



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 04:38 PM EDT

PDB ID : 7UNV / pdb_00007unv
EMDB ID : EMD-26634
Title : Pseudomonas aeruginosa 70S ribosome initiation complex bound to IF2-GDPCP (structure II-A)
Authors : Basu, R.S.; Sherman, M.B.; Gagnon, M.G.
Deposited on : 2022-04-11
Resolution : 2.70 Å (reported)
Based on initial models : 6SPG, 3JCJ

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

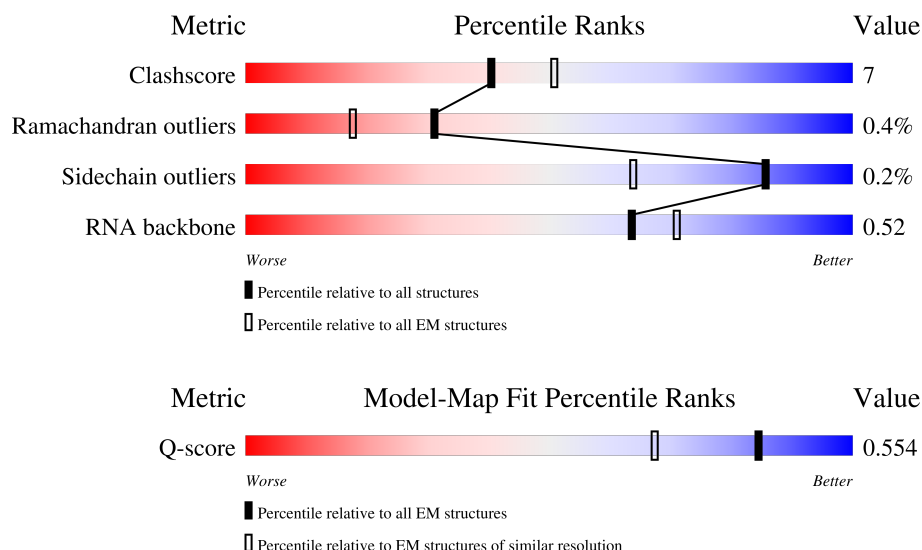
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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.



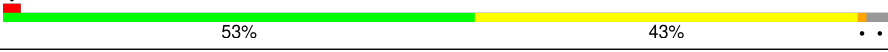
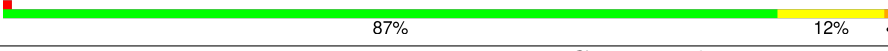
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 (2.20 - 3.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a	1536	
2	b	246	
3	c	228	

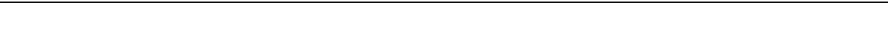
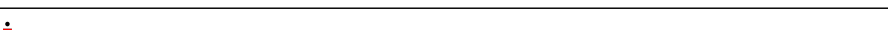
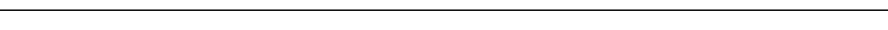
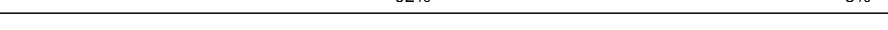
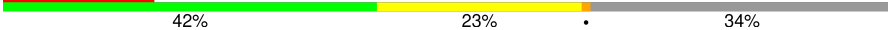
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Mol	Chain	Length	Quality of chain
4	d	206	
5	e	166	
6	f	139	
7	g	156	
8	h	130	
9	i	130	
10	j	103	
11	k	129	
12	l	123	
13	m	118	
14	n	101	
15	o	89	
16	p	83	
17	q	88	
18	r	76	
19	s	91	
20	t	91	
21	u	71	
22	v	77	
23	w	24	
24	x	840	
25	A	2891	
26	B	120	
27	C	273	
28	D	211	

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Mol	Chain	Length	Quality of chain
29	E	200	
30	F	179	
31	G	177	
32	H	148	
33	I	166	
34	J	143	
35	L	142	
36	M	122	
37	N	144	
38	O	137	
39	P	129	
40	Q	116	
41	R	116	
42	S	118	
43	T	103	
44	U	110	
45	V	99	
46	W	104	
47	X	204	
48	Y	85	
49	Z	78	
50	1	63	
51	2	58	
52	3	71	
53	4	60	

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Mol	Chain	Length	Quality of chain
54	5	51	96%
55	6	44	91% 9%
56	7	64	89% 9%
57	8	38	89% 11%

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 149599 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
1	a	1522	Total	C	N	O	P	0	0
			32675	14581	5999	10574	1521		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	224	Total	C	N	O	S	0	0
			1751	1104	320	317	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	208	Total	C	N	O	S	0	0
			1656	1047	313	291	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	205	Total	C	N	O	S	0	0
			1617	998	313	301	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	154	Total	C	N	O	S	0	0
			1134	711	210	207	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	106	Total	C	N	O	S	0	0
			857	534	159	158	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	152	Total	C	N	O	S	0	0
			1187	743	231	208	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	129	Total	C	N	O	S	0	0
			982	618	173	185	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	127	Total	C	N	O	S	0	0
			1010	625	203	181	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	99	Total	C	N	O	S	0	0
			787	493	147	146	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	119	Total	C	N	O	S	0	0
			879	545	171	161	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	122	Total	C	N	O	S	0	0
			959	588	198	169	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			892	544	182	162	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			800	494	167	136	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			703	434	139	129	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	81	Total	C	N	O	S	0	0
			636	397	125	113	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			645	404	124	115	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	62	Total	C	N	O	0	0
			480	307	85	88		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	83	Total	C	N	O	S	0	0
			663	422	129	109	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	87	Total	C	N	O	S	0	0
			671	414	138	117	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	62	Total	C	N	O	S	0	0
			506	316	103	86	1		

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

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

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	w	6	Total	C	N	O	P	0	0
			131	59	27	39	6		

- Molecule 24 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	x	593	Total	C	N	O	S	0	0
			4275	2676	773	810	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A	2884	Total	C	N	O	P	0	0
			61891	27621	11346	20041	2883		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	117	Total	C	N	O	P	0	0
			2495	1114	448	816	117		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	C	272	Total	C	N	O	S	0	0
			2072	1276	426	364	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	D	211	Total	C	N	O	S	0	0
			1588	981	304	297	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	E	200	Total	C	N	O	S	0	0
			1521	955	283	280	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	176	Total	C	N	O	S	0	0
			1406	899	249	254	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	G	175	Total	C	N	O	S	0	0
			1323	834	244	243	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	H	72	Total	C	N	O	S	0	0
			513	321	92	99	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
33	I	118	Total	C	N	O	0	0
			587	349	118	120		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	J	134	Total	C	N	O	S	0	0
			689	415	134	138	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L	142	Total	C	N	O	S	0	0
			1130	718	206	202	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	N	144	Total	C	N	O	S	0	0
			1066	654	215	194	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	O	137	Total	C	N	O	S	0	0
			1085	689	211	181	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	P	120	Total	C	N	O	S	0	0
			959	600	192	162	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Q	115	Total	C	N	O	S	0	0
			881	544	174	161	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	R	114	Total	C	N	O	S	0	0
			902	568	171	162	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
42	S	117	Total	C	N	O	0	0
			933	591	196	146		

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	T	103	Total	C	N	O	S	0	0
			822	521	156	143	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	U	110	Total	C	N	O	S	0	0
			833	515	161	153	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	V	94	Total	C	N	O	S	0	0
			739	472	134	132	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	W	103	Total	C	N	O	S	0	0
			786	494	150	141	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	X	190	Total	C	N	O	S	0	0
			1445	915	262	265	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
48	Y	76	Total	C	N	O	0	0
			575	364	111	100		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Z	77	Total	C	N	O	S	0	0
			630	391	134	103	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	1	61	Total	C	N	O	S	0	0
			490	301	96	91	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	2	57	Total	C	N	O	S	0	0
			445	277	87	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	3	47	Total	C	N	O	S	0	0
			356	222	60	68	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	4	55	Total	C	N	O	S	0	0
			440	264	93	82	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	5	51	Total	C	N	O	S	0	0
			426	272	78	75	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	6	44	Total	C	N	O	S	0	0
			365	222	87	54	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
56	7	63	Total	C	N	O	S	0	0
			506	314	108	81	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	8	38	Total	C	N	O	S	0	0
			307	186	69	48	4		

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

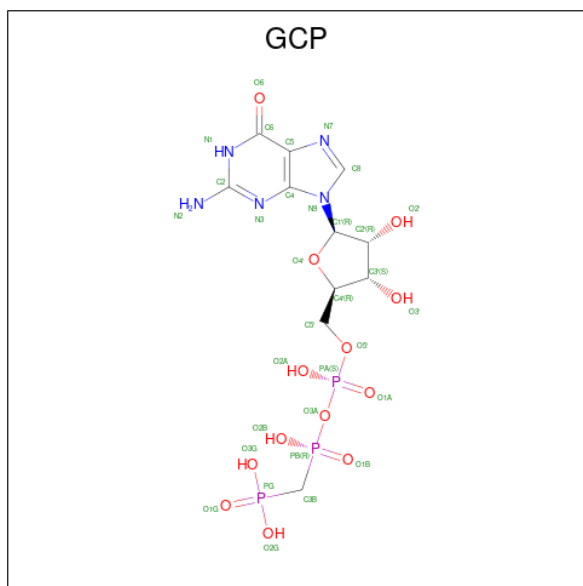
Mol	Chain	Residues	Atoms		AltConf
58	a	121	Total	Mg	0
			121	121	
58	q	1	Total	Mg	0
			1	1	
58	t	1	Total	Mg	0
			1	1	
58	v	1	Total	Mg	0
			1	1	
58	w	1	Total	Mg	0
			1	1	
58	x	1	Total	Mg	0
			1	1	
58	A	455	Total	Mg	0
			455	455	
58	B	4	Total	Mg	0
			4	4	
58	C	3	Total	Mg	0
			3	3	
58	D	2	Total	Mg	0
			2	2	
58	E	1	Total	Mg	0
			1	1	
58	P	1	Total	Mg	0
			1	1	
58	Y	1	Total	Mg	0
			1	1	
58	4	1	Total	Mg	0
			1	1	
58	7	1	Total	Mg	0
			1	1	

- Molecule 59 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).



Mol	Chain	Residues	Atoms					AltConf
59	v	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 60 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
60	x	1	Total	C	N	O	P	0
			32	11	5	13	3	

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	3	1	Total 1	Zn 1	0
61	8	1	Total 1	Zn 1	0

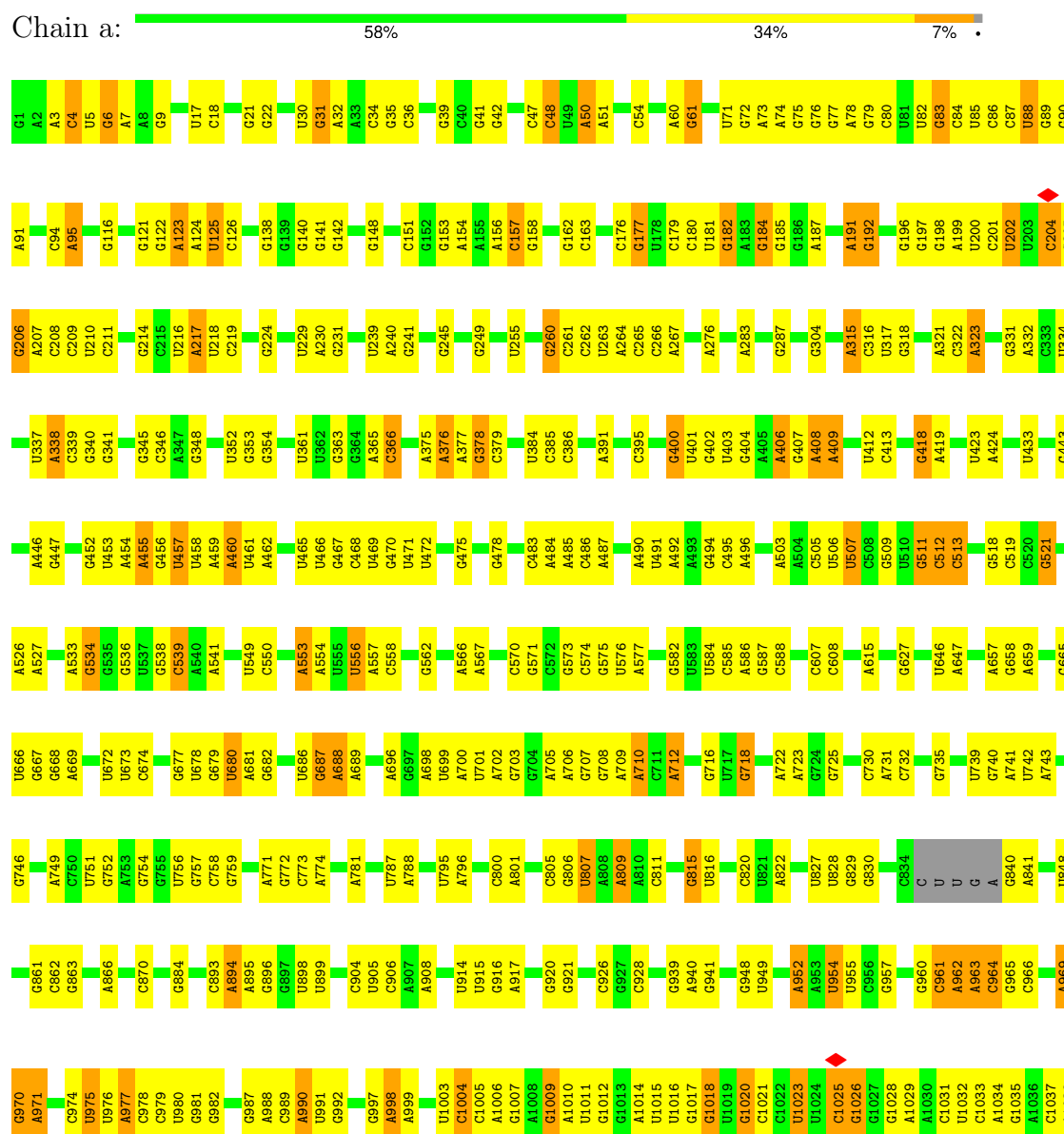
- Molecule 62 is water.

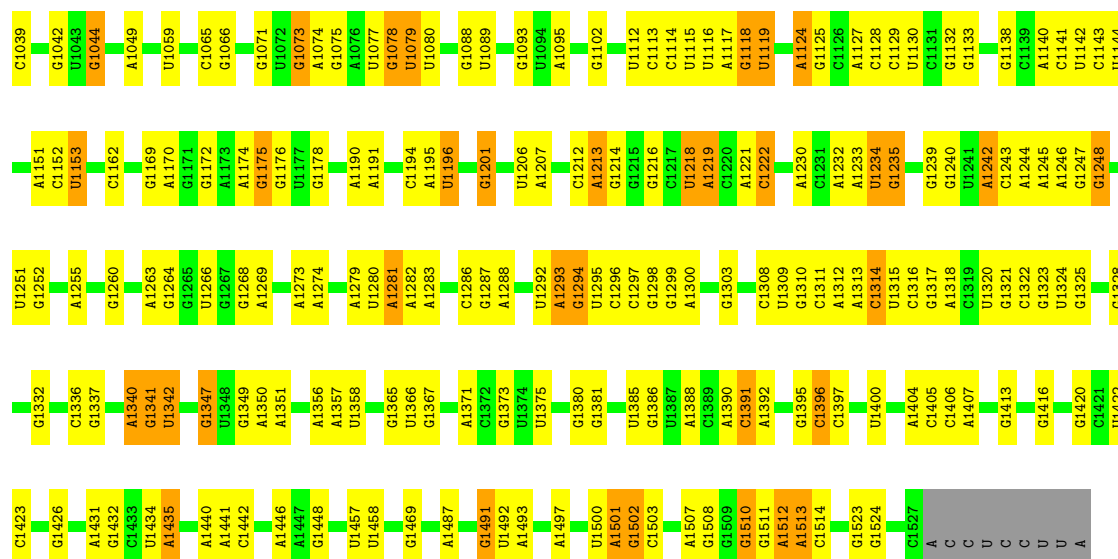
Mol	Chain	Residues	Atoms		AltConf
62	a	46	Total 46	O 46	0
62	k	1	Total 1	O 1	0
62	v	1	Total 1	O 1	0
62	w	1	Total 1	O 1	0
62	x	1	Total 1	O 1	0
62	A	238	Total 238	O 238	0
62	B	1	Total 1	O 1	0
62	C	2	Total 2	O 2	0
62	N	1	Total 1	O 1	0
62	4	2	Total 2	O 2	0
62	6	1	Total 1	O 1	0

3 Residue-property plots

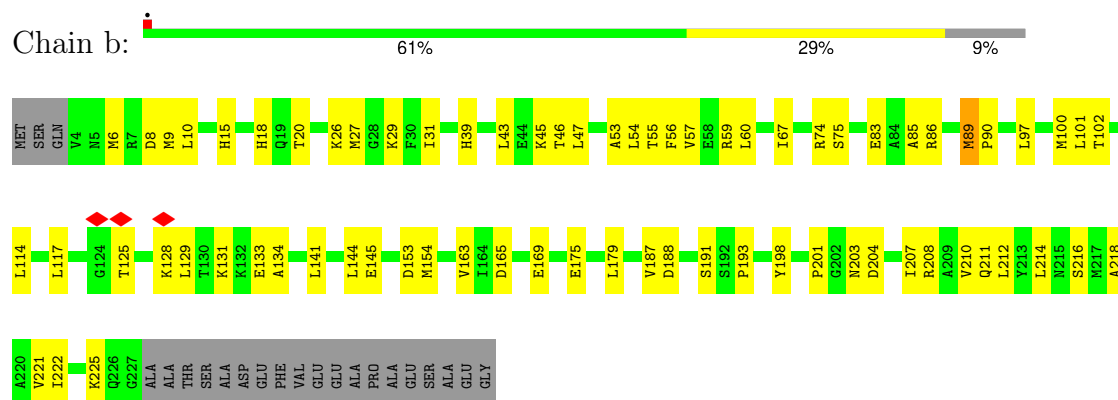
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

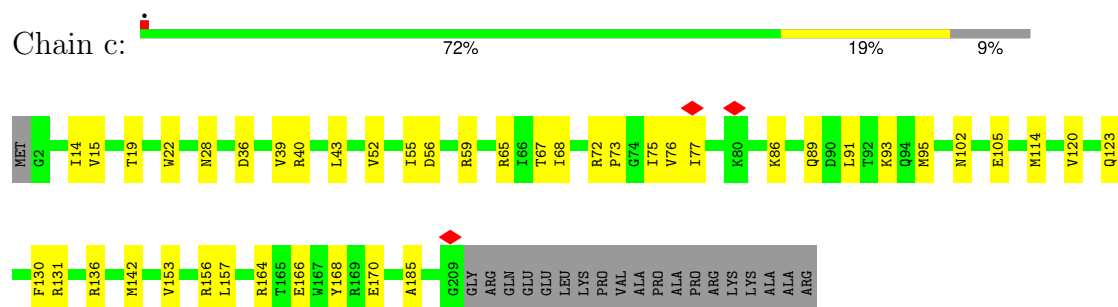




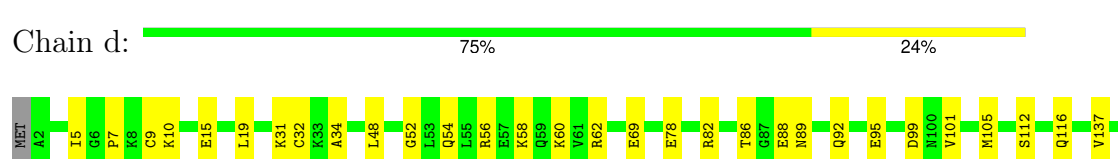
• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3

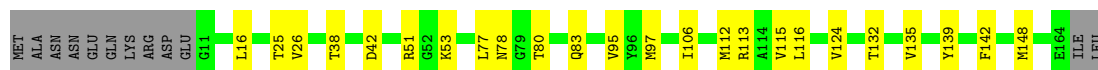
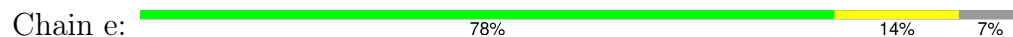


