C:C6	2.40	0.56
1:a:459:A:H2'	1:a:460:A:H8	1.69	0.56
1:a:1175:G:H2'	1:a:1176:A:H8	1.70	0.56
7:g:69:VAL:HG21	7:g:104:ILE:HD11	1.88	0.56
38:Q:94:ARG:NH1	38:Q:97:PHE:O	2.35	0.56
1:a:269:C:H2'	1:a:270:A:C8	2.40	0.56
1:a:946:A:H2'	1:a:947:G:H8	1.70	0.56
4:d:104:ARG:HH21	4:d:171:LEU:HD23	1.71	0.56
25:A:2190:G:H2'	25:A:2191:A:C8	2.40	0.56
1:a:458:U:O2	1:a:474:G:N2	2.31	0.56
6:f:19:PRO:O	6:f:22:ILE:HB	2.05	0.56
1:a:154:U:H2'	1:a:155:A:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:D:1:MET:HE2	28:D:205:PRO:HG2	1.88	0.55
29:E:1:MET:N	29:E:14:VAL:O	2.40	0.55
11:k:112:ASP:HB3	21:u:2:PRO:HD2	1.87	0.55
25:A:2180:U:O5'	25:A:2180:U:H6	1.90	0.55
25:A:776:G:N2	60:A:3613:HOH:O	2.34	0.55
1:a:475:C:H2'	1:a:476:U:C6	2.42	0.55
25:A:2120:G:H2'	25:A:2121:G:C8	2.41	0.55
25:A:2139:U:H2'	25:A:2140:G:C8	2.42	0.55
25:A:2189:U:H2'	25:A:2190:G:C8	2.40	0.55
25:A:2305:U:C2	30:F:151:GLY:HA3	2.41	0.55
1:a:65:A:N7	1:a:381:C:N4	2.54	0.55
1:a:1027:C:H2'	1:a:1028:C:C5	2.42	0.55
25:A:1469:A:H2'	25:A:1470:A:C8	2.41	0.55
1:a:460:A:H2'	1:a:461:A:H8	1.73	0.54
25:A:2295:C:OP1	38:Q:10:ARG:NH1	2.40	0.54
25:A:2547:A:H2'	25:A:2548:U:C6	2.43	0.54
25:A:2112:G:H5'	25:A:2113:U:C5	2.42	0.54
25:A:2327:A:H2'	25:A:2328:A:C8	2.41	0.54
1:a:82:G:O2'	1:a:83:C:O4'	2.18	0.54
25:A:1007:C:OP1	33:L:37:ARG:NH1	2.40	0.54
1:a:385:C:H2'	1:a:386:C:C6	2.43	0.54
1:a:1034:G:H2'	1:a:1035:A:H5'	1.90	0.54
22:w:43:C:H2'	22:w:44:G:C8	2.42	0.54
4:d:170:TRP:CE2	4:d:186:PRO:HB3	2.43	0.54
5:e:115:LEU:HD13	5:e:123:VAL:HG11	1.88	0.54
1:a:1378:C:H5"	7:g:5:ARG:HH12	1.72	0.54
25:A:285:G:O6	25:A:355:U:O2	2.25	0.54
25:A:1590:A:H2'	25:A:1591:A:C8	2.43	0.54
44:W:50:PRO:HA	44:W:54:GLN:HG3	1.89	0.54
50:3:41:HIS:CD2	50:3:43:PHE:H	2.25	0.54
1:a:1167:A:O2'	1:a:1169:A:N7	2.40	0.54
8:h:22:LYS:O	8:h:65:TYR:OH	2.24	0.54
39:R:43:PHE:CE2	39:R:63:LYS:HE2	2.43	0.54
25:A:1141:U:H4'	25:A:1142:A:O4'	2.07	0.54
2:b:119:THR:O	2:b:123:ASP:CB	2.55	0.53
31:G:7:ALA:O	31:G:69:ARG:HD2	2.08	0.53
8:h:29:SER:HB3	8:h:57:PRO:HB2	1.91	0.53
1:a:1035:A:O2'	1:a:1037:C:N4	2.41	0.53
30:F:11:GLU:HA	30:F:14:LYS:HE2	1.90	0.53
46:Y:65:GLY:HA2	46:Y:85:GLU:HB2	1.90	0.53
10:j:28:THR:HA	10:j:31:ARG:HE	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:545:C:H5'	4:d:69:GLU:HG3	1.91	0.53
25:A:358:U:H2'	25:A:359:G:C8	2.44	0.53
19:s:35:SER:OG	19:s:38:SER:OG	2.26	0.53
25:A:713:G:N2	25:A:718:A:H62	2.01	0.53
1:a:80:A:H1'	1:a:81:A:C2	2.43	0.53
1:a:382:A:H2'	1:a:383:A:C8	2.44	0.53
1:a:478:A:H2'	1:a:479:U:O4'	2.09	0.53
4:d:62:ARG:HH21	4:d:68:LEU:HA	1.74	0.53
5:e:13:GLU:HG2	5:e:39:VAL:HG12	1.91	0.52
13:m:52:GLN:O	13:m:56:LEU:HD13	2.10	0.52
1:a:77:A:H2'	1:a:78:A:C8	2.44	0.52
6:f:88:MET:HE3	18:r:65:LEU:HD13	1.90	0.52
25:A:2135:A:N6	25:A:2156:G:O2'	2.42	0.52
26:B:76:G:OP1	45:X:9:ARG:NH1	2.38	0.52
30:F:38:MET:HE3	30:F:53:ALA:HB1	1.90	0.52
1:a:202:G:H2'	1:a:203:G:H8	1.74	0.52
5:e:36:LEU:HD22	5:e:134:ILE:HD13	1.92	0.52
25:A:2181:U:H6	25:A:2181:U:O5'	1.92	0.52
26:B:32:U:C2	26:B:51:G:N2	2.78	0.52
31:G:73:ASN:O	31:G:76:VAL:HG12	2.10	0.52
33:L:58:ASN:HD21	33:L:128:ASN:ND2	2.04	0.52
25:A:279:A:N6	25:A:361:G:O2'	2.42	0.52
25:A:2144:G:C2	25:A:2146:C:H1'	2.45	0.52
34:M:70:ARG:HG2	34:M:76:VAL:HG12	1.92	0.52
1:a:1314:C:H2'	1:a:1315:U:H6	1.75	0.52
10:j:41:PRO:HA	10:j:72:ARG:HG2	1.91	0.52
29:E:106:LYS:HG2	29:E:200:LEU:HD13	1.91	0.52
3:c:86:LYS:O	3:c:90:VAL:HG23	2.10	0.52
3:c:114:LYS:HD3	3:c:185:ASN:ND2	2.25	0.52
32:H:12:LEU:HD13	32:H:19:VAL:HG21	1.92	0.52
1:a:538:G:OP2	12:l:112:GLN:NE2	2.42	0.52
3:c:47:LEU:HD21	3:c:87:LEU:HD21	1.91	0.52
9:i:84:THR:HG21	9:i:103:PHE:HB3	1.90	0.52
16:p:48:GLU:OE1	16:p:51:ARG:NH2	2.39	0.52
25:A:277:G:H4'	25:A:278:A:O5'	2.10	0.52
25:A:593:U:H2'	25:A:594:U:C6	2.44	0.52
25:A:2113:U:O4	25:A:2119:A:N6	2.43	0.52
1:a:76:G:N1	1:a:93:U:C2	2.77	0.52
4:d:50:ASP:OD2	4:d:54:GLN:NE2	2.29	0.52
50:3:57:VAL:O	50:3:61:ASN:ND2	2.43	0.52
4:d:118:VAL:HG22	4:d:123:ILE:HG13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:45:ARG:NH1	5:e:73:ASN:OD1	2.43	0.52
5:e:105:ILE:HD13	5:e:123:VAL:HG12	1.92	0.52
18:r:42:SER:HB2	18:r:52:GLN:HE21	1.74	0.52
25:A:2190:G:H2'	25:A:2191:A:H8	1.75	0.52
1:a:73:C:H2'	1:a:74:A:C8	2.45	0.52
2:b:68:LEU:HD23	2:b:161:LEU:HD21	1.92	0.52
25:A:1114:C:H2'	25:A:1115:G:C8	2.44	0.52
9:i:19:VAL:HG22	9:i:65:ILE:HG12	1.92	0.51
25:A:2127:G:H21	25:A:2173:A:H1'	1.75	0.51
1:a:728:A:H2'	1:a:729:A:C8	2.45	0.51
2:b:6:MET:HG2	2:b:43:LEU:HD22	1.92	0.51
25:A:2108:A:H2'	25:A:2109:U:O4'	2.10	0.51
25:A:2120:G:H1	25:A:2179:C:N4	2.07	0.51
1:a:216:U:H2'	1:a:217:C:C6	2.45	0.51
51:4:46:ASP:OD1	51:4:46:ASP:N	2.41	0.51
1:a:216:U:H2'	1:a:217:C:H6	1.75	0.51
1:a:520:A:O2'	12:l:70:GLU:OE2	2.17	0.51
25:A:1542:U:H2'	25:A:1543:G:O4'	2.10	0.51
25:A:2328:A:H2'	25:A:2329:U:C6	2.45	0.51
25:A:1:G:H2'	25:A:2:G:H8	1.75	0.51
1:a:269:C:H2'	1:a:270:A:H8	1.75	0.51
26:B:1:U:H2'	26:B:2:G:C8	2.44	0.51
10:j:5:ARG:HH12	10:j:7:ARG:HE	1.57	0.51
25:A:364:C:H2'	25:A:365:U:C6	2.46	0.51
25:A:414:C:H2'	25:A:415:A:C8	2.45	0.51
1:a:409:U:OP1	4:d:23:SER:OG	2.22	0.51
1:a:993:G:O2'	1:a:995:C:N4	2.30	0.51
6:f:88:MET:HE2	18:r:64:TYR:CD2	2.46	0.51
22:w:64:A:O2'	22:w:65:G:OP1	2.24	0.51
25:A:2131:U:O5'	25:A:2133:G:H4'	2.11	0.51
25:A:2291:U:H2'	25:A:2292:U:C6	2.46	0.51
1:a:5:U:OP1	1:a:5:U:H6	1.92	0.51
1:a:999:C:H2'	1:a:1000:A:H8	1.76	0.51
1:a:144:G:H2'	1:a:145:G:C8	2.46	0.50
4:d:140:ASN:N	4:d:182:PHE:O	2.40	0.50
7:g:47:LEU:HB3	7:g:58:GLU:HG2	1.93	0.50
7:g:136:LYS:NZ	7:g:140:ASP:OD1	2.38	0.50
1:a:1009:U:O4	1:a:1020:G:O6	2.28	0.50
25:A:2106:U:H2'	25:A:2107:G:H8	1.76	0.50
25:A:2189:U:O2'	25:A:2190:G:OP1	2.25	0.50
25:A:2191:A:H2'	25:A:2192:U:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:F:147:ASP:OD1	30:F:148:ARG:N	2.43	0.50
39:R:5:ILE:O	39:R:9:GLU:HG3	2.12	0.50
7:g:78:ARG:NH1	7:g:79:ARG:O	2.44	0.50
25:A:1028:A:H2'	25:A:1029:A:C8	2.47	0.50
1:a:714:G:H2'	1:a:715:A:C8	2.47	0.50
25:A:2106:U:H2'	25:A:2107:G:C8	2.46	0.50
27:C:161:TYR:HB3	27:C:194:GLU:HG2	1.94	0.50
1:a:626:G:H2'	1:a:627:G:C8	2.47	0.50
1:a:1073:U:O2	2:b:103:ASN:ND2	2.45	0.50
25:A:2144:G:N2	25:A:2146:C:O2'	2.44	0.50
1:a:193:C:H2'	1:a:194:C:H6	1.77	0.50
2:b:4:VAL:HG11	2:b:50:PHE:HE2	1.75	0.50
25:A:2074:U:H2'	25:A:2075:U:C6	2.47	0.50
30:F:119:ALA:O	30:F:167:ARG:NH1	2.33	0.50
1:a:1023:U:H2'	1:a:1024:G:N7	2.27	0.50
4:d:34:ILE:HD12	4:d:34:ILE:H	1.76	0.50
15:o:18:ASP:HB3	15:o:21:ASP:HB2	1.93	0.50
1:a:212:G:C2	1:a:213:G:C8	3.00	0.49
1:a:1030:U:H5'	1:a:1031:C:H5"	1.93	0.49
27:C:69:ARG:HB3	27:C:129:THR:HG21	1.94	0.49
4:d:57:GLU:OE1	4:d:200:ILE:HG13	2.12	0.49
25:A:2243:U:H2'	25:A:2244:U:C6	2.47	0.49
25:A:1353:A:H2'	25:A:1354:A:C8	2.48	0.49
1:a:1062:U:H2'	1:a:1063:C:C6	2.47	0.49
1:a:1071:C:H2'	1:a:1072:G:H8	1.78	0.49
44:W:41:LEU:HD23	44:W:62:GLU:HG3	1.94	0.49
20:t:29:ARG:O	20:t:33:LYS:HG2	2.12	0.49
25:A:272:A:H2'	25:A:273:G:C8	2.47	0.49
1:a:539:A:H2'	1:a:540:G:C8	2.48	0.49
1:a:1530:G:N7	21:u:46:LYS:NZ	2.61	0.49
2:b:31:ILE:HG21	2:b:39:HIS:HD2	1.77	0.49
10:j:10:LEU:HD22	10:j:98:VAL:HG22	1.95	0.49
29:E:168:ASP:OD1	29:E:170:ARG:NH1	2.45	0.49
1:a:427:U:P	4:d:13:ARG:HH22	2.35	0.49
1:a:1218:C:H2'	1:a:1219:A:H8	1.76	0.49
1:a:1287:A:H2'	1:a:1288:A:C8	2.47	0.49
20:t:20:HIS:CE1	20:t:24:ARG:HH12	2.30	0.49
30:F:131:GLY:HA2	30:F:153:ASP:HA	1.93	0.49
25:A:877:A:H1'	25:A:900:A:H61	1.78	0.49
25:A:2795:C:H2'	25:A:2796:U:C6	2.47	0.49
1:a:1147:C:O2	9:i:18:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1518:MA6:H92	1:a:1519:MA6:N6	2.28	0.49
10:j:7:ARG:HD3	10:j:75:ASP:OD1	2.12	0.49
25:A:359:G:H2'	25:A:360:U:O4'	2.12	0.49
1:a:1008:U:H3'	1:a:1009:U:H5"	1.95	0.49
1:a:1020:G:H2'	1:a:1021:A:H8	1.78	0.49
22:w:23:A:H2'	22:w:24:G:H8	1.76	0.49
25:A:948:C:H1'	25:A:984:A:C8	2.48	0.49
1:a:131:A:H2'	1:a:132:C:C6	2.48	0.48
1:a:1314:C:H2'	1:a:1315:U:C6	2.48	0.48
25:A:2123:G:H1'	25:A:2176:A:N1	2.28	0.48
27:C:29:PRO:HG2	27:C:34:LEU:HD11	1.95	0.48
27:C:71:LYS:NZ	27:C:100:GLU:OE1	2.46	0.48
1:a:1273:C:H2'	1:a:1274:A:O4'	2.13	0.48
57:a:3133:T8B:O6	57:a:3133:T8B:O7	2.31	0.48
2:b:20:THR:HA	2:b:39:HIS:HE1	1.76	0.48
7:g:27:VAL:HG22	7:g:43:VAL:HG11	1.95	0.48
25:A:627:A:OP1	35:N:78:ARG:NH2	2.30	0.48
1:a:634:C:H2'	1:a:635:A:C8	2.47	0.48
4:d:170:TRP:CZ3	4:d:190:ASP:HB3	2.48	0.48
25:A:276:U:O2'	25:A:277:G:O4'	2.29	0.48
25:A:2102:G:H22	25:A:2187:U:H3	1.62	0.48
28:D:183:GLU:HG3	28:D:184:ARG:HG3	1.96	0.48
38:Q:80:GLU:O	38:Q:84:GLU:HG2	2.14	0.48
11:k:20:VAL:HG23	11:k:83:GLU:HB2	1.95	0.48
11:k:64:GLN:HG3	11:k:99:ALA:HB2	1.94	0.48
25:A:61:C:OP2	48:1:47:ARG:NH2	2.46	0.48
25:A:2111:U:H1'	25:A:2118:U:H4'	1.94	0.48
11:k:109:ASN:OD1	11:k:110:ILE:N	2.46	0.48
26:B:51:G:OP1	38:Q:63:LYS:NZ	2.45	0.48
1:a:70:U:O2'	1:a:94:G:N7	2.36	0.48
2:b:67:ILE:HG22	2:b:160:ALA:HB3	1.95	0.48
17:q:44:LEU:HD21	17:q:73:TRP:CG	2.49	0.48
25:A:191:A:H2'	25:A:192:C:C6	2.49	0.48
1:a:1178:G:OP2	9:i:95:ARG:NH1	2.47	0.48
57:a:3133:T8B:H18	57:a:3133:T8B:O12	2.14	0.48
22:w:75:C:H2'	22:w:76:A:C8	2.49	0.48
1:a:1002:G:C2	1:a:1003:G:H1'	2.49	0.47
25:A:881:G:O6	25:A:895:U:C4	2.67	0.47
25:A:2788:C:H2'	25:A:2789:C:C6	2.48	0.47
30:F:13:VAL:O	30:F:17:MET:HG2	2.14	0.47
55:8:2:LYS:NZ	55:8:32:LYS:O	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:121:THR:HG23	3:c:189:ALA:HB2	1.96	0.47
1:a:1121:U:H2'	1:a:1122:U:C6	2.49	0.47
1:a:1144:G:N2	1:a:1146:A:H62	2.12	0.47
26:B:48:U:H2'	26:B:49:C:C6	2.49	0.47
36:O:11:LYS:NZ	36:O:87:GLY:O	2.44	0.47
1:a:373:A:C2	1:a:374:A:C8	3.02	0.47
1:a:401:C:O2'	1:a:621:A:N3	2.38	0.47
8:h:54:ASP:OD1	8:h:54:ASP:N	2.48	0.47
1:a:147:G:H2'	1:a:148:G:C8	2.49	0.47
1:a:219:U:H2'	1:a:220:G:H8	1.79	0.47
1:a:908:A:H2'	1:a:909:A:C8	2.50	0.47
1:a:999:C:H2'	1:a:1000:A:C8	2.50	0.47
1:a:1153:G:OP1	10:j:16:ARG:NH2	2.47	0.47
2:b:55:ALA:HA	2:b:58:ASN:HD21	1.80	0.47
1:a:17:U:H2'	1:a:18:C:C6	2.49	0.47
1:a:1026:G:C6	1:a:1035:A:N1	2.81	0.47
1:a:1316:G:N1	1:a:1319:A:OP2	2.40	0.47
4:d:85:ASN:HB2	4:d:88:GLU:OE1	2.14	0.47
20:t:82:GLN:O	20:t:85:LYS:HG2	2.15	0.47
1:a:1530:G:O6	21:u:46:LYS:NZ	2.45	0.47
9:i:52:LEU:HD22	9:i:63:LEU:HD11	1.95	0.47
25:A:544:C:H4'	25:A:545:U:C4	2.50	0.47
25:A:1032:A:H1'	55:8:23:ILE:HD13	1.96	0.47
25:A:1153:C:OP1	40:S:92:ARG:NH2	2.40	0.47
25:A:1746:A:H2'	25:A:1747:U:C6	2.49	0.47
46:Y:11:ARG:NH1	46:Y:12:ASN:OD1	2.47	0.47
1:a:344:A:H5"	1:a:345:C:H5	1.79	0.47
1:a:1176:A:H2'	1:a:1177:G:C8	2.50	0.47
1:a:1356:G:H2'	1:a:1357:A:H8	1.77	0.47
1:a:1437:A:H5"	20:t:29:ARG:HH12	1.79	0.47
10:j:66:GLU:HB2	14:n:99:ALA:HB2	1.96	0.47
25:A:144:A:H2'	25:A:145:C:C6	2.50	0.47
30:F:116:GLY:O	30:F:178:ARG:NH1	2.48	0.47
25:A:1405:U:H2'	25:A:1406:U:C6	2.50	0.47
31:G:4:VAL:O	31:G:69:ARG:HD3	2.14	0.47
49:2:23:THR:HG23	49:2:47:MET:HB2	1.97	0.47
1:a:1121:U:H2'	1:a:1122:U:H6	1.78	0.47
1:a:1253:G:H2'	1:a:1254:A:H8	1.79	0.47
5:e:41:ASP:HB2	5:e:45:ARG:HB2	1.96	0.47
5:e:76:LEU:HA	5:e:82:GLN:HE21	1.80	0.47
28:D:1:MET:HG2	28:D:2:ILE:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8:16:ILE:HD13	55:8:25:VAL:HG22	1.96	0.47
1:a:945:G:C2	1:a:946:A:C8	3.03	0.46
4:d:29:ASP:HA	4:d:34:ILE:HD11	1.97	0.46
25:A:2105:U:H2'	25:A:2106:U:H6	1.77	0.46
2:b:97:LEU:HD21	2:b:147:SER:HB2	1.98	0.46
3:c:112:ASP:O	3:c:116:VAL:HG23	2.15	0.46
25:A:849:A:H2'	25:A:850:U:C6	2.51	0.46
1:a:270:A:H2'	1:a:271:C:C6	2.50	0.46
1:a:456:A:H2'	1:a:457:G:H8	1.78	0.46
4:d:73:ARG:HD3	4:d:77:LYS:NZ	2.31	0.46
25:A:2146:C:O2'	25:A:2147:A:N7	2.46	0.46
1:a:626:G:H2'	1:a:627:G:H8	1.80	0.46
25:A:1294:U:O2'	37:P:23:ASN:ND2	2.48	0.46
25:A:1720:U:H2'	25:A:1721:G:O4'	2.16	0.46
34:M:1:MET:HG3	34:M:67:LYS:HD3	1.97	0.46
20:t:78:ASN:O	20:t:82:GLN:HG2	2.15	0.46
25:A:1590:A:H2'	25:A:1591:A:H8	1.80	0.46
25:A:1771:C:H2'	25:A:1772:A:C8	2.51	0.46
1:a:524:G:H2'	1:a:525:C:C6	2.51	0.46
8:h:76:GLN:HE21	8:h:128:TYR:HD2	1.62	0.46
12:l:59:ASN:OD1	12:l:61:PHE:HD2	1.99	0.46
31:G:9:VAL:HG22	31:G:50:LEU:HB2	1.97	0.46
25:A:1682:G:H2'	25:A:1683:U:C6	2.51	0.46
25:A:2820:A:N3	25:A:2820:A:H2'	2.30	0.46
2:b:6:MET:SD	2:b:10:LEU:HD23	2.56	0.46
1:a:102:G:H2'	1:a:103:U:H6	1.81	0.46
1:a:377:G:H2'	1:a:378:G:C8	2.50	0.46
14:n:39:GLU:OE2	14:n:43:ASN:ND2	2.44	0.46
25:A:891:G:H2'	25:A:892:A:H8	1.81	0.46
1:a:175:C:H2'	1:a:176:C:H6	1.79	0.46
1:a:476:U:H2'	1:a:477:C:C6	2.51	0.46
4:d:73:ARG:HD3	4:d:77:LYS:HZ2	1.79	0.46
5:e:105:ILE:HG13	5:e:116:GLU:OE1	2.16	0.46
25:A:2147:A:H2'	25:A:2148:G:O4'	2.16	0.46
2:b:117:LEU:HD13	2:b:141:LEU:HD22	1.98	0.45
25:A:2064:C:H2'	25:A:2065:C:C6	2.51	0.45
25:A:2124:G:C5	25:A:2125:G:H1'	2.51	0.45
34:M:106:GLU:OE1	34:M:106:GLU:N	2.49	0.45
1:a:193:C:H2'	1:a:194:C:C6	2.52	0.45
1:a:1027:C:H2'	1:a:1028:C:H5	1.81	0.45
2:b:4:VAL:HG11	2:b:50:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:o:8:THR:O	15:o:12:VAL:HG23	2.16	0.45
34:M:66:LYS:HB3	34:M:66:LYS:HE2	1.71	0.45
11:k:84:VAL:HB	11:k:110:ILE:HD13	1.98	0.45
25:A:422:A:OP2	60:A:3601:HOH:O	2.21	0.45
28:D:1:MET:HG2	28:D:2:ILE:N	2.31	0.45
29:E:149:ILE:HB	29:E:188:MET:HG2	1.97	0.45
1:a:202:G:H2'	1:a:203:G:C8	2.51	0.45
1:a:381:C:H2'	1:a:382:A:C8	2.51	0.45
14:n:23:LYS:O	14:n:26:GLU:HG3	2.17	0.45
1:a:131:A:H2'	1:a:132:C:H6	1.81	0.45
4:d:105:MET:HB2	4:d:173:VAL:HG21	1.96	0.45
6:f:14:GLN:OE1	6:f:17:GLN:NE2	2.49	0.45
6:f:18:VAL:HG21	6:f:58:HIS:CD2	2.52	0.45
10:j:84:VAL:HA	10:j:87:LEU:HD12	1.98	0.45
25:A:155:A:H2'	25:A:156:A:C8	2.52	0.45
25:A:2126:A:N1	25:A:2163:A:O2'	2.40	0.45
29:E:44:ARG:NH1	60:E:301:HOH:O	2.39	0.45
44:W:49:VAL:HG13	44:W:52:LEU:O	2.16	0.45
1:a:150:U:H2'	1:a:151:A:H8	1.81	0.45
15:o:26:GLU:OE2	15:o:26:GLU:N	2.50	0.45
2:b:111:ILE:HD13	2:b:148:LEU:HD13	1.99	0.45
7:g:88:PRO:HG2	7:g:152:ALA:HB2	1.97	0.45
13:m:83:LEU:HD21	19:s:65:GLU:HB3	1.97	0.45
25:A:813:U:H2'	25:A:814:C:C6	2.52	0.45
25:A:1266:G:O2'	25:A:2012:G:O6	2.33	0.45
31:G:78:GLY:HA2	31:G:82:GLY:HA2	1.98	0.45
1:a:64:G:H4'	1:a:65:A:H3'	1.99	0.45
1:a:1402:4OC:HM22	1:a:1403:C:H5'	1.98	0.45
1:a:1005:A:O5'	1:a:1005:A:H8	2.00	0.45
13:m:93:ARG:NH1	25:A:888:C:OP1	2.50	0.45
25:A:2653:U:H5"	25:A:2654:A:H2'	1.99	0.45
25:A:2820:A:O2'	25:A:2821:A:OP1	2.28	0.45
1:a:161:A:H2'	1:a:162:A:C8	2.52	0.44
1:a:560:A:H4'	1:a:561:U:H5"	1.99	0.44
3:c:51:SER:HB3	3:c:115:LEU:HD11	1.99	0.44
3:c:55:ILE:HD12	3:c:68:ILE:HG22	2.00	0.44
25:A:2152:G:H2'	25:A:2153:C:C6	2.52	0.44
1:a:77:A:H2'	1:a:78:A:H8	1.79	0.44
1:a:501:C:H2'	1:a:502:A:C8	2.51	0.44
1:a:1412:C:H2'	1:a:1413:A:C8	2.51	0.44
1:a:221:C:H2'	1:a:222:C:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2186:G:H2'	25:A:2187:U:C6	2.52	0.44
1:a:951:G:OP2	13:m:101:ARG:NH2	2.48	0.44
10:j:11:LYS:HG3	10:j:71:LEU:HD13	1.99	0.44
25:A:2158:A:H4'	25:A:2159:G:O4'	2.18	0.44
29:E:124:PHE:HE1	29:E:141:MET:HE1	1.81	0.44
1:a:429:U:H3'	4:d:9:LEU:HD12	1.99	0.44
1:a:1130:A:OP1	9:i:18:ARG:NH2	2.49	0.44
25:A:1386:C:H2'	25:A:1387:A:C8	2.52	0.44
32:H:3:VAL:O	32:H:18:GLN:HA	2.16	0.44
34:M:30:ARG:NH2	34:M:37:ASP:OD1	2.51	0.44
1:a:463:U:H3	1:a:469:C:H42	1.66	0.44
1:a:1302:C:N4	13:m:14:HIS:HD2	2.15	0.44
4:d:56:ARG:NH2	4:d:59:GLN:HG2	2.33	0.44
4:d:183:LYS:HD2	4:d:184:ARG:HD2	2.00	0.44
20:t:50:ALA:HA	20:t:53:GLU:CD	2.42	0.44
25:A:544:C:H4'	25:A:545:U:C5	2.53	0.44
25:A:1027:A:C2	25:A:2488:G:H5'	2.53	0.44
25:A:2071:A:H2'	25:A:2072:C:C6	2.52	0.44
44:W:98:SER:OG	44:W:98:SER:O	2.35	0.44
1:a:203:G:N2	1:a:204:G:O6	2.48	0.44
1:a:309:A:O2'	1:a:607:A:N1	2.48	0.44
1:a:1124:G:N2	1:a:1125:U:O4	2.38	0.44
2:b:161:LEU:HD23	2:b:161:LEU:HA	1.89	0.44
4:d:76:TYR:CG	4:d:204:TYR:HD2	2.35	0.44
14:n:80:SER:O	14:n:84:VAL:HG23	2.18	0.44
25:A:608:A:H2'	25:A:609:A:C8	2.52	0.44
30:F:8:TYR:HB2	30:F:173:PHE:HZ	1.83	0.44
1:a:59:A:H5'	1:a:387:U:H5"	2.00	0.44
1:a:381:C:H2'	1:a:382:A:O4'	2.17	0.44
1:a:403:C:H2'	1:a:404:G:H8	1.82	0.44
1:a:687:A:C2	1:a:704:A:C5	3.06	0.44
1:a:1283:U:H2'	1:a:1284:C:O4'	2.17	0.44
1:a:1311:A:OP1	50:3:59:ARG:NH1	2.51	0.44
6:f:21:MET:O	6:f:24:ARG:HB2	2.18	0.44
25:A:3:U:H2'	25:A:4:U:C6	2.52	0.44
25:A:1816:C:N4	27:C:35:GLU:OE1	2.50	0.44
1:a:635:A:H2'	1:a:636:U:H6	1.83	0.44
25:A:612:G:H2'	25:A:614:A:OP2	2.18	0.44
25:A:958:U:H2'	26:B:89:U:H6	1.83	0.44
30:F:36:LEU:HB3	30:F:152:LEU:HD11	2.00	0.44
30:F:122:PHE:HB3	30:F:163:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:L:65:THR:O	33:L:68:LYS:HG2	2.18	0.44
35:N:109:LYS:HE2	35:N:128:THR:HG22	2.00	0.44
1:a:102:G:H2'	1:a:103:U:C6	2.53	0.43
1:a:109:A:C6	1:a:326:G:C6	3.06	0.43
1:a:1163:A:H2'	1:a:1164:G:H8	1.81	0.43
1:a:1253:G:H2'	1:a:1254:A:C8	2.52	0.43
2:b:4:VAL:HG21	2:b:50:PHE:HD2	1.83	0.43
5:e:94:VAL:HB	5:e:111:MET:HE3	1.99	0.43
5:e:153:VAL:HA	5:e:156:LYS:HG2	2.00	0.43
7:g:54:SER:HB2	7:g:56:LYS:NZ	2.33	0.43
25:A:1856:U:H2'	25:A:1857:G:O4'	2.18	0.43
30:F:57:LEU:HD12	30:F:57:LEU:HA	1.86	0.43
30:F:127:ASN:HB2	30:F:156:ILE:O	2.18	0.43
45:X:35:GLU:OE1	45:X:35:GLU:N	2.50	0.43
1:a:976:G:OP2	1:a:1358:U:O2'	2.36	0.43
3:c:114:LYS:HB2	3:c:185:ASN:HD22	1.83	0.43
25:A:549:G:H2'	25:A:550:C:C6	2.53	0.43
25:A:558:U:P	33:L:113:PRO:HG2	2.58	0.43
1:a:335:C:H2'	1:a:336:A:C8	2.52	0.43
1:a:461:A:H2'	1:a:462:G:H8	1.83	0.43
7:g:69:VAL:O	7:g:138:ARG:HG3	2.19	0.43
25:A:1:G:H2'	25:A:2:G:C8	2.52	0.43
55:8:38:GLY:OXT	60:8:201:HOH:O	2.21	0.43
1:a:1024:G:H2'	1:a:1025:U:O4'	2.19	0.43
9:i:54:LEU:HD23	9:i:98:LEU:HD23	2.00	0.43
20:t:9:LYS:NZ	20:t:13:GLN:OE1	2.35	0.43
20:t:49:LYS:O	20:t:53:GLU:OE1	2.36	0.43
25:A:273:G:C6	25:A:274:C:N4	2.86	0.43
25:A:479:A:N3	25:A:481:G:H5"	2.33	0.43
25:A:645:C:H2'	25:A:647:G:N7	2.33	0.43
26:B:42:C:C5	30:F:66:LEU:HD22	2.54	0.43
1:a:337:G:H2'	1:a:338:A:C8	2.53	0.43
25:A:5:A:H2'	25:A:6:A:C8	2.54	0.43
27:C:78:VAL:HG21	27:C:110:LEU:HD21	2.00	0.43
1:a:1106:G:H5"	3:c:172:ARG:HG2	2.01	0.43
23:x:75:C:H2'	23:x:76:A:O4'	2.18	0.43
25:A:2484:G:OP1	36:O:44:ARG:HD2	2.19	0.43
30:F:38:MET:HE1	30:F:53:ALA:O	2.18	0.43
1:a:664:G:H22	1:a:741:G:H1	1.66	0.43
1:a:1435:G:H2'	1:a:1436:U:C6	2.53	0.43
17:q:19:LYS:O	17:q:19:LYS:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:364:C:H2'	25:A:365:U:H6	1.84	0.43
25:A:1263:U:OP1	51:4:13:ARG:NH1	2.52	0.43
2:b:73:LYS:HB2	2:b:76:ALA:HB3	2.00	0.43
12:l:39:THR:HG22	12:l:51:LYS:HG3	2.01	0.43
25:A:639:U:H2'	25:A:640:C:C6	2.54	0.43
25:A:784:G:H5'	25:A:785:G:OP1	2.18	0.43
25:A:2144:G:O2'	25:A:2147:A:N1	2.43	0.43
36:O:30:SER:OG	36:O:106:ASP:OD1	2.30	0.43
45:X:67:GLY:C	45:X:68:LYS:HD2	2.44	0.43
1:a:403:C:H2'	1:a:404:G:C8	2.52	0.43
1:a:608:A:H2'	1:a:609:A:O4'	2.19	0.43
4:d:95:GLU:OE1	4:d:104:ARG:NH1	2.52	0.43
4:d:104:ARG:HH22	4:d:170:TRP:NE1	2.16	0.43
9:i:98:LEU:HD22	9:i:103:PHE:HD2	1.84	0.43
25:A:250:G:H2'	25:A:251:A:C8	2.54	0.43
25:A:1045:C:H4'	25:A:1047:G:H5"	2.00	0.43
25:A:1545:A:H2'	25:A:1546:G:O4'	2.19	0.43
25:A:2134:A:N6	25:A:2156:G:N3	2.67	0.43
25:A:2847:U:H2'	25:A:2848:G:O4'	2.19	0.43
30:F:37:ASN:HB3	30:F:153:ASP:OD2	2.17	0.43
1:a:159:G:N2	1:a:161:A:H3'	2.34	0.43
1:a:231:U:H2'	1:a:232:G:H8	1.84	0.43
6:f:10:VAL:HG12	6:f:84:VAL:HA	2.00	0.43
25:A:1864:U:OP1	25:A:2410:G:O2'	2.31	0.43
25:A:2107:G:H1	25:A:2182:U:H3	1.67	0.43
25:A:2136:G:N2	25:A:2156:G:O2'	2.52	0.43
1:a:1071:C:H2'	1:a:1072:G:C8	2.54	0.42
1:a:1518:MA6:O5'	1:a:1518:MA6:H8	2.18	0.42
2:b:78:GLU:O	2:b:81:LYS:HG3	2.19	0.42
3:c:87:LEU:O	3:c:91:VAL:HG23	2.18	0.42
19:s:68:GLY:HA3	50:3:56:ARG:HH21	1.84	0.42
25:A:1715:G:O2'	25:A:1743:G:O6	2.25	0.42
25:A:2191:A:O2'	25:A:2192:U:OP1	2.33	0.42
25:A:2591:C:H2'	25:A:2592:G:C8	2.54	0.42
34:M:2:ILE:HD12	34:M:8:LEU:HD21	2.00	0.42
39:R:25:THR:HG22	39:R:88:ARG:HB3	2.00	0.42
52:5:11:LEU:HD21	52:5:34:LEU:HD23	2.00	0.42
1:a:642:A:C8	8:h:107:SER:HA	2.54	0.42
1:a:674:G:H2'	1:a:675:A:H8	1.84	0.42
4:d:104:ARG:HH21	4:d:171:LEU:CD2	2.31	0.42
25:A:518:G:H2'	25:A:519:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:35:C:H2'	26:B:36:C:H5'	2.01	0.42
31:G:95:ARG:HD2	31:G:128:GLN:NE2	2.33	0.42
1:a:509:A:N3	1:a:543:U:O2'	2.44	0.42
1:a:983:A:H5'	1:a:984:C:OP2	2.19	0.42
1:a:1035:A:H1'	1:a:1036:A:H2	1.84	0.42
2:b:7:ARG:CZ	2:b:11:LYS:HD3	2.49	0.42
25:A:1843:C:H4'	27:C:251:GLN:NE2	2.32	0.42
30:F:66:LEU:O	30:F:87:CYS:HA	2.19	0.42
1:a:151:A:C5	1:a:152:A:C8	3.07	0.42
1:a:662:U:H2'	1:a:663:A:C8	2.54	0.42
1:a:875:U:O2'	8:h:15:ARG:NH1	2.52	0.42
1:a:1025:U:H5"	1:a:1026:G:O5'	2.19	0.42
17:q:20:SER:OG	17:q:71:LYS:NZ	2.35	0.42
25:A:2680:U:O2'	25:A:2681:C:H5'	2.19	0.42
44:W:96:PHE:CE2	44:W:103:ILE:HG12	2.54	0.42
1:a:86:G:H5'	1:a:87:C:H6	1.85	0.42
1:a:162:A:O5'	1:a:162:A:H8	2.02	0.42
1:a:398:U:H2'	1:a:399:G:C8	2.54	0.42
1:a:501:C:OP1	12:l:114:ARG:NH2	2.42	0.42
1:a:1288:A:H2'	1:a:1289:A:C8	2.55	0.42
4:d:95:GLU:CD	4:d:100:ASN:HD21	2.28	0.42
4:d:174:ASP:HB3	4:d:179:GLU:HG3	1.99	0.42
12:l:19:SER:OG	12:l:20:ASN:N	2.51	0.42
21:u:4:ILE:HD12	21:u:18:ARG:HG2	2.02	0.42
25:A:84:A:N1	25:A:98:G:O2'	2.43	0.42
25:A:358:U:H2'	25:A:359:G:N7	2.35	0.42
25:A:2845:U:H5"	39:R:52:ASN:O	2.19	0.42
1:a:151:A:C5	1:a:171:A:N6	2.87	0.42
25:A:634:C:H2'	25:A:635:C:C6	2.54	0.42
25:A:2120:G:N1	25:A:2179:C:C4	2.88	0.42
26:B:3:C:H2'	26:B:4:C:H6	1.84	0.42
28:D:32:ASN:HD22	28:D:52:THR:HB	1.84	0.42
1:a:623:C:H2'	1:a:624:C:H6	1.83	0.42
1:a:745:G:H2'	1:a:746:A:C8	2.55	0.42
1:a:1119:C:P	9:i:85:ARG:HH22	2.42	0.42
13:m:79:ARG:HH11	13:m:79:ARG:HB2	1.85	0.42
20:t:20:HIS:CE1	20:t:24:ARG:NH1	2.88	0.42
25:A:288:U:H2'	25:A:289:G:C8	2.55	0.42
25:A:360:U:H3'	25:A:361:G:C8	2.55	0.42
25:A:645:C:H2'	25:A:647:G:C8	2.55	0.42
25:A:721:A:H2'	25:A:722:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2636:C:O2'	28:D:45:TYR:OH	2.32	0.42
25:A:2812:G:H2'	25:A:2813:A:C8	2.54	0.42
30:F:125:ARG:HE	30:F:125:ARG:HB3	1.65	0.42
33:L:23:LYS:HE2	33:L:142:ILE:OXT	2.19	0.42
37:P:82:GLU:O	37:P:86:ARG:HG3	2.20	0.42
1:a:991:U:C4	1:a:1212:U:H1'	2.54	0.42
25:A:414:C:H2'	25:A:415:A:H8	1.83	0.42
25:A:1357:C:H2'	25:A:1358:G:O4'	2.19	0.42
25:A:2189:U:HO2'	25:A:2190:G:P	2.40	0.42
25:A:2661:G:H8	25:A:2661:G:OP2	2.03	0.42
42:U:83:LYS:HB3	42:U:95:ARG:HD2	2.01	0.42
1:a:1004:A:C8	1:a:1025:U:H1'	2.55	0.42
1:a:1518:MA6:H103	1:a:1519:MA6:H102	2.02	0.42
2:b:7:ARG:NH1	2:b:11:LYS:HD3	2.35	0.42
2:b:54:LEU:O	2:b:58:ASN:ND2	2.52	0.42
23:x:21:A:H61	23:x:46:G:H2'	1.84	0.42
25:A:891:G:H2'	25:A:892:A:C8	2.55	0.42
25:A:1673:G:O6	28:D:134:HIS:HD2	2.02	0.42
25:A:2092:U:OP2	32:H:27:ARG:NH1	2.51	0.42
34:M:40:LYS:HE3	34:M:57:VAL:HG12	2.01	0.42
1:a:73:C:H2'	1:a:74:A:H8	1.83	0.42
1:a:1307:U:OP1	13:m:100:GLN:NE2	2.52	0.42
5:e:13:GLU:OE2	5:e:68:ARG:NH1	2.52	0.42
13:m:25:VAL:HG22	13:m:29:ARG:HD2	2.01	0.42
25:A:577:G:H2'	25:A:578:G:C8	2.55	0.42
25:A:2117:A:N6	25:A:2170:A:H61	2.18	0.42
1:a:1496:C:H2'	1:a:1497:G:O4'	2.20	0.41
5:e:12:GLN:HE21	5:e:117:VAL:HA	1.85	0.41
14:n:97:LYS:HB2	14:n:97:LYS:HE2	1.89	0.41
20:t:46:ALA:HA	20:t:49:LYS:HG2	2.01	0.41
25:A:1721:G:O2'	25:A:1739:A:N6	2.48	0.41
25:A:2498:OMC:HM22	25:A:2499:C:H5'	2.02	0.41
39:R:6:LYS:O	39:R:10:GLN:HG2	2.19	0.41
50:3:41:HIS:HB3	50:3:44:PHE:HD1	1.85	0.41
1:a:75:G:H2'	1:a:75:G:N3	2.34	0.41
1:a:464:U:H3	1:a:468:A:H62	1.68	0.41
1:a:1408:A:C2	57:a:3133:T8B:H5	2.56	0.41
11:k:18:ASP:OD1	11:k:18:ASP:N	2.51	0.41
12:l:79:VAL:HG22	12:l:103:ASP:OD2	2.20	0.41
25:A:832:U:H2'	25:A:833:A:C8	2.55	0.41
31:G:164:TYR:HB2	31:G:167:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:L:125:TYR:OH	33:L:132:HIS:NE2	2.53	0.41
1:a:76:G:C2	1:a:93:U:O2	2.74	0.41
1:a:219:U:H2'	1:a:220:G:C8	2.55	0.41
1:a:373:A:O2'	1:a:451:A:N7	2.53	0.41
1:a:1163:A:H2'	1:a:1164:G:C8	2.55	0.41
1:a:1355:G:H2'	1:a:1356:G:H8	1.85	0.41
14:n:83:LYS:HD3	14:n:83:LYS:HA	1.83	0.41
30:F:8:TYR:O	30:F:13:VAL:HG23	2.21	0.41
30:F:38:MET:CE	30:F:53:ALA:HB1	2.49	0.41
30:F:163:ASP:O	30:F:167:ARG:HG3	2.19	0.41
36:O:127:LYS:HE3	36:O:127:LYS:HB2	1.89	0.41
1:a:453:G:H2'	1:a:454:G:C8	2.55	0.41
1:a:642:A:N7	8:h:107:SER:HA	2.35	0.41
3:c:107:ARG:HG2	3:c:108:LYS:HG3	2.03	0.41
3:c:154:SER:HB3	3:c:165:THR:HG23	2.03	0.41
20:t:44:LYS:HB2	20:t:44:LYS:HE3	1.74	0.41
25:A:2038:G:H2'	25:A:2039:U:O4'	2.21	0.41
31:G:101:ASN:O	31:G:117:LEU:HG	2.20	0.41
32:H:4:ILE:HA	32:H:17:ASP:O	2.20	0.41
35:N:123:ARG:HG2	35:N:143:GLU:HB2	2.02	0.41
1:a:107:G:O6	20:t:10:ARG:NE	2.37	0.41
1:a:440:C:C2	1:a:441:A:C8	3.09	0.41
1:a:618:C:H1'	16:p:14:ARG:HH12	1.85	0.41
16:p:56:ARG:HD2	16:p:56:ARG:HA	1.79	0.41
22:w:64:A:HO2'	22:w:65:G:P	2.42	0.41
25:A:157:C:H2'	25:A:158:U:O4'	2.21	0.41
25:A:2020:A:H5'	51:4:9:THR:CG2	2.51	0.41
5:e:94:VAL:HB	5:e:111:MET:CE	2.51	0.41
6:f:43:GLY:HA2	6:f:58:HIS:CE1	2.56	0.41
9:i:80:ARG:O	9:i:84:THR:HG23	2.21	0.41
25:A:700:G:O2'	25:A:1632:A:N3	2.48	0.41
25:A:894:U:H2'	25:A:895:U:O4'	2.19	0.41
25:A:2849:U:H4'	25:A:2868:A:C2	2.55	0.41
26:B:57:A:H4'	30:F:27:GLN:HE21	1.85	0.41
27:C:107:PRO:HD2	27:C:110:LEU:HD22	2.03	0.41
34:M:63:VAL:HG12	34:M:107:LEU:HD11	2.01	0.41
44:W:24:LYS:HE2	44:W:24:LYS:HB2	1.89	0.41
1:a:204:G:H2'	1:a:205:A:C8	2.55	0.41
1:a:592:G:H2'	1:a:593:U:C6	2.55	0.41
1:a:868:C:H2'	1:a:869:G:O4'	2.20	0.41
6:f:96:VAL:HG12	6:f:96:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:r:48:ARG:HB2	18:r:51:TYR:HD2	1.86	0.41
25:A:286:U:C2	25:A:287:G:C8	3.09	0.41
25:A:307:G:N1	25:A:310:A:OP2	2.48	0.41
25:A:2820:A:C5	37:P:4:ARG:HD2	2.55	0.41
30:F:37:ASN:OD1	30:F:38:MET:N	2.53	0.41
30:F:49:LEU:HD22	30:F:148:ARG:HH12	1.86	0.41
49:2:41:THR:HG22	49:2:43:ALA:H	1.86	0.41
1:a:1026:G:HO2'	1:a:1027:C:P	2.44	0.41
4:d:99:ASP:OD1	4:d:99:ASP:N	2.53	0.41
25:A:1645:G:H5"	25:A:1646:C:H5'	2.03	0.41
25:A:1889:A:H2'	25:A:1890:A:C8	2.55	0.41
25:A:2107:G:H2'	25:A:2108:A:C8	2.56	0.41
35:N:108:ALA:HB3	35:N:125:LEU:HD22	2.03	0.41
38:Q:115:LEU:HA	38:Q:115:LEU:HD23	1.83	0.41
41:T:6:GLN:HB3	41:T:11:GLN:HG2	2.01	0.41
1:a:197:A:N3	1:a:198:G:H1'	2.36	0.41
1:a:299:G:H2'	1:a:300:A:C8	2.55	0.41
5:e:88:VAL:HG22	5:e:93:ARG:HG3	2.03	0.41
8:h:50:LYS:HG2	8:h:60:GLU:OE2	2.21	0.41
18:r:55:LEU:O	18:r:59:ILE:HG13	2.20	0.41
25:A:1883:U:H2'	25:A:1884:G:O4'	2.20	0.41
25:A:2103:C:H2'	25:A:2104:C:C6	2.56	0.41
25:A:2176:A:H2'	25:A:2177:C:C6	2.55	0.41
25:A:2783:U:H2'	25:A:2784:U:C6	2.55	0.41
37:P:45:ARG:O	37:P:49:GLU:HG3	2.21	0.41
40:S:41:LYS:HA	40:S:44:GLN:HE21	1.86	0.41
47:Z:43:GLU:OE2	47:Z:45:ARG:HD3	2.20	0.41
48:1:12:GLU:HG3	48:1:13:GLU:N	2.36	0.41
1:a:1103:C:H5"	2:b:97:LEU:HD12	2.02	0.41
1:a:1410:A:H2'	1:a:1411:C:C6	2.56	0.41
2:b:104:TRP:HA	2:b:107:VAL:HG22	2.02	0.41
7:g:12:ILE:HG23	7:g:21:GLU:OE1	2.21	0.41
10:j:29:ALA:O	10:j:32:THR:OG1	2.37	0.41
14:n:6:MET:HB3	14:n:63:ARG:NH1	2.36	0.41
16:p:21:VAL:HG11	16:p:60:TRP:CE2	2.56	0.41
25:A:1000:A:H2'	25:A:1001:A:C8	2.56	0.41
25:A:2273:A:H2'	25:A:2274:A:C8	2.56	0.41
32:H:19:VAL:HG13	32:H:21:VAL:HG23	2.03	0.41
1:a:203:G:C2	1:a:215:C:C2	3.09	0.40
25:A:172:A:H2'	25:A:173:A:C8	2.56	0.40
29:E:191:ASP:O	29:E:195:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:F:65:PRO:HA	30:F:89:VAL:HG12	2.03	0.40
34:M:23:LYS:HE2	34:M:23:LYS:HB2	1.90	0.40
44:W:45:HIS:CD2	44:W:58:ILE:HG12	2.56	0.40
1:a:324:G:N2	1:a:327:A:C8	2.90	0.40
1:a:1023:U:N3	1:a:1024:G:O6	2.55	0.40
1:a:1314:C:N4	19:s:2:PRO:O	2.47	0.40
1:a:1530:G:H2'	1:a:1531:A:C8	2.57	0.40
2:b:9:MET:HB3	2:b:43:LEU:HD11	2.02	0.40
4:d:97:ARG:HG3	4:d:99:ASP:OD1	2.21	0.40
14:n:73:PHE:HE2	14:n:75:ARG:HA	1.86	0.40
16:p:21:VAL:HG21	16:p:60:TRP:CD1	2.56	0.40
20:t:79:LEU:HA	20:t:79:LEU:HD23	1.81	0.40
27:C:167:ARG:HG3	27:C:172:VAL:HG12	2.03	0.40
1:a:374:A:C4	1:a:375:U:C5	3.09	0.40
2:b:78:GLU:HG2	2:b:79:ALA:N	2.36	0.40
4:d:56:ARG:HH21	4:d:59:GLN:HG2	1.86	0.40
13:m:90:ARG:HD2	13:m:90:ARG:HA	1.79	0.40
25:A:1495:A:H2'	25:A:1496:A:C8	2.56	0.40
25:A:2308:G:N3	25:A:2308:G:H2'	2.36	0.40
35:N:13:LYS:HD3	35:N:13:LYS:HA	1.83	0.40
35:N:20:GLY:O	35:N:21:ARG:HD2	2.22	0.40
45:X:4:ILE:HD12	45:X:61:LEU:HD13	2.03	0.40
1:a:259:G:C4	1:a:260:G:C8	3.10	0.40
1:a:1161:C:H2'	1:a:1162:C:H6	1.86	0.40
25:A:546:U:H2'	25:A:548:G:N2	2.37	0.40
25:A:1156:A:C8	40:S:51:ARG:HG2	2.56	0.40
29:E:145:ASP:HB3	29:E:184:ASP:HB2	2.02	0.40
30:F:52:ASN:HD22	30:F:52:ASN:HA	1.69	0.40
47:Z:37:ARG:NH1	60:Z:101:HOH:O	2.50	0.40
1:a:390:U:H2'	1:a:391:G:H8	1.87	0.40
4:d:54:GLN:HB3	4:d:203:LEU:HB2	2.02	0.40
6:f:9:MET:HA	6:f:58:HIS:O	2.21	0.40
6:f:24:ARG:O	6:f:27:ALA:HB3	2.22	0.40
29:E:1:MET:HB3	29:E:2:GLU:H	1.75	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%)	205 (92%)	17 (8%)	0	100	100
3	c	204/233 (88%)	194 (95%)	10 (5%)	0	100	100
4	d	203/206 (98%)	197 (97%)	6 (3%)	0	100	100
5	e	154/167 (92%)	149 (97%)	5 (3%)	0	100	100
6	f	101/131 (77%)	92 (91%)	9 (9%)	0	100	100
7	g	150/156 (96%)	141 (94%)	9 (6%)	0	100	100
8	h	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
9	i	125/130 (96%)	121 (97%)	4 (3%)	0	100	100
10	j	96/103 (93%)	92 (96%)	3 (3%)	1 (1%)	12	32
11	k	113/129 (88%)	103 (91%)	10 (9%)	0	100	100
12	l	118/124 (95%)	113 (96%)	5 (4%)	0	100	100
13	m	113/118 (96%)	107 (95%)	6 (5%)	0	100	100
14	n	98/101 (97%)	98 (100%)	0	0	100	100
15	o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	p	79/82 (96%)	70 (89%)	9 (11%)	0	100	100
17	q	77/84 (92%)	73 (95%)	4 (5%)	0	100	100
18	r	52/75 (69%)	49 (94%)	3 (6%)	0	100	100
19	s	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
20	t	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
21	u	53/71 (75%)	51 (96%)	2 (4%)	0	100	100
27	C	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
28	D	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	24	48
29	E	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
30	F	175/179 (98%)	163 (93%)	12 (7%)	0	100	100
31	G	174/177 (98%)	164 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	H	39/149 (26%)	34 (87%)	5 (13%)	0	100	100
33	L	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
34	M	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
35	N	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
36	O	132/136 (97%)	127 (96%)	5 (4%)	0	100	100
37	P	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
38	Q	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
39	R	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
40	S	115/118 (98%)	115 (100%)	0	0	100	100
41	T	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
42	U	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
43	V	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
44	W	100/104 (96%)	95 (95%)	5 (5%)	0	100	100
45	X	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
46	Y	82/85 (96%)	81 (99%)	1 (1%)	0	100	100
47	Z	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
48	1	59/63 (94%)	57 (97%)	2 (3%)	0	100	100
49	2	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
50	3	56/70 (80%)	51 (91%)	5 (9%)	0	100	100
51	4	53/57 (93%)	53 (100%)	0	0	100	100
52	5	49/55 (89%)	46 (94%)	3 (6%)	0	100	100
53	6	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
54	7	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
55	8	36/38 (95%)	36 (100%)	0	0	100	100
All	All	5454/5886 (93%)	5227 (96%)	225 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	D	149	ASN
10	j	57	VAL