• Molecule 4: 30S ribosomal protein S4

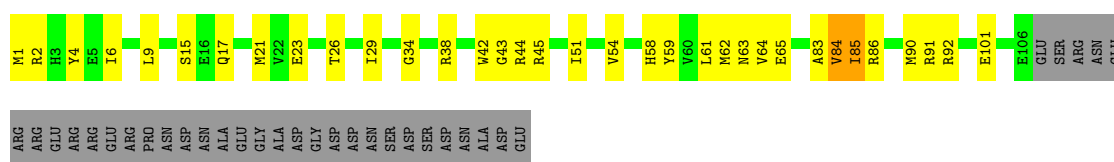




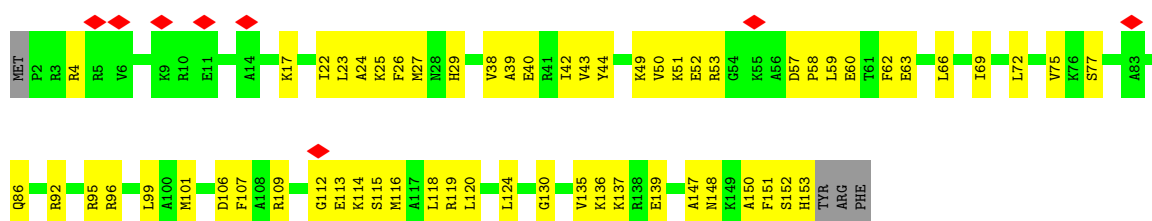
- Molecule 5: 30S ribosomal protein S5



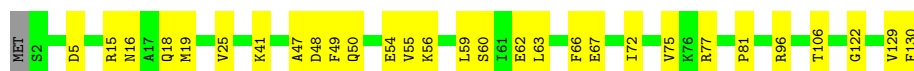
- Molecule 6: 30S ribosomal protein S6



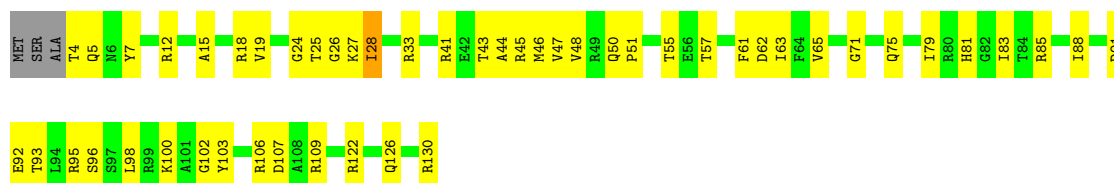
- Molecule 7: 30S ribosomal protein S7



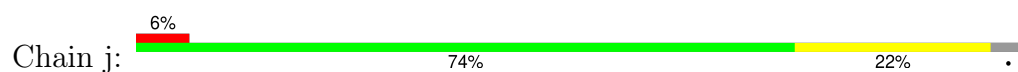
- Molecule 8: 30S ribosomal protein S8



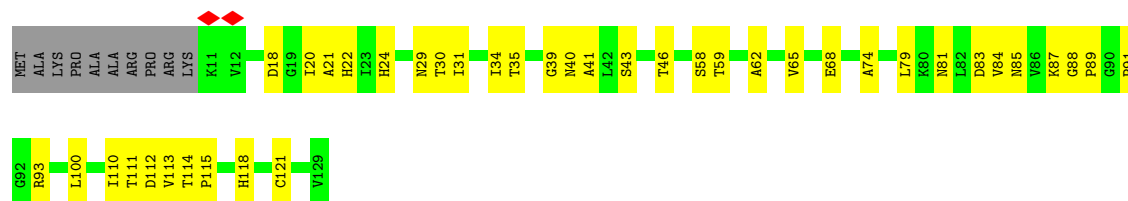
- Molecule 9: 30S ribosomal protein S9



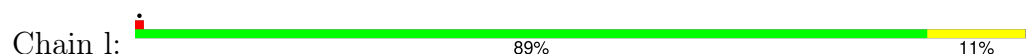
- Molecule 10: 30S ribosomal protein S10



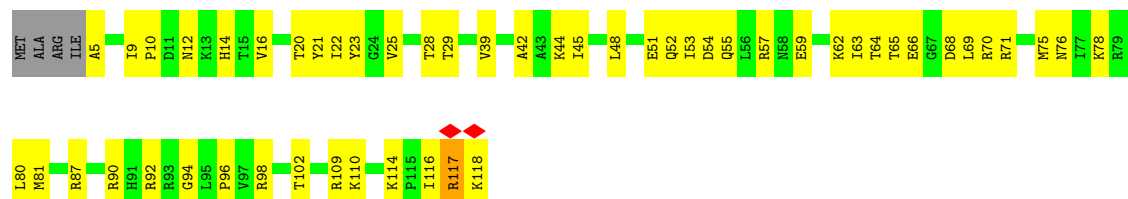
- Molecule 11: 30S ribosomal protein S11



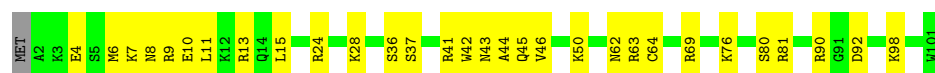
- Molecule 12: 30S ribosomal protein S12



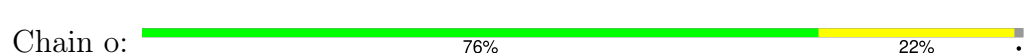
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15



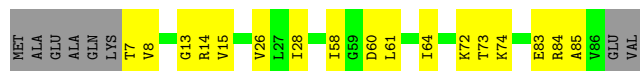
- Molecule 16: 30S ribosomal protein S16

Chain p:  83% 14%



- Molecule 17: 30S ribosomal protein S17

Chain q:  72% 19% 9%



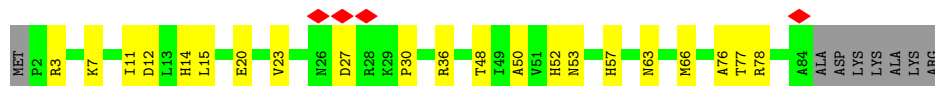
- Molecule 18: 30S ribosomal protein S18

Chain r:  7% 61% 21% 11%



- Molecule 19: 30S ribosomal protein S19

Chain s:  68% 23% 9%



- Molecule 20: 30S ribosomal protein S20

Chain t:  85% 11%



- Molecule 21: 30S ribosomal protein S21

Chain u:  70% 17% 13%



- Molecule 22: P-site initiator tRNA

Chain v:  47% 39% 12%



- Molecule 23: mRNA

GGCCAAAGGAAGGUAA13H18GUUCA

Chain x:

NET	THR	GLN	VAL	VAL	LYS	GLU	GLU	ALA	GLN	VAL	VAL	VAL	ASP	THR	PRO	VAL	VAL	GLU	ARG	ARG	ASP	ALA	GLY	LEU	LEU	LEU	LEU	GLN	MET	MET	ARG	ASP	ALA	ALA	LEU	LEU	PRO	PRO	HIS	THR	THR	SER	ALA	ALA	GLU	GLU	LYS	GLN	ALA	LEU	LEU	LEU	THR	THR	HIS	HIS	LEU	HIS	LYS	GLY	GLY	SER	SER	ASP	ARG	ALA	ALA	SER	SER	GLU	GLU
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PRO	ARG	LYS	ILE	THR	LEU	GLN	ARG	LYS	THR	THR	THR	THR	LYS	VAL	GLY	GLY	SER	LYS	THR	THR	SER	SER	VAL	VAL	GLU	GLU	VAL	VAL	ARG	LYS	LYS	LYS	LYS	THR	TYR	THR	VAL	VAL	LYS	LYS	ARG	ARG	PRO	ASP	GLU	GLU	ILE	GLU	GLU	ALA	ALA	ALA	ALA	GLU	GLU	GLU	GLN	GLN	ARG	ARG	GLU	GLU	LEU	LEU	GLU	GLU	ALA	ALA	GLU	GLU	LEU	LEU	ARG	LEU
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LYS	GLU	GLU	ALA	ALA	ARG	GLN	ARG	ALA	GLU	GLU	ALA	ALA	GLU	GLU	LYS	ALA	ALA	ALA	GLN	GLU	ALA	ALA	ALA	THR	ALA	VAL	VAL	ASP	VAL	ALA	VAL	VAL	ALA	GLU	GLU	PRO	VAL	ALA	ALA	LYS	PRO	ALA	ALA	ALA	VAL	VAL	GLU	GLU	ARG	LYS
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LYS	GLU	GLU	PRO	ARG	ARG	VAL	LYS	ASP	GLU	ASP	ASP	ASP	ARG	ARG	ASP	ARG	LYS	HIS	THR	HIS	GLN	ARG	ARG	PRO	PRO	VAL	VAL	LYS	GLY	LYS	LYS	VAL	VAL	PRO	PRO	ALA	ALA	ARG	ARG	SER	ARG	THR	ASP	GLU	GLU	SER	SER	ASP	GLY	TYR	ARG	ARG	GLY	GLY	GLY	ARG	GLY	LYS	SER
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LYS	LEU	LYS	ARG	ASN	GLN	P248	R259	S277	P287	P293	V294	E337	V345	H350	V351	R362	H363	G354	K355	D360	R363	V367	E371	V384	E385	T386	E387	R388	G389	H399	R406	T413	D414	I415	L418	V419	M427	Q428	Q429	T430
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V434 V446
V447 V448
K462 L465
E473 E474
W475 P480
F481 V482
P483 W484
S485 A486
K487 K488
L488 L496
A497 A498
V499 V498
L500 L500
T511 R517
V520 V521
E522 E529
T534 T535
V535 D539
R543 I552
V553 V554
R558 G564
N565 K566
E570 L580

G581	G582	D583	G584	F607	R608	G611	G627	T628	F629	F630	N631	M632	G633	G634	E635	F636	G637	K638	T639	L644	G648	R649	G650	L655	L662	G663	N664	Q668	T680	D683	A684	F695	R717	T718	T719	L725	L726	E727	D728	S739	D740	L741	L745
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R752	R753	R754	R776	R777	R778	R779	R780	R781	R782	R785	R792	R801	R807	R819	R822	R823	R824	R828	R829	R830	R831	R838	R839	R840
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Chain A: 64% 30% 6%

G1	G2	U3	C4	A5	A6	G9	G15	G16	G17	C18	C24	G27	A28	U34	G35	G36	C37	A38	G43	A44	A45	A46	U50	G58	G61	U62	G70	A71	A74	G75	G79	G80	G81	G82	G83	A84	G85	U86	C87	A92	A93	C94	A95	G96	A97	C98	A99
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U99	U100	U101	G102	G110	U114	C115	A118	A119	U120	G124	G125	A131	U134	A135	A141	C142	U150	U155	A156	C157	A160	C163	C164	A165	U166	A181	A191	C192	A196	A197	C198	A199	G205	U206	A207	C208	C209	G215	A216	G220	A221
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A222	A223	A224	G230	A233	A240	G242	U243	A244	G247	G248	G249	G250	G251	G252	A255	G261	A265	G266	U271	A272	A273	G274	G275	U276	U277	G288	A289	G290	G291	G292	A293	A294	G295	G296	G299	U300	G301	A304	A305	G306	A314	U315	A316	G317	U318	G319
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G320	G321	G322	G323	G324	C331	C337	A344	U345	U348	U349	G350	A351	A356	A357	A358	U359	G371	A372	G373	C374	A375	C376	G377	A380	A381	A382	G387	U396	G397	G400	G401	G402	A403	C404	C405	A406	U407	A426	A434	A435	U439	A444	A445	C446	C447
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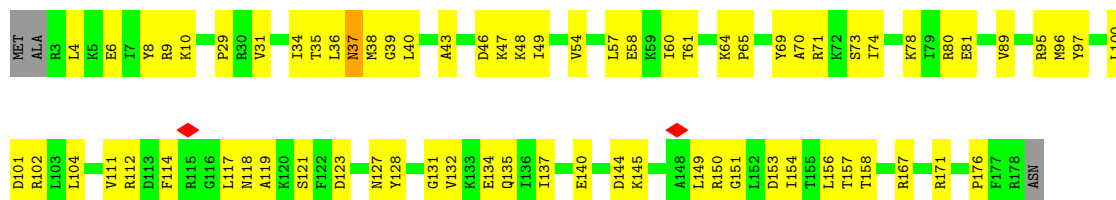
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G2012	G2013	G1871	G1751	U1637	A1509	G1419	C1307	U1185	A1077	A974	C874	A772	A658	G568	G459
U2013	U2014	A1876	U1756	U1638	U1510	G1420	A1308	U1186	A1078	C977	A875	A773	G659	U570	G460
A2017	A2018	G1877	A1760	G1640	G1511	A1421	U1316	G1193	C1082	A986	C878	G775	G664	G572	A461
G2019	G2020	A1878	G1761	G1641	U1512	C1424	U1331	G1199	U1083	A990	C879	A779	A665	G573	A462
A2023	A2024	G1890	U1762	A1642	U1517	U1425	U1334	G1211	U1084	A991	C880	A780	A666	G574	A463
G2025	G2026	G1891	G1763	G1643	C1518	U1426	G1334	G1212	A1085	A992	A881	G786	A667	G575	G464
U2027	U2028	G1892	U1766	G1650	U1519	C1430	U1339	A1211	A1086	G992	C882	G787	C686	C466	G465
G2030	G2031	G1893	A1771	A1654	U1520	G1432	U1340	A1214	U1087	G993	C883	A788	A675	C577	G467
A2034	A2035	G1894	A1772	G1657	U1522	C1433	A1341	G1225	U1088	U994	U884	A792	U676	U578	A470
G2036	G2037	G1897	A1773	G1664	U	U1434	C1344	G1226	G1089	C395	A885	U793	A686	A580	A471
U2039	U2040	A1900	A1774	G1665	U	U1435	C1345	G1227	U1090	C396	C886	G795	U687	U581	G472
A2044	A2045	G1901	C1777	G1672	G1526	G1439	A1346	A1233	C1094	A999	A888	G799	C688	U584	G482
G2047	G2048	U1902	A1778	G1673	G1527	U1446	G1347	A1234	U1095	U1002	A889	U800	U693	C585	G485
A2049	A2050	G1906	C1782	A1674	U1528	U1447	G1348	G1237	A1096	U1003	A890	U801	G694	A586	G487
G2051	G2052	G1909	C1783	G1675	U1529	U1448	C1349	G1238	U1097	G1007	C903	U802	U700	G587	U495
U2055	U2056	A1915	C1784	G1676	A1531	C1449	A1352	U1242	U1098	G1008	C904	U803	A701	G594	A496
G2057	G2058	G1916	U1785	A1680	U1537	G1452	A1353	G1243	G1101	A1011	U908	U817	C713	A598	A499
A2061	A2062	G1917	C1787	G1685	U1538	U1453	A1354	G1244	G1102	G1012	C911	U818	U714	A599	A500
G2067	G2068	U1918	A1788	G1686	U1539	U1454	C1357	A1249	G1105	U1016	C912	U819	G715	G600	A501
U2069	U2070	G1919	C1789	G1687	U1540	U1455	G1358	G1250	G1106	A1017	G913	U820	G716	G601	A502
A2073	A2074	A1923	A1790	G1688	U1541	U1456	A1359	G1251	G1107	A1018	G914	U821	A717	G602	A503
G2077	G2078	G1926	U1795	G1689	U1542	U1457	A1360	G1252	G1108	A1019	G915	U822	G718	G603	A504
U2081	U2082	U1927	A1796	G1690	U1543	U1458	A1361	G1253	G1109	U1023	A916	U823	G719	U604	U512
A2085	A2086	G1928	C1797	G1691	U1544	U1459	C1362	G1254	G1110	U1024	G917	U824	A720	U605	G513
G2087	G2088	U1929	A1798	G1692	U1545	U1460	A1363	G1255	G1111	U1025	G918	U825	C728	G608	A517
U2091	U2092	C1945	G1799	G1693	U1546	G1461	C1364	G1256	G1112	A1030	G919	U826	C729	A518	A519
A2095	A2096	G1949	C1803	G1694	U1547	U1462	A1365	G1257	G1113	G1037	G920	U827	U731	A520	A521
G2099	G2100	C1954	G1811	G1695	U1548	A1470	A1366	G1258	G1114	U1042	G921	U828	C732	G623	G522
U2103	U2104	U1957	A1816	G1696	U1549	A1471	A1367	G1259	G1115	A1043	G922	U829	C733	G624	A523
A2107	A2108	U1958	G1817	G1697	U1550	A1472	A1368	G1260	G1116	U1044	G923	U830	G734	G625	G524
G2109	G2110	G1959	C1822	G1698	U1551	U1473	A1369	G1261	G1117	A1045	G924	U831	G735	G626	G525
U2113	U2114	U1960	G1829	G1699	U1552	U1474	U1392	G1262	A1118	A1046	G925	U832	U736	G627	U536
A2117	A2118	G1974	G1834	G1700	U1553	A1475	U1393	G1263	G1119	A1047	G926	U833	G737	U537	U538
U2121	U2122	U1975	A1835	G1701	U1554	U1476	U1394	G1264	G1120	A1048	G927	U834	G738	U539	U540
G2125	G2126	C1978	G1836	G1702	U1555	U1477	U1395	G1265	G1121	U1049	G928	U835	U739	U541	A541
A2129	A2130	U1979	U1837	G1703	U1556	U1478	U1396	G1266	G1122	A1050	G929	U836	G740	G628	U542
U2133	U2134	G1980	C1838	G1704	U1557	U1479	U1397	G1267	G1123	A1051	G930	U837	G741	U543	U544
G2137	G2138	U1981	G1839	G1705	U1558	U1480	U1398	G1268	G1124	U1052	G931	U838	G742	G629	A545
U2141	U2142	U1982	A1840	G1706	U1559	U1481	U1399	G1269	G1125	G1053	G932	U839	G743	U546	U547
A2145	A2146	G1983	U1841	G1707	U1560	U1482	U1400	G1270	G1126	A1054	G933	U840	G744	U548	U549
G2149	G2150	C1984	G1842	G1708	U1561	U1483	U1401	G1271	G1127	U1055	G934	U841	G745	U549	U550
U2153	U2154	U1985	A1843	G1709	U1562	U1484	U1402	G1272	G1128	A1056	G935	U842	U746	G630	A551
G2157	G2158	G1986	U1844	G1710	U1563	U1485	U1403	G1273	G1129	A1057	G936	U843	G747	G631	U552
U2161	U2162	U1987	C1845	G1711	U1564	U1486	U1404	G1274	G1130	U1058	G937	U844	G748	G632	U553
A2165	A2166	C1987	G1846	G1712	U1565	U1487	U1405	G1275	G1131	A1059	G938	U845	G749	G633	U554
G2169	G2170	U1988	U1847	G1713	U1566	U1488	U1406	G1276	G1132	U1060	G939	U846	G750	U555	U556
U2173	U2174	G1989	A1848	G1714	U1567	U1489	U1407	G1277	G1133	A1061	G940	U847	G751	U556	U557
A2177	A2178	U1990	G1849	G1715	U1568	U1490	U1408	G1278	G1134	U1062	G941	U848	G752	U557	U558
G2181	G2182	C1990	U1850	G1716	U1569	U1491	U1409	G1279	G1135	A1063	G942	U849	G753	U558	U559
U2185	U2186	G1991	C1851	U1717	U1570	U1492	U1410	G1280	G1136	A1064	G943	U850	G754	U559	U560
A2189	A2190	U1992	G1852	G1718	U1571	U1493	U1411	G1281	G1137	U1065	G944	U851	G755	U560	U561
G2193	G2194	C1993	U1853	G1719	U1572	U1494	U1412	G1282	G1138	A1066	G945	U852	G756	U561	U562
U2197	U2198	U1994	A1854	G1720	U1573	U1495	U1413	G1283	G1139	A1067	G946	U853	G757	U562	U563
A2201	A2202	G1995	G1855	G1721	U1574	U1496	U1414	G1284	G1140	U1068	G947	U854	G758	U563	U564
U2205	U2206	U1996	C1856	G1722	U1575	U1497	U1415	G1285	G1141	A1069	G948	U855	G759	U564	U565
G2209	G2210	C1997	U1857	G1723	U1576	U1498	U1416	G1286	G1142	U1070	G949	U856	G760	U565	U566
U2213	U2214	U1998	G1858	G1724	U1577	U1499	U1417	G1287	G1143	A1071	G950	U857	G761	U566	U567
A2217	A2218	G1999	A1859	G1725	U1578	U1500	U1418	G1288	G1144	U1072	G951	U858	G762	U567	U568
G2221	G2222	C1999	U1860	G1726	U1579	U1501	U1419	G1289	G1145	A1073	G952	U859	G763	U568	U569
U2225	U2226	U1999	G1861	G1727	U1580	U1502	U1420	G1290	G1146	U1074	G953	U860	G764	U569	U570
A2229	A2230	G2000	C1862	G1728	U1581	U1503	U1421	G1291	G1147	A1075	G954	U861	G765	U570	U571
G2233	G2234	U2000	U1863	G1729	U1582	U1504	U1422	G1292	G1148	U1076	G955	U862	G766	U571	U572
U2237	U2238	C2000	G1864	G1730	U1583	U1505	U1423	G1293	G1149	A1077	G956	U863	G767	U572	U573
A2241	A2242	G2001	A1865	G1731	U1584	U1506	U1424	G1294	G1150	U1078	G957	U864	G768	U573	U574
G2245	G2246	U2002	U1866	G1732	U1585	U1507	U1425	G1295	G1151	A1079	G958	U865	G769	U574	U575
U2249	U2250	C2002	G1867	G1733	U1586	U1508	U1426	G1296	G1152	U1080	G959	U866	G770	U575	U576
A2253	A2254	U2003	A1868	G1734	U1587	U1509	U1427	G1297	G1153	A1081	G960	U867	G771	U576	U577
G2257	G2258	G2004	U1869	G1735	U1588	U1510	U1428	G1298	G1154	U1082	G961	U868	G772	U577	U578
U2261	U2262	C2005	G1870	G1736	U1589	U1511	U1429	G1299	G1155	A1083	G962	U869	G773	U578	U579
A2265	A2266	U2006	A1871	G1737	U1590	U1512	U1430	G1300	G1156	U1084	G963	U870	G774	U579	U580
G2269	G2270	U2007	U1872	G1738	U1591	U1513	U1431	G1301	G1157	A1085	G964	U871	G775	U580	U581
U2273	U2274	C2008	G1873	G1739	U1592	U1514	U1432	G1302	G1158	U1086	G965	U872	G776	U581	U582
A2277	A2278	U2009	A1874	G1740	U1593	U1515	U1433	G1303	G1159	A1087	G966	U873	G777	U582	U583
G2281	G2282	G2009	U1875	G1741	U1594	U1516	U1434	G1304	G1160	U1088	G967	U874	G778	U583	U584
U2285	U2286	C2010	G1876	G1742	U1595	U1517	U1435	G1305	G1161	U1089	G968	U875	G779	U584	U585
A2289	A2290	U2010	A1877	G1743	U1596	U1518	U1436	G1306	G1162	A1089	G969	U876	G780	U585	U586
G2293	G2294	G2011	U1878	G1744	U1597	U1519	U1437	G1307	G1163	U1090	G970	U877	G781	U586	U587
U2297	U2298	C2012	G1879	G1745	U1598	U1520	U1438	G1308	G1164	A1091	G971	U878	G782	U587	U588
A2301	A2302	U2013	A1880	G1746	U1599	U1521	U1439	G1309	G1165	U1091	G972	U879	G783	U588	U589
G2305	G2306	G2014	U1881	G1747	U1600	U1522	U1440	G1310	G1166	A1092	G973	U880	G784	U589	U590
U2309	U2310	C2015	G1882	G1748	U1601	U1523	U1441	G1311	G1167	U1092	G974	U881	G785	U590	U591
A2313	A2314														

Chain E:  87% 12%



- Molecule 30: 50S ribosomal protein L5

Chain F:  59% 39% ..