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
20	t	65/66 (98%)	65 (100%)	0	100	100
21	u	48/61 (79%)	48 (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	32/114 (28%)	32 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	L	116/116 (100%)	116 (100%)	0	100	100
34	M	104/104 (100%)	104 (100%)	0	100	100
35	N	103/103 (100%)	103 (100%)	0	100	100
36	O	107/107 (100%)	107 (100%)	0	100	100
37	P	98/103 (95%)	98 (100%)	0	100	100
38	Q	86/87 (99%)	86 (100%)	0	100	100
39	R	99/100 (99%)	99 (100%)	0	100	100
40	S	89/90 (99%)	89 (100%)	0	100	100
41	T	84/84 (100%)	84 (100%)	0	100	100
42	U	93/93 (100%)	93 (100%)	0	100	100
43	V	80/84 (95%)	80 (100%)	0	100	100
44	W	83/85 (98%)	83 (100%)	0	100	100
45	X	78/78 (100%)	78 (100%)	0	100	100
46	Y	62/63 (98%)	62 (100%)	0	100	100
47	Z	67/68 (98%)	67 (100%)	0	100	100
48	1	54/55 (98%)	54 (100%)	0	100	100
49	2	48/49 (98%)	48 (100%)	0	100	100
50	3	53/62 (86%)	53 (100%)	0	100	100
51	4	46/48 (96%)	46 (100%)	0	100	100
52	5	46/49 (94%)	46 (100%)	0	100	100
53	6	38/38 (100%)	38 (100%)	0	100	100
54	7	51/52 (98%)	51 (100%)	0	100	100
55	8	34/34 (100%)	34 (100%)	0	100	100
All	All	4549/4803 (95%)	4549 (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 (87) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	39	HIS
2	b	58	ASN
2	b	89	GLN
3	c	140	ASN

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Mol	Chain	Res	Type
4	d	41	HIS
4	d	74	ASN
4	d	85	ASN
4	d	131	ASN
4	d	152	GLN
5	e	12	GLN
5	e	19	ASN
5	e	43	ASN
5	e	82	GLN
5	e	122	ASN
6	f	3	HIS
6	f	58	HIS
7	g	68	ASN
7	g	86	GLN
7	g	130	ASN
8	h	67	GLN
8	h	76	GLN
9	i	32	GLN
9	i	37	GLN
9	i	126	GLN
10	j	58	ASN
11	k	28	ASN
12	l	112	GLN
13	m	14	HIS
13	m	105	ASN
14	n	35	ASN
14	n	60	GLN
15	o	51	HIS
16	p	9	HIS
17	q	50	ASN
18	r	52	GLN
19	s	14	HIS
19	s	52	HIS
19	s	83	HIS
20	t	20	HIS
20	t	21	ASN
27	C	90	ASN
27	C	143	ASN
27	C	239	ASN
27	C	260	ASN
28	D	36	GLN
28	D	49	GLN

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Mol	Chain	Res	Type
28	D	134	HIS
28	D	136	ASN
29	E	97	ASN
29	E	136	GLN
29	E	165	HIS
30	F	5	HIS
30	F	27	GLN
30	F	52	ASN
31	G	111	HIS
31	G	128	GLN
32	H	28	ASN
33	L	40	HIS
33	L	58	ASN
36	O	22	GLN
36	O	45	GLN
36	O	60	GLN
37	P	23	ASN
38	Q	19	GLN
38	Q	29	HIS
38	Q	100	HIS
38	Q	104	GLN
39	R	15	GLN
39	R	115	ASN
40	S	20	GLN
40	S	44	GLN
42	U	7	HIS
42	U	9	HIS
42	U	40	ASN
42	U	57	ASN
44	W	66	GLN
45	X	5	ASN
45	X	49	ASN
46	Y	50	ASN
46	Y	76	ASN
47	Z	6	GLN
48	1	15	ASN
50	3	41	HIS
53	6	6	GLN
53	6	29	GLN
54	7	28	ASN
55	8	35	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1526/1542 (98%)	194 (12%)	0
22	w	72/76 (94%)	16 (22%)	0
23	x	75/77 (97%)	8 (10%)	0
24	v	11/24 (45%)	2 (18%)	0
25	A	2842/2904 (97%)	397 (13%)	14 (0%)
26	B	119/120 (99%)	15 (12%)	2 (1%)
All	All	4645/4743 (97%)	632 (13%)	16 (0%)

All (632) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	U
1	a	5	U
1	a	6	G
1	a	19	A
1	a	22	G
1	a	32	A
1	a	39	G
1	a	47	C
1	a	48	C
1	a	50	A
1	a	51	A
1	a	58	C
1	a	59	A
1	a	71	A
1	a	79	G
1	a	81	A
1	a	82	G
1	a	84	U
1	a	85	U
1	a	86	G
1	a	94	G
1	a	95	C
1	a	122	G
1	a	130	A
1	a	131	A
1	a	141	G
1	a	163	C
1	a	174	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	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	266	G
1	a	267	C
1	a	269	C
1	a	280	C
1	a	281	G
1	a	289	G
1	a	321	A
1	a	328	C
1	a	344	A
1	a	347	G
1	a	351	G
1	a	352	C
1	a	353	A
1	a	354	G
1	a	367	U
1	a	372	C
1	a	373	A
1	a	384	G
1	a	388	G
1	a	397	A
1	a	406	G
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
1	a	429	U
1	a	435	A
1	a	444	G