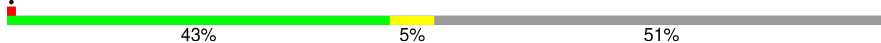


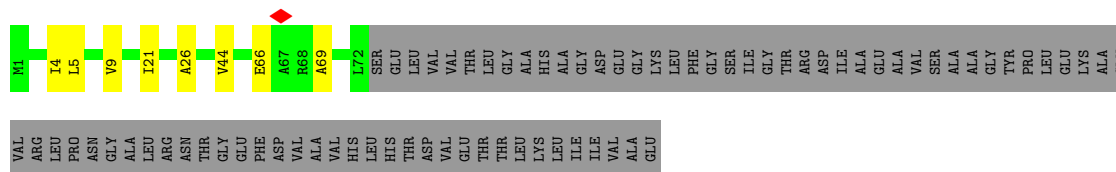
- Molecule 31: 50S ribosomal protein L6

Chain G:  89% 10% .



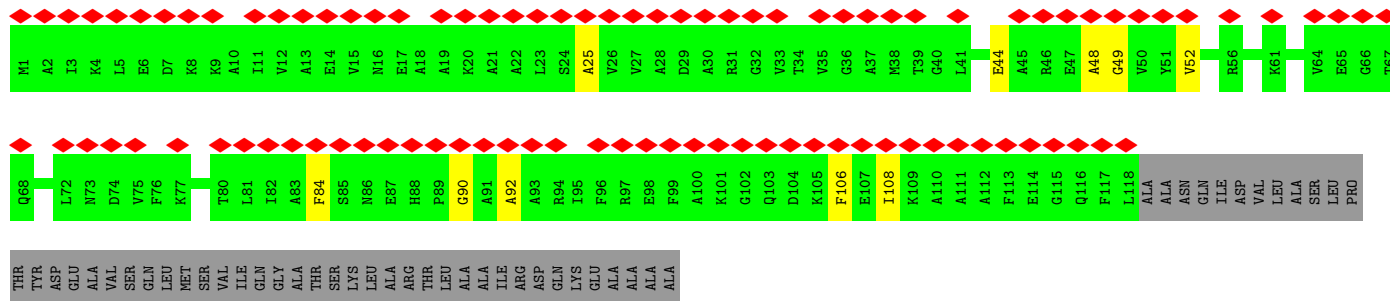
- Molecule 32: 50S ribosomal protein L9

Chain H:  43% 5% 51%



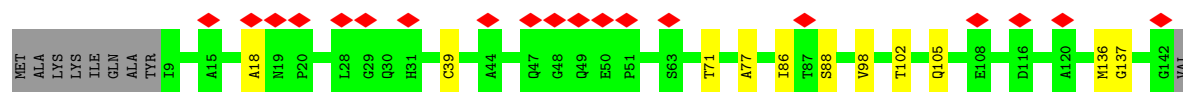
- Molecule 33: 50S ribosomal protein L10

Chain I:  57% 65% 6% 29%

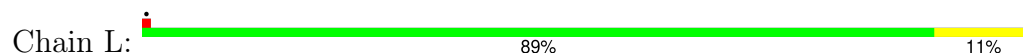


- Molecule 34: 50S ribosomal protein L11

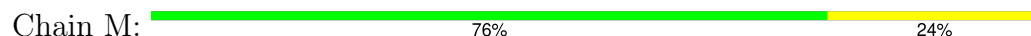
Chain J:  13% 86% 8% 6%



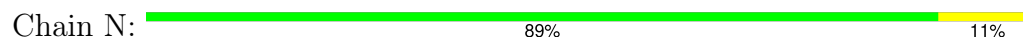
- Molecule 35: 50S ribosomal protein L13



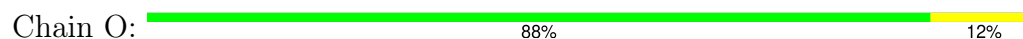
- Molecule 36: 50S ribosomal protein L14



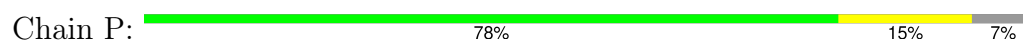
- Molecule 37: 50S ribosomal protein L15



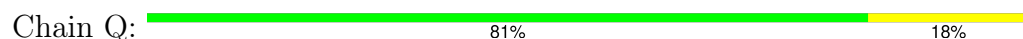
- Molecule 38: 50S ribosomal protein L16



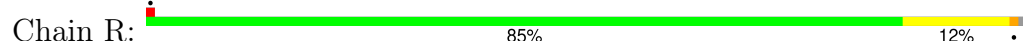
- Molecule 39: 50S ribosomal protein L17



- Molecule 40: 50S ribosomal protein L18



- Molecule 41: 50S ribosomal protein L19





- Molecule 42: 50S ribosomal protein L20

Chain S: 92% 8%



- Molecule 43: 50S ribosomal protein L21

Chain T: 88% 10%



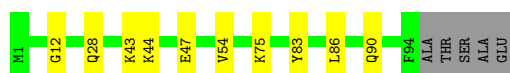
- Molecule 44: 50S ribosomal protein L22

Chain U: 90% 10%



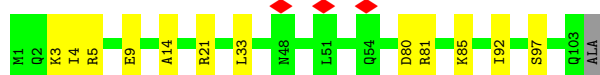
- Molecule 45: 50S ribosomal protein L23

Chain V: 85% 10% 5%



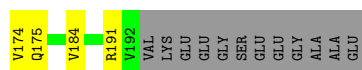
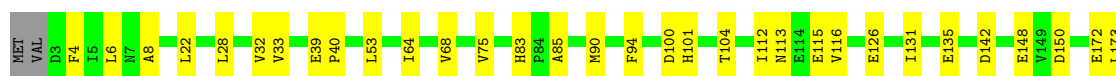
- Molecule 46: 50S ribosomal protein L24

Chain W: 88% 12%



- Molecule 47: 50S ribosomal protein L25

Chain X: 75% 18% 7%



• Molecule 48: 50S ribosomal protein L27

Chain Y:  80% 9% 11%

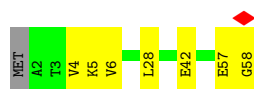
• Molecule 49: 50S ribosomal protein L28

Chain Z:  90% 9% .

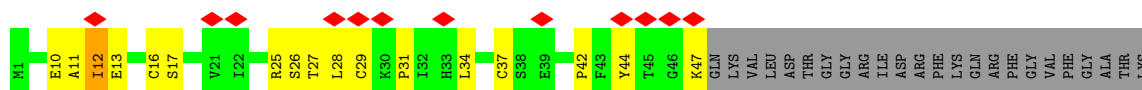
• Molecule 50: 50S ribosomal protein L29

Chain 1:  79% 17% .

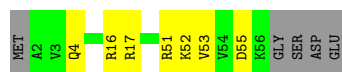
• Molecule 51: 50S ribosomal protein L30

Chain 2:  86% 12% .

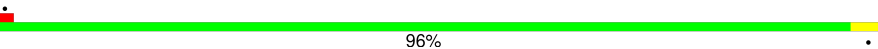
• Molecule 52: 50S ribosomal protein L31

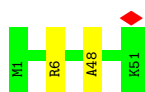
Chain 3:  17% 42% 23% 34%

• Molecule 53: 50S ribosomal protein L32

Chain 4:  80% 12% 8%

• Molecule 54: 50S ribosomal protein L33

Chain 5:  96% .



- Molecule 55: 50S ribosomal protein L34

Chain 6:  91% 9%



- Molecule 56: 50S ribosomal protein L35

Chain 7:  89% 9% .



- Molecule 57: 50S ribosomal protein L36

Chain 8:  89% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	73337	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	31	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.999	Depositor
Minimum map value	-0.674	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, OMC, 4OC, GCP, MG, 5MU, 5MC, 2MG, 2MA, 4SU, 1MG, PSU, OMG, OMU, FME, 7MG, 6MZ, ZN, MA6

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	0.15	0/36354	0.29	0/56707
2	b	0.15	0/1779	0.46	0/2392
3	c	0.15	0/1685	0.33	0/2270
4	d	0.17	0/1636	0.35	0/2189
5	e	0.16	0/1148	0.40	0/1544
6	f	0.18	0/871	0.47	0/1172
7	g	0.13	0/1204	0.38	0/1609
8	h	0.14	0/993	0.33	0/1332
9	i	0.12	0/1022	0.36	0/1365
10	j	0.24	0/797	0.40	0/1076
11	k	0.14	0/895	0.33	0/1209
12	l	0.14	0/973	0.36	0/1303
13	m	0.15	0/901	0.44	0/1209
14	n	0.14	0/812	0.41	0/1082
15	o	0.17	0/710	0.39	0/947
16	p	0.14	0/647	0.36	0/870
17	q	0.12	0/653	0.34	0/881
18	r	0.13	0/488	0.34	0/660
19	s	0.10	0/678	0.28	0/912
20	t	0.14	0/678	0.26	0/904
21	u	0.12	0/513	0.31	0/680
22	v	0.23	0/1725	0.35	2/2689 (0.1%)
23	w	0.12	0/147	0.18	0/227
24	x	0.14	0/4325	0.37	0/5861
25	A	0.19	0/68977	0.31	2/107590 (0.0%)
26	B	0.13	0/2789	0.25	0/4345
27	C	0.16	0/2108	0.33	0/2831
28	D	0.19	0/1611	0.39	0/2167
29	E	0.20	0/1541	0.38	0/2075
30	F	0.16	0/1427	0.48	0/1917
31	G	0.13	0/1341	0.31	0/1805

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	H	0.10	0/516	0.30	0/696
33	I	0.08	0/586	0.34	0/813
34	J	0.10	0/688	0.35	0/953
35	L	0.15	0/1156	0.31	0/1559
36	M	0.16	0/947	0.33	0/1268
37	N	0.16	0/1078	0.39	0/1436
38	O	0.16	0/1105	0.31	0/1476
39	P	0.16	0/975	0.34	0/1304
40	Q	0.11	0/888	0.28	0/1183
41	R	0.24	0/911	0.36	0/1218
42	S	0.16	0/943	0.29	0/1253
43	T	0.15	0/835	0.29	0/1117
44	U	0.14	0/837	0.27	0/1114
45	V	0.14	0/749	0.29	0/1002
46	W	0.14	0/794	0.34	0/1062
47	X	0.13	0/1468	0.29	0/1987
48	Y	0.24	0/583	0.39	0/774
49	Z	0.20	0/641	0.34	0/854
50	1	0.12	0/491	0.22	0/654
51	2	0.13	0/449	0.26	0/602
52	3	0.11	0/364	0.31	0/494
53	4	0.15	0/446	0.32	0/594
54	5	0.12	0/433	0.27	0/576
55	6	0.18	0/368	0.39	0/482
56	7	0.15	0/511	0.26	0/668
57	8	0.15	0/308	0.29	0/404
All	All	0.17	0/160498	0.32	4/239363 (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
28	D	0	1
43	T	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1094	C	OP1-P-O3'	-8.98	81.05	108.00
22	v	76	A	O4'-C1'-N9	8.16	120.44	108.20
25	A	1094	C	OP2-P-O3'	-8.08	83.77	108.00
22	v	75	C	OP2-P-O3'	-5.84	90.47	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	D	151	THR	Peptide
43	T	51	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	32675	0	16461	416	0
2	b	1751	0	1785	48	0
3	c	1656	0	1706	26	0
4	d	1617	0	1650	35	0
5	e	1134	0	1181	18	0
6	f	857	0	836	33	0
7	g	1187	0	1244	42	0
8	h	982	0	1036	19	0
9	i	1010	0	1052	37	0
10	j	787	0	822	22	0
11	k	879	0	896	35	0
12	l	959	0	1009	10	0
13	m	892	0	933	38	0
14	n	800	0	837	26	0
15	o	703	0	727	12	0
16	p	636	0	646	8	0
17	q	645	0	689	11	0
18	r	480	0	488	11	0
19	s	663	0	697	18	0
20	t	671	0	722	9	0
21	u	506	0	537	8	0
22	v	1625	0	828	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	w	131	0	66	0	0
24	x	4275	0	4235	71	0
25	A	61891	0	31145	529	0
26	B	2495	0	1263	17	0
27	C	2072	0	2152	22	0
28	D	1588	0	1603	23	0
29	E	1521	0	1581	18	0
30	F	1406	0	1467	53	0
31	G	1323	0	1386	12	0
32	H	513	0	514	4	0
33	I	587	0	322	4	0
34	J	689	0	416	5	0
35	L	1130	0	1160	11	0
36	M	938	0	1012	18	0
37	N	1066	0	1112	13	0
38	O	1085	0	1157	13	0
39	P	959	0	1005	17	0
40	Q	881	0	920	14	0
41	R	902	0	960	11	0
42	S	933	0	1023	10	0
43	T	822	0	858	9	0
44	U	833	0	897	7	0
45	V	739	0	788	7	0
46	W	786	0	836	7	0
47	X	1445	0	1486	23	0
48	Y	575	0	598	5	0
49	Z	630	0	653	5	0
50	1	490	0	520	7	0
51	2	445	0	472	4	0
52	3	356	0	342	13	0
53	4	440	0	437	6	0
54	5	426	0	457	1	0
55	6	365	0	409	3	0
56	7	506	0	569	4	0
57	8	307	0	342	3	0
58	4	1	0	0	0	0
58	7	1	0	0	0	0
58	A	455	0	0	0	0
58	B	4	0	0	0	0
58	C	3	0	0	0	0
58	D	2	0	0	0	0
58	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	P	1	0	0	0	0
58	Y	1	0	0	0	0
58	a	121	0	0	0	0
58	q	1	0	0	0	0
58	t	1	0	0	0	0
58	v	1	0	0	0	0
58	w	1	0	0	0	0
58	x	1	0	0	0	0
59	v	10	0	10	0	0
60	x	32	0	14	2	0
61	3	1	0	0	0	0
61	8	1	0	0	0	0
62	4	2	0	0	0	0
62	6	1	0	0	0	0
62	A	238	0	0	2	0
62	B	1	0	0	0	0
62	C	2	0	0	0	0
62	N	1	0	0	0	0
62	a	46	0	0	0	0
62	k	1	0	0	0	0
62	v	1	0	0	0	0
62	w	1	0	0	0	0
62	x	1	0	0	0	0
All	All	149599	0	100969	1713	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 7.

All (1713) 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:74:A:H62	1:a:89:G:N2	1.49	1.10
1:a:1020:G:H1	1:a:1029:A:N6	1.50	1.08
25:A:2175:U:H3'	25:A:2176:U:C5	1.88	1.08
1:a:74:A:N6	1:a:89:G:H21	1.52	1.06
25:A:2154:U:H3	25:A:2158:A:N6	1.56	1.03
1:a:75:G:H1	1:a:88:U:H3	1.02	0.98
25:A:1519:G:H2'	25:A:1520:U:C6	2.04	0.92
25:A:2175:U:H3'	25:A:2176:U:C6	2.07	0.88
25:A:2172:U:H2'	25:A:2173:G:H8	1.38	0.87
10:j:52:LEU:HB2	14:n:81:ARG:HD2	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:458:U:H2'	1:a:459:A:H2'	1.59	0.85
25:A:2175:U:H3'	25:A:2176:U:H5	1.37	0.84
13:m:25:VAL:HG23	13:m:29:THR:HG23	1.60	0.83
24:x:558:ARG:HE	24:x:581:GLY:HA2	1.46	0.81
1:a:1117:A:H4'	10:j:38:GLY:HA3	1.63	0.81
25:A:2175:U:C5	25:A:2176:U:C4	2.70	0.80
25:A:1050:U:H4'	25:A:1051:U:H5'	1.64	0.79
11:k:88:GLY:H	11:k:114:THR:HG22	1.46	0.79
25:A:845:G:H2'	25:A:846:G:C8	2.18	0.79
4:d:172:GLU:HG3	4:d:183:LYS:HZ2	1.49	0.78
1:a:1017:G:C6	1:a:1018:G:O6	2.38	0.77
1:a:709:A:H2'	1:a:710:A:C8	2.20	0.77
1:a:1212:C:H2'	1:a:1213:A:H8	1.49	0.77
4:d:95:GLU:HG2	4:d:186:PRO:HG2	1.67	0.77
1:a:1033:C:H2'	1:a:1034:A:H8	1.51	0.76
48:Y:31:VAL:HG21	48:Y:82:ILE:HD12	1.68	0.76
10:j:42:LEU:HB2	10:j:71:LYS:HB2	1.66	0.75
6:f:84:VAL:HG13	6:f:85:ILE:H	1.51	0.75
1:a:708:G:H2'	1:a:709:A:C8	2.22	0.75
6:f:44:ARG:H	6:f:58:HIS:HA	1.52	0.75
25:A:466:C:O2	25:A:470:A:N6	2.20	0.74
25:A:1519:G:H1	25:A:1529:U:H3	1.35	0.74
30:F:111:VAL:HG13	30:F:112:ARG:H	1.51	0.74
17:q:61:LEU:HB3	17:q:83:GLU:HB2	1.68	0.74
29:E:52:SER:O	29:E:73:ARG:HD2	1.88	0.74
1:a:74:A:H62	1:a:89:G:H21	0.80	0.73
1:a:538:G:OP1	4:d:56:ARG:NH2	2.22	0.73
25:A:2470:C:O2'	38:O:52:ARG:NH2	2.20	0.73
39:P:37:THR:HG22	39:P:39:PRO:HD2	1.68	0.73
3:c:131:ARG:NH1	3:c:168:TYR:OH	2.22	0.73
7:g:50:VAL:HG21	7:g:124:LEU:HD23	1.71	0.73
25:A:686:A:HO2'	25:A:687:G:H8	1.37	0.73
1:a:709:A:H2'	1:a:710:A:H8	1.53	0.72
25:A:27:G:N2	25:A:503:G:O2'	2.22	0.72
52:3:11:ALA:HA	52:3:25:ARG:HA	1.71	0.72
1:a:707:G:H2'	1:a:708:G:C8	2.25	0.72
25:A:2300:C:H2'	25:A:2301:G:H8	1.54	0.72
16:p:4:ILE:HG12	16:p:21:VAL:HG22	1.72	0.72
1:a:536:G:OP1	4:d:10:LYS:NZ	2.23	0.71
25:A:1288:A:H2	25:A:1616:G:H21	1.38	0.71
1:a:1311:C:OP1	14:n:24:ARG:NH2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2315:A:H2'	25:A:2316:A:C8	2.25	0.71
24:x:473:GLU:HB2	24:x:480:PRO:HA	1.71	0.71
2:b:46:THR:HG22	2:b:201:PRO:HG2	1.73	0.71
13:m:116:ILE:O	13:m:118:LYS:N	2.22	0.71
25:A:1587:A:H5''	25:A:1588:A:H5'	1.72	0.71
1:a:556:U:OP2	12:l:14:ARG:NH1	2.24	0.70
25:A:2175:U:C3'	25:A:2176:U:C6	2.73	0.70
31:G:16:GLU:HB3	31:G:27:LYS:HB3	1.73	0.70
1:a:1075:G:OP2	5:e:53:LYS:NZ	2.24	0.70
25:A:2175:U:C5	25:A:2176:U:O4	2.43	0.70
41:R:35:GLU:O	41:R:35:GLU:HG2	1.90	0.70
1:a:969:A:H4'	1:a:970:G:H5''	1.72	0.70
25:A:1017:A:O2'	25:A:1116:A:N6	2.24	0.70
25:A:2172:U:O2'	25:A:2173:G:H5'	1.91	0.70
1:a:315:A:N6	1:a:323:A:OP2	2.24	0.70
25:A:2175:U:H2'	25:A:2176:U:C6	2.28	0.69
1:a:1020:G:H1	1:a:1029:A:H61	0.76	0.69
8:h:5:ASP:OD1	8:h:77:ARG:NH1	2.26	0.69
24:x:355:LYS:HB3	24:x:419:VAL:HG11	1.75	0.69
25:A:2102:G:H21	25:A:2158:A:H2	1.41	0.69
3:c:123:GLN:OE1	3:c:136:ARG:NH2	2.26	0.68
1:a:1350:A:H2'	1:a:1351:A:H8	1.58	0.68
36:M:65:THR:HG23	36:M:68:GLY:H	1.58	0.68
1:a:1141:C:O2	9:i:18:ARG:NH1	2.27	0.68
11:k:85:ASN:ND2	11:k:111:THR:OG1	2.27	0.68
25:A:2414:C:H5''	25:A:2416:G:H5'	1.75	0.68
1:a:740:G:H2'	1:a:741:A:C8	2.28	0.68
5:e:83:GLN:H	5:e:148:MET:HE3	1.59	0.68
27:C:165:VAL:HG21	27:C:181:MET:HE1	1.75	0.68
6:f:23:GLU:HA	6:f:26:THR:HG22	1.75	0.68
24:x:363:ARG:HG2	24:x:384:VAL:HG11	1.76	0.68
25:A:562:A:OP2	43:T:80:ARG:NH2	2.27	0.68
2:b:114:LEU:HD13	2:b:144:LEU:HB3	1.76	0.68
25:A:2175:U:C4	25:A:2176:U:C4	2.82	0.68
5:e:116:LEU:HD13	5:e:124:VAL:HG11	1.76	0.67
1:a:459:A:O2'	1:a:460:A:O5'	2.13	0.67
35:L:45:THR:HG22	42:S:64:ARG:HH21	1.58	0.67
1:a:153:G:N2	1:a:156:A:OP2	2.28	0.67
11:k:93:ARG:NH2	21:u:23:CYS:SG	2.67	0.67
37:N:15:GLU:O	37:N:16:LYS:HG2	1.95	0.67
53:4:52:LYS:HE2	53:4:55:ASP:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:26:LYS:HE3	2:b:193:PRO:HD2	1.76	0.67
25:A:1521:C:O5'	25:A:1521:C:H6	1.78	0.67
25:A:2154:U:O4	25:A:2158:A:N7	2.28	0.67
8:h:15:ARG:HG2	8:h:19:MET:HE3	1.76	0.67
1:a:486:C:H2'	1:a:487:A:C8	2.29	0.66
17:q:60:ASP:OD2	17:q:84:ARG:NH2	2.28	0.66
51:2:4:VAL:HG23	51:2:58:GLY:HA2	1.77	0.66
25:A:2155:G:N1	25:A:2158:A:OP2	2.28	0.66
1:a:73:A:OP2	1:a:90:G:N2	2.27	0.66
1:a:157:C:H2'	1:a:158:G:H8	1.60	0.66
24:x:739:SER:OG	24:x:740:ASP:N	2.23	0.66
24:x:807:ARG:NH1	25:A:2447:U:O2'	2.29	0.66
30:F:100:LEU:O	30:F:104:LEU:N	2.25	0.66
1:a:1117:A:C4'	10:j:38:GLY:HA3	2.25	0.66
37:N:88:ASP:H	37:N:118:ARG:HH12	1.43	0.66
8:h:75:VAL:HG23	8:h:129:VAL:HG22	1.77	0.66
25:A:575:G:N7	42:S:6:ARG:NH2	2.43	0.66
1:a:974:C:O2'	14:n:13:ARG:NH1	2.29	0.66
1:a:1349:G:H2'	1:a:1350:A:H8	1.59	0.66
8:h:54:GLU:O	8:h:56:LYS:N	2.21	0.65
48:Y:40:GLN:NE2	48:Y:45:PHE:H	1.93	0.65
11:k:35:THR:HG22	11:k:41:ALA:HA	1.79	0.65
25:A:2278:U:H2'	25:A:2279:G:C8	2.31	0.65
30:F:117:LEU:N	30:F:176:PRO:O	2.28	0.65
5:e:97:MET:HE3	5:e:116:LEU:HD21	1.79	0.65
10:j:82:LYS:HG3	10:j:85:ASP:HB2	1.78	0.65
25:A:873:U:O2'	25:A:882:C:N3	2.28	0.65
25:A:1519:G:H2'	25:A:1520:U:H6	1.57	0.65
9:i:25:THR:H	9:i:27:LYS:HZ3	1.44	0.65
19:s:30:PRO:HA	19:s:48:THR:O	1.95	0.65
1:a:940:A:H2'	1:a:941:G:H8	1.61	0.65
15:o:26:GLU:HG3	15:o:81:LEU:HD22	1.78	0.65
46:W:85:LYS:HE3	46:W:92:ILE:HD11	1.78	0.65
1:a:1260:G:N2	1:a:1263:A:OP2	2.28	0.65
22:v:8:4SU:O2	22:v:21:A:H2	1.79	0.65
25:A:2102:G:O2'	25:A:2158:A:N6	2.30	0.65
1:a:4:C:N4	1:a:607:C:OP1	2.28	0.65
1:a:672:U:H2'	1:a:673:U:H6	1.61	0.65
25:A:1116:A:H4'	25:A:1117:A:H5''	1.79	0.65
1:a:1320:U:H2'	1:a:1321:G:H8	1.60	0.65
25:A:1030:A:H61	25:A:1105:G:H1	1.42	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2167:U:O2	25:A:2168:G:N2	2.30	0.65
13:m:66:GLU:HA	13:m:70:ARG:HH11	1.61	0.64
25:A:1522:U:O5'	25:A:1522:U:H6	1.79	0.64
26:B:75:G:H1'	47:X:32:VAL:HG21	1.79	0.64
7:g:62:PHE:HA	7:g:124:LEU:HD11	1.80	0.64
25:A:871:G:O6	25:A:884:U:C2	2.51	0.64
25:A:929:G:OP1	56:7:64:ARG:NH2	2.29	0.64
1:a:1065:C:H2'	1:a:1066:G:H8	1.62	0.64
1:a:453:U:H2'	1:a:454:A:H8	1.62	0.64
1:a:1268:G:HO2'	1:a:1269:A:H8	1.44	0.64
4:d:62:ARG:NH1	4:d:69:GLU:OE1	2.30	0.64
25:A:358:A:O2'	25:A:359:U:O2	2.15	0.64
1:a:678:U:O2	11:k:41:ALA:N	2.30	0.64
11:k:87:LYS:HB2	11:k:113:VAL:HG23	1.80	0.64
25:A:1237:G:H5''	42:S:6:ARG:HD3	1.80	0.64
25:A:1766:U:OP2	25:A:1771:A:N6	2.28	0.64
25:A:1789:A:H2'	25:A:1790:A:C8	2.32	0.64
45:V:28:GLN:HE21	45:V:83:TYR:HB3	1.61	0.64
1:a:339:C:OP1	41:R:38:ARG:NH1	2.31	0.64
1:a:1212:C:H2'	1:a:1213:A:C8	2.32	0.64
4:d:86:THR:HA	4:d:89:ASN:HB2	1.79	0.64
7:g:51:LYS:HD3	7:g:58:PRO:HD3	1.78	0.64
21:u:58:LYS:HE2	21:u:62:ARG:HH12	1.63	0.64
25:A:2228:A:H2'	25:A:2229:G:C8	2.33	0.64
30:F:73:SER:HA	30:F:80:ARG:HA	1.78	0.64
30:F:140:GLU:HG3	52:3:28:LEU:HG	1.80	0.64
22:v:18:G:C4	22:v:58:A:C2	2.86	0.63
25:A:2111:G:H22	25:A:2161:C:H2'	1.62	0.63
1:a:1371:A:OP1	7:g:92:ARG:NH2	2.31	0.63
1:a:701:U:H2'	1:a:702:A:H8	1.62	0.63
9:i:19:VAL:HG21	9:i:83:ILE:HG22	1.80	0.63
2:b:29:LYS:O	2:b:45:LYS:NZ	2.26	0.63
13:m:63:ILE:HG22	13:m:64:THR:HG22	1.80	0.63
14:n:36:SER:H	14:n:41:ARG:HH12	1.44	0.63
26:B:30:C:H1'	26:B:57:A:H61	1.62	0.63
25:A:28:A:N6	25:A:503:G:H1'	2.14	0.63
13:m:45:ILE:HG13	13:m:48:LEU:HD12	1.81	0.63
3:c:65:ARG:NH2	3:c:102:ASN:OD1	2.32	0.63
50:1:1:MET:SD	50:1:17:GLN:NE2	2.71	0.63
25:A:2133:C:H4'	25:A:2134:A:H5'	1.79	0.63
25:A:2143:G:O2'	25:A:2145:A:N7	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1216:G:H5'	19:s:78:ARG:HH11	1.64	0.62
30:F:34:ILE:HG13	30:F:96:MET:HE3	1.79	0.62
4:d:15:GLU:OE2	4:d:56:ARG:NH1	2.32	0.62
7:g:113:GLU:O	7:g:119:ARG:NH2	2.33	0.62
9:i:130:ARG:NH2	22:v:33:U:OP2	2.32	0.62
25:A:1572:C:O2'	25:A:1573:U:OP1	2.16	0.62
25:A:2286:G:OP2	30:F:71:ARG:NH2	2.32	0.62
1:a:454:A:H2'	1:a:455:A:H8	1.64	0.62
25:A:462:A:OP1	29:E:78:ARG:NH2	2.31	0.62
48:Y:40:GLN:HE22	48:Y:45:PHE:H	1.46	0.62
24:x:287:MET:HG3	24:x:294:VAL:HG22	1.80	0.62
25:A:100:U:O4	46:W:5:ARG:NH2	2.33	0.62
9:i:43:THR:HA	9:i:46:MET:HE2	1.82	0.62
25:A:1018:A:H2'	25:A:1019:A:C8	2.35	0.62
1:a:1028:G:H2'	1:a:1029:A:H8	1.64	0.62
25:A:2175:U:C2'	25:A:2176:U:C6	2.83	0.62
27:C:261:ASN:ND2	27:C:264:THR:OG1	2.32	0.62
51:2:5:LYS:HB2	51:2:57:GLU:HB2	1.81	0.62
24:x:637:LYS:NZ	24:x:664:ASN:O	2.32	0.62
25:A:288:A:O2'	25:A:289:G:O4'	2.17	0.62
25:A:1044:A:H62	25:A:1095:U:H3	1.47	0.61
7:g:27:MET:SD	7:g:43:VAL:HG11	2.40	0.61
25:A:2102:G:N2	25:A:2105:U:O2'	2.29	0.61
42:S:87:ALA:HB1	43:T:52:PRO:HD3	1.81	0.61
1:a:141:G:H2'	1:a:142:G:C8	2.35	0.61
2:b:55:THR:HG23	2:b:59:ARG:HH12	1.66	0.61
9:i:91:ASP:O	9:i:93:THR:N	2.29	0.61
24:x:499:VAL:HG13	24:x:500:LEU:HD12	1.83	0.61
12:l:68:GLY:O	12:l:99:ARG:NH1	2.32	0.61
12:l:114:ARG:HB2	12:l:119:ALA:HB3	1.82	0.61
35:L:117:ASP:OD1	35:L:120:ARG:NH1	2.34	0.61
13:m:110:LYS:O	13:m:114:LYS:NZ	2.30	0.61
25:A:2087:G:C6	25:A:2177:G:C6	2.89	0.61
29:E:148:VAL:HB	29:E:187:VAL:HG12	1.82	0.61
35:L:6:ALA:H	35:L:45:THR:HG21	1.66	0.61
52:3:16:CYS:HA	52:3:34:LEU:HB2	1.83	0.61
7:g:151:PHE:O	7:g:153:HIS:N	2.34	0.61
25:A:2175:U:C3'	25:A:2176:U:C5	2.77	0.61
30:F:101:ASP:OD1	30:F:102:ARG:N	2.34	0.61
25:A:2300:C:H2'	25:A:2301:G:C8	2.35	0.60
1:a:1349:G:H2'	1:a:1350:A:C8	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:207:ILE:O	2:b:210:VAL:HG22	2.01	0.60
25:A:1572:C:O2'	25:A:1573:U:O4'	2.19	0.60
1:a:669:A:H1'	11:k:118:HIS:ND1	2.16	0.60
2:b:6:MET:SD	2:b:47:LEU:HD22	2.42	0.60
14:n:90:ARG:NH1	14:n:92:ASP:OD2	2.33	0.60
25:A:1058:G:N2	25:A:1085:A:O2'	2.35	0.60
36:M:38:ILE:HD11	36:M:111:PHE:HZ	1.66	0.60
1:a:966:C:OP2	10:j:59:LYS:NZ	2.30	0.60
1:a:672:U:H2'	1:a:673:U:C6	2.35	0.60
1:a:1350:A:H2'	1:a:1351:A:C8	2.36	0.60
13:m:16:VAL:O	13:m:20:THR:HG23	2.01	0.60
25:A:197:A:N6	25:A:2417:A:O2'	2.34	0.60
1:a:1396:4OC:HM22	1:a:1397:C:H5'	1.82	0.60
11:k:20:ILE:HG22	11:k:83:ASP:HB2	1.83	0.60
28:D:181:ASP:OD2	28:D:184:ARG:NE	2.32	0.60
1:a:204:C:O2'	1:a:206:G:N7	2.29	0.60
34:J:18:ALA:HA	34:J:39:CYS:HB2	1.82	0.60
1:a:1169:G:H2'	1:a:1170:A:H8	1.67	0.60
24:x:552:ILE:HG22	24:x:608:ARG:HB3	1.83	0.60
25:A:1373:C:H2'	25:A:1374:A:C8	2.36	0.60
25:A:1468:U:O2	25:A:1497:G:O6	2.20	0.60
1:a:157:C:H2'	1:a:158:G:C8	2.37	0.59
25:A:1672:G:H2'	25:A:1673:C:C6	2.37	0.59
25:A:2177:G:C2	25:A:2178:A:C5	2.90	0.59
1:a:75:G:O6	1:a:88:U:O4	2.20	0.59
1:a:1341:G:H4'	1:a:1342:U:O5'	2.01	0.59
3:c:124:LEU:HD11	3:c:130:PHE:HB3	1.83	0.59
39:P:2:ARG:O	39:P:2:ARG:HD2	2.02	0.59
15:o:7:GLU:O	15:o:11:ILE:HG13	2.03	0.59
1:a:916:G:H4'	5:e:26:VAL:HA	1.83	0.59
1:a:926:C:H5''	7:g:4:ARG:HE	1.67	0.59
22:v:47:U:H5'	22:v:48:C:H5'	1.85	0.59
31:G:164:TYR:HB2	31:G:167:GLU:HB2	1.84	0.59
32:H:4:ILE:HD11	32:H:44:VAL:HG12	1.84	0.59
1:a:1117:A:O3'	10:j:38:GLY:HA3	2.03	0.59
1:a:1281:A:H2	1:a:1347:G:H1'	1.67	0.59
18:r:71:THR:HG22	18:r:73:SER:H	1.66	0.59
24:x:259:ARG:NH1	24:x:277:SER:OG	2.35	0.59
1:a:759:G:N2	1:a:807:U:OP2	2.31	0.59
1:a:1314:C:O2	19:s:36:ARG:NH2	2.36	0.59
14:n:64:CYS:HB2	14:n:80:SER:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:805:C:O2'	1:a:895:A:N1	2.34	0.59
8:h:41:LYS:NZ	8:h:47:ALA:O	2.35	0.59
30:F:70:ALA:HB3	30:F:81:GLU:HA	1.85	0.59
25:A:571:C:H2'	25:A:572:A:C8	2.38	0.59
1:a:666:U:O2'	18:r:64:TYR:OH	2.20	0.58
25:A:2154:U:H3	25:A:2158:A:H62	0.72	0.58
1:a:1385:U:H2'	1:a:1386:G:C8	2.37	0.58
7:g:22:ILE:HG23	7:g:101:MET:HE2	1.85	0.58
22:v:52:G:H5''	30:F:80:ARG:NH1	2.17	0.58
25:A:2177:G:N2	25:A:2178:A:C4	2.71	0.58
1:a:304:G:H5''	16:p:31:ARG:HB3	1.86	0.58
22:v:43:A:H2'	22:v:44:A:C8	2.38	0.58
1:a:1141:C:O2'	9:i:7:TYR:OH	2.21	0.58
11:k:21:ALA:HB3	11:k:84:VAL:HG12	1.86	0.58
13:m:75:MET:HA	13:m:78:LYS:HE3	1.85	0.58
25:A:2098:U:OP1	25:A:2132:C:N4	2.36	0.58
2:b:54:LEU:HD21	2:b:216:SER:HB3	1.85	0.58
6:f:43:GLY:HA2	6:f:59:TYR:H	1.68	0.58
11:k:31:ILE:HG12	11:k:46:THR:HG22	1.85	0.58
25:A:1834:A:O2'	25:A:1835:A:H8	1.86	0.58
12:l:14:ARG:HE	12:l:15:MET:H	1.49	0.58