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Mol	Chain	Res	Type
1	a	464	U
1	a	467	U
1	a	468	A
1	a	478	A
1	a	479	U
1	a	484	G
1	a	486	U
1	a	509	A
1	a	511	C
1	a	512	U
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	564	C
1	a	572	A
1	a	573	A
1	a	576	C
1	a	577	G
1	a	579	A
1	a	596	A
1	a	633	G
1	a	653	U
1	a	665	A
1	a	723	U
1	a	724	G
1	a	746	A
1	a	747	A
1	a	748	G
1	a	755	G
1	a	760	G
1	a	777	A
1	a	793	U
1	a	794	A
1	a	815	A
1	a	817	C
1	a	821	G
1	a	890	G
1	a	914	A
1	a	926	G

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Mol	Chain	Res	Type
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	978	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	1024	G
1	a	1027	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	1036	A
1	a	1038	C
1	a	1039	G
1	a	1042	A
1	a	1044	A
1	a	1053	G
1	a	1065	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1137	C
1	a	1139	G
1	a	1159	U
1	a	1167	A
1	a	1168	U
1	a	1171	A
1	a	1196	A
1	a	1197	A
1	a	1213	A

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Mol	Chain	Res	Type
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	1322	C
1	a	1338	G
1	a	1363	A
1	a	1364	U
1	a	1378	C
1	a	1379	G
1	a	1388	C
1	a	1401	G
1	a	1419	G
1	a	1432	G
1	a	1441	A
1	a	1446	A
1	a	1448	C
1	a	1453	G
1	a	1487	G
1	a	1492	A
1	a	1494	G
1	a	1499	A
1	a	1503	A
1	a	1506	U
1	a	1517	G
1	a	1529	G
1	a	1530	G
22	w	9	A
22	w	19	G
22	w	20	U
22	w	24	G

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Mol	Chain	Res	Type
22	w	41	C
22	w	45	U
22	w	46	G7M
22	w	48	C
22	w	50	U
22	w	57	G
22	w	58	A
22	w	63	G
22	w	65	G
22	w	67	C
22	w	70	G
22	w	74	C
23	x	9	G
23	x	21	A
23	x	38	A
23	x	47	U
23	x	58	A
23	x	70	G
23	x	75	C
23	x	76	A
24	v	16	A
24	v	24	A
25	A	4	U
25	A	6	A
25	A	10	A
25	A	12	U
25	A	14	A
25	A	15	G
25	A	34	U
25	A	35	G
25	A	42	A
25	A	45	G
25	A	58	G
25	A	68	G
25	A	71	A
25	A	74	A
25	A	75	G
25	A	100	U
25	A	101	A
25	A	118	A
25	A	119	A
25	A	120	U

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Mol	Chain	Res	Type
25	A	139	U
25	A	140	C
25	A	142	A
25	A	181	A
25	A	186	G
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	269	C
25	A	271	G
25	A	272	A
25	A	274	C
25	A	276	U
25	A	277	G
25	A	278	A
25	A	281	C
25	A	282	A
25	A	311	A
25	A	329	G
25	A	330	A
25	A	345	A
25	A	354	A
25	A	356	G
25	A	360	U
25	A	361	G
25	A	362	A
25	A	363	G
25	A	367	G
25	A	385	C
25	A	386	G
25	A	396	G
25	A	404	A
25	A	411	G
25	A	412	A
25	A	428	A

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Mol	Chain	Res	Type
25	A	456	C
25	A	481	G
25	A	491	G
25	A	504	A
25	A	505	A
25	A	508	A
25	A	509	C
25	A	530	G
25	A	532	A
25	A	538	A
25	A	545	U
25	A	546	U
25	A	547	A
25	A	549	G
25	A	563	A
25	A	573	U
25	A	574	A
25	A	575	A
25	A	586	A
25	A	592	A
25	A	603	A
25	A	614	A
25	A	615	U
25	A	618	G
25	A	627	A
25	A	637	A
25	A	645	C
25	A	647	G
25	A	653	U
25	A	654	A
25	A	655	A
25	A	686	U
25	A	709	U
25	A	710	U
25	A	716	A
25	A	725	G
25	A	726	G
25	A	730	A
25	A	736	C
25	A	747	5MU
25	A	758	C
25	A	764	A

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Mol	Chain	Res	Type
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	792	A
25	A	794	A
25	A	798	G
25	A	805	G
25	A	807	U
25	A	812	C
25	A	827	U
25	A	828	U
25	A	845	A
25	A	846	U
25	A	847	U
25	A	859	G
25	A	866	A
25	A	883	G
25	A	884	U
25	A	888	C
25	A	890	C
25	A	891	G
25	A	893	C
25	A	895	U
25	A	896	A
25	A	900	A
25	A	910	A
25	A	914	G
25	A	915	C
25	A	927	A
25	A	931	U
25	A	946	C
25	A	961	C
25	A	968	C
25	A	974	G
25	A	983	A
25	A	985	C
25	A	996	A
25	A	1009	A
25	A	1012	U

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Mol	Chain	Res	Type
25	A	1013	C
25	A	1026	G
25	A	1027	A
25	A	1032	A
25	A	1033	U
25	A	1036	G
25	A	1038	G
25	A	1039	A
25	A	1040	A
25	A	1045	C
25	A	1047	G
25	A	1108	U
25	A	1110	G
25	A	1111	A
25	A	1112	G
25	A	1115	G
25	A	1119	U
25	A	1130	U
25	A	1132	U
25	A	1135	C
25	A	1141	U
25	A	1142	A
25	A	1187	G
25	A	1206	G
25	A	1212	G
25	A	1241	A
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	1289	C
25	A	1300	G
25	A	1301	A
25	A	1321	A
25	A	1352	U
25	A	1365	A
25	A	1379	U
25	A	1383	A

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Mol	Chain	Res	Type
25	A	1395	A
25	A	1416	G
25	A	1420	A
25	A	1428	C
25	A	1429	G
25	A	1452	G
25	A	1453	A
25	A	1482	G
25	A	1483	G
25	A	1493	C
25	A	1508	A
25	A	1509	A
25	A	1510	G
25	A	1515	A
25	A	1524	G
25	A	1529	G
25	A	1534	U
25	A	1535	A
25	A	1536	C
25	A	1537	G
25	A	1566	A
25	A	1569	A
25	A	1578	U
25	A	1583	A
25	A	1584	U
25	A	1585	C
25	A	1609	A
25	A	1647	U
25	A	1648	U
25	A	1674	G
25	A	1715	G
25	A	1729	U
25	A	1730	C
25	A	1731	G
25	A	1733	G
25	A	1738	G
25	A	1744	A
25	A	1764	C
25	A	1773	A
25	A	1786	A
25	A	1800	C
25	A	1801	A

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Mol	Chain	Res	Type
25	A	1808	A
25	A	1816	C
25	A	1829	A
25	A	1848	A
25	A	1858	A
25	A	1871	A
25	A	1872	A
25	A	1879	C
25	A	1905	C
25	A	1906	G
25	A	1913	A
25	A	1915	3TD
25	A	1929	G
25	A	1930	G
25	A	1937	A
25	A	1938	A
25	A	1941	C
25	A	1955	U
25	A	1964	G
25	A	1967	C
25	A	1970	A
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	2030	6MZ
25	A	2031	A
25	A	2033	A
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	2076	U
25	A	2093	G
25	A	2098	U

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Mol	Chain	Res	Type
25	A	2100	G
25	A	2104	C
25	A	2108	A
25	A	2109	U
25	A	2110	G
25	A	2111	U
25	A	2112	G
25	A	2113	U
25	A	2115	G
25	A	2116	G
25	A	2118	U
25	A	2119	A
25	A	2126	A
25	A	2131	U
25	A	2132	U
25	A	2133	G
25	A	2136	G
25	A	2145	C
25	A	2147	A
25	A	2157	G
25	A	2162	G
25	A	2164	C
25	A	2168	G
25	A	2170	A
25	A	2172	U
25	A	2173	A
25	A	2179	C
25	A	2182	U
25	A	2183	A
25	A	2187	U
25	A	2189	U
25	A	2190	G
25	A	2192	U
25	A	2194	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	2259	U
25	A	2268	A

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Mol	Chain	Res	Type
25	A	2273	A
25	A	2283	C
25	A	2287	A
25	A	2305	U
25	A	2308	G
25	A	2322	A
25	A	2325	G
25	A	2333	A
25	A	2335	A
25	A	2339	C
25	A	2350	C
25	A	2361	G
25	A	2377	A
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
25	A	2435	A
25	A	2441	U
25	A	2448	A
25	A	2469	A
25	A	2474	U
25	A	2476	A
25	A	2477	U
25	A	2478	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	2556	C
25	A	2566	A
25	A	2567	G

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Mol	Chain	Res	Type
25	A	2572	A
25	A	2573	C
25	A	2574	G
25	A	2582	G
25	A	2602	A
25	A	2608	G
25	A	2609	U
25	A	2613	U
25	A	2615	U
25	A	2629	U
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	2749	A
25	A	2750	A
25	A	2765	A
25	A	2778	A
25	A	2796	U
25	A	2798	U
25	A	2800	A
25	A	2820	A
25	A	2821	A
25	A	2835	A
25	A	2836	U
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	2900	A
25	A	2902	C
26	B	4	C

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Mol	Chain	Res	Type
26	B	13	G
26	B	35	C
26	B	44	G
26	B	45	A
26	B	52	A
26	B	53	A
26	B	56	G
26	B	57	A
26	B	65	U
26	B	67	G
26	B	89	U
26	B	91	C
26	B	105	G
26	B	109	A

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	3	U
25	A	271	G
25	A	277	G
25	A	784	G
25	A	1026	G
25	A	1031	G
25	A	1037	G
25	A	2097	A
25	A	2189	U
25	A	2191	A
25	A	2430	A
25	A	2473	U
25	A	2538	C
25	A	2799	A
26	B	3	C
26	B	66	A

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

51 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	MIA	w	37	22	28,31,32	2.33	7 (25%)	38,44,47	2.82	14 (36%)
22	PSU	w	39	22	18,21,22	1.26	3 (16%)	21,30,33	2.37	4 (19%)
22	PSU	w	55	22	18,21,22	1.44	4 (22%)	21,30,33	2.17	3 (14%)
25	5MU	A	747	25	19,22,23	1.41	5 (26%)	27,32,35	2.23	9 (33%)
1	MA6	a	1519	1	23,26,27	1.47	5 (21%)	33,38,41	2.49	13 (39%)
1	5MC	a	967	1	19,22,23	1.47	3 (15%)	26,32,35	1.16	2 (7%)
25	PSU	A	1911	25	18,21,22	1.49	4 (22%)	21,30,33	2.17	5 (23%)
25	PSU	A	2504	25	18,21,22	1.51	4 (22%)	21,30,33	2.08	3 (14%)
25	OMU	A	2552	25	19,22,23	1.39	3 (15%)	25,31,34	2.01	5 (20%)
23	PSU	x	55	23	18,21,22	1.35	3 (16%)	21,30,33	2.04	4 (19%)
1	UR3	a	1498	1	19,22,23	0.93	1 (5%)	26,32,35	1.80	5 (19%)
1	PSU	a	516	1,56	18,21,22	1.41	5 (27%)	21,30,33	2.05	4 (19%)
23	5MU	x	54	23	19,22,23	1.39	5 (26%)	27,32,35	2.23	6 (22%)
1	2MG	a	1516	1	23,26,27	1.27	4 (17%)	33,38,41	2.33	10 (30%)
25	5MU	A	1939	25	19,22,23	1.45	4 (21%)	27,32,35	2.30	6 (22%)
25	PSU	A	2604	25	18,21,22	1.51	4 (22%)	21,30,33	2.20	5 (23%)
25	2MA	A	2503	25,56	22,25,26	1.41	5 (22%)	32,37,40	2.33	9 (28%)
36	MS6	O	82	36	5,7,8	0.57	0	2,7,9	0.99	0
12	D2T	l	89	12	8,9,10	1.78	1 (12%)	6,11,13	2.69	3 (50%)
25	OMC	A	2498	25,56	19,22,23	0.85	1 (5%)	25,31,34	1.15	1 (4%)
23	4SU	x	8	23	18,21,22	1.87	4 (22%)	25,30,33	2.27	5 (20%)
23	5MC	x	32	23	19,22,23	1.45	3 (15%)	26,32,35	1.24	3 (11%)
36	4D4	O	81	36	9,11,12	2.56	3 (33%)	7,13,15	1.02	0
25	1MG	A	745	25	23,26,27	1.11	2 (8%)	33,39,42	1.76	5 (15%)
25	PSU	A	2580	25,56	18,21,22	1.59	6 (33%)	21,30,33	2.06	5 (23%)
22	5MU	w	54	22	19,22,23	1.39	4 (21%)	27,32,35	2.05	6 (22%)
1	MA6	a	1518	1	23,26,27	1.42	5 (21%)	33,38,41	2.48	13 (39%)
25	2MG	A	2445	25,56	23,26,27	1.36	5 (21%)	33,38,41	2.29	7 (21%)
25	H2U	A	2449	25	18,21,22	1.22	2 (11%)	19,30,33	1.05	2 (10%)
22	PSU	w	32	22	18,21,22	1.41	4 (22%)	21,30,33	2.07	4 (19%)
22	4SU	w	8	22	18,21,22	1.96	4 (22%)	25,30,33	1.86	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	3TD	A	1915	25,56	19,22,23	4.10	7 (36%)	23,32,35	1.86	3 (13%)
25	G7M	A	2069	25,56	23,26,27	1.58	4 (17%)	34,39,42	1.79	5 (14%)
25	PSU	A	746	25,56	18,21,22	1.54	4 (22%)	21,30,33	2.03	4 (19%)
1	2MG	a	1207	1	23,26,27	1.28	3 (13%)	33,38,41	2.16	5 (15%)
25	6MZ	A	2030	25	22,25,26	1.43	4 (18%)	29,36,39	2.25	9 (31%)
28	MEQ	D	150	28	8,9,10	0.51	0	5,10,12	0.43	0
25	5MC	A	1962	25	19,22,23	1.33	3 (15%)	26,32,35	1.17	3 (11%)
11	IAS	k	119	11	6,7,8	0.99	0	3,8,10	1.32	1 (33%)
22	G7M	w	46	22	23,26,27	2.40	5 (21%)	34,39,42	3.00	10 (29%)
1	2MG	a	966	1	23,26,27	1.32	4 (17%)	33,38,41	2.22	7 (21%)
1	G7M	a	527	1	23,26,27	1.56	3 (13%)	34,39,42	1.76	5 (14%)
25	PSU	A	955	25	18,21,22	1.53	4 (22%)	21,30,33	2.20	5 (23%)
1	5MC	a	1407	1	19,22,23	1.42	3 (15%)	26,32,35	1.18	3 (11%)
1	4OC	a	1402	1,56	20,23,24	0.76	1 (5%)	25,32,35	1.01	2 (8%)
25	PSU	A	2457	25	18,21,22	1.61	5 (27%)	21,30,33	2.29	6 (28%)
25	PSU	A	1917	25	18,21,22	1.52	4 (22%)	21,30,33	2.10	4 (19%)
25	OMG	A	2251	23,25,56	23,26,27	1.29	3 (13%)	32,38,41	2.16	6 (18%)
25	2MG	A	1835	25	23,26,27	1.34	4 (17%)	33,38,41	2.19	6 (18%)
25	PSU	A	2605	25	18,21,22	1.53	4 (22%)	21,30,33	2.12	4 (19%)
25	6MZ	A	1618	25	22,25,26	1.42	5 (22%)	29,36,39	2.25	9 (31%)

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	MIA	w	37	22	-	2/15/33/34	0/3/3/3
22	PSU	w	39	22	-	0/7/25/26	0/2/2/2
22	PSU	w	55	22	-	1/7/25/26	0/2/2/2
25	5MU	A	747	25	-	0/7/25/26	0/2/2/2
1	MA6	a	1519	1	-	3/11/29/30	0/3/3/3
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
25	PSU	A	1911	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2504	25	-	1/7/25/26	0/2/2/2
25	OMU	A	2552	25	-	0/9/27/28	0/2/2/2
23	PSU	x	55	23	-	0/7/25/26	0/2/2/2
1	UR3	a	1498	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	a	516	1,56	-	0/7/25/26	0/2/2/2
23	5MU	x	54	23	-	0/7/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/9/27/28	0/3/3/3
25	5MU	A	1939	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2604	25	-	0/7/25/26	0/2/2/2
25	2MA	A	2503	25,56	-	0/7/25/26	0/3/3/3
36	MS6	O	82	36	-	2/4/6/8	-
12	D2T	l	89	12	-	4/7/12/14	-
25	OMC	A	2498	25,56	-	1/9/27/28	0/2/2/2
23	4SU	x	8	23	-	0/7/25/26	0/2/2/2
23	5MC	x	32	23	-	0/7/25/26	0/2/2/2
36	4D4	O	81	36	-	3/11/12/14	-
25	1MG	A	745	25	-	0/7/25/26	0/3/3/3
25	PSU	A	2580	25,56	-	1/7/25/26	0/2/2/2
22	5MU	w	54	22	-	0/7/25/26	0/2/2/2
1	MA6	a	1518	1	-	2/11/29/30	0/3/3/3
25	2MG	A	2445	25,56	-	0/9/27/28	0/3/3/3
25	H2U	A	2449	25	-	0/7/38/39	0/2/2/2
22	PSU	w	32	22	-	0/7/25/26	0/2/2/2
22	4SU	w	8	22	-	0/7/25/26	0/2/2/2
25	3TD	A	1915	25,56	-	2/7/25/26	0/2/2/2
25	G7M	A	2069	25,56	-	0/7/25/26	0/3/3/3
25	PSU	A	746	25,56	-	2/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	0/9/27/28	0/3/3/3
25	6MZ	A	2030	25	-	2/9/27/28	0/3/3/3
28	MEQ	D	150	28	-	2/8/9/11	-
25	5MC	A	1962	25	-	0/7/25/26	0/2/2/2
11	IAS	k	119	11	-	0/7/7/8	-
22	G7M	w	46	22	-	0/7/25/26	0/3/3/3
1	2MG	a	966	1	-	0/9/27/28	0/3/3/3
1	G7M	a	527	1	-	2/7/25/26	0/3/3/3
25	PSU	A	955	25	-	0/7/25/26	0/2/2/2
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
1	4OC	a	1402	1,56	-	3/9/29/30	0/2/2/2
25	PSU	A	2457	25	-	0/7/25/26	0/2/2/2
25	PSU	A	1917	25	-	2/7/25/26	0/2/2/2
25	OMG	A	2251	23,25,56	-	0/9/27/28	0/3/3/3
25	2MG	A	1835	25	-	0/9/27/28	0/3/3/3
25	PSU	A	2605	25	-	0/7/25/26	0/2/2/2
25	6MZ	A	1618	25	-	0/9/27/28	0/3/3/3

All (183) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1915	3TD	C6-C5	12.38	1.49	1.35
25	A	1915	3TD	C2-N1	9.34	1.48	1.37
22	w	46	G7M	C8-N7	7.79	1.46	1.33
22	w	37	MIA	C2-S10	-7.79	1.69	1.75
22	w	37	MIA	C13-C14	6.71	1.52	1.32
36	O	81	4D4	CZ-NE	5.74	1.44	1.33
25	A	1915	3TD	C6-N1	5.50	1.45	1.36
25	A	2069	G7M	C5-N7	-5.23	1.33	1.39
22	w	46	G7M	C5-N7	-5.16	1.33	1.39
1	a	527	G7M	C5-N7	-5.16	1.33	1.39
1	a	967	5MC	C5-C4	5.14	1.48	1.44
23	x	32	5MC	C5-C4	5.00	1.47	1.44
23	x	8	4SU	C4-S4	-5.00	1.59	1.68
22	w	8	4SU	C4-S4	-4.97	1.59	1.68
1	a	1407	5MC	C5-C4	4.83	1.47	1.44
25	A	1915	3TD	C2-N3	4.52	1.48	1.38
25	A	1962	5MC	C5-C4	4.37	1.47	1.44
22	w	8	4SU	C4-N3	-4.22	1.33	1.37
1	a	1519	MA6	C5-C4	4.20	1.46	1.39
12	l	89	D2T	CB-CA	-4.13	1.53	1.54
1	a	1518	MA6	C5-C4	4.01	1.46	1.39
22	w	46	G7M	C8-N9	3.98	1.46	1.35
22	w	37	MIA	C5-C4	3.97	1.46	1.39
25	A	2030	6MZ	C5-C4	3.86	1.46	1.39
25	A	1618	6MZ	C5-C4	3.82	1.45	1.39
25	A	2503	2MA	C5-C4	3.76	1.45	1.39
25	A	2457	PSU	C4-N3	-3.72	1.31	1.38
36	O	81	4D4	CZ-NH2	3.58	1.45	1.32
23	x	8	4SU	C4-N3	-3.55	1.33	1.37
25	A	2605	PSU	C4-N3	-3.52	1.32	1.38
25	A	955	PSU	C4-N3	-3.49	1.32	1.38
25	A	2445	2MG	C6-N1	-3.48	1.32	1.38
22	w	46	G7M	C5-C4	3.48	1.47	1.38
25	A	2552	OMU	C4-N3	-3.47	1.32	1.38
25	A	2580	PSU	C4-N3	-3.43	1.32	1.38
25	A	1939	5MU	C4-N3	-3.42	1.32	1.38
25	A	2604	PSU	C4-N3	-3.41	1.32	1.38
25	A	1835	2MG	C6-N1	-3.39	1.32	1.38
25	A	2552	OMU	C2-N3	-3.38	1.32	1.38
25	A	1911	PSU	C4-N3	-3.34	1.32	1.38
25	A	2504	PSU	C4-N3	-3.31	1.32	1.38
25	A	746	PSU	C4-N3	-3.30	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	2251	OMG	C6-N1	-3.29	1.32	1.38
25	A	2069	G7M	C6-N1	-3.27	1.32	1.38
25	A	2449	H2U	C2-N3	-3.20	1.32	1.38
25	A	1917	PSU	C6-C5	3.14	1.38	1.35
25	A	2605	PSU	C2-N3	-3.12	1.32	1.37
25	A	1917	PSU	C4-N3	-3.08	1.33	1.38
1	a	966	2MG	C5-C4	3.07	1.47	1.38
23	x	8	4SU	C5-C4	-3.06	1.38	1.42
25	A	747	5MU	C4-N3	-3.04	1.33	1.38
22	w	55	PSU	C4-N3	-3.04	1.33	1.38
1	a	527	G7M	C5-C4	3.01	1.45	1.38
22	w	32	PSU	C4-N3	-3.01	1.33	1.38
22	w	54	5MU	C4-N3	-3.00	1.33	1.38
25	A	1939	5MU	C2-N3	-3.00	1.32	1.38
1	a	1518	MA6	C5-N7	-2.99	1.33	1.39
1	a	966	2MG	C6-N1	-2.99	1.33	1.38
25	A	2030	6MZ	C5-N7	-2.98	1.33	1.39
1	a	1207	2MG	C5-C4	2.94	1.46	1.38
23	x	55	PSU	C6-C5	2.94	1.38	1.35
25	A	2449	H2U	C4-N3	-2.93	1.32	1.37
23	x	54	5MU	C4-N3	-2.92	1.33	1.38
25	A	746	PSU	C6-C5	2.92	1.38	1.35
22	w	8	4SU	C5-C4	-2.91	1.39	1.42
25	A	1618	6MZ	C5-N7	-2.91	1.33	1.39
1	a	1207	2MG	C6-N1	-2.90	1.33	1.38
25	A	1915	3TD	O2-C2	-2.89	1.17	1.23
1	a	1516	2MG	C6-N1	-2.88	1.33	1.38
1	a	516	PSU	C4-N3	-2.87	1.33	1.38
25	A	2251	OMG	C5-N7	-2.81	1.33	1.39
22	w	8	4SU	C2-N3	-2.79	1.33	1.38
23	x	55	PSU	C4-N3	-2.79	1.33	1.38
25	A	2457	PSU	C2-N3	-2.77	1.32	1.37
25	A	747	5MU	C6-N1	-2.76	1.33	1.38
1	a	1519	MA6	C5-C6	2.76	1.48	1.41
25	A	1962	5MC	C6-N1	-2.76	1.33	1.38
25	A	2457	PSU	C2-N1	-2.75	1.33	1.36
23	x	32	5MC	C6-N1	-2.75	1.33	1.38
25	A	2504	PSU	C2-N3	-2.74	1.33	1.37
1	a	1516	2MG	C5-C4	2.72	1.46	1.38
25	A	2580	PSU	C2-N3	-2.72	1.33	1.37
1	a	516	PSU	C6-C5	2.72	1.38	1.35
25	A	745	1MG	C5-C4	2.71	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	w	55	PSU	C6-C5	2.71	1.38	1.35
25	A	1911	PSU	C6-C5	2.70	1.38	1.35
1	a	527	G7M	C6-N1	-2.69	1.33	1.38
25	A	2251	OMG	C5-C4	2.69	1.46	1.38
25	A	1939	5MU	C6-N1	-2.68	1.33	1.38
22	w	54	5MU	C2-N3	-2.67	1.33	1.38
25	A	1835	2MG	C5-C4	2.67	1.46	1.38
25	A	955	PSU	C2-N3	-2.66	1.33	1.37
25	A	2069	G7M	C5-C4	2.65	1.44	1.38
25	A	746	PSU	C2-N3	-2.64	1.33	1.37
25	A	2503	2MA	C5-N7	-2.63	1.34	1.39
25	A	745	1MG	C5-N7	-2.63	1.33	1.39
22	w	39	PSU	C6-C5	2.62	1.38	1.35
25	A	2604	PSU	C6-C5	2.62	1.38	1.35
22	w	54	5MU	C6-N1	-2.62	1.33	1.38
25	A	1835	2MG	C5-N7	-2.61	1.33	1.39
25	A	747	5MU	C2-N3	-2.61	1.33	1.38
22	w	32	PSU	C6-C5	2.60	1.38	1.35
25	A	2604	PSU	C2-N3	-2.57	1.33	1.37
22	w	46	G7M	C6-N1	-2.55	1.34	1.38
25	A	1618	6MZ	C5-C6	2.55	1.48	1.41
25	A	1917	PSU	C2-N3	-2.55	1.33	1.37
25	A	2030	6MZ	C5-C6	2.54	1.48	1.41
36	O	81	4D4	CZ-NH1	-2.54	1.25	1.34
22	w	37	MIA	C5-N7	-2.54	1.34	1.39
1	a	967	5MC	C6-N1	-2.54	1.33	1.38
23	x	54	5MU	C6-N1	-2.53	1.33	1.38
25	A	746	PSU	C2-N1	-2.52	1.33	1.36
25	A	2580	PSU	C2-N1	-2.52	1.33	1.36
25	A	2503	2MA	C5-C6	2.51	1.48	1.41
1	a	1407	5MC	C6-N1	-2.50	1.33	1.38
25	A	2504	PSU	C6-C5	2.50	1.38	1.35
25	A	2605	PSU	C2-N1	-2.49	1.33	1.36
1	a	1519	MA6	C5-N7	-2.49	1.34	1.39
25	A	1911	PSU	C2-N3	-2.47	1.33	1.37
25	A	955	PSU	C6-C5	2.47	1.38	1.35
25	A	2580	PSU	O4'-C1'	-2.46	1.40	1.43
25	A	1939	5MU	C6-C5	2.46	1.38	1.34
25	A	2445	2MG	C5-C4	2.45	1.45	1.38
25	A	2504	PSU	C2-N1	-2.45	1.33	1.36
1	a	1407	5MC	C6-C5	2.43	1.38	1.34
25	A	1618	6MZ	C8-N9	-2.43	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	2552	OMU	C5-C4	-2.41	1.38	1.43
25	A	2445	2MG	C5-N7	-2.39	1.34	1.39
22	w	32	PSU	C2-N3	-2.39	1.33	1.37
25	A	2604	PSU	C2-N1	-2.39	1.33	1.36
25	A	1915	3TD	C4-N3	2.37	1.45	1.40
1	a	966	2MG	C5-N7	-2.37	1.34	1.39
22	w	55	PSU	C2-N3	-2.37	1.33	1.37
23	x	54	5MU	C2-N3	-2.36	1.33	1.38
25	A	1915	3TD	O4-C4	-2.36	1.18	1.23
23	x	54	5MU	C6-C5	2.36	1.38	1.34
25	A	1917	PSU	C2-N1	-2.35	1.33	1.36
23	x	8	4SU	C2-N3	-2.34	1.33	1.38
1	a	1519	MA6	C4-N9	-2.34	1.32	1.37
22	w	37	MIA	C5-C6	2.34	1.47	1.41
1	a	967	5MC	C6-C5	2.33	1.38	1.34
1	a	516	PSU	C2-N3	-2.30	1.33	1.37
23	x	32	5MC	C6-C5	2.30	1.38	1.34
25	A	2457	PSU	C6-C5	2.29	1.37	1.35
1	a	1518	MA6	C5-C6	2.29	1.47	1.41
22	w	39	PSU	C4-N3	-2.27	1.34	1.38
25	A	2030	6MZ	C4-N9	-2.27	1.33	1.37
25	A	1911	PSU	C2-N1	-2.27	1.33	1.36
25	A	2457	PSU	C6-N1	-2.26	1.32	1.36
1	a	966	2MG	C2-N3	2.26	1.36	1.32
1	a	1516	2MG	C5-N7	-2.25	1.34	1.39
1	a	516	PSU	C2-N1	-2.25	1.33	1.36
1	a	1518	MA6	C8-N9	-2.25	1.33	1.37
25	A	955	PSU	C2-N1	-2.25	1.33	1.36
25	A	1962	5MC	C6-C5	2.24	1.38	1.34
22	w	37	MIA	C4-N9	-2.24	1.33	1.37
1	a	1518	MA6	C4-N9	-2.22	1.33	1.37
25	A	2580	PSU	C6-C5	2.21	1.37	1.35
25	A	2503	2MA	C4-N9	-2.21	1.33	1.37
25	A	1618	6MZ	C4-N9	-2.20	1.33	1.37
22	w	55	PSU	C2-N1	-2.20	1.33	1.36
23	x	55	PSU	C2-N3	-2.20	1.33	1.37
1	a	1207	2MG	C5-N7	-2.18	1.34	1.39
25	A	2445	2MG	C2-N1	-2.17	1.33	1.36
23	x	54	5MU	C4-C5	2.16	1.48	1.44
22	w	54	5MU	C6-C5	2.14	1.38	1.34
25	A	2498	OMC	C6-N1	-2.13	1.33	1.38
1	a	1519	MA6	C8-N7	2.11	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	w	32	PSU	C2-N1	-2.11	1.33	1.36
1	a	1498	UR3	C5-C4	-2.10	1.38	1.43
25	A	2445	2MG	C4-N9	-2.08	1.32	1.38
1	a	1402	4OC	C6-N1	-2.08	1.33	1.38
25	A	747	5MU	C6-C5	2.07	1.38	1.34
22	w	37	MIA	C8-N7	2.06	1.35	1.31
25	A	1835	2MG	C2-N1	-2.05	1.33	1.36
25	A	2503	2MA	C8-N9	-2.03	1.34	1.37
22	w	39	PSU	C2-N1	-2.03	1.34	1.36
25	A	2069	G7M	C4-N9	-2.03	1.32	1.38
25	A	2605	PSU	C6-C5	2.03	1.37	1.35
25	A	747	5MU	C4-C5	2.02	1.48	1.44
25	A	2580	PSU	C6-N1	-2.01	1.33	1.36
1	a	516	PSU	O4'-C1'	-2.01	1.41	1.43
1	a	1516	2MG	C4-N9	-2.01	1.33	1.38