22:v:8:4SU:O2	22:v:21:A:C2	2.57	0.58
38:O:78:PRO:HG2	38:O:81:VAL:HG21	1.86	0.58
1:a:483:C:H2'	1:a:484:A:H8	1.69	0.58
7:g:66:LEU:HA	7:g:69:ILE:HG22	1.85	0.58
25:A:1253:G:OP1	53:4:16:ARG:NH1	2.37	0.58
1:a:83:G:H2'	1:a:84:C:H6	1.67	0.58
25:A:571:C:H2'	25:A:572:A:H8	1.68	0.58
25:A:2178:A:O2'	25:A:2179:G:H5'	2.04	0.58
30:F:144:ASP:OD1	30:F:145:LYS:N	2.36	0.58
1:a:658:G:H22	1:a:735:G:H1	1.52	0.58
1:a:1117:A:H4'	10:j:38:GLY:CA	2.33	0.58
3:c:19:THR:O	3:c:40:ARG:NH2	2.37	0.58
25:A:1:G:O6	25:A:2890:A:N6	2.37	0.58
25:A:5:A:H2'	25:A:6:A:C8	2.39	0.58
30:F:31:VAL:HA	30:F:158:THR:HG22	1.85	0.58
1:a:453:U:H2'	1:a:454:A:C8	2.38	0.57
1:a:1247:G:H2'	1:a:1248:G:H8	1.69	0.57
4:d:162:CYS:HA	4:d:165:ARG:HE	1.69	0.57
24:x:583:ASP:OD1	24:x:584:GLY:N	2.37	0.57
12:l:50:ARG:HG3	12:l:90:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:o:25:PRO:O	15:o:29:VAL:HG23	2.04	0.57
25:A:2177:G:C2	25:A:2178:A:C4	2.91	0.57
35:L:45:THR:OG1	35:L:48:VAL:HG12	2.03	0.57
25:A:2096:U:C2	25:A:2168:G:C6	2.92	0.57
1:a:1119:U:H4'	10:j:7:ARG:HH22	1.70	0.57
1:a:940:A:H2'	1:a:941:G:C8	2.38	0.57
2:b:18:HIS:NE2	2:b:188:ASP:OD2	2.37	0.57
11:k:24:HIS:O	11:k:30:THR:HA	2.04	0.57
13:m:39:VAL:HG12	13:m:52:GLN:HG2	1.86	0.57
25:A:1456:A:H2'	25:A:1457:A:C8	2.39	0.57
1:a:404:G:OP2	4:d:31:LYS:NZ	2.37	0.57
8:h:48:ASP:OD1	8:h:50:GLN:NE2	2.38	0.57
25:A:247:G:OP2	25:A:249:C:N4	2.35	0.57
31:G:27:LYS:HD2	31:G:32:ALA:HB1	1.85	0.57
2:b:6:MET:HE1	2:b:47:LEU:HB2	1.86	0.57
25:A:439:U:O4'	29:E:78:ARG:NH1	2.38	0.57
22:v:8:4SU:O5'	22:v:8:4SU:H6	2.05	0.57
25:A:2233:G:H2'	25:A:2234:A:C8	2.40	0.57
1:a:78:A:H2'	1:a:79:G:C8	2.40	0.57
2:b:55:THR:OG1	2:b:59:ARG:NH2	2.37	0.57
1:a:677:G:N2	11:k:39:GLY:O	2.38	0.56
25:A:1084:U:H1'	25:A:1087:U:H5	1.70	0.56
24:x:355:LYS:NZ	60:x:902:GCP:O3G	2.36	0.56
25:A:98:C:N4	25:A:99:U:O4	2.38	0.56
25:A:2175:U:C6	25:A:2176:U:C5	2.93	0.56
30:F:61:THR:O	30:F:95:ARG:NH2	2.38	0.56
30:F:127:ASN:HD22	30:F:157:THR:HA	1.70	0.56
31:G:158:LYS:HD2	31:G:160:LYS:HD2	1.87	0.56
36:M:58:MET:HE2	36:M:86:LEU:HB3	1.87	0.56
1:a:255:U:OP2	20:t:74:ARG:NH2	2.37	0.56
1:a:1406:C:H2'	1:a:1407:A:C8	2.41	0.56
24:x:485:SER:O	24:x:487:LYS:N	2.38	0.56
25:A:300:U:H2'	25:A:301:G:O4'	2.05	0.56
29:E:116:ARG:NH2	37:N:1:MET:O	2.36	0.56
41:R:21:PHE:O	41:R:51:LYS:NZ	2.38	0.56
1:a:1219:A:OP1	13:m:102:THR:OG1	2.23	0.56
24:x:639:THR:HG22	24:x:668:GLN:HE21	1.71	0.56
1:a:83:G:H2'	1:a:84:C:C6	2.40	0.56
1:a:263:U:H2'	1:a:264:A:C8	2.40	0.56
25:A:459:G:N7	55:6:39:ARG:NH2	2.46	0.56
25:A:871:G:O6	25:A:884:U:O2	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:W:80:ASP:OD2	46:W:97:SER:OG	2.24	0.56
1:a:229:U:H2'	1:a:230:A:H8	1.69	0.56
1:a:741:A:H2'	1:a:742:U:C6	2.40	0.56
25:A:191:A:H2'	25:A:192:C:C6	2.40	0.56
25:A:997:C:OP1	35:L:37:ARG:NH1	2.37	0.56
30:F:167:ARG:O	30:F:171:ARG:N	2.38	0.56
41:R:89:ARG:NH2	41:R:111:ILE:O	2.33	0.56
47:X:104:THR:HG22	47:X:135:GLU:OE2	2.04	0.56
25:A:840:U:H2'	25:A:841:C:H6	1.70	0.56
25:A:1420:A:H2'	25:A:1421:A:C8	2.41	0.56
25:A:1373:C:H2'	25:A:1374:A:H8	1.71	0.56
1:a:916:G:H2'	1:a:917:A:C8	2.41	0.56
25:A:867:A:N6	25:A:888:A:O2'	2.39	0.56
25:A:2559:A:N7	28:D:150:GLN:HG3	2.21	0.56
25:A:2571:U:H2'	25:A:2572:U:H2'	1.88	0.56
30:F:119:ALA:HB1	30:F:167:ARG:HE	1.71	0.56
33:I:44:GLU:O	33:I:49:GLY:N	2.39	0.56
47:X:6:LEU:HD11	47:X:53:LEU:HD13	1.87	0.56
13:m:117:ARG:NH1	13:m:118:LYS:OXT	2.39	0.55
17:q:72:LYS:HG3	17:q:73:THR:HG23	1.86	0.55
25:A:2191:G:OP2	27:C:147:LYS:NZ	2.37	0.55
1:a:125:U:H2'	1:a:126:C:C6	2.42	0.55
1:a:84:C:H2'	1:a:85:U:H6	1.70	0.55
14:n:4:GLU:HA	14:n:7:LYS:HE2	1.88	0.55
25:A:5:A:H2'	25:A:6:A:H8	1.71	0.55
25:A:1786:G:OP1	27:C:259:ARG:NH1	2.33	0.55
25:A:2135:G:H2'	25:A:2136:U:C6	2.42	0.55
1:a:41:G:H2'	1:a:42:G:H8	1.72	0.55
1:a:1380:G:H2'	1:a:1381:G:H8	1.70	0.55
14:n:10:GLU:HG2	14:n:63:ARG:HH11	1.72	0.55
25:A:1:G:H2'	25:A:2:G:H8	1.71	0.55
25:A:272:A:H2'	25:A:273:A:C8	2.42	0.55
28:D:116:LYS:HB2	28:D:165:LEU:HB2	1.89	0.55
1:a:409:A:O2'	24:x:277:SER:O	2.25	0.55
6:f:83:ALA:O	6:f:85:ILE:N	2.40	0.55
12:l:73:ASN:ND2	12:l:105:SER:OG	2.39	0.55
22:v:54:5MU:HN3	22:v:58:A:H62	1.55	0.55
25:A:2175:U:C3'	25:A:2176:U:H6	2.20	0.55
52:3:16:CYS:SG	52:3:37:CYS:HB3	2.47	0.55
1:a:1118:G:OP1	10:j:38:GLY:N	2.40	0.55
22:v:67:C:H2'	22:v:68:C:H6	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1095:U:H2'	25:A:1096:A:C8	2.42	0.55
25:A:2057:A:H2'	25:A:2058:A:H8	1.71	0.55
25:A:2233:G:H2'	25:A:2234:A:H8	1.71	0.55
1:a:687:G:O2'	1:a:688:A:OP1	2.23	0.55
1:a:1138:G:N2	1:a:1140:A:H62	2.04	0.55
25:A:2057:A:H2'	25:A:2058:A:C8	2.42	0.55
25:A:2151:C:H5''	25:A:2158:A:H8	1.70	0.55
33:I:90:GLY:O	33:I:92:ALA:N	2.38	0.55
1:a:87:C:H2'	1:a:88:U:H6	1.72	0.55
25:A:540:U:H2'	25:A:541:A:H8	1.72	0.55
25:A:517:A:N7	62:A:3517:HOH:O	2.33	0.55
25:A:2102:G:N1	25:A:2106:A:OP2	2.40	0.55
25:A:2142:U:OP2	25:A:2143:G:N2	2.40	0.55
32:H:21:ILE:HD11	32:H:26:ALA:HB2	1.88	0.55
33:I:25:ALA:HA	33:I:84:PHE:HA	1.88	0.55
39:P:24:MET:HE1	39:P:40:LYS:HD3	1.88	0.55
10:j:63:ASP:OD1	14:n:98:LYS:NZ	2.40	0.54
11:k:34:ILE:HD11	11:k:43:SER:HB3	1.88	0.54
27:C:135:ILE:O	27:C:167:ARG:NH2	2.37	0.54
13:m:55:GLN:O	13:m:59:GLU:HG2	2.06	0.54
25:A:971:A:OP2	25:A:972:C:N4	2.31	0.54
30:F:43:ALA:HB1	30:F:47:LYS:HA	1.89	0.54
30:F:176:PRO:HG3	52:3:44:TYR:HE1	1.72	0.54
47:X:172:GLU:CD	47:X:174:VAL:H	2.15	0.54
1:a:1028:G:H2'	1:a:1029:A:C8	2.42	0.54
13:m:80:LEU:HD13	13:m:87:ARG:HD3	1.88	0.54
25:A:629:U:H2'	25:A:630:C:C6	2.42	0.54
45:V:86:LEU:HB3	45:V:90:GLN:HE21	1.72	0.54
1:a:375:A:O2'	1:a:376:A:O5'	2.25	0.54
25:A:1295:A:N7	62:A:3518:HOH:O	2.33	0.54
17:q:7:THR:OG1	17:q:8:VAL:N	2.40	0.54
25:A:1639:G:O2'	39:P:106:ASP:OD2	2.21	0.54
25:A:1876:A:H2'	25:A:1877:A:C8	2.42	0.54
4:d:196:ASN:HB3	4:d:199:LEU:HD13	1.89	0.54
25:A:405:C:H2'	25:A:406:A:C8	2.43	0.54
25:A:1340:A:H2'	25:A:1341:A:C8	2.43	0.54
1:a:75:G:H2'	1:a:76:G:C8	2.43	0.54
1:a:210:U:H2'	1:a:211:C:C6	2.42	0.54
11:k:112:ASP:N	21:u:2:PRO:O	2.35	0.54
25:A:876:U:N3	25:A:880:G:O6	2.41	0.54
25:A:1352:A:OP1	49:Z:3:ARG:HD2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2122:A:H5''	25:A:2140:C:H41	1.73	0.54
25:A:2177:G:N3	25:A:2178:A:C8	2.75	0.54
25:A:2177:G:N1	25:A:2178:A:C5	2.75	0.54
25:A:2300:C:O2'	30:F:37:ASN:ND2	2.41	0.54
1:a:978:C:N3	1:a:1216:G:N2	2.55	0.54
1:a:1242:A:H4'	9:i:33:ARG:HH12	1.73	0.54
8:h:49:PHE:HB2	8:h:59:LEU:HD11	1.88	0.54
13:m:68:ASP:OD1	13:m:71:ARG:NH2	2.41	0.54
22:v:57:A:H2'	22:v:58:A:H5'	1.89	0.54
52:3:10:GLU:OE2	52:3:29:CYS:N	2.41	0.54
1:a:263:U:H2'	1:a:264:A:H8	1.72	0.54
1:a:352:U:H2'	1:a:353:G:C8	2.43	0.54
9:i:107:ASP:OD2	9:i:109:ARG:NH2	2.41	0.54
22:v:71:C:H2'	22:v:72:A:C8	2.43	0.54
24:x:520:VAL:HG22	24:x:535:VAL:HG12	1.89	0.54
25:A:2230:U:H2'	25:A:2231:U:C6	2.43	0.54
1:a:702:A:H2'	1:a:703:G:H8	1.73	0.54
1:a:1282:A:H2'	1:a:1283:A:C8	2.43	0.54
1:a:1303:G:OP2	13:m:98:ARG:NH1	2.41	0.54
24:x:388:ARG:HH12	24:x:497:GLU:HB2	1.72	0.54
1:a:352:U:H2'	1:a:353:G:H8	1.72	0.53
1:a:1033:C:H2'	1:a:1034:A:C8	2.38	0.53
24:x:745:ILE:HD11	24:x:829:GLU:HG2	1.91	0.53
26:B:9:G:C2	26:B:10:A:C8	2.96	0.53
31:G:39:PRO:HG3	31:G:64:MET:HE2	1.89	0.53
34:J:102:THR:HG23	34:J:105:GLN:H	1.74	0.53
1:a:904:C:OP2	12:l:18:LYS:NZ	2.37	0.53
25:A:304:A:O2'	25:A:306:G:N7	2.35	0.53
2:b:83:GLU:HG2	2:b:214:LEU:HB3	1.90	0.53
2:b:187:VAL:HG13	2:b:191:SER:HB2	1.90	0.53
24:x:287:MET:HB3	24:x:293:PRO:HA	1.91	0.53
25:A:2100:U:H3'	25:A:2101:A:H8	1.74	0.53
1:a:1247:G:H2'	1:a:1248:G:C8	2.42	0.53
22:v:51:C:H2'	22:v:52:G:H8	1.72	0.53
25:A:2301:G:H5'	30:F:35:THR:HG21	1.89	0.53
1:a:87:C:H2'	1:a:88:U:C6	2.44	0.53
1:a:971:A:N6	1:a:1218:U:OP1	2.42	0.53
1:a:1292:U:H1'	1:a:1293:A:C6	2.42	0.53
1:a:1390:A:H4'	1:a:1391:C:H5''	1.90	0.53
2:b:15:HIS:O	2:b:15:HIS:ND1	2.41	0.53
7:g:112:GLY:H	7:g:119:ARG:HE	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:47:ALA:HB3	8:h:62:GLU:HB2	1.90	0.53
10:j:47:GLU:OE1	14:n:76:LYS:NZ	2.41	0.53
11:k:21:ALA:O	11:k:84:VAL:HA	2.08	0.53
15:o:36:ILE:O	15:o:40:GLN:HG2	2.09	0.53
25:A:2094:C:O2'	25:A:2095:U:O4'	2.27	0.53
30:F:34:ILE:HG12	30:F:156:LEU:HD13	1.91	0.53
36:M:25:LEU:HD12	36:M:38:ILE:HG22	1.90	0.53
4:d:78:GLU:OE2	4:d:82:ARG:NE	2.40	0.53
25:A:700:U:H2'	25:A:701:A:H8	1.73	0.53
25:A:1083:G:H21	25:A:1088:A:H62	1.57	0.53
35:L:19:ASP:OD1	35:L:58:ASN:ND2	2.26	0.53
6:f:9:LEU:HD12	6:f:85:ILE:HG23	1.91	0.53
25:A:1642:A:O2'	25:A:1643:G:OP1	2.23	0.53
25:A:2245:C:O2'	25:A:2414:C:OP2	2.27	0.53
1:a:772:G:O2'	11:k:121:CYS:HB3	2.09	0.53
1:a:1216:G:OP1	19:s:78:ARG:NH1	2.42	0.53
1:a:1317:G:H2'	1:a:1318:A:H8	1.74	0.53
6:f:92:ARG:NH2	18:r:22:ASP:OD1	2.42	0.53
13:m:116:ILE:O	13:m:117:ARG:HD3	2.09	0.53
25:A:694:G:H1'	25:A:717:A:H61	1.74	0.53
25:A:1529:U:H2'	25:A:1530:G:C8	2.44	0.53
38:O:61:GLY:O	47:X:191:ARG:NH2	2.32	0.53
1:a:705:A:H2'	1:a:706:A:C8	2.43	0.53
1:a:706:A:H2'	1:a:707:G:C8	2.43	0.53
22:v:51:C:H2'	22:v:52:G:C8	2.43	0.53
24:x:558:ARG:NE	24:x:581:GLY:HA2	2.18	0.53
25:A:840:U:H2'	25:A:841:C:C6	2.44	0.53
25:A:1811:G:O2'	27:C:253:THR:HG21	2.09	0.53
25:A:1845:A:H61	25:A:1871:G:H1'	1.73	0.53
25:A:2051:C:H2'	25:A:2052:C:C6	2.43	0.53
35:L:23:GLN:HE22	35:L:142:ILE:HD12	1.73	0.53
1:a:1317:G:H2'	1:a:1318:A:C8	2.44	0.53
2:b:15:HIS:HB3	2:b:43:LEU:HD11	1.91	0.53
6:f:17:GLN:O	6:f:21:MET:N	2.42	0.53
14:n:11:LEU:O	14:n:15:LEU:HD12	2.09	0.53
14:n:46:VAL:O	14:n:50:LYS:HG2	2.08	0.52
25:A:653:G:H5''	37:N:17:HIS:NE2	2.23	0.52
25:A:1095:U:H2'	25:A:1096:A:H8	1.74	0.52
25:A:2175:U:C6	25:A:2176:U:C4	2.98	0.52
43:T:5:ILE:HG22	43:T:38:VAL:HG22	1.90	0.52
43:T:6:VAL:HG22	43:T:11:GLN:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:73:A:N6	1:a:90:G:O2'	2.36	0.52
1:a:1512:MA6:H92	1:a:1513:MA6:N6	2.24	0.52
25:A:1018:A:N3	25:A:2473:C:O2'	2.41	0.52
25:A:2315:A:H2'	25:A:2316:A:H8	1.73	0.52
1:a:200:U:H2'	1:a:201:C:C6	2.44	0.52
1:a:952:A:N6	19:s:77:THR:O	2.43	0.52
25:A:837:C:H2'	25:A:838:A:H8	1.74	0.52
1:a:41:G:H2'	1:a:42:G:C8	2.44	0.52
1:a:210:U:H2'	1:a:211:C:H6	1.74	0.52
1:a:840:G:H2'	1:a:841:A:C8	2.44	0.52
7:g:23:LEU:O	7:g:27:MET:HG2	2.10	0.52
25:A:949:A:H2'	25:A:950:A:C8	2.45	0.52
25:A:1783:U:H2'	25:A:1784:C:H6	1.74	0.52
25:A:2775:A:H2'	25:A:2776:C:C6	2.44	0.52
28:D:208:LYS:O	28:D:210:ARG:HG2	2.09	0.52
1:a:1071:G:N2	1:a:1074:A:OP2	2.32	0.52
27:C:145:GLU:HG2	27:C:189:ARG:H	1.74	0.52
28:D:116:LYS:HG2	28:D:123:LYS:HE2	1.91	0.52
1:a:84:C:H2'	1:a:85:U:C6	2.44	0.52
1:a:893:C:O2'	1:a:894:A:OP1	2.26	0.52
25:A:823:A:H2'	25:A:824:G:C8	2.45	0.52
25:A:2291:G:H22	25:A:2299:U:H3	1.55	0.52
1:a:331:G:H2'	1:a:332:A:C8	2.45	0.52
22:v:18:G:C2	22:v:58:A:C4	2.97	0.52
24:x:337:GLU:HB3	24:x:511:THR:HB	1.90	0.52
24:x:414:ASP:O	24:x:415:ILE:HG13	2.10	0.52
24:x:752:ARG:HA	24:x:824:VAL:HG23	1.92	0.52
24:x:819:TYR:CE2	24:x:822:VAL:HG12	2.44	0.52
25:A:467:G:N1	25:A:470:A:OP2	2.40	0.52
25:A:1783:U:H2'	25:A:1784:C:C6	2.45	0.52
1:a:553:A:H4'	1:a:554:A:H3'	1.92	0.52
1:a:679:G:H2'	1:a:680:U:C6	2.45	0.52
3:c:39:VAL:HG23	3:c:91:LEU:HD22	1.90	0.52
6:f:51:ILE:O	6:f:54:VAL:HG22	2.10	0.52
24:x:529:ARG:HB2	24:x:580:LEU:HD11	1.90	0.52
24:x:741:LEU:HD23	24:x:741:LEU:O	2.10	0.52
25:A:879:C:H3'	25:A:880:G:C8	2.45	0.52
25:A:990:A:H2'	25:A:991:A:C8	2.43	0.52
26:B:37:C:O2	40:Q:99:HIS:NE2	2.43	0.52
29:E:180:ILE:HG12	37:N:1:MET:HE3	1.92	0.52
56:7:16:LYS:NZ	56:7:17:THR:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:153:ASP:CG	2:b:154:MET:H	2.18	0.52
24:x:351:VAL:O	60:x:902:GCP:O3G	2.28	0.52
25:A:700:U:H2'	25:A:701:A:C8	2.45	0.52
25:A:1276:C:H2'	25:A:1277:A:H8	1.75	0.52
25:A:1420:A:H2'	25:A:1421:A:H8	1.75	0.52
25:A:2124:C:H2'	25:A:2125:G:C8	2.44	0.52
25:A:2536:G:H2'	25:A:2537:G:H8	1.74	0.52
32:H:66:GLU:HA	32:H:69:ALA:HB3	1.92	0.52
1:a:533:A:H2'	1:a:534:G:C8	2.45	0.52
9:i:44:ALA:HA	9:i:47:VAL:HG12	1.91	0.52
25:A:1348:G:H2'	25:A:1349:C:C6	2.45	0.52
1:a:21:G:H2'	1:a:22:G:C8	2.45	0.51
1:a:318:G:N1	1:a:321:A:OP2	2.41	0.51
1:a:1042:G:O2'	1:a:1044:G:OP1	2.28	0.51
1:a:1286:C:H2'	1:a:1287:G:C8	2.45	0.51
25:A:1766:U:H5	25:A:1771:A:N7	2.07	0.51