All (262) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	w	37	MIA	C12-C13-C14	-9.62	109.74	127.01
25	A	2503	2MA	C5-C4-N3	-8.46	118.27	127.18
22	w	37	MIA	C5-C4-N3	-7.74	119.03	127.18
22	w	46	G7M	CN7-N7-C8	-7.63	113.24	124.79
25	A	2445	2MG	C2-N3-C4	7.59	121.49	112.00
1	a	1516	2MG	C2-N3-C4	7.47	121.34	112.00
25	A	2457	PSU	N1-C2-N3	7.32	122.89	115.17
25	A	1835	2MG	C2-N3-C4	7.21	121.01	112.00
25	A	2604	PSU	N1-C2-N3	7.15	122.71	115.17
1	a	1207	2MG	C2-N3-C4	7.11	120.90	112.00
25	A	2251	OMG	C5-C4-N3	-7.04	117.19	128.39
25	A	955	PSU	N1-C2-N3	7.03	122.59	115.17
1	a	966	2MG	C2-N3-C4	7.00	120.76	112.00
22	w	46	G7M	N9-C8-N7	-6.98	95.53	112.48
1	a	1498	UR3	C4-N3-C2	-6.97	118.97	124.58
25	A	1911	PSU	N1-C2-N3	6.88	122.43	115.17
22	w	39	PSU	N1-C2-N3	6.85	122.40	115.17
22	w	55	PSU	N1-C2-N3	6.82	122.36	115.17
22	w	46	G7M	C8-N7-C5	6.81	116.30	107.78
23	x	8	4SU	C4-N3-C2	-6.75	120.84	127.31
1	a	966	2MG	C5-C4-N3	-6.63	117.83	128.39
25	A	1917	PSU	N1-C2-N3	6.62	122.15	115.17
22	w	32	PSU	N1-C2-N3	6.45	121.97	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	2504	PSU	N1-C2-N3	6.45	121.97	115.17
25	A	2580	PSU	N1-C2-N3	6.45	121.97	115.17
25	A	2445	2MG	C5-C4-N3	-6.44	118.14	128.39
25	A	1835	2MG	C5-C4-N3	-6.42	118.18	128.39
25	A	2605	PSU	N1-C2-N3	6.35	121.86	115.17
22	w	46	G7M	N9-C4-N3	6.26	138.48	125.95
23	x	55	PSU	N1-C2-N3	6.26	121.77	115.17
25	A	2503	2MA	N3-C4-N9	6.26	134.93	126.99
25	A	746	PSU	N1-C2-N3	6.23	121.74	115.17
1	a	1207	2MG	C5-C4-N3	-6.20	118.52	128.39
25	A	1618	6MZ	C5-C4-N3	-6.19	118.19	126.72
1	a	1516	2MG	C5-C4-N3	-6.19	118.55	128.39
1	a	516	PSU	N1-C2-N3	6.15	121.66	115.17
1	a	1518	MA6	C5-C4-N3	-6.03	118.41	126.72
22	w	37	MIA	N3-C4-N9	5.94	134.53	126.99
25	A	1915	3TD	N1-C2-N3	5.93	120.44	116.13
1	a	1519	MA6	C5-C4-N3	-5.70	118.87	126.72
25	A	2251	OMG	C2-N3-C4	5.69	122.11	112.30
25	A	1939	5MU	N3-C2-N1	5.63	122.22	114.89
25	A	2030	6MZ	C5-C4-N3	-5.63	118.97	126.72
25	A	1939	5MU	C4-N3-C2	-5.62	119.97	127.34
23	x	54	5MU	C4-N3-C2	-5.57	120.04	127.34
22	w	46	G7M	C5-C4-N3	-5.55	117.67	128.15
25	A	745	1MG	C5-C4-N3	-5.53	119.59	128.39
25	A	2069	G7M	C5-C4-N3	-5.51	117.74	128.15
1	a	527	G7M	N9-C4-N3	5.51	136.97	125.95
1	a	527	G7M	C5-C4-N3	-5.49	117.77	128.15
25	A	2069	G7M	N9-C4-N3	5.39	136.73	125.95
25	A	2552	OMU	C4-N3-C2	-5.38	119.94	126.61
25	A	747	5MU	C4-N3-C2	-5.36	120.31	127.34
22	w	39	PSU	C4-N3-C2	-5.32	119.04	126.37
25	A	747	5MU	N3-C2-N1	5.31	121.81	114.89
23	x	8	4SU	C5-C4-N3	5.30	119.69	114.75
23	x	54	5MU	N3-C2-N1	5.30	121.80	114.89
1	a	966	2MG	N9-C4-N3	5.18	136.30	125.95
22	w	8	4SU	C4-N3-C2	-5.17	122.36	127.31
22	w	8	4SU	C5-C4-N3	5.15	119.54	114.75
25	A	2552	OMU	N3-C2-N1	5.13	121.57	114.89
25	A	2251	OMG	N9-C4-N3	5.13	136.21	125.95
25	A	2069	G7M	C2-N3-C4	5.13	121.13	112.30
1	a	1518	MA6	N3-C4-N9	5.00	135.66	127.17
25	A	1835	2MG	N9-C4-N3	4.99	135.94	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	w	54	5MU	C4-N3-C2	-4.94	120.86	127.34
25	A	1939	5MU	C5-C4-N3	4.86	119.55	115.32
1	a	527	G7M	C2-N3-C4	4.85	120.66	112.30
25	A	1618	6MZ	N3-C4-N9	4.82	135.36	127.17
22	w	54	5MU	N3-C2-N1	4.81	121.16	114.89
1	a	1518	MA6	C10-N6-C6	-4.80	108.30	120.52
25	A	2445	2MG	N9-C4-N3	4.77	135.48	125.95
23	x	54	5MU	C5-C4-N3	4.73	119.43	115.32
1	a	1519	MA6	C9-N6-C6	-4.72	108.50	120.52
22	w	39	PSU	O2-C2-N1	-4.68	117.96	122.79
25	A	2457	PSU	C4-N3-C2	-4.65	119.96	126.37
1	a	1207	2MG	N9-C4-N3	4.61	135.16	125.95
25	A	2605	PSU	C4-N3-C2	-4.58	120.07	126.37
22	w	54	5MU	C5-C4-N3	4.57	119.30	115.32
1	a	1519	MA6	C10-N6-C6	-4.51	109.04	120.52
25	A	745	1MG	C2-N3-C4	4.49	122.08	111.98
25	A	955	PSU	C4-N3-C2	-4.47	120.21	126.37
22	w	46	G7M	C2-N3-C4	4.47	120.00	112.30
23	x	8	4SU	N3-C2-N1	4.46	120.70	114.89
25	A	745	1MG	N9-C4-N3	4.45	134.85	125.95
25	A	2604	PSU	C4-N3-C2	-4.44	120.26	126.37
22	w	55	PSU	C4-N3-C2	-4.41	120.29	126.37
1	a	1516	2MG	N9-C4-N3	4.38	134.70	125.95
25	A	747	5MU	C5-C4-N3	4.38	119.13	115.32
25	A	2552	OMU	C5-C4-N3	4.38	120.93	114.80
25	A	1939	5MU	C5-C6-N1	-4.36	118.57	123.31
22	w	46	G7M	C8-N9-C4	4.34	117.83	107.09
25	A	1911	PSU	C4-N3-C2	-4.33	120.40	126.37
1	a	1519	MA6	C2-N1-C6	4.33	122.41	111.83
25	A	2504	PSU	C4-N3-C2	-4.30	120.45	126.37
25	A	1915	3TD	C4-N3-C2	-4.28	120.08	124.61
1	a	1518	MA6	N1-C6-N6	4.25	122.04	116.86
23	x	55	PSU	C4-N3-C2	-4.25	120.52	126.37
22	w	32	PSU	C4-N3-C2	-4.24	120.54	126.37
25	A	2030	6MZ	C9-N6-C6	-4.20	118.96	122.85
25	A	746	PSU	C4-N3-C2	-4.18	120.61	126.37
22	w	37	MIA	C16-C14-C13	-4.18	110.12	122.66
23	x	8	4SU	C5-C4-S4	-4.14	119.58	124.31
25	A	1939	5MU	O4-C4-C5	-4.12	120.21	124.92
25	A	2030	6MZ	C6-C5-N7	4.11	136.91	132.43
1	a	1519	MA6	C4-C5-N7	-4.11	105.88	110.58
1	a	516	PSU	C4-N3-C2	-4.08	120.75	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	89	D2T	CB1-SB-CB	4.05	109.65	102.36
25	A	2030	6MZ	N3-C4-N9	4.03	134.02	127.17
25	A	1618	6MZ	C2-N3-C4	4.02	121.66	111.83
23	x	54	5MU	O4-C4-C5	-4.01	120.32	124.92
25	A	747	5MU	O4-C4-C5	-4.00	120.34	124.92
1	a	1518	MA6	C2-N1-C6	3.99	121.58	111.83
25	A	1917	PSU	C4-N3-C2	-3.98	120.89	126.37
12	l	89	D2T	OD2-CG-CB	3.98	121.74	113.15
1	a	1519	MA6	N3-C4-N9	3.97	133.92	127.17
22	w	55	PSU	O2-C2-N1	-3.96	118.71	122.79
25	A	2580	PSU	C4-N3-C2	-3.95	120.93	126.37
1	a	1519	MA6	C2-N3-C4	3.90	121.35	111.83
23	x	54	5MU	C5-C6-N1	-3.88	119.10	123.31
25	A	2030	6MZ	C2-N3-C4	3.85	121.25	111.83
22	w	37	MIA	C15-C14-C13	-3.78	111.30	122.66
1	a	1518	MA6	C9-N6-C6	-3.78	110.90	120.52
25	A	2457	PSU	O2-C2-N1	-3.74	118.93	122.79
25	A	2503	2MA	C4-C5-N7	-3.74	106.30	110.58
1	a	1518	MA6	C2-N3-C4	3.74	120.97	111.83
22	w	54	5MU	O4-C4-C5	-3.70	120.68	124.92
22	w	37	MIA	C6-C5-N7	3.70	136.46	132.43
22	w	46	G7M	C1'-N9-C8	-3.70	114.25	126.74
25	A	2030	6MZ	C4-C5-N7	-3.69	106.37	110.58
1	a	1516	2MG	C6-C5-N7	3.66	136.96	130.29
25	A	1911	PSU	O2-C2-N1	-3.66	119.02	122.79
1	a	1519	MA6	N1-C2-N3	-3.63	123.09	128.58
25	A	1917	PSU	O2-C2-N1	-3.61	119.06	122.79
22	w	8	4SU	N3-C2-N1	3.60	119.58	114.89
25	A	1618	6MZ	C4-C5-N7	-3.58	106.49	110.58
25	A	2604	PSU	O2-C2-N1	-3.57	119.10	122.79
23	x	32	5MC	C5-C6-N1	-3.57	119.44	123.31
25	A	747	5MU	C5-C6-N1	-3.55	119.45	123.31
1	a	1407	5MC	C5-C6-N1	-3.53	119.47	123.31
25	A	1939	5MU	O2-C2-N1	-3.51	118.23	122.80
22	w	37	MIA	C2-N3-C4	3.51	121.47	112.29
25	A	2030	6MZ	N1-C2-N3	-3.50	123.28	128.58
25	A	955	PSU	O2-C2-N1	-3.50	119.18	122.79
1	a	516	PSU	O2-C2-N1	-3.49	119.19	122.79
25	A	1618	6MZ	C6-C5-N7	3.48	136.23	132.43
25	A	2445	2MG	C6-C5-N7	3.48	136.62	130.29
22	w	37	MIA	C4-C5-N7	-3.45	106.64	110.58
22	w	32	PSU	O2-C2-N1	-3.44	119.24	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1498	UR3	C5-C4-N3	3.44	119.56	115.04
25	A	1618	6MZ	N1-C2-N3	-3.43	123.39	128.58
25	A	2504	PSU	O2-C2-N1	-3.36	119.32	122.79
1	a	1519	MA6	C10-N6-C9	-3.33	105.48	116.18
25	A	746	PSU	O2-C2-N1	-3.26	119.42	122.79
1	a	1518	MA6	N1-C2-N3	-3.25	123.67	128.58
1	a	1518	MA6	C5-C6-N6	-3.24	120.21	125.33
25	A	2580	PSU	O2-C2-N1	-3.23	119.46	122.79
1	a	1207	2MG	C6-C5-N7	3.22	136.15	130.29
25	A	2498	OMC	O2-C2-N3	-3.20	117.28	122.33
23	x	55	PSU	O2-C2-N1	-3.19	119.50	122.79
25	A	2251	OMG	C6-C5-N7	3.17	136.06	130.29
22	w	54	5MU	C5-C6-N1	-3.16	119.88	123.31
1	a	967	5MC	C5-C6-N1	-3.02	120.03	123.31
1	a	1518	MA6	C4-C5-N7	-3.01	107.14	110.58
23	x	54	5MU	O2-C2-N1	-2.98	118.92	122.80
22	w	46	G7M	CN7-N7-C5	2.94	130.46	126.80
23	x	32	5MC	C5-C4-N3	-2.92	118.76	121.75
25	A	2605	PSU	O2-C2-N1	-2.92	119.77	122.79
25	A	1962	5MC	C5-C4-N3	-2.91	118.77	121.75
25	A	1835	2MG	C6-C5-N7	2.89	135.55	130.29
1	a	1516	2MG	C4-C5-N7	-2.85	106.15	110.67
25	A	1618	6MZ	C9-N6-C6	-2.81	120.24	122.85
22	w	37	MIA	C4-N9-C8	2.74	108.61	105.74
25	A	1962	5MC	C5-C6-N1	-2.72	120.36	123.31
25	A	2251	OMG	C4-C5-N7	-2.70	106.39	110.67
25	A	2503	2MA	C5-N7-C8	2.69	107.67	103.45
1	a	967	5MC	C5-C4-N3	-2.68	119.01	121.75
1	a	1519	MA6	C5-N7-C8	2.66	107.63	103.45
25	A	2445	2MG	C4-C5-N7	-2.66	106.46	110.67
1	a	1407	5MC	C5-C4-N3	-2.65	119.03	121.75
22	w	8	4SU	C5-C4-S4	-2.64	121.29	124.31
1	a	1516	2MG	N1-C2-N2	2.62	119.24	116.56
25	A	2552	OMU	O4-C4-C5	-2.62	120.65	125.16
1	a	966	2MG	C6-C5-N7	2.61	135.03	130.29
22	w	46	G7M	O6-C6-C5	-2.59	122.24	128.01
25	A	746	PSU	C6-C5-C4	-2.58	116.43	118.17
25	A	2030	6MZ	C5-N7-C8	2.57	107.48	103.45
25	A	1618	6MZ	C5-N7-C8	2.52	107.42	103.45
22	w	37	MIA	N3-C2-N1	-2.52	122.40	127.00
22	w	37	MIA	C5-N7-C8	2.52	107.40	103.45
1	a	1207	2MG	C4-C5-N7	-2.51	106.69	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	745	1MG	C6-C5-N7	2.51	134.93	129.36
25	A	2580	PSU	O4'-C1'-C2'	2.50	108.61	105.15
1	a	1407	5MC	O2-C2-N3	-2.50	118.39	122.33
1	a	1519	MA6	C6-C5-N7	2.49	137.41	133.43
1	a	1402	4OC	O2-C2-N3	-2.48	118.42	122.33
25	A	2503	2MA	C4-N9-C8	2.47	108.33	105.74
25	A	2503	2MA	C6-C5-N7	2.46	136.83	132.09
25	A	2069	G7M	C5-C6-N1	2.45	116.91	111.84
25	A	2605	PSU	C5-C6-N1	-2.44	118.75	122.14
25	A	2503	2MA	N6-C6-N1	2.44	120.32	117.03
1	a	1518	MA6	C4-N9-C8	2.42	108.27	105.74
1	a	966	2MG	C2-N1-C6	-2.37	121.69	124.55
1	a	527	G7M	O6-C6-C5	-2.36	122.74	128.01
1	a	516	PSU	O4'-C1'-C2'	2.35	108.41	105.15
25	A	955	PSU	C5-C6-N1	-2.35	118.88	122.14
25	A	2552	OMU	O2-C2-N1	-2.35	119.74	122.80
23	x	8	4SU	C1'-N1-C2	2.35	121.81	117.59
1	a	1518	MA6	C10-N6-C9	-2.35	108.64	116.18
25	A	2069	G7M	O6-C6-C5	-2.34	122.78	128.01
25	A	745	1MG	C4-C5-N7	-2.33	106.98	110.67
1	a	1498	UR3	C6-N1-C2	-2.32	119.91	121.80
25	A	747	5MU	C1'-N1-C2	2.32	121.75	117.59
25	A	1618	6MZ	C4-N9-C8	2.31	108.16	105.74
25	A	2503	2MA	C2-N1-C6	2.30	121.64	118.10
25	A	2449	H2U	C5-C4-N3	2.30	119.14	116.69
22	w	54	5MU	C5M-C5-C4	2.29	121.23	118.78
22	w	37	MIA	C11-S10-C2	-2.27	100.55	102.25
23	x	55	PSU	C5-C6-N1	-2.27	118.99	122.14
25	A	1835	2MG	C4-C5-N7	-2.27	107.08	110.67
25	A	2580	PSU	C5-C6-N1	-2.24	119.03	122.14
1	a	966	2MG	C4-C5-N7	-2.24	107.12	110.67
22	w	39	PSU	C5-C6-N1	-2.21	119.07	122.14
25	A	2449	H2U	N3-C2-N1	2.21	118.87	116.65
1	a	966	2MG	O6-C6-C5	-2.21	120.70	126.53
22	w	37	MIA	C2-N1-C6	2.21	121.73	117.54
1	a	1518	MA6	C5-N7-C8	2.21	106.92	103.45
1	a	1519	MA6	C4-N9-C8	2.21	108.05	105.74
1	a	527	G7M	C5-C6-N1	2.20	116.39	111.84
25	A	2445	2MG	C5-C6-N1	2.20	118.86	113.25
25	A	2457	PSU	C5-C6-N1	-2.19	119.10	122.14
11	k	119	IAS	OD1-CG-CB	-2.17	119.06	125.38
1	a	1402	4OC	C6-C5-C4	2.17	119.61	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	2604	PSU	C5-C6-N1	-2.16	119.14	122.14
25	A	747	5MU	O2-C2-N1	-2.16	119.98	122.80
25	A	1911	PSU	C5-C6-N1	-2.14	119.17	122.14
22	w	37	MIA	N9-C8-N7	-2.14	110.90	113.94
25	A	2503	2MA	N9-C8-N7	-2.14	110.90	113.94
25	A	747	5MU	C5M-C5-C4	2.13	121.06	118.78
1	a	1498	UR3	C3U-N3-C2	2.13	121.05	117.33
25	A	2251	OMG	C5-C6-N1	2.13	118.68	113.25
1	a	1519	MA6	N1-C6-N6	2.11	119.42	116.86
12	l	89	D2T	OD2-CG-OD1	-2.11	119.30	124.08
25	A	747	5MU	C1'-N1-C6	-2.10	117.70	121.15
25	A	1911	PSU	O4'-C1'-C2'	2.09	108.05	105.15
1	a	1516	2MG	CM2-N2-C2	-2.09	119.16	123.65
25	A	2445	2MG	C2-N1-C6	-2.09	122.03	124.55
25	A	1915	3TD	C1'-C5-C4	2.08	120.77	117.61
23	x	32	5MC	O2-C2-N3	-2.08	119.05	122.33
25	A	1835	2MG	O6-C6-C5	-2.08	121.05	126.53
25	A	1962	5MC	N1-C2-N3	2.07	122.40	118.80
25	A	2457	PSU	O2-C2-N3	-2.07	118.18	121.86
25	A	2604	PSU	O2-C2-N3	-2.07	118.19	121.86
25	A	1917	PSU	C6-C5-C4	-2.06	116.78	118.17
25	A	2030	6MZ	C2-N1-C6	2.06	122.06	115.24
1	a	1516	2MG	C5-C6-N1	2.06	118.49	113.25
1	a	1516	2MG	C2-N1-C6	-2.05	122.07	124.55
25	A	955	PSU	O2-C2-N3	-2.04	118.23	121.86
1	a	1498	UR3	C1'-N1-C2	2.04	120.38	117.04
22	w	32	PSU	C5-C6-N1	-2.03	119.32	122.14
25	A	2457	PSU	O4'-C1'-C2'	2.01	107.94	105.15
1	a	1516	2MG	O6-C6-C5	-2.01	121.23	126.53

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	527	G7M	O4'-C4'-C5'-O5'
1	a	1518	MA6	C5-C6-N6-C9
1	a	1519	MA6	C5-C6-N6-C9
12	l	89	D2T	CA-CB-CG-OD1
12	l	89	D2T	CA-CB-CG-OD2
22	w	37	MIA	C12-C13-C14-C15
22	w	37	MIA	C12-C13-C14-C16
25	A	1915	3TD	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	a	527	G7M	C3'-C4'-C5'-O5'
25	A	1915	3TD	C3'-C4'-C5'-O5'
25	A	1917	PSU	C3'-C4'-C5'-O5'
25	A	1917	PSU	O4'-C4'-C5'-O5'
28	D	150	MEQ	OE1-CD-CG-CB
28	D	150	MEQ	NE2-CD-CG-CB
1	a	1402	4OC	O4'-C4'-C5'-O5'
1	a	1519	MA6	N1-C6-N6-C9
25	A	2030	6MZ	O4'-C4'-C5'-O5'
25	A	2030	6MZ	C3'-C4'-C5'-O5'
36	O	82	MS6	CB-CG-SD-CE
1	a	1518	MA6	N1-C6-N6-C9
25	A	2498	OMC	O4'-C4'-C5'-O5'
25	A	2504	PSU	O4'-C4'-C5'-O5'
22	w	55	PSU	O4'-C1'-C5-C4
36	O	81	4D4	OB-CB-CG-CD
25	A	2580	PSU	O4'-C4'-C5'-O5'
1	a	1402	4OC	C3'-C2'-O2'-CM2
1	a	1402	4OC	C3'-C4'-C5'-O5'
1	a	1519	MA6	O4'-C4'-C5'-O5'
12	l	89	D2T	SB-CB-CG-OD2
25	A	746	PSU	O4'-C1'-C5-C6
36	O	82	MS6	CA-CB-CG-SD
12	l	89	D2T	CG-CB-SB-CB1
25	A	746	PSU	C2'-C1'-C5-C6
36	O	81	4D4	O-C-CA-CB
36	O	81	4D4	CA-CB-CG-CD

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	a	1519	MA6	2	0
25	A	2498	OMC	1	0
1	a	1518	MA6	3	0
1	a	1402	4OC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 718 ligands modelled in this entry, 716 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	PHE	w	102	22	10,11,12	1.66	1 (10%)	8,13,15	0.55	0
57	T8B	a	3133	-	48,48,48	2.73	10 (20%)	63,71,71	1.73	17 (26%)

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
58	PHE	w	102	22	-	0/5/6/8	0/1/1/1
57	T8B	a	3133	-	-	0/26/26/26	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	a	3133	T8B	C27-C26	-10.06	1.40	1.48
57	a	3133	T8B	C2-C3	-8.83	1.39	1.51
57	a	3133	T8B	C25-C26	7.67	1.52	1.38
58	w	102	PHE	CB-CG	-5.08	1.39	1.51
57	a	3133	T8B	C10-C11	4.57	1.38	1.33
57	a	3133	T8B	C11-C12	-4.36	1.39	1.48
57	a	3133	T8B	C23-C24	-3.76	1.39	1.49
57	a	3133	T8B	C15-C14	-3.04	1.39	1.46
57	a	3133	T8B	C25-C24	2.97	1.53	1.43
57	a	3133	T8B	C9-C10	-2.80	1.38	1.43
57	a	3133	T8B	C15-C9	-2.70	1.38	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	a	3133	T8B	O5-C14-O6	4.74	122.11	116.45
57	a	3133	T8B	C21-C23-C24	-4.44	120.00	125.09
57	a	3133	T8B	C13-O4-C12	-3.69	109.01	115.85
57	a	3133	T8B	O11-C26-C27	3.37	118.98	113.95
57	a	3133	T8B	C26-C25-C24	-3.25	116.24	120.81
57	a	3133	T8B	C32-C27-C26	3.14	126.74	121.69
57	a	3133	T8B	C11-O5-C14	-3.12	119.04	121.54
57	a	3133	T8B	C19-O8-C18	-2.60	108.41	113.92
57	a	3133	T8B	C15-C16-C17	2.58	123.16	121.13
57	a	3133	T8B	O4-C12-C11	2.46	115.21	111.77
57	a	3133	T8B	O10-C24-C23	2.34	123.25	119.31
57	a	3133	T8B	C4-C5-C6	-2.33	118.25	122.13
57	a	3133	T8B	O11-C26-C25	-2.20	118.20	121.09
57	a	3133	T8B	C9-C15-C14	2.16	122.28	120.07
57	a	3133	T8B	O7-C16-C15	-2.09	117.07	121.29
57	a	3133	T8B	O6-C14-C15	-2.01	119.34	124.45
57	a	3133	T8B	O2-C1-C2	-2.01	116.87	122.94

There are no chirality outliers.

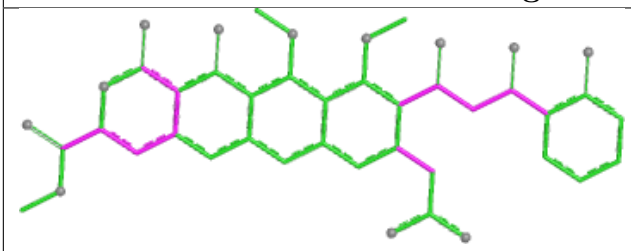
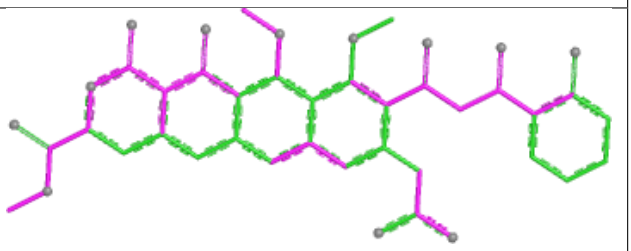
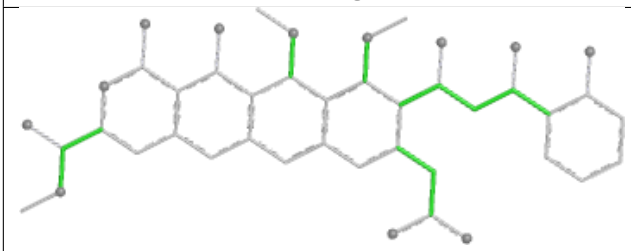
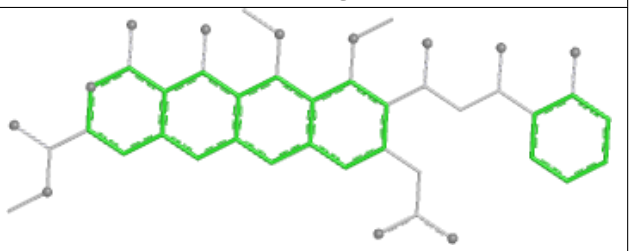
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	a	3133	T8B	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand T8B a 3133	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

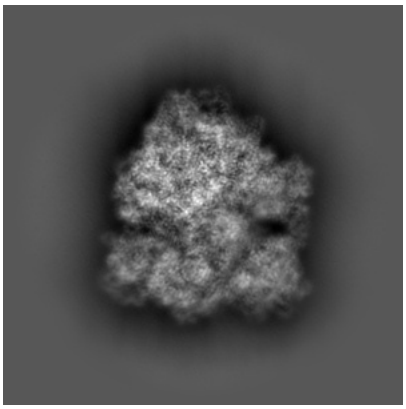
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-28197. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

6.1.1 Primary map



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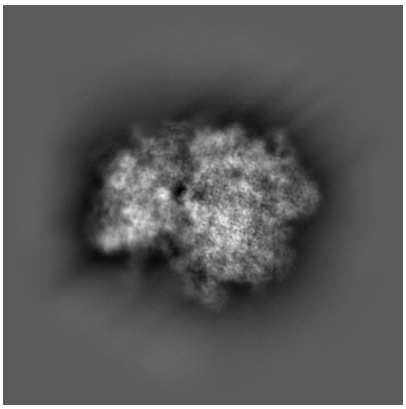

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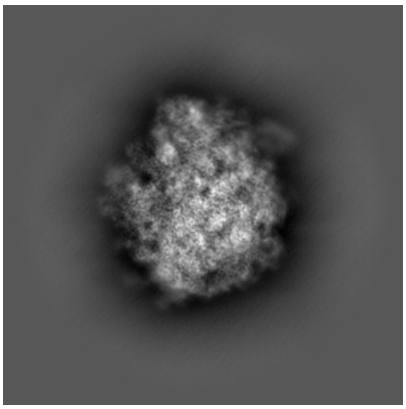
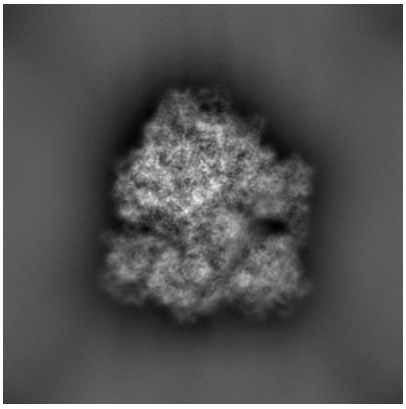
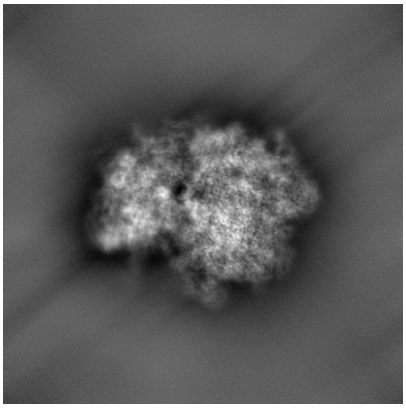