25:A:2177:G:C2	25:A:2178:A:C8	2.98	0.51
1:a:454:A:H2'	1:a:455:A:C8	2.45	0.51
24:x:753:ASP:OD1	24:x:754:VAL:N	2.42	0.51
25:A:786:U:H2'	25:A:787:C:C6	2.45	0.51
25:A:1424:C:H2'	25:A:1425:U:C6	2.45	0.51
25:A:1425:U:H2'	25:A:1426:A:C8	2.46	0.51
30:F:111:VAL:HG13	30:F:112:ARG:N	2.23	0.51
7:g:95:ARG:HG2	7:g:99:LEU:HD23	1.92	0.51
13:m:51:GLU:O	13:m:55:GLN:NE2	2.42	0.51
22:v:14:A:H61	22:v:21:A:H2	1.59	0.51
25:A:92:A:H2'	25:A:93:A:C8	2.45	0.51
48:Y:25:LEU:HD13	48:Y:31:VAL:HG12	1.93	0.51
9:i:41:ARG:H	9:i:45:ARG:HH22	1.58	0.51
30:F:96:MET:HG3	30:F:97:TYR:HD1	1.75	0.51
30:F:135:GLN:HE22	30:F:149:LEU:HA	1.75	0.51
1:a:1194:C:H5''	1:a:1195:A:H3'	1.92	0.51
25:A:1344:C:H2'	25:A:1345:G:O4'	2.10	0.51
25:A:1781:A:H2'	25:A:1782:C:C6	2.46	0.51
40:Q:67:ILE:HD13	40:Q:101:ARG:HG2	1.92	0.51
41:R:101:LEU:HD11	41:R:111:ILE:HD11	1.92	0.51
1:a:1336:C:H2'	1:a:1337:G:H8	1.76	0.51
14:n:45:GLN:CD	19:s:7:LYS:HD2	2.36	0.51
20:t:44:LEU:HG	20:t:48:GLN:HE22	1.76	0.51
25:A:4:C:H2'	25:A:5:A:H8	1.75	0.51
25:A:165:A:HO2'	25:A:166:U:H6	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:822:U:H2'	25:A:823:A:H8	1.74	0.51
25:A:880:G:C5	25:A:881:A:H1'	2.45	0.51
25:A:1302:C:O2'	25:A:1379:A:N3	2.40	0.51
35:L:45:THR:HG22	42:S:64:ARG:NH2	2.25	0.51
41:R:34:LYS:HD2	41:R:39:GLN:HE22	1.76	0.51
1:a:384:U:H2'	1:a:385:C:C6	2.45	0.51
1:a:400:G:H5'	4:d:5:ILE:HG21	1.92	0.51
1:a:954:U:H2'	1:a:1219:A:H62	1.76	0.51
1:a:1172:G:OP1	9:i:95:ARG:NH2	2.43	0.51
5:e:95:VAL:HG13	5:e:112:MET:HE3	1.93	0.51
25:A:2498:U:H5''	28:D:128:ARG:HG3	1.93	0.51
42:S:97:ASP:OD1	42:S:101:ASN:ND2	2.40	0.51
1:a:182:G:N7	1:a:184:G:N2	2.59	0.51
1:a:607:C:H2'	1:a:608:C:C6	2.46	0.51
1:a:1080:U:H3	1:a:1093:G:H22	1.58	0.51
2:b:208:ARG:HA	2:b:211:GLN:NE2	2.25	0.51
7:g:52:GLU:OE2	7:g:53:ARG:NH2	2.42	0.51
11:k:59:THR:HG23	11:k:62:ALA:H	1.76	0.51
25:A:27:G:H1'	25:A:504:A:N6	2.26	0.51
25:A:687:G:H2'	25:A:688:C:C6	2.46	0.51
50:1:32:LYS:HD2	50:1:43:LEU:HD11	1.93	0.51
1:a:981:G:H2'	1:a:982:G:H8	1.76	0.51
25:A:191:A:H2'	25:A:192:C:H6	1.76	0.51
25:A:570:U:H2'	25:A:571:C:C6	2.46	0.51
25:A:1741:A:O2'	25:A:1742:A:OP1	2.28	0.51
1:a:1078:G:H5''	1:a:1079:U:H2'	1.93	0.51
5:e:106:ILE:O	5:e:113:ARG:NH2	2.43	0.51
9:i:4:THR:OG1	9:i:5:GLN:N	2.44	0.51
22:v:52:G:H2'	22:v:53:G:H8	1.76	0.51
25:A:2417:A:H2'	25:A:2417:A:N3	2.26	0.51
39:P:103:ARG:NH2	39:P:106:ASP:OD2	2.41	0.51
1:a:78:A:H2'	1:a:79:G:H8	1.76	0.50
7:g:72:LEU:HA	7:g:96:ARG:HH12	1.76	0.50
25:A:371:G:H5'	49:Z:18:ILE:HD13	1.93	0.50
26:B:48:U:H4'	40:Q:99:HIS:HD2	1.76	0.50
54:5:6:ARG:O	54:5:48:ALA:N	2.44	0.50
1:a:1169:G:H2'	1:a:1170:A:C8	2.47	0.50
1:a:1239:G:C6	1:a:1240:G:O6	2.64	0.50
1:a:1239:G:H2'	1:a:1240:G:C8	2.47	0.50
9:i:71:GLY:O	9:i:75:GLN:HG3	2.11	0.50
25:A:570:U:H2'	25:A:571:C:H6	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:772:A:C2	27:C:225:MET:HG2	2.46	0.50
25:A:822:U:H2'	25:A:823:A:C8	2.47	0.50
25:A:2793:C:O2'	25:A:2794:U:OP1	2.29	0.50
39:P:29:PHE:O	39:P:78:LYS:NZ	2.42	0.50
1:a:1006:A:N6	1:a:1012:G:O6	2.45	0.50
30:F:36:LEU:O	30:F:37:ASN:OD1	2.30	0.50
47:X:22:LEU:HD22	47:X:28:LEU:HD12	1.92	0.50
7:g:107:PHE:HZ	7:g:137:LYS:HD3	1.77	0.50
22:v:18:G:C6	22:v:58:A:N1	2.79	0.50
24:x:496:LEU:HA	24:x:499:VAL:HG12	1.94	0.50
25:A:899:A:C5	38:O:13:MET:HG3	2.46	0.50
34:J:77:ALA:HA	34:J:136:MET:HE1	1.93	0.50
1:a:86:C:H2'	1:a:87:C:H6	1.76	0.50
1:a:1321:G:H2'	1:a:1322:C:H6	1.77	0.50
5:e:115:VAL:HG13	5:e:142:PHE:HE1	1.77	0.50
26:B:49:C:H2'	26:B:50:A:H8	1.76	0.50
28:D:149:CYS:SG	28:D:150:GLN:N	2.78	0.50
46:W:4:ILE:HG21	46:W:33:LEU:HD11	1.94	0.50
3:c:43:LEU:HD21	3:c:68:ILE:HD11	1.94	0.50
13:m:12:ASN:HA	13:m:44:LYS:HD3	1.94	0.50
24:x:386:THR:OG1	24:x:389:GLY:O	2.28	0.50
25:A:2273:G:H4'	25:A:2274:A:O5'	2.12	0.50
40:Q:75:GLN:NE2	40:Q:79:GLU:OE2	2.35	0.50
1:a:1298:G:N2	1:a:1328:G:O6	2.44	0.50
17:q:13:GLY:HA3	17:q:28:ILE:HD13	1.94	0.50
25:A:1042:C:O2'	25:A:1043:U:OP1	2.30	0.50
25:A:1425:U:H2'	25:A:1426:A:H8	1.75	0.50
25:A:2300:C:H4'	30:F:37:ASN:HD22	1.76	0.50
33:I:44:GLU:O	33:I:48:ALA:N	2.44	0.50
1:a:181:U:H3'	1:a:182:G:H5''	1.93	0.50
4:d:172:GLU:HG3	4:d:183:LYS:NZ	2.23	0.50
6:f:29:ILE:HD11	6:f:65:GLU:H	1.76	0.50
7:g:72:LEU:HA	7:g:96:ARG:HH22	1.77	0.50
25:A:871:G:H2'	25:A:872:G:O4'	2.11	0.50
25:A:1399:U:H2'	25:A:1400:A:C8	2.47	0.50
25:A:1399:U:H2'	25:A:1400:A:H8	1.76	0.50
25:A:2118:U:O2'	25:A:2144:G:O3'	2.29	0.50
25:A:2170:C:H2'	25:A:2171:A:C8	2.47	0.50
47:X:173:LEU:O	47:X:175:GLN:N	2.45	0.50
49:Z:33:LEU:HA	49:Z:52:SER:HA	1.94	0.50
25:A:1456:A:H2'	25:A:1457:A:H8	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2098:U:O4	25:A:2135:G:N2	2.37	0.50
25:A:2461:U:O2'	25:A:2462:C:OP1	2.27	0.50
28:D:118:PHE:HA	28:D:164:HIS:H	1.77	0.50
31:G:121:ILE:HD11	31:G:144:VAL:HG21	1.94	0.50
1:a:576:U:H2'	1:a:577:A:H8	1.76	0.49
7:g:107:PHE:CZ	7:g:137:LYS:HD3	2.47	0.49
8:h:5:ASP:HB2	8:h:81:PRO:HG3	1.94	0.49
8:h:18:GLN:HE21	8:h:63:LEU:HB3	1.77	0.49
24:x:350:HIS:O	24:x:355:LYS:NZ	2.39	0.49
25:A:1419:G:H2'	25:A:1420:A:C8	2.46	0.49
25:A:1450:A:H2'	25:A:1451:A:C8	2.47	0.49
1:a:668:G:H2'	1:a:669:A:H8	1.77	0.49
1:a:975:U:OP1	14:n:9:ARG:NH2	2.36	0.49
1:a:1416:G:H5'	36:M:48:PRO:HB3	1.93	0.49
2:b:89:MET:HE2	2:b:89:MET:N	2.27	0.49
2:b:153:ASP:OD1	2:b:154:MET:N	2.41	0.49
6:f:6:ILE:HG23	6:f:62:MET:SD	2.52	0.49
25:A:837:C:H2'	25:A:838:A:C8	2.46	0.49
25:A:2316:A:H2'	25:A:2317:G:C8	2.47	0.49
30:F:43:ALA:HB2	30:F:49:ILE:HG12	1.94	0.49
1:a:722:A:H2'	1:a:723:A:C8	2.47	0.49
1:a:989:C:O4'	14:n:8:ASN:ND2	2.46	0.49
6:f:84:VAL:HG13	6:f:85:ILE:N	2.22	0.49
25:A:2087:G:C6	25:A:2177:G:O6	2.65	0.49
1:a:17:U:H2'	1:a:18:C:C6	2.48	0.49
9:i:26:GLY:N	9:i:61:PHE:O	2.46	0.49
38:O:51:ARG:O	38:O:55:THR:HG23	2.11	0.49
1:a:206:G:C4	1:a:207:A:C8	3.01	0.49
1:a:820:C:O2	8:h:16:ASN:ND2	2.46	0.49
1:a:1049:A:N3	3:c:156:ARG:NH1	2.58	0.49
1:a:1308:C:H2'	1:a:1309:U:C6	2.46	0.49
1:a:1336:C:H2'	1:a:1337:G:C8	2.48	0.49
2:b:129:LEU:HD11	2:b:133:GLU:OE2	2.12	0.49
25:A:1756:U:O2'	25:A:1945:C:OP1	2.29	0.49
25:A:2121:A:H1'	25:A:2145:A:H2'	1.94	0.49
25:A:2292:U:H5''	30:F:131:GLY:HA3	1.95	0.49
27:C:98:ASP:OD1	27:C:98:ASP:N	2.45	0.49
1:a:677:G:H2'	1:a:678:U:H6	1.78	0.49
1:a:1501:A:H2'	1:a:1502:G:C8	2.47	0.49
2:b:20:THR:HA	2:b:39:HIS:CD2	2.47	0.49
10:j:69:THR:HG22	10:j:71:LYS:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:o:29:VAL:HG11	15:o:67:LEU:HD21	1.94	0.49
24:x:360:ASP:OD1	24:x:367:VAL:HG22	2.12	0.49
25:A:331:C:OP2	46:W:3:LYS:NZ	2.38	0.49
25:A:1016:U:O2'	25:A:1017:A:OP1	2.28	0.49
25:A:1627:A:H2'	25:A:1628:C:C6	2.47	0.49
25:A:2293:C:N4	30:F:39:GLY:O	2.46	0.49
26:B:55:U:H2'	26:B:56:G:C8	2.48	0.49
47:X:100:ASP:O	47:X:101:HIS:ND1	2.45	0.49
1:a:471:U:H2'	1:a:472:U:C6	2.48	0.49
1:a:699:U:C4	1:a:700:A:N7	2.80	0.49
1:a:751:U:H2'	1:a:752:G:O4'	2.13	0.49
1:a:800:C:H2'	1:a:801:A:H8	1.76	0.49
4:d:32:CYS:SG	4:d:34:ALA:HB2	2.53	0.49
26:B:59:A:HO2'	40:Q:2:SER:N	2.10	0.49
30:F:135:GLN:HE21	30:F:150:ARG:HH21	1.61	0.49
52:3:42:PRO:HB3	52:3:47:LYS:HE2	1.95	0.49
1:a:829:G:O2'	1:a:830:G:H5''	2.12	0.49
1:a:586:A:H2'	1:a:587:G:H8	1.78	0.49
1:a:1065:C:H2'	1:a:1066:G:C8	2.46	0.49
4:d:19:LEU:HD12	4:d:60:LYS:HG3	1.95	0.49
8:h:18:GLN:HG2	8:h:63:LEU:HD13	1.95	0.49
14:n:6:MET:HE2	14:n:63:ARG:NH2	2.28	0.49
25:A:686:A:O2'	25:A:687:G:H8	1.93	0.49
25:A:2274:A:O2'	25:A:2275:A:O5'	2.26	0.49
28:D:151:THR:HG22	28:D:152:PRO:HD3	1.95	0.49
25:A:625:C:O2'	25:A:629:U:OP1	2.30	0.49
25:A:1434:U:H2'	25:A:1435:U:C6	2.47	0.49
25:A:1711:A:H62	25:A:1723:G:H21	1.60	0.49
25:A:2061:U:H2'	25:A:2062:U:C6	2.47	0.49
25:A:2665:A:H2'	25:A:2666:A:C8	2.47	0.49
25:A:2851:G:HO2'	25:A:2852:U:P	2.36	0.49
30:F:123:ASP:OD1	30:F:127:ASN:HB2	2.13	0.49
1:a:506:U:O2'	1:a:507:U:OP1	2.29	0.48
1:a:840:G:H2'	1:a:841:A:H8	1.78	0.48
1:a:1233:A:H4'	1:a:1234:U:O5'	2.12	0.48
14:n:41:ARG:O	14:n:45:GLN:HG3	2.12	0.48
17:q:60:ASP:OD1	17:q:85:ALA:N	2.39	0.48
25:A:4:C:H2'	25:A:5:A:C8	2.48	0.48
25:A:43:G:C2'	25:A:44:A:H5'	2.43	0.48
25:A:2578:C:H2'	25:A:2579:G:C8	2.48	0.48
57:8:16:ILE:HD13	57:8:25:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:317:U:H2'	1:a:318:G:O4'	2.13	0.48
1:a:1009:G:O2'	1:a:1010:A:O4'	2.19	0.48
1:a:1294:G:H1'	1:a:1297:C:N4	2.28	0.48
8:h:54:GLU:C	8:h:56:LYS:H	2.17	0.48
25:A:1519:G:C5	25:A:1520:U:C4	3.01	0.48
25:A:2568:G:OP2	25:A:2568:G:N2	2.43	0.48
1:a:229:U:H2'	1:a:230:A:C8	2.46	0.48
13:m:94:GLY:O	13:m:109:ARG:HB3	2.13	0.48
15:o:29:VAL:HG13	15:o:63:ARG:HG3	1.94	0.48
25:A:150:U:H2'	25:A:151:C:H6	1.78	0.48
25:A:1096:A:H2'	25:A:1097:G:H8	1.79	0.48
25:A:1105:G:H2'	25:A:1106:G:H8	1.77	0.48
29:E:2:GLN:HB3	29:E:10:ALA:HB1	1.95	0.48
1:a:31:G:O2'	1:a:48:C:N4	2.47	0.48
1:a:187:A:O2'	20:t:59:ASP:OD2	2.28	0.48
1:a:378:G:H2'	1:a:379:C:C6	2.48	0.48
1:a:395:C:O2'	1:a:615:A:N3	2.43	0.48
1:a:998:A:H2'	1:a:999:A:C8	2.48	0.48
1:a:1020:G:H2'	1:a:1020:G:N3	2.28	0.48
3:c:76:VAL:HG23	3:c:77:ILE:HG13	1.93	0.48
7:g:115:SER:O	7:g:119:ARG:HG3	2.12	0.48
15:o:81:LEU:HD12	15:o:85:LEU:HD23	1.94	0.48
19:s:53:ASN:ND2	19:s:76:ALA:O	2.35	0.48
25:A:665:A:H4'	29:E:61:GLN:HE21	1.78	0.48
25:A:803:U:H5''	43:T:86:ARG:HH21	1.77	0.48
25:A:1781:A:H2'	25:A:1782:C:H6	1.79	0.48
25:A:1796:A:H2'	25:A:1797:A:C8	2.48	0.48
25:A:2278:U:H2'	25:A:2279:G:H8	1.78	0.48
29:E:105:ARG:NH1	29:E:199:LEU:O	2.46	0.48
1:a:707:G:H2'	1:a:708:G:H8	1.77	0.48
25:A:629:U:H2'	25:A:630:C:H6	1.77	0.48
40:Q:44:ASP:N	40:Q:44:ASP:OD1	2.46	0.48
43:T:51:LEU:O	43:T:53:VAL:N	2.46	0.48
1:a:315:A:H2'	1:a:316:C:C6	2.48	0.48
22:v:9:G:O2'	22:v:10:G:N7	2.43	0.48
25:A:1099:C:O2'	25:A:1100:G:OP1	2.25	0.48
47:X:112:ILE:HD13	47:X:148:GLU:OE2	2.14	0.48
1:a:365:A:H2'	1:a:366:C:O4'	2.14	0.48
1:a:518:G:H2'	1:a:519:C:C6	2.49	0.48
4:d:54:GLN:HB3	4:d:203:LEU:HB2	1.94	0.48
11:k:74:ALA:HB1	11:k:79:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:o:75:VAL:O	15:o:79:THR:HG23	2.13	0.48
22:v:52:G:H2'	22:v:53:G:C8	2.49	0.48
25:A:3:U:H2'	25:A:4:C:C6	2.49	0.48
25:A:567:G:O2'	25:A:1241:A:OP1	2.32	0.48
25:A:860:U:H2'	25:A:861:U:C6	2.49	0.48
25:A:2624:U:H2'	25:A:2625:G:O4'	2.14	0.48
31:G:30:LYS:HD2	31:G:30:LYS:O	2.13	0.48
1:a:1292:U:H5''	1:a:1293:A:OP1	2.14	0.48
2:b:85:ALA:O	2:b:86:ARG:HG2	2.13	0.48
9:i:24:GLY:HA3	9:i:62:ASP:HB2	1.96	0.48
18:r:32:TYR:CD1	18:r:55:LEU:HD11	2.49	0.48
19:s:30:PRO:HB3	19:s:48:THR:HG22	1.94	0.48
22:v:18:G:N1	22:v:58:A:C6	2.82	0.48
24:x:399:HIS:O	24:x:406:ARG:NH1	2.37	0.48
24:x:719:TYR:CD2	24:x:725:ILE:HG12	2.49	0.48
25:A:624:G:H2'	25:A:625:C:C6	2.49	0.48
25:A:1273:A:O2'	25:A:1275:A:OP2	2.21	0.48
25:A:1657:G:O2'	25:A:1978:U:O4	2.26	0.48
30:F:121:SER:HG	30:F:128:TYR:HE1	1.61	0.48
1:a:197:G:H1'	1:a:459:A:H61	1.78	0.48
2:b:10:LEU:HD12	2:b:15:HIS:CD2	2.49	0.48
7:g:130:GLY:HA2	7:g:135:VAL:HG11	1.96	0.48
25:A:2554:G:H2'	25:A:2555:U:C6	2.49	0.48
30:F:38:MET:HE3	30:F:40:LEU:HD11	1.96	0.48
44:U:48:LYS:O	44:U:52:GLU:HG3	2.13	0.48
1:a:1073:G:H5'	5:e:51:ARG:CZ	2.44	0.48
1:a:1243:C:O2'	9:i:75:GLN:OE1	2.23	0.48
2:b:8:ASP:OD1	2:b:9:MET:N	2.47	0.48
11:k:18:ASP:HA	11:k:81:ASN:HB2	1.96	0.48
22:v:50:U:H2'	22:v:51:C:C6	2.49	0.48
25:A:150:U:H2'	25:A:151:C:C6	2.49	0.48
25:A:2685:U:H2'	25:A:2686:C:C6	2.49	0.48
25:A:2727:A:H2'	25:A:2728:A:C8	2.48	0.48
25:A:2835:G:O2'	25:A:2854:G:N2	2.43	0.48
1:a:809:A:N7	1:a:1503:C:O2'	2.42	0.47
11:k:22:HIS:NE2	11:k:85:ASN:OD1	2.47	0.47
25:A:869:G:C5	25:A:870:G:H1'	2.49	0.47
25:A:1530:G:H2'	25:A:1531:A:C8	2.49	0.47
25:A:2391:U:H2'	25:A:2392:G:O4'	2.14	0.47
25:A:2834:U:H2'	25:A:2835:G:O4'	2.14	0.47
28:D:1:MET:HE3	28:D:207:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:230:A:H2'	1:a:231:G:C8	2.49	0.47
1:a:495:C:H2'	1:a:496:A:H8	1.79	0.47
1:a:732:C:P	6:f:91:ARG:HH11	2.37	0.47
1:a:1321:G:H2'	1:a:1322:C:C6	2.49	0.47
2:b:117:LEU:HD22	2:b:141:LEU:HD13	1.95	0.47
10:j:63:ASP:OD2	10:j:65:TYR:OH	2.32	0.47
25:A:579:U:H2'	25:A:580:A:C8	2.49	0.47
25:A:598:A:H2'	25:A:599:A:C8	2.49	0.47
25:A:1673:C:H2'	25:A:1674:A:C8	2.49	0.47
25:A:2177:G:O2'	25:A:2178:A:H5'	2.14	0.47