Z

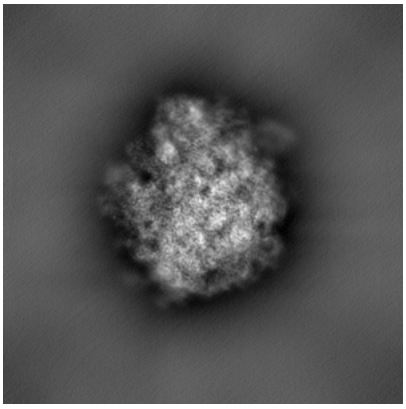
6.1.2 Raw map



X



Y

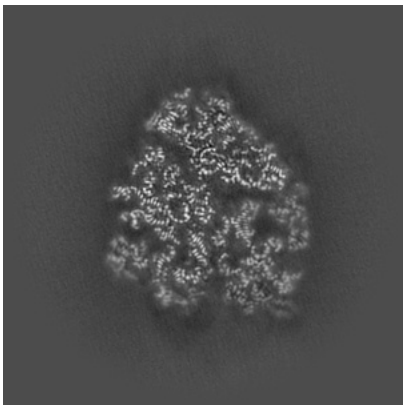


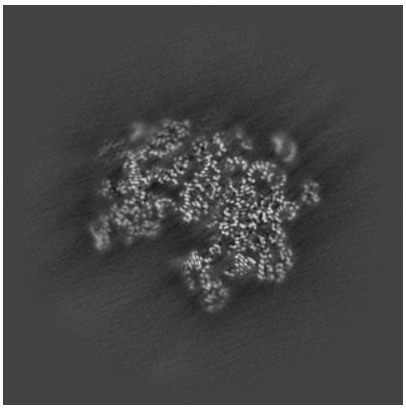
Z

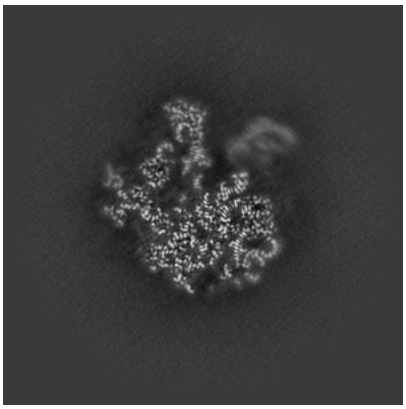
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

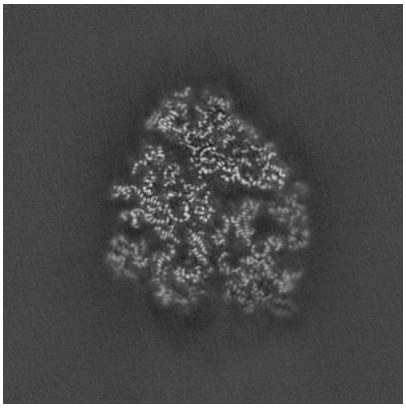
6.2.1 Primary map

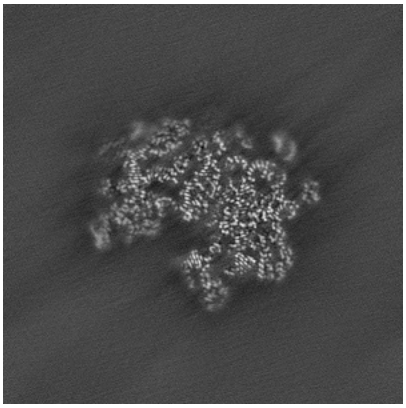

X Index: 256

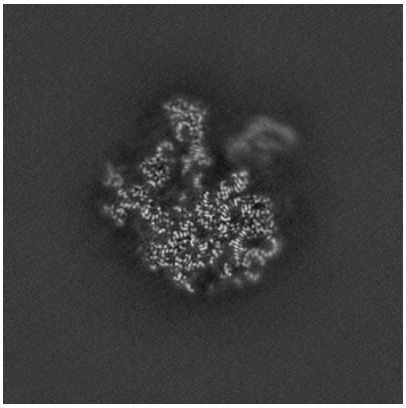

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256

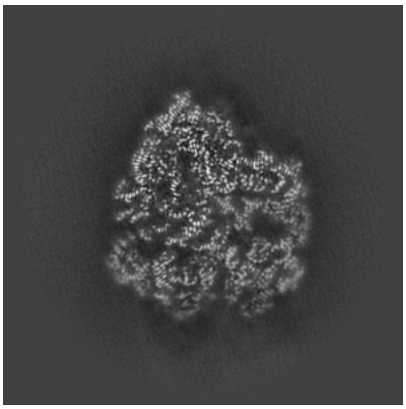

Y Index: 256


Z Index: 256

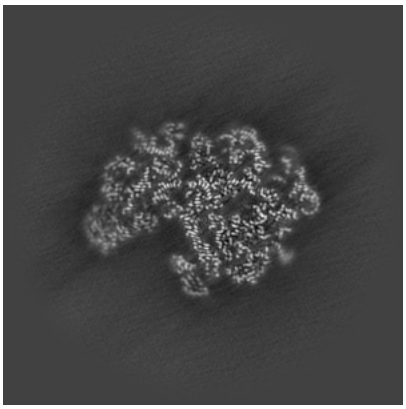
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

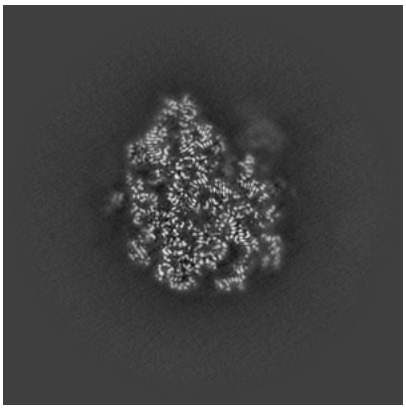
6.3.1 Primary map



X Index: 247

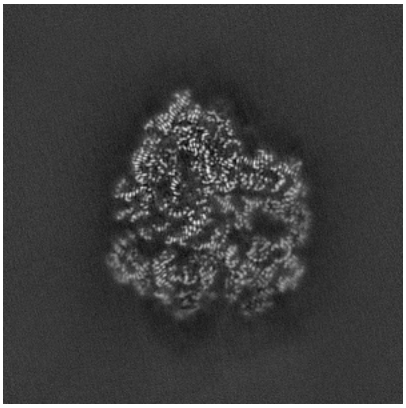


Y Index: 237

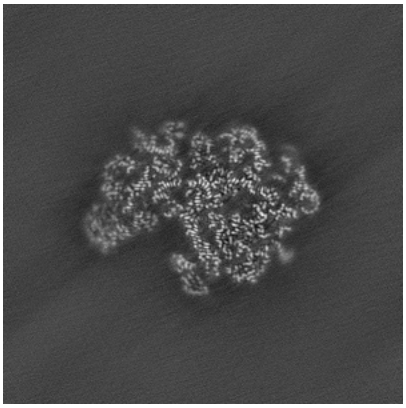


Z Index: 288

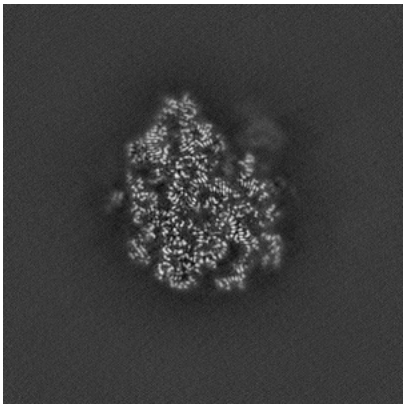
6.3.2 Raw map



X Index: 247



Y Index: 237

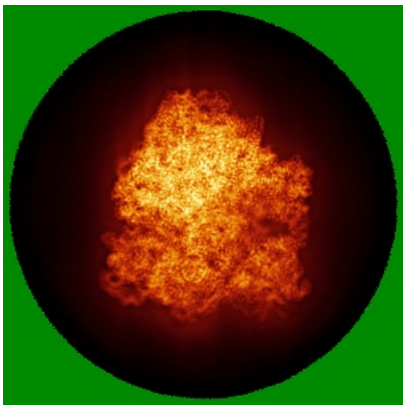


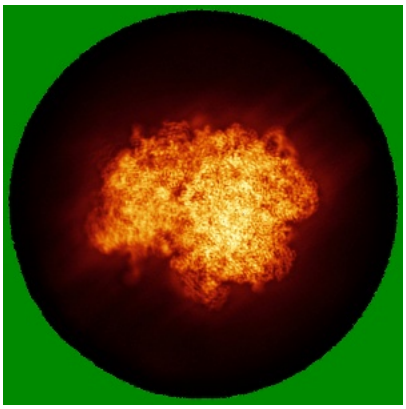
Z Index: 288

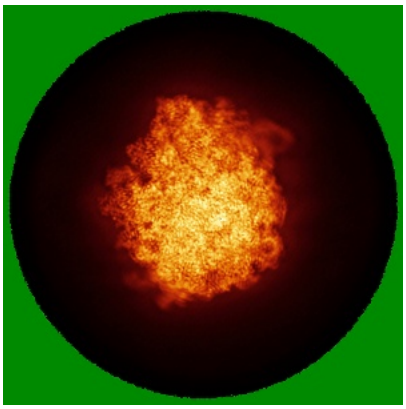
The images above show the largest variance slices of the map in three orthogonal directions.

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

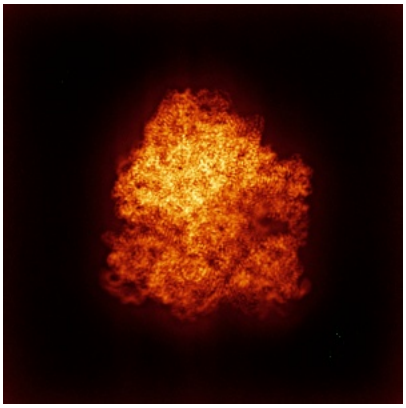
6.4.1 Primary map

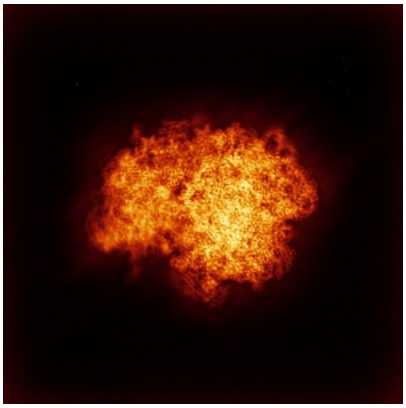

X

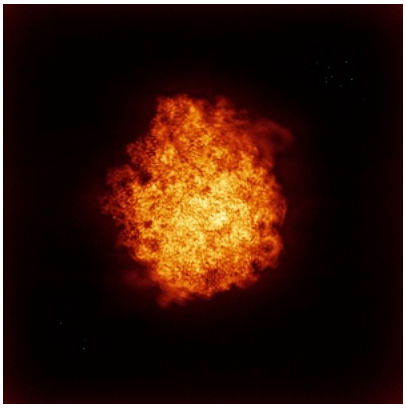

Y


Z

6.4.2 Raw map


X

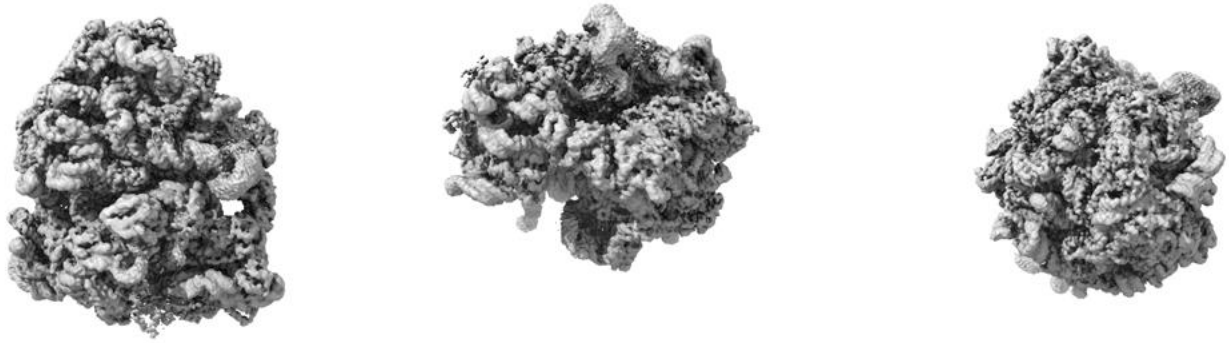

Y


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.

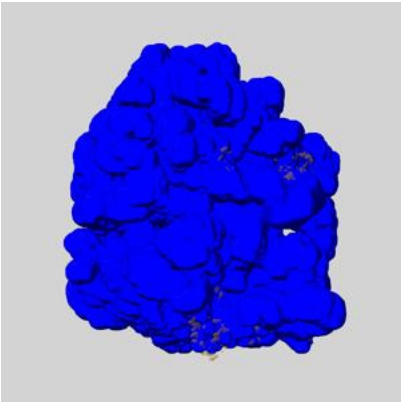
6.6 Mask visualisation (i)

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

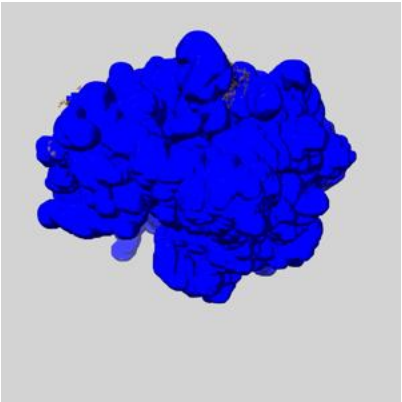
A mask typically either:

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

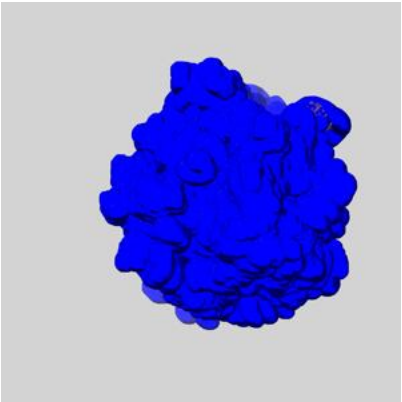
6.6.1 emd_28197_msk_1.map (i)



X



Y

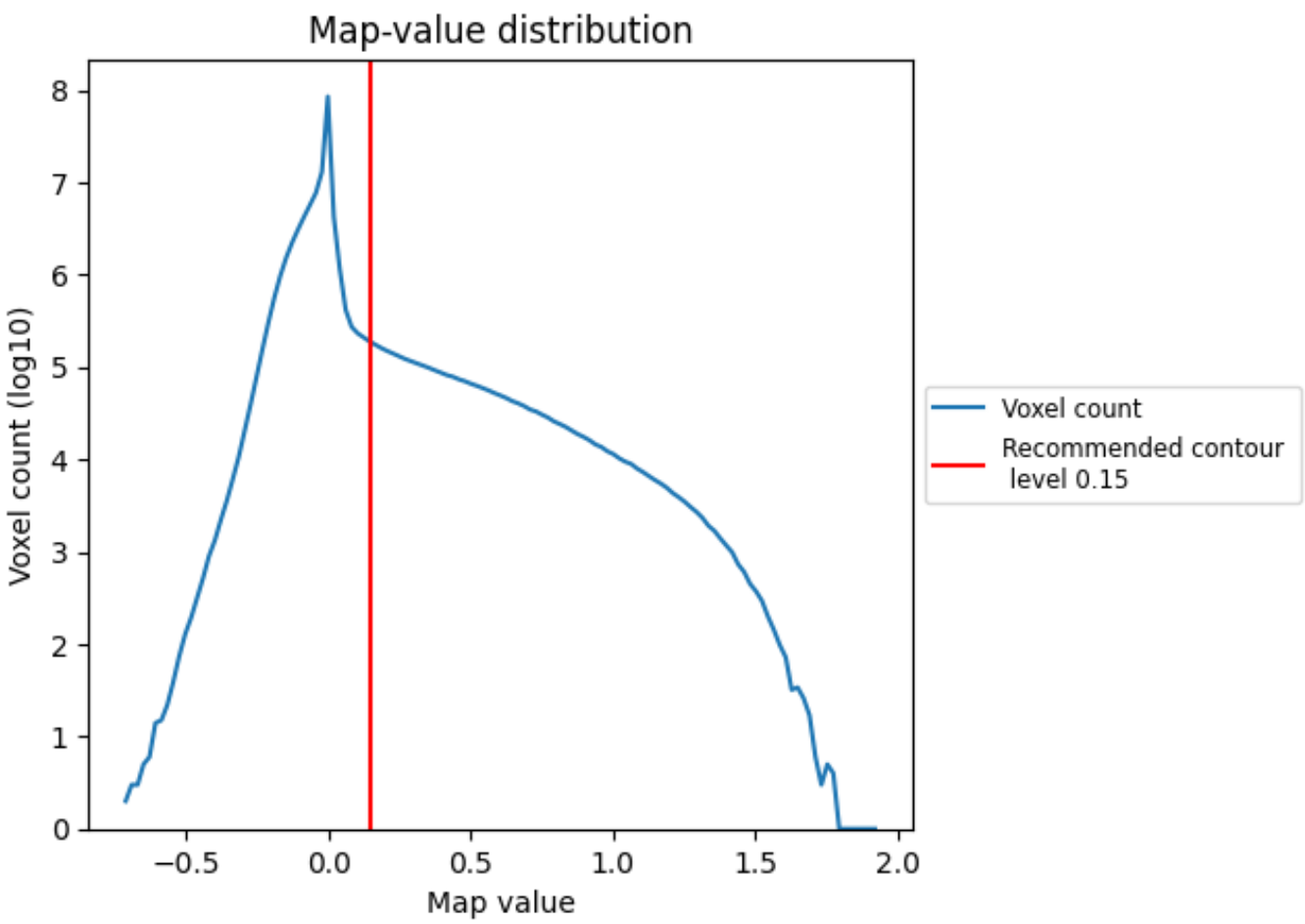


Z

7 Map analysis (i)

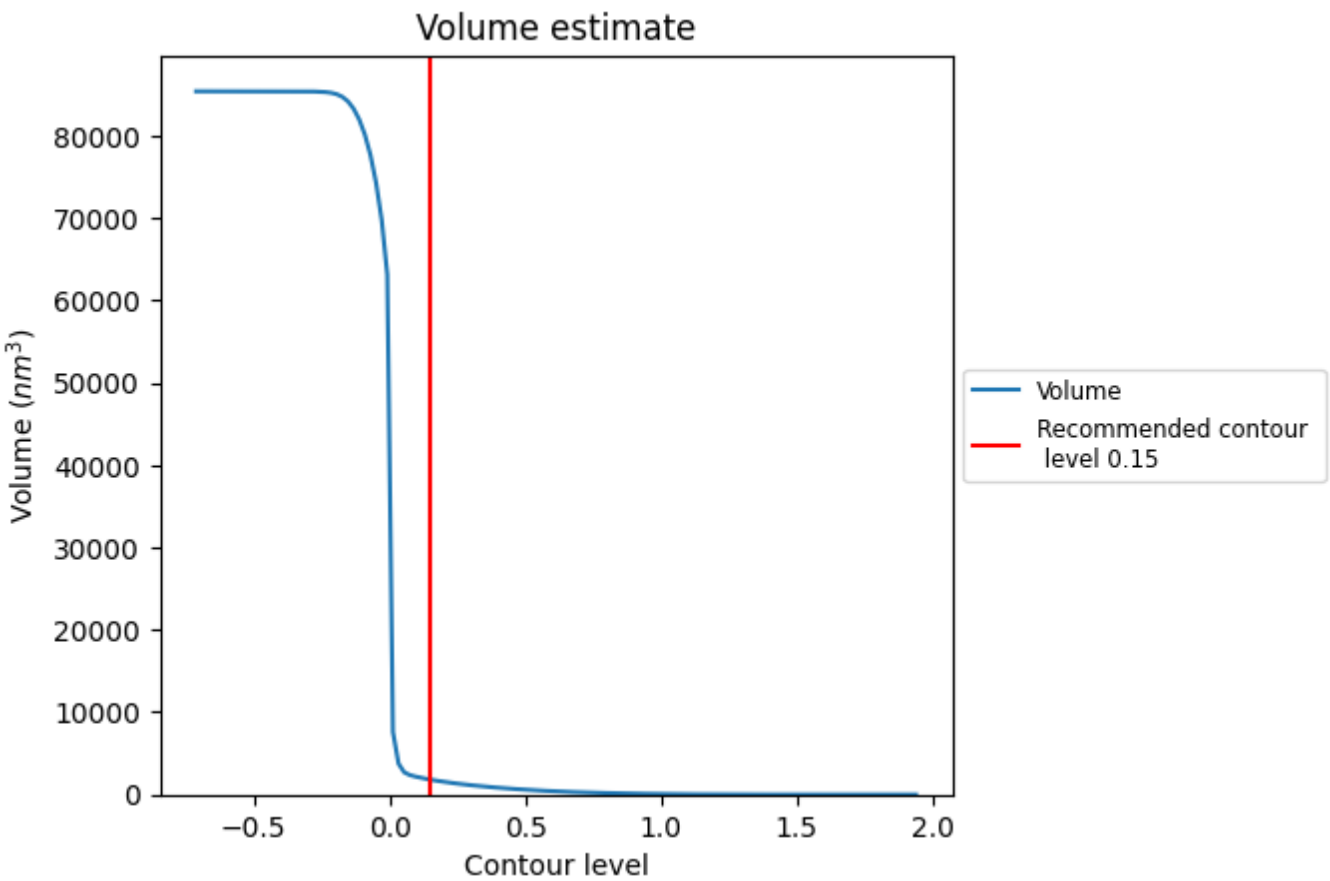
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