1:a:376:A:H2'	1:a:377:A:C8	2.50	0.47
1:a:1281:A:H2'	1:a:1282:A:C8	2.49	0.47
22:v:18:G:C2	22:v:58:A:C2	3.02	0.47
25:A:693:U:H2'	25:A:694:G:O4'	2.14	0.47
15:o:9:ALA:HA	15:o:12:VAL:HG22	1.97	0.47
25:A:2012:C:H2'	25:A:2013:U:C6	2.49	0.47
30:F:153:ASP:OD2	30:F:154:ILE:N	2.48	0.47
1:a:5:U:H4'	1:a:6:G:O5'	2.15	0.47
1:a:470:G:H2'	1:a:471:U:C6	2.48	0.47
1:a:549:U:H2'	1:a:550:C:C6	2.49	0.47
1:a:657:A:H2'	1:a:658:G:C8	2.50	0.47
1:a:699:U:C2	1:a:700:A:C8	3.02	0.47
1:a:939:G:C2	1:a:940:A:C8	3.03	0.47
1:a:970:G:O2'	1:a:1356:A:N1	2.41	0.47
4:d:7:PRO:HB2	4:d:10:LYS:HD3	1.95	0.47
24:x:462:LYS:HG2	24:x:481:PHE:CE2	2.49	0.47
25:A:27:G:O2'	25:A:28:A:O5'	2.33	0.47
25:A:963:A:H5'	25:A:1175:U:H1'	1.97	0.47
25:A:1025:U:OP1	31:G:59:GLN:NE2	2.46	0.47
25:A:1519:G:C4	25:A:1520:U:C5	3.03	0.47
25:A:2191:G:H4'	27:C:150:LYS:HD3	1.96	0.47
25:A:2718:G:H2'	25:A:2719:G:C8	2.49	0.47
24:x:543:ARG:NH1	24:x:570:GLU:OE2	2.47	0.47
24:x:780:ARG:HB2	24:x:831:PHE:HE2	1.80	0.47
25:A:1074:A:H2'	25:A:1075:A:C8	2.49	0.47
25:A:1185:U:H2'	25:A:1186:U:C6	2.50	0.47
25:A:1303:U:H2'	25:A:1304:G:H8	1.79	0.47
25:A:1520:U:H2'	25:A:1521:C:C6	2.49	0.47
27:C:180:GLU:OE2	27:C:268:ILE:HG23	2.14	0.47
1:a:198:G:C8	1:a:459:A:N1	2.83	0.47
1:a:539:C:OP1	4:d:58:LYS:NZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:646:U:O4	1:a:746:G:O2'	2.25	0.47
1:a:1175:G:O2'	1:a:1176:G:N7	2.43	0.47
1:a:1234:U:O2'	1:a:1235:G:OP1	2.32	0.47
4:d:48:LEU:HD12	4:d:52:GLY:HA3	1.97	0.47
6:f:42:TRP:CD1	6:f:45:ARG:HH11	2.33	0.47
9:i:46:MET:O	9:i:50:GLN:HG3	2.14	0.47
25:A:586:A:H2'	25:A:587:G:C8	2.49	0.47
25:A:817:U:O2'	25:A:2055:U:N3	2.48	0.47
25:A:836:U:H5	25:A:923:A:N7	2.13	0.47
25:A:899:A:N7	38:O:13:MET:HG3	2.29	0.47
25:A:2175:U:C4	25:A:2176:U:N3	2.83	0.47
25:A:2215:G:H2'	25:A:2216:U:C6	2.49	0.47
50:1:26:PHE:CE1	50:1:30:MET:HE3	2.49	0.47
52:3:26:SER:OG	52:3:27:THR:N	2.48	0.47
7:g:60:GLU:HA	7:g:63:GLU:HG3	1.96	0.47
25:A:1641:G:H5'	39:P:39:PRO:HG2	1.96	0.47
25:A:2100:U:H3'	25:A:2101:A:C8	2.50	0.47
38:O:51:ARG:HD3	38:O:66:ILE:HD11	1.97	0.47
1:a:4:C:H41	1:a:607:C:H5''	1.79	0.47
3:c:56:ASP:HB2	3:c:67:THR:OG1	2.15	0.47
4:d:88:GLU:O	4:d:92:GLN:HG2	2.15	0.47
7:g:49:LYS:NZ	7:g:118:LEU:HB2	2.29	0.47
13:m:10:PRO:HG3	13:m:21:TYR:CE2	2.50	0.47
14:n:69:ARG:NH2	14:n:81:ARG:HH21	2.13	0.47
17:q:14:ARG:NH1	17:q:61:LEU:HB2	2.29	0.47
24:x:413:THR:OG1	24:x:415:ILE:O	2.28	0.47
25:A:1276:C:H2'	25:A:1277:A:C8	2.49	0.47
25:A:2001:A:H2'	25:A:2002:A:C8	2.49	0.47
1:a:957:G:N2	10:j:57:VAL:HG11	2.29	0.47
25:A:579:U:H2'	25:A:580:A:H8	1.79	0.47
25:A:694:G:O2'	25:A:717:A:N6	2.47	0.47
25:A:1018:A:H2'	25:A:1019:A:H8	1.79	0.47
25:A:1491:U:H2'	25:A:1492:U:H6	1.79	0.47
47:X:113:ASN:HB2	47:X:116:VAL:HG22	1.97	0.47
47:X:115:GLU:HG2	47:X:116:VAL:HG13	1.97	0.47
1:a:731:A:H2'	1:a:732:C:C6	2.50	0.46
1:a:1124:A:H2'	1:a:1125:G:H8	1.79	0.46
1:a:1507:A:H2'	1:a:1508:G:C8	2.50	0.46
25:A:319:G:H2'	25:A:320:G:H8	1.80	0.46
56:7:30:HIS:ND1	56:7:31:ILE:HG13	2.30	0.46
1:a:176:C:H3'	1:a:177:G:H21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:182:G:N7	1:a:184:G:C2	2.83	0.46
1:a:467:G:H2'	1:a:468:C:O4'	2.16	0.46
2:b:131:LYS:HA	2:b:134:ALA:HB3	1.96	0.46
2:b:222:ILE:HD13	2:b:225:LYS:HE3	1.96	0.46
10:j:81:ASP:HB3	10:j:83:THR:HG23	1.97	0.46
13:m:54:ASP:OD1	13:m:54:ASP:N	2.44	0.46
25:A:247:G:O6	56:7:12:LYS:NZ	2.49	0.46
25:A:1453:U:O3'	25:A:1536:G:O2'	2.33	0.46
25:A:2096:U:O2	25:A:2168:G:C6	2.68	0.46
25:A:2128:G:H1	25:A:2137:U:H3	1.62	0.46
28:D:85:LEU:HD13	28:D:88:GLU:H	1.79	0.46
39:P:12:ARG:HB3	39:P:16:HIS:HB3	1.97	0.46
1:a:122:G:HO2'	1:a:123:A:H8	1.61	0.46
1:a:705:A:H2'	1:a:706:A:H8	1.80	0.46
1:a:712:A:C5	11:k:118:HIS:CD2	3.04	0.46
3:c:142:MET:HE2	3:c:170:GLU:OE1	2.15	0.46
4:d:170:TRP:CD1	4:d:171:VAL:HG13	2.51	0.46
22:v:18:G:C6	22:v:58:A:C6	3.03	0.46
25:A:405:C:H2'	25:A:406:A:H8	1.79	0.46
25:A:1052:G:H2'	25:A:1053:G:H8	1.81	0.46
25:A:2295:G:O2'	25:A:2297:A:OP2	2.32	0.46
1:a:1233:A:O2'	7:g:114:LYS:O	2.34	0.46
4:d:105:MET:HG2	4:d:173:VAL:HG22	1.98	0.46
24:x:448:VAL:HG23	24:x:483:PRO:HA	1.96	0.46
43:T:6:VAL:HB	43:T:37:ARG:HG2	1.98	0.46
1:a:512:C:H4'	1:a:513:C:O5'	2.15	0.46
1:a:686:U:O2'	1:a:688:A:N7	2.34	0.46
2:b:218:ALA:O	2:b:221:VAL:HG12	2.16	0.46
4:d:95:GLU:HG2	4:d:186:PRO:CG	2.44	0.46
6:f:15:SER:O	6:f:15:SER:OG	2.30	0.46
9:i:75:GLN:O	9:i:79:ILE:HG12	2.14	0.46
25:A:2524:U:H2'	25:A:2525:C:C6	2.50	0.46
25:A:2724:G:H2'	25:A:2725:A:C8	2.51	0.46
41:R:16:LYS:NZ	41:R:77:THR:O	2.40	0.46
1:a:218:U:H2'	1:a:219:C:H6	1.80	0.46
1:a:1007:G:N2	1:a:1010:A:OP2	2.36	0.46
1:a:1112:U:OP1	9:i:106:ARG:NH1	2.47	0.46
5:e:83:GLN:H	5:e:148:MET:CE	2.25	0.46
8:h:66:PHE:CD2	8:h:67:GLU:HG2	2.51	0.46
22:v:66:C:H2'	22:v:67:C:C6	2.50	0.46
24:x:779:ILE:HG23	24:x:792:GLU:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:9:G:O2'	25:A:2616:U:O4	2.29	0.46
25:A:938:C:H2'	25:A:939:G:H8	1.79	0.46
25:A:1030:A:N6	25:A:1105:G:H1	2.11	0.46
25:A:1494:C:H2'	25:A:1495:A:C8	2.51	0.46
25:A:2584:G:H2'	25:A:2585:A:C8	2.50	0.46
38:O:35:LYS:NZ	47:X:85:ALA:O	2.42	0.46
49:Z:33:LEU:HD13	49:Z:50:ARG:HG2	1.97	0.46
7:g:17:LYS:HE3	7:g:44:TYR:CZ	2.51	0.46
11:k:65:VAL:O	11:k:68:GLU:HG3	2.15	0.46
24:x:522:GLU:HG3	24:x:534:THR:HB	1.97	0.46
25:A:134:U:H2'	25:A:135:A:H8	1.81	0.46
25:A:536:U:O2	25:A:536:U:H2'	2.14	0.46
25:A:1392:U:H2'	25:A:1393:U:C6	2.51	0.46
25:A:2169:G:H2'	25:A:2170:C:C6	2.50	0.46
25:A:2292:U:C2	30:F:151:GLY:HA3	2.51	0.46
25:A:2536:G:O2'	25:A:2537:G:OP1	2.27	0.46
25:A:2687:A:H2'	25:A:2688:C:C6	2.50	0.46
1:a:179:C:H2'	1:a:180:C:C6	2.51	0.46
1:a:533:A:H2'	1:a:534:G:H8	1.81	0.46
1:a:1004:C:C4	1:a:1014:A:N6	2.84	0.46
3:c:39:VAL:HG21	3:c:95:MET:HE3	1.97	0.46
25:A:319:G:H2'	25:A:320:G:C8	2.51	0.46
25:A:871:G:C6	25:A:884:U:O2	2.69	0.46
25:A:1491:U:H2'	25:A:1492:U:C6	2.51	0.46
25:A:2237:G:OP1	38:O:85:LYS:NZ	2.41	0.46
25:A:2278:U:OP1	25:A:2367:U:O2'	2.31	0.46
25:A:2295:G:O2'	25:A:2296:A:O5'	2.34	0.46
36:M:38:ILE:HD11	36:M:111:PHE:CZ	2.50	0.46
36:M:104:ARG:HH22	41:R:35:GLU:HB2	1.81	0.46
1:a:459:A:O2'	1:a:460:A:O4'	2.32	0.46
1:a:961:5MC:H2'	1:a:962:A:C2	2.51	0.46
4:d:153:LEU:O	4:d:156:ALA:N	2.49	0.46
7:g:27:MET:HE1	7:g:40:GLU:HA	1.98	0.46
25:A:45:G:H5'	25:A:46:G:OP1	2.16	0.46
25:A:913:A:H2'	25:A:914:G:C8	2.51	0.46
27:C:200:HIS:O	27:C:203:ARG:HG2	2.15	0.46
28:D:1:MET:SD	28:D:204:ARG:NH1	2.89	0.46
42:S:9:ILE:HD12	42:S:12:ARG:HH21	1.81	0.46
52:3:12:ILE:HG21	52:3:28:LEU:HB2	1.98	0.46
1:a:198:G:H2'	1:a:199:A:C8	2.51	0.46
1:a:981:G:H2'	1:a:982:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1286:C:H2'	1:a:1287:G:H8	1.80	0.46
1:a:1303:G:P	13:m:87:ARG:HH21	2.39	0.46
3:c:73:PRO:HG3	3:c:105:GLU:HG3	1.97	0.46
6:f:38:ARG:HH21	6:f:63:ASN:HD21	1.64	0.46
11:k:89:PRO:HB3	21:u:32:VAL:HG11	1.97	0.46
13:m:90:ARG:NH2	13:m:96:PRO:O	2.44	0.46
25:A:2127:G:C6	25:A:2139:G:C6	3.04	0.46
25:A:2301:G:H2'	25:A:2302:G:H8	1.81	0.46
28:D:116:LYS:HG3	39:P:1:MET:SD	2.56	0.46
39:P:12:ARG:HE	39:P:16:HIS:CE1	2.33	0.46
47:X:126:GLU:OE1	47:X:126:GLU:N	2.49	0.46
1:a:205:G:C6	1:a:206:G:H1'	2.51	0.45
1:a:1017:G:O6	1:a:1018:G:O6	2.34	0.45
9:i:96:SER:O	9:i:100:LYS:HG2	2.16	0.45
12:l:14:ARG:HE	12:l:15:MET:N	2.14	0.45
18:r:63:ARG:HD3	18:r:70:TYR:HA	1.98	0.45
24:x:487:LYS:HD2	24:x:488:LEU:HD22	1.98	0.45
24:x:695:PHE:HE1	24:x:717:ARG:HD3	1.79	0.45
24:x:776:ASN:O	24:x:777:ARG:NH1	2.45	0.45
25:A:880:G:H2'	25:A:881:A:H4'	1.97	0.45
27:C:199:GLU:CD	27:C:199:GLU:H	2.23	0.45
1:a:862:C:H2'	1:a:863:G:O4'	2.16	0.45
2:b:101:LEU:HB3	2:b:179:LEU:HD12	1.98	0.45
4:d:176:ASP:N	4:d:176:ASP:OD1	2.46	0.45
9:i:98:LEU:O	9:i:102:GLY:N	2.48	0.45
9:i:98:LEU:HD12	9:i:103:TYR:HB2	1.98	0.45
13:m:76:ASN:O	13:m:80:LEU:HG	2.16	0.45
24:x:648:VAL:HG12	24:x:650:GLY:H	1.80	0.45
25:A:291:G:H2'	25:A:292:G:O4'	2.15	0.45
25:A:652:G:H5'	37:N:16:LYS:HB3	1.97	0.45
25:A:694:G:H2'	25:A:716:G:H22	1.81	0.45
25:A:1915:A:H2'	25:A:1916:G:O4'	2.16	0.45
45:V:75:LYS:HE2	45:V:75:LYS:HB2	1.80	0.45
25:A:512:U:H2'	25:A:513:G:C8	2.51	0.45
25:A:657:U:H2'	25:A:658:A:O4'	2.17	0.45
25:A:2000:A:O2'	44:U:94:ASP:OD1	2.23	0.45
25:A:2067:G:H5'	49:Z:19:SER:HB2	1.98	0.45
27:C:63:ARG:HD3	27:C:84:ASP:OD1	2.16	0.45
53:4:51:ARG:HH21	53:4:53:VAL:HG12	1.82	0.45
1:a:86:C:H2'	1:a:87:C:C6	2.52	0.45
2:b:97:LEU:O	2:b:100:MET:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:47:VAL:HA	9:i:50:GLN:HG3	1.98	0.45
13:m:23:TYR:CE1	13:m:69:LEU:HD23	2.51	0.45
14:n:62:ASN:OD1	14:n:62:ASN:N	2.50	0.45
25:A:160:A:N3	25:A:2195:C:O2'	2.43	0.45
25:A:470:A:N3	25:A:472:G:H5''	2.32	0.45
25:A:626:G:H5''	37:N:128:THR:HB	1.98	0.45
25:A:920:C:N4	25:A:1170:C:OP2	2.33	0.45
25:A:1561:A:H2'	25:A:1562:A:C8	2.51	0.45
25:A:2578:C:H2'	25:A:2579:G:H8	1.82	0.45
30:F:134:GLU:HB3	30:F:137:ILE:HD11	1.98	0.45
31:G:39:PRO:HG2	31:G:42:GLU:OE1	2.17	0.45
1:a:732:C:OP1	6:f:91:ARG:NH1	2.50	0.45
1:a:971:A:H1'	1:a:976:U:O4	2.16	0.45
1:a:1037:C:H2'	1:a:1038:A:C8	2.51	0.45
5:e:132:THR:HG22	5:e:132:THR:O	2.17	0.45
25:A:1357:C:H2'	25:A:1358:G:O4'	2.16	0.45
25:A:2789:U:H2'	25:A:2790:C:H6	1.82	0.45
40:Q:27:LEU:HD23	40:Q:91:PHE:HD1	1.81	0.45
1:a:1310:G:OP1	14:n:28:LYS:NZ	2.49	0.45
19:s:50:ALA:HB1	19:s:57:HIS:HB3	1.99	0.45
27:C:211:THR:HG22	27:C:216:VAL:HB	1.99	0.45
27:C:235:GLY:HA3	27:C:239:THR:HG21	1.97	0.45
30:F:58:GLU:OE1	30:F:64:LYS:HA	2.16	0.45
36:M:17:ARG:CZ	36:M:47:ILE:HD11	2.46	0.45
1:a:218:U:H2'	1:a:219:C:C6	2.52	0.45
1:a:587:G:H2'	1:a:588:C:H6	1.82	0.45
1:a:772:G:O5'	1:a:772:G:H8	1.98	0.45
1:a:1245:A:H2'	1:a:1246:A:C8	2.52	0.45
4:d:164:GLN:O	4:d:164:GLN:HG2	2.17	0.45
6:f:34:GLY:HA3	6:f:65:GLU:O	2.16	0.45
6:f:42:TRP:CZ3	6:f:61:LEU:HD23	2.52	0.45
7:g:26:PHE:HE2	7:g:120:LEU:HD11	1.81	0.45
17:q:26:VAL:HG11	17:q:64:ILE:HD13	1.99	0.45
25:A:27:G:H22	25:A:503:G:C2'	2.29	0.45
25:A:295:C:O5'	46:W:81:ARG:NH2	2.50	0.45
25:A:558:U:H1'	25:A:2017:6MZ:H9C1	1.97	0.45
25:A:2228:A:H2'	25:A:2229:G:H8	1.78	0.45
34:J:86:ILE:HG22	34:J:88:SER:H	1.81	0.45
47:X:142:ASP:OD2	47:X:142:ASP:N	2.50	0.45
1:a:79:G:H2'	1:a:80:C:C6	2.52	0.45
1:a:893:C:H2'	1:a:894:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1510:2MG:N2	1:a:1513:MA6:OP2	2.46	0.45
5:e:77:LEU:HD13	5:e:80:THR:H	1.82	0.45
6:f:9:LEU:HD22	6:f:59:TYR:CZ	2.52	0.45
14:n:36:SER:O	14:n:37:SER:OG	2.34	0.45
24:x:350:HIS:CG	24:x:351:VAL:H	2.35	0.45
25:A:1430:C:H2'	25:A:1431:A:C8	2.51	0.45
28:D:2:THR:HB	28:D:85:LEU:HA	1.99	0.45
28:D:10:CYS:SG	41:R:5:ILE:HD11	2.56	0.45
44:U:73:THR:HB	44:U:106:LYS:HD2	1.99	0.45
1:a:687:G:HO2'	1:a:688:A:P	2.38	0.45
1:a:1244:A:H2'	1:a:1245:A:C8	2.52	0.45
25:A:586:A:H2'	25:A:587:G:H8	1.81	0.45
25:A:792:A:O2'	25:A:793:U:OP1	2.32	0.45
25:A:872:G:H3'	25:A:873:U:H6	1.82	0.45
25:A:2087:G:N1	25:A:2177:G:N7	2.65	0.45
25:A:2108:G:O6	25:A:2165:C:N4	2.50	0.45
26:B:41:C:N4	30:F:69:TYR:OH	2.50	0.45
30:F:8:TYR:OH	30:F:29:PRO:O	2.35	0.45
50:1:18:LEU:HB2	50:1:53:VAL:HG11	1.99	0.45
1:a:483:C:H2'	1:a:484:A:C8	2.50	0.44
1:a:742:U:H2'	1:a:743:A:C8	2.52	0.44
1:a:1300:A:N6	1:a:1325:G:O2'	2.49	0.44
2:b:89:MET:HE2	2:b:89:MET:H	1.81	0.44
2:b:169:GLU:OE1	2:b:169:GLU:N	2.50	0.44
18:r:50:LYS:O	18:r:54:GLN:HG2	2.17	0.44
25:A:937:A:H2'	25:A:938:C:C6	2.52	0.44
25:A:1303:U:H2'	25:A:1304:G:C8	2.52	0.44
25:A:2051:C:H2'	25:A:2052:C:H6	1.81	0.44
26:B:49:C:H2'	26:B:50:A:C8	2.51	0.44
27:C:116:LEU:HD22	27:C:127:GLY:HA3	1.98	0.44
36:M:64:ARG:HG2	36:M:79:PHE:CG	2.51	0.44
36:M:88:ASN:HD21	36:M:92:GLU:HB2	1.80	0.44
2:b:90:PRO:CG	2:b:154:MET:HG2	2.47	0.44
24:x:345:VAL:HG12	24:x:415:ILE:HB	1.98	0.44
25:A:938:C:H1'	25:A:974:A:C8	2.52	0.44
25:A:1075:A:H4'	25:A:1094:C:O2'	2.16	0.44
3:c:72:ARG:HG2	3:c:75:ILE:HG22	1.98	0.44
6:f:86:ARG:NH1	18:r:64:TYR:O	2.50	0.44
7:g:49:LYS:HZ2	7:g:118:LEU:HB2	1.82	0.44
7:g:77:SER:HA	7:g:86:GLN:HA	2.00	0.44
10:j:6:ILE:HG22	10:j:103:GLY:HA2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:v:23:C:H2'	22:v:24:U:H6	1.83	0.44
25:A:860:U:H2'	25:A:861:U:H6	1.81	0.44
25:A:1075:A:H2'	25:A:1076:A:C4	2.52	0.44
25:A:1393:U:H2'	25:A:1394:C:C6	2.52	0.44
25:A:1471:A:H2'	25:A:1472:A:C8	2.52	0.44
25:A:2025:G:H2'	25:A:2026:U:O4'	2.17	0.44
25:A:2294:G:H5''	25:A:2295:G:OP2	2.18	0.44
1:a:240:A:C2	1:a:276:A:C5	3.06	0.44
1:a:976:U:H4'	1:a:977:A:O5'	2.17	0.44
1:a:1239:G:C6	1:a:1240:G:C6	3.05	0.44
3:c:89:GLN:O	3:c:93:LYS:HG2	2.17	0.44
7:g:116:MET:HA	7:g:119:ARG:HB2	1.99	0.44
11:k:87:LYS:HG3	11:k:114:THR:HA	1.99	0.44
24:x:644:LEU:HD21	24:x:655:LEU:HB3	1.99	0.44
25:A:899:A:H2'	25:A:900:A:C8	2.53	0.44
25:A:1517:U:H2'	25:A:1518:C:C6	2.53	0.44
25:A:2179:G:H2'	25:A:2180:G:H8	1.82	0.44
28:D:123:LYS:HG2	28:D:165:LEU:HD11	1.98	0.44
1:a:34:C:H2'	1:a:35:G:H8	1.82	0.44
1:a:495:C:H2'	1:a:496:A:C8	2.52	0.44
1:a:1282:A:H2'	1:a:1283:A:H8	1.81	0.44
1:a:1309:U:H2'	1:a:1310:G:O4'	2.17	0.44
1:a:1340:A:OP1	9:i:122:ARG:NH1	2.44	0.44
1:a:1395:G:H2'	1:a:1396:4OC:O4'	2.18	0.44
3:c:43:LEU:HD23	3:c:55:ILE:HD13	1.99	0.44
11:k:87:LYS:HD2	11:k:115:PRO:HD3	1.98	0.44
14:n:43:ASN:OD1	14:n:44:ALA:N	2.51	0.44
14:n:80:SER:OG	14:n:81:ARG:N	2.50	0.44
24:x:739:SER:HB3	24:x:838:ARG:NE	2.32	0.44
25:A:584:U:H2'	25:A:585:C:C6	2.52	0.44
25:A:1497:G:HO2'	25:A:1498:G:P	2.40	0.44
25:A:2534:A:H2'	25:A:2535:U:C6	2.53	0.44
25:A:2862:C:H4'	41:R:3:ASN:HB3	2.00	0.44
45:V:47:GLU:HG3	45:V:54:VAL:HG12	1.99	0.44
1:a:35:G:H2'	1:a:36:C:C6	2.53	0.44
1:a:401:U:H5''	4:d:112:SER:HB3	1.98	0.44
1:a:1114:C:H2'	1:a:1115:U:H6	1.83	0.44
2:b:208:ARG:O	2:b:212:LEU:HG	2.17	0.44
4:d:101:VAL:HG21	4:d:137:VAL:HG21	1.99	0.44
6:f:2:ARG:HD2	6:f:91:ARG:CZ	2.47	0.44
14:n:36:SER:H	14:n:41:ARG:NH1	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:p:43:ALA:O	16:p:44:THR:OG1	2.27	0.44
24:x:430:THR:O	24:x:434:VAL:HG13	2.18	0.44
25:A:731:U:H2'	25:A:732:C:C6	2.53	0.44
25:A:916:A:C2	51:2:42:GLU:HB3	2.52	0.44
28:D:78:ARG:O	28:D:78:ARG:HG3	2.16	0.44
37:N:56:PRO:O	37:N:60:ARG:HB2	2.16	0.44
1:a:337:U:O2'	1:a:340:G:O6	2.22	0.44
1:a:587:G:H2'	1:a:588:C:C6	2.53	0.44
2:b:53:ALA:O	2:b:57:VAL:HG12	2.18	0.44
2:b:163:VAL:HG12	2:b:165:ASP:H	1.83	0.44
24:x:418:LEU:HB3	24:x:446:VAL:HG12	1.98	0.44
25:A:801:U:H2'	37:N:21:ARG:HA	2.00	0.44
25:A:1016:U:HO2'	25:A:1017:A:P	2.40	0.44
25:A:2119:U:C5	25:A:2121:A:H4'	2.52	0.44
25:A:2220:U:H2'	25:A:2221:G:C8	2.53	0.44
25:A:2465:A:OP1	57:8:32:ARG:NH2	2.47	0.44
27:C:21:ASN:HB3	27:C:24:LEU:HG	2.00	0.44
29:E:1:MET:HG3	29:E:13:VAL:HG23	2.00	0.44
1:a:512:C:H5''	1:a:513:C:C6	2.52	0.44
1:a:699:U:N3	1:a:700:A:C8	2.86	0.44
1:a:905:U:H2'	1:a:906:C:C6	2.53	0.44
1:a:1441:A:OP1	1:a:1442:C:N4	2.38	0.44
6:f:4:TYR:CE2	6:f:91:ARG:HB2	2.53	0.44
14:n:7:LYS:O	14:n:10:GLU:HG3	2.18	0.44
19:s:27:ASP:OD1	19:s:27:ASP:N	2.51	0.44
24:x:517:ARG:HB3	24:x:539:ASP:OD1	2.18	0.44
25:A:61:G:H2'	25:A:62:U:C6	2.53	0.44
25:A:198:C:H2'	25:A:199:A:H5''	2.00	0.44
25:A:272:A:H2'	25:A:273:A:H8	1.81	0.44
25:A:664:G:O2'	29:E:68:ARG:HD2	2.17	0.44
25:A:744:G:H2'	25:A:745:U:C6	2.53	0.44
1:a:3:A:H5''	1:a:4:C:H6	1.81	0.44
3:c:114:MET:HE2	3:c:185:ALA:HB1	2.00	0.44
6:f:1:MET:SD	6:f:2:ARG:N	2.91	0.44
7:g:39:ALA:O	7:g:43:VAL:HG12	2.18	0.44
8:h:25:VAL:O	8:h:60:SER:HA	2.18	0.44
13:m:66:GLU:HA	13:m:70:ARG:NH1	2.30	0.44
16:p:50:LEU:HD22	16:p:74:LEU:HD22	1.98	0.44
21:u:21:ARG:O	21:u:25:LYS:HG2	2.18	0.44
24:x:350:HIS:HA	24:x:429:GLN:HB2	2.00	0.44
24:x:564:ASN:OD1	24:x:566:LYS:HE3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1615:C:H2'	25:A:1616:G:O4'	2.17	0.44
25:A:1840:A:H2'	25:A:1841:A:C8	2.52	0.44
25:A:2674:U:H2'	25:A:2675:G:O4'	2.17	0.44
1:a:1023:U:H2'	1:a:1025:C:C4	2.53	0.43
5:e:115:VAL:HG13	5:e:142:PHE:CE1	2.53	0.43
10:j:14:ASP:OD1	10:j:14:ASP:N	2.50	0.43
24:x:683:ASP:OD1	24:x:684:ALA:N	2.51	0.43
25:A:713:C:H2'	25:A:714:U:O4'	2.18	0.43
25:A:871:G:H1	25:A:884:U:H1'	1.82	0.43
25:A:2126:U:O3'	25:A:2127:G:H8	2.01	0.43
52:3:13:GLU:HB2	52:3:31:PRO:HB3	2.00	0.43
2:b:89:MET:HA	2:b:90:PRO:HD3	1.85	0.43
4:d:116:GLN:HG2	4:d:154:ARG:HH12	1.84	0.43
22:v:44:A:H2'	22:v:45:G:O4'	2.17	0.43
22:v:54:5MU:O4	22:v:58:A:N7	2.51	0.43
25:A:694:G:H1'	25:A:717:A:N6	2.32	0.43
25:A:2170:C:N4	25:A:2171:A:H62	2.15	0.43
25:A:2351:C:H2'	25:A:2352:G:O4'	2.19	0.43
26:B:37:C:N4	26:B:49:C:H1'	2.34	0.43
26:B:48:U:H2'	26:B:49:C:C6	2.52	0.43
28:D:105:GLN:O	28:D:107:VAL:HG13	2.17	0.43
30:F:6:GLU:O	30:F:10:LYS:HG2	2.16	0.43
40:Q:41:ILE:HG21	40:Q:45:GLY:HA2	1.99	0.43
1:a:230:A:H2'	1:a:231:G:H8	1.84	0.43
1:a:700:A:C5	1:a:701:U:C6	3.06	0.43
1:a:1112:U:H2'	1:a:1113:C:H6	1.83	0.43
1:a:1341:G:OP2	9:i:109:ARG:HG2	2.18	0.43
5:e:78:ASN:HB2	5:e:83:GLN:OE1	2.18	0.43
6:f:90:MET:O	6:f:91:ARG:C	2.61	0.43
22:v:18:G:N3	22:v:58:A:C2	2.86	0.43
25:A:719:G:H5'	25:A:720:A:H5''	2.00	0.43
25:A:1052:G:H2'	25:A:1053:G:C8	2.53	0.43
36:M:12:ASP:OD2	36:M:85:VAL:HG13	2.18	0.43
50:1:10:SER:OG	50:1:12:GLU:OE1	2.33	0.43
1:a:424:A:OP1	4:d:9:CYS:HB3	2.17	0.43
1:a:708:G:H2'	1:a:709:A:H8	1.81	0.43
1:a:948:G:H2'	1:a:949:U:C6	2.54	0.43
1:a:1195:A:H1'	1:a:1196:U:OP2	2.19	0.43
2:b:56:PHE:CG	2:b:198:TYR:HE2	2.36	0.43
7:g:106:ASP:HA	7:g:109:ARG:HD2	2.01	0.43
25:A:299:C:H2'	25:A:300:U:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:350:G:H2'	25:A:351:A:C8	2.53	0.43
25:A:2447:U:C2	25:A:2448:A:C8	3.07	0.43
30:F:78:LYS:O	30:F:78:LYS:HG3	2.17	0.43
39:P:114:GLU:OE1	39:P:118:ARG:NH2	2.51	0.43
8:h:96:ARG:HG3	8:h:130:PHE:CG	2.52	0.43
9:i:28:ILE:HD13	9:i:63:ILE:HB	2.00	0.43
10:j:52:LEU:HD23	10:j:62:ARG:HE	1.84	0.43
13:m:59:GLU:HA	13:m:62:LYS:HE2	2.00	0.43
24:x:462:LYS:HG2	24:x:481:PHE:HE2	1.83	0.43
24:x:739:SER:HB3	24:x:838:ARG:CZ	2.48	0.43
25:A:141:A:OP1	45:V:44:LYS:NZ	2.34	0.43
25:A:1643:G:OP1	25:A:2809:G:N2	2.41	0.43
25:A:1795:A:H3'	25:A:1796:A:C8	2.54	0.43
25:A:2415:G:N2	37:N:54:GLN:HE21	2.17	0.43
26:B:55:U:H2'	26:B:56:G:H8	1.84	0.43
1:a:264:A:H2'	1:a:265:C:H6	1.84	0.43
1:a:718:G:OP2	1:a:848:U:O2'	2.36	0.43
1:a:1322:C:OP1	13:m:28:THR:HG21	2.19	0.43
7:g:147:ALA:C	7:g:148:ASN:HD22	2.26	0.43
11:k:34:ILE:HD13	11:k:74:ALA:HB2	2.00	0.43
13:m:65:THR:OG1	13:m:66:GLU:OE1	2.18	0.43
25:A:694:G:H2'	25:A:716:G:N2	2.33	0.43
25:A:1331:U:O2	25:A:1372:A:H5''	2.18	0.43
25:A:2536:G:H2'	25:A:2537:G:C8	2.54	0.43
30:F:60:ILE:HG13	30:F:61:THR:HG23	2.00	0.43
36:M:53:LYS:HB3	36:M:53:LYS:HE2	1.82	0.43
47:X:75:VAL:HG11	47:X:94:PHE:HB3	2.00	0.43
47:X:131:ILE:HD11	47:X:184:VAL:HG22	2.01	0.43
1:a:456:G:O2'	1:a:457:U:H6	2.01	0.43
9:i:19:VAL:HA	9:i:65:VAL:HG12	2.00	0.43
15:o:33:SER:O	15:o:37:ASN:ND2	2.52	0.43
15:o:40:GLN:O	15:o:44:LYS:HG2	2.19	0.43
18:r:73:SER:OG	18:r:74:HIS:N	2.50	0.43
25:A:1074:A:O2'	25:A:1075:A:H5'	2.19	0.43
25:A:1419:G:O2'	25:A:1420:A:H5'	2.18	0.43
25:A:2851:G:H2'	25:A:2852:U:C6	2.54	0.43
28:D:15:ILE:HD11	28:D:178:VAL:HG11	1.99	0.43
36:M:16:ALA:HB2	36:M:52:VAL:HG21	2.01	0.43
42:S:87:ALA:CB	43:T:52:PRO:HD3	2.46	0.43
1:a:94:C:O2'	1:a:95:A:N7	2.51	0.43
1:a:406:A:N3	1:a:406:A:H2'	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:452:G:H2'	1:a:453:U:C6	2.54	0.43
1:a:914:U:H2'	1:a:915:U:C6	2.54	0.43
3:c:22:TRP:HB3	3:c:59:ARG:HB2	2.00	0.43
5:e:135:VAL:HG22	5:e:139:TYR:CE2	2.54	0.43
6:f:84:VAL:O	6:f:86:ARG:N	2.42	0.43
6:f:86:ARG:HD3	6:f:86:ARG:HA	1.74	0.43
13:m:14:HIS:CD2	13:m:42:ALA:HA	2.54	0.43
25:A:156:A:H2'	25:A:157:C:C6	2.54	0.43
25:A:665:A:N3	25:A:2430:C:O2'	2.48	0.43
43:T:7:THR:HG23	43:T:22:VAL:HG21	2.00	0.43
47:X:39:GLU:CD	47:X:40:PRO:HD2	2.44	0.43
1:a:61:G:N7	20:t:6:SER:OG	2.50	0.43
1:a:667:G:H2'	1:a:668:G:C8	2.53	0.43
1:a:815:G:H2'	1:a:816:U:C6	2.53	0.43
1:a:1255:A:N6	1:a:1268:G:H1'	2.34	0.43
1:a:1312:A:H5''	19:s:3:ARG:NH1	2.34	0.43
1:a:1315:U:O2	19:s:36:ARG:NH1	2.52	0.43
2:b:179:LEU:HD23	2:b:179:LEU:HA	1.85	0.43
3:c:164:ARG:NE	3:c:166:GLU:OE1	2.44	0.43
8:h:5:ASP:CG	8:h:77:ARG:HH12	2.27	0.43
18:r:36:THR:HG23	18:r:38:LYS:HG3	2.01	0.43
19:s:20:GLU:O	19:s:23:VAL:HG22	2.19	0.43
20:t:24:LEU:HD22	20:t:61:MET:HE1	2.00	0.43
24:x:350:HIS:HB3	24:x:353:HIS:CD2	2.53	0.43
25:A:1483:A:H2'	25:A:1485:C:C5	2.54	0.43
25:A:1535:A:H2'	25:A:1536:G:O4'	2.19	0.43
25:A:2687:A:H2'	25:A:2688:C:H6	1.82	0.43
26:B:33:G:O6	26:B:50:A:N6	2.52	0.43
39:P:87:TYR:OH	39:P:115:LEU:HB3	2.19	0.43
52:3:42:PRO:HA	52:3:47:LYS:HZ3	1.83	0.43
1:a:154:A:N6	1:a:340:G:N7	2.66	0.43
1:a:979:C:H2'	1:a:980:U:C6	2.54	0.43
3:c:52:VAL:HG23	3:c:68:ILE:HG23	2.01	0.43
9:i:41:ARG:H	9:i:45:ARG:NH2	2.17	0.43
9:i:48:VAL:O	9:i:51:PRO:HD2	2.19	0.43
11:k:29:ASN:OD1	11:k:30:THR:N	2.51	0.43
25:A:1:G:H2'	25:A:2:G:C8	2.53	0.43
25:A:580:A:H2'	25:A:581:U:C6	2.54	0.43
25:A:853:G:H2'	25:A:854:C:C6	2.53	0.43
25:A:2095:U:H2'	25:A:2096:U:H5'	2.01	0.43
25:A:2636:C:H2'	25:A:2637:U:H6	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:D:184:ARG:NH1	41:R:8:GLN:HG2	2.34	0.43
40:Q:76:LEU:HG	40:Q:80:ARG:HE	1.84	0.43
1:a:198:G:H2'	1:a:199:A:H8	1.83	0.42
1:a:576:U:H2'	1:a:577:A:C8	2.53	0.42
1:a:712:A:N7	11:k:118:HIS:HD2	2.17	0.42
1:a:898:U:H2'	1:a:899:U:C6	2.53	0.42
1:a:1005:C:H2'	1:a:1006:A:H8	1.84	0.42
20:t:24:LEU:HD22	20:t:61:MET:CE	2.49	0.42
25:A:1519:G:H2'	25:A:1520:U:C5	2.51	0.42
25:A:2153:U:H2'	25:A:2154:U:O4'	2.19	0.42
25:A:2154:U:C2	25:A:2158:A:N6	2.86	0.42
27:C:273:LYS:HA	27:C:273:LYS:HD3	1.85	0.42
30:F:132:VAL:HG12	30:F:134:GLU:H	1.84	0.42
1:a:418:G:H2'	1:a:419:A:C8	2.54	0.42
1:a:469:U:H2'	1:a:470:G:H8	1.84	0.42
1:a:668:G:H2'	1:a:669:A:C8	2.54	0.42
1:a:1281:A:C2	1:a:1347:G:H1'	2.52	0.42
1:a:1322:C:C2	1:a:1323:G:C8	3.07	0.42
1:a:1457:U:H2'	1:a:1458:U:C6	2.54	0.42
15:o:79:THR:HA	15:o:82:ILE:HG22	2.01	0.42
25:A:373:G:H2'	25:A:374:C:O4'	2.19	0.42
25:A:2485:OMC:HM22	25:A:2486:C:H5'	2.01	0.42
30:F:118:ASN:OD1	30:F:118:ASN:N	2.52	0.42
1:a:315:A:H2'	1:a:316:C:H6	1.83	0.42
1:a:465:U:H2'	1:a:466:U:C6	2.53	0.42
1:a:963:A:O2'	1:a:964:C:OP1	2.37	0.42
1:a:1128:C:H2'	1:a:1129:C:O4'	2.19	0.42
2:b:125:THR:O	2:b:128:LYS:HG3	2.20	0.42
25:A:750:G:H2'	25:A:751:A:O4'	2.18	0.42
25:A:1424:C:H2'	25:A:1425:U:H6	1.84	0.42
29:E:72:ILE:HG13	29:E:73:ARG:HG2	2.01	0.42
36:M:1:MET:HB2	36:M:32:TYR:HB3	2.02	0.42
1:a:191:A:H4'	1:a:192:G:H5'	2.01	0.42
1:a:197:G:O2'	1:a:198:G:H8	2.03	0.42
1:a:378:G:H2'	1:a:379:C:H6	1.84	0.42
1:a:698:A:C5	1:a:699:U:C5	3.06	0.42
1:a:1423:C:H4'	25:A:1693:G:O2'	2.20	0.42
2:b:219:GLU:HA	2:b:222:ILE:HB	2.01	0.42
3:c:153:VAL:HG12	3:c:157:LEU:HD21	2.02	0.42
4:d:170:TRP:CE2	4:d:186:PRO:HG3	2.55	0.42
6:f:51:ILE:HG22	6:f:85:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:25:LYS:HG3	7:g:29:HIS:CE1	2.54	0.42
7:g:113:GLU:OE2	7:g:118:LEU:HG	2.19	0.42
25:A:359:U:O2	25:A:359:U:H2'	2.19	0.42
25:A:1018:A:N6	25:A:1115:G:H2'	2.34	0.42
25:A:1268:G:H2'	25:A:1269:U:C6	2.53	0.42
25:A:1527:G:H2'	25:A:1528:A:C8	2.53	0.42
25:A:1673:C:H2'	25:A:1674:A:H8	1.83	0.42
25:A:1679:A:H2'	25:A:1680:A:C8	2.55	0.42
47:X:75:VAL:CG1	47:X:94:PHE:HB3	2.49	0.42
1:a:402:G:H2'	1:a:403:U:C6	2.54	0.42
1:a:412:U:H2'	1:a:413:C:C6	2.54	0.42
1:a:484:A:H2'	1:a:485:A:H8	1.83	0.42
1:a:678:U:H1'	11:k:40:ASN:HB3	2.02	0.42
2:b:102:THR:HG23	2:b:175:GLU:HB2	2.01	0.42
7:g:136:LYS:O	7:g:139:GLU:HG3	2.19	0.42
25:A:1761:C:O2	25:A:1761:C:H2'	2.18	0.42
29:E:51:VAL:HG12	29:E:73:ARG:HD3	2.01	0.42
35:L:69:THR:HG22	35:L:90:GLU:HG3	2.01	0.42
39:P:32:GLU:HB3	39:P:118:ARG:HD3	2.00	0.42
1:a:375:A:O2'	1:a:376:A:C8	2.70	0.42
1:a:586:A:H2'	1:a:587:G:C8	2.54	0.42
1:a:665:G:H2'	1:a:666:U:C6	2.55	0.42
1:a:673:U:H2'	1:a:674:C:H6	1.84	0.42
1:a:795:U:H2'	1:a:796:A:H8	1.84	0.42
1:a:1153:U:O4'	1:a:1176:G:N2	2.53	0.42
22:v:23:C:H2'	22:v:24:U:C6	2.55	0.42
25:A:28:A:H61	25:A:503:G:H1'	1.85	0.42
25:A:872:G:N2	25:A:883:U:O2	2.49	0.42
25:A:2034:C:H2'	25:A:2035:G:H8	1.84	0.42
25:A:2096:U:C2	25:A:2168:G:O6	2.73	0.42
25:A:2364:A:H2'	25:A:2365:A:C8	2.54	0.42
25:A:2524:U:H2'	25:A:2525:C:H6	1.84	0.42
32:H:5:LEU:HD11	32:H:9:VAL:HG12	2.01	0.42
1:a:1141:C:H2'	1:a:1142:U:C6	2.54	0.42
7:g:24:ALA:O	7:g:27:MET:HB2	2.20	0.42
13:m:5:ALA:HB1	13:m:9:ILE:HG22	2.00	0.42
22:v:18:G:N2	22:v:58:A:C4	2.88	0.42
25:A:37:C:H2'	25:A:38:A:C8	2.54	0.42
25:A:2119:U:O4	25:A:2121:A:O2'	2.37	0.42
27:C:133:ARG:HB