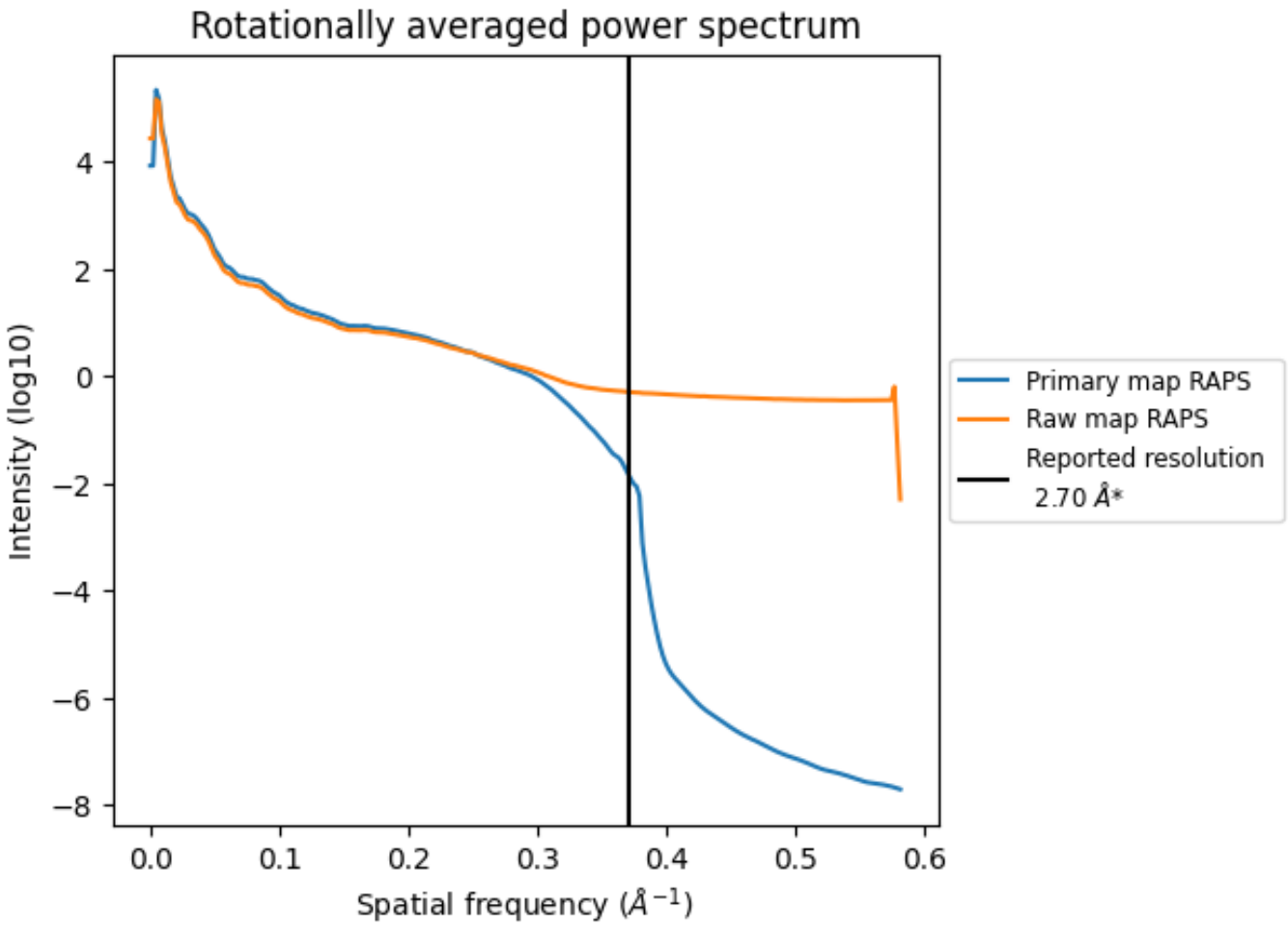
7.2 Volume estimate (i)



The volume at the recommended contour level is 1815 nm^3; this corresponds to an approximate mass of 1640 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)

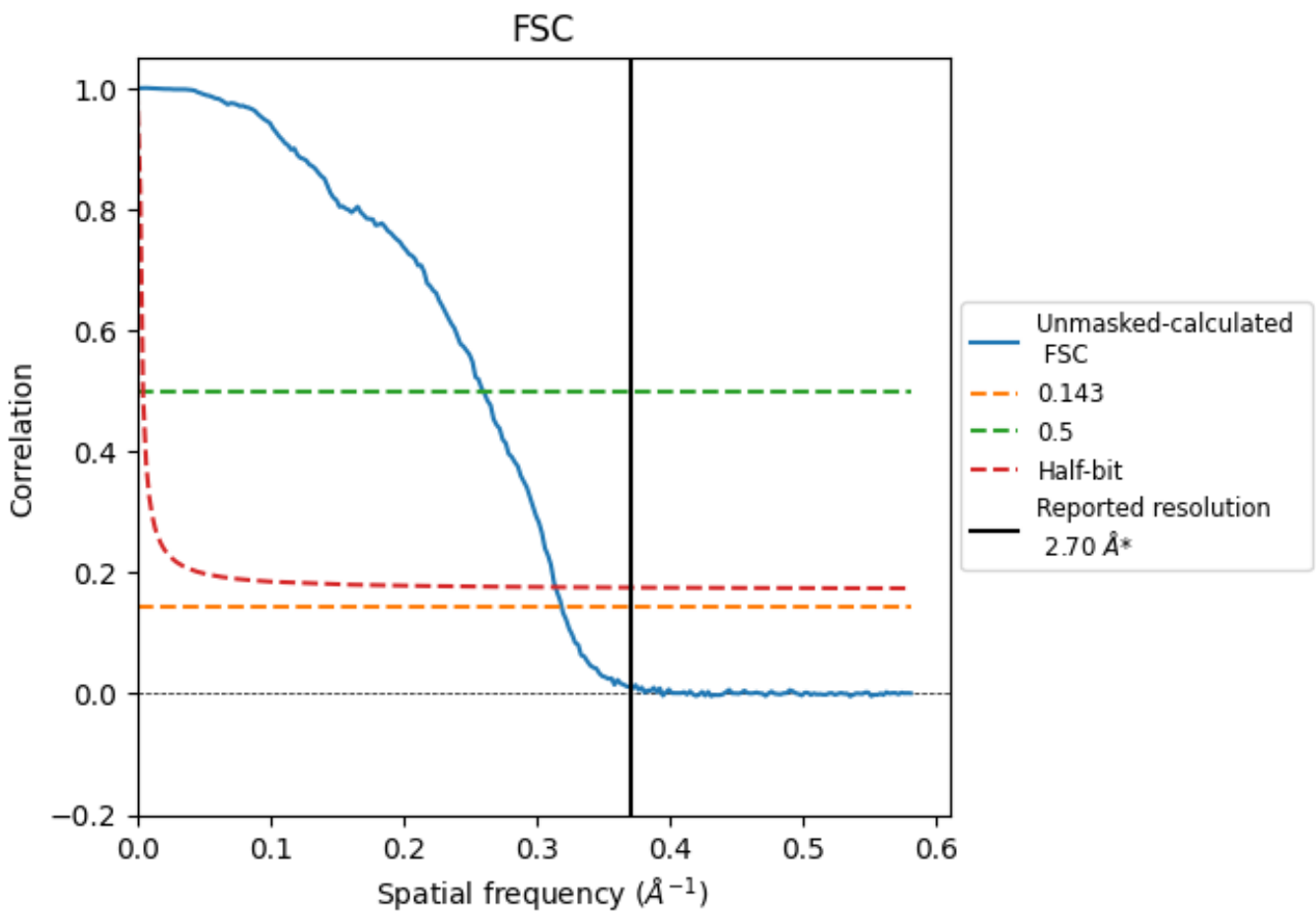


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

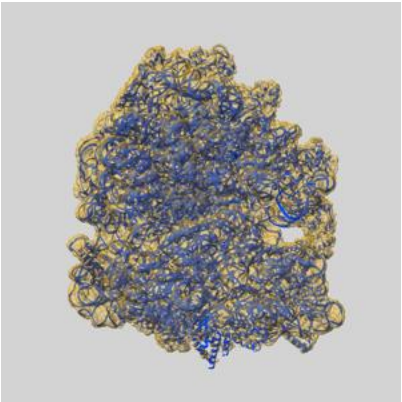
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.13	3.85	3.18

*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 3.13 differs from the reported value 2.7 by more than 10 %

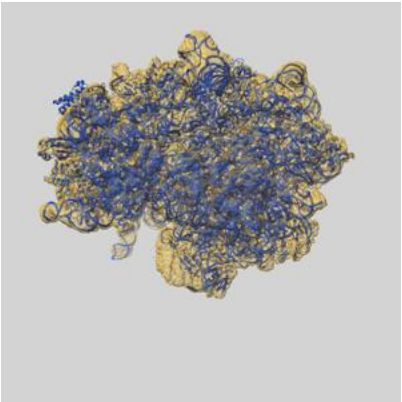
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-28197 and PDB model 8EKC. Per-residue inclusion information can be found in section 3 on page 18.

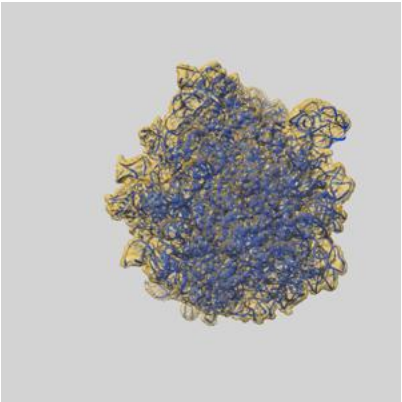
9.1 Map-model overlay (i)



X



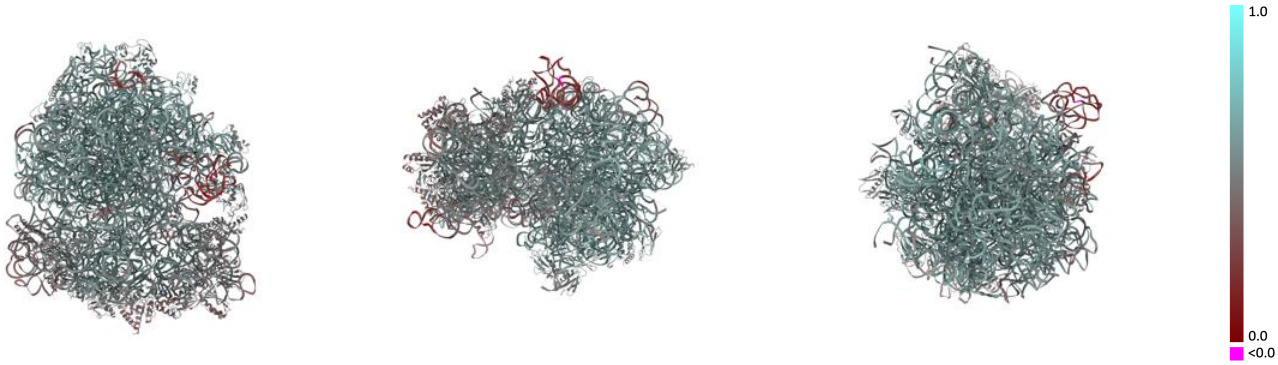
Y



Z

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

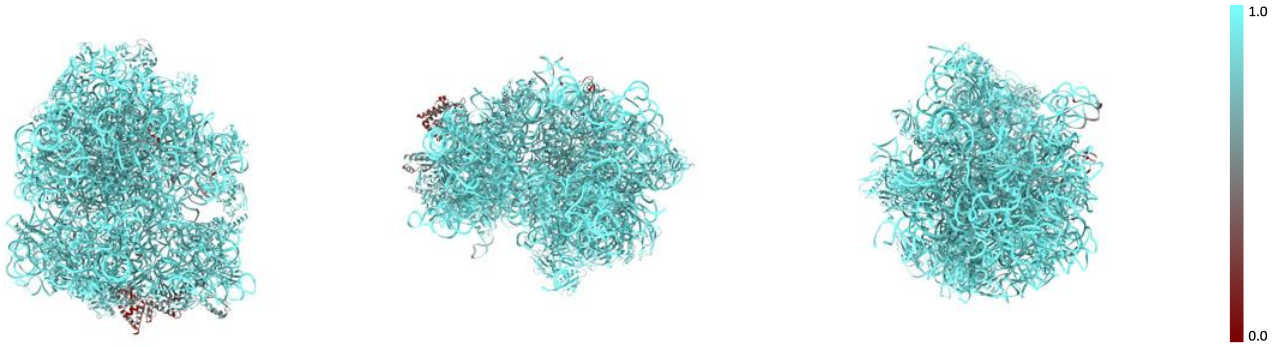
9.2 Q-score mapped to coordinate model (i)



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.

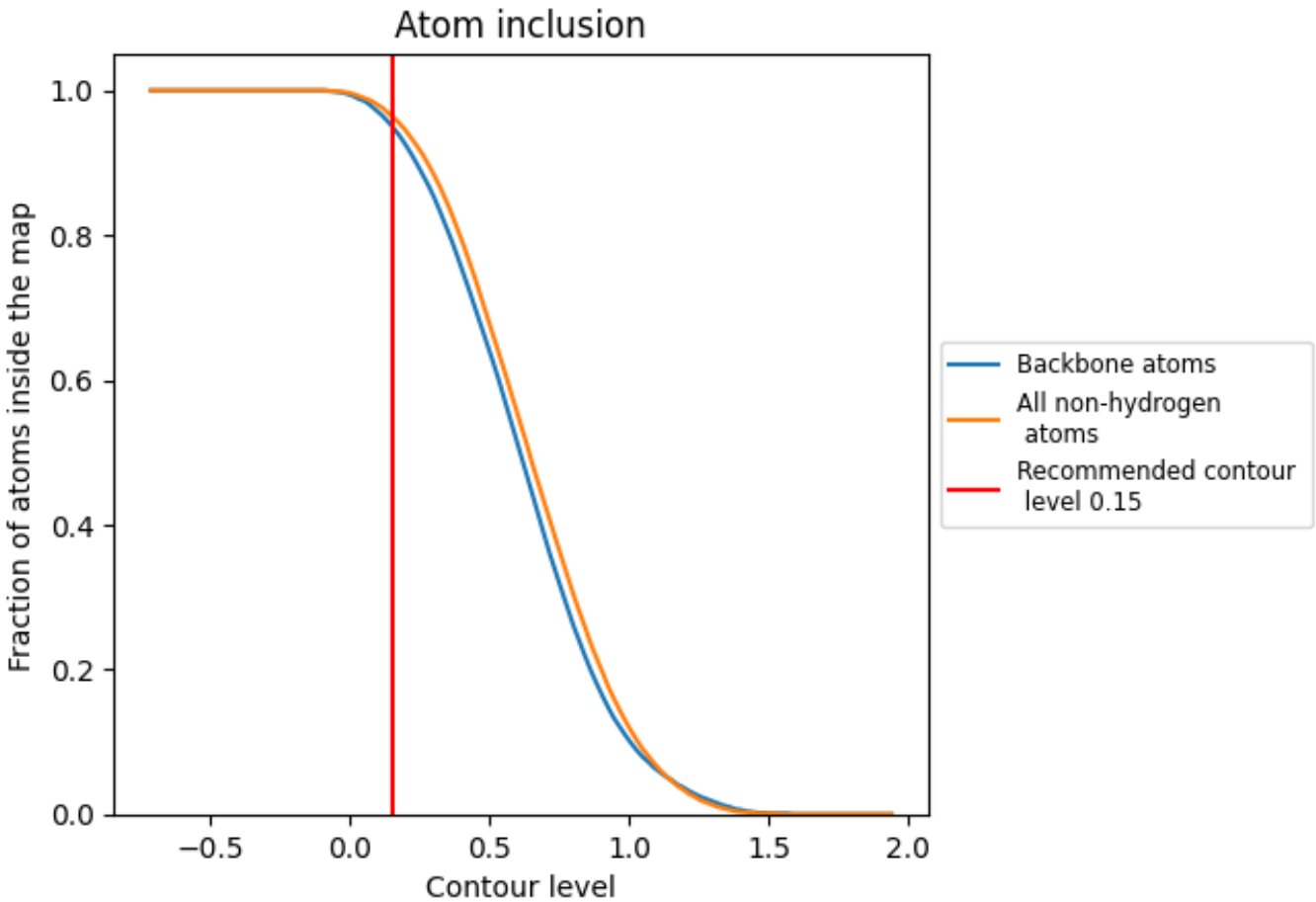
9.3 Atom inclusion mapped to coordinate model (i)



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, 95% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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

Chain	Atom inclusion	Q-score
All	0.9640	0.5530
1	0.9380	0.5330
2	0.9660	0.5820
3	0.8810	0.4830
4	0.9710	0.6010
5	0.9410	0.5680
6	0.9780	0.6150
7	0.9740	0.6120
8	0.9690	0.6010
A	0.9920	0.5800
B	0.9980	0.5580
C	0.9720	0.6060
D	0.9760	0.5990
E	0.9350	0.5670
F	0.9520	0.5160
G	0.9340	0.5210
H	0.2870	0.4390
L	0.9760	0.5970
M	0.9730	0.5960
N	0.9530	0.5880
O	0.9670	0.5960
P	0.9890	0.6060
Q	0.9660	0.5500
R	0.9540	0.5880
S	0.9860	0.6030
T	0.9500	0.5820
U	0.9570	0.5950
V	0.9360	0.5650
W	0.9530	0.5450
X	0.9540	0.5630
Y	0.9530	0.5960
Z	0.9680	0.5930
a	0.9930	0.5200
b	0.3340	0.4180
c	0.8060	0.5120

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	0.8690	0.4470
e	0.9410	0.5460
f	0.9020	0.4790
g	0.8730	0.4640
h	0.9540	0.5480
i	0.9140	0.4820
j	0.7150	0.4530
k	0.9450	0.5230
l	0.9450	0.5550
m	0.9420	0.5000
n	0.8620	0.5050
o	0.9520	0.5190
p	0.9020	0.4690
q	0.9390	0.5030
r	0.9600	0.5300
s	0.9160	0.4810
t	0.9160	0.4550
u	0.6900	0.4750
v	0.9960	0.5750
w	0.9920	0.5330
x	0.9930	0.5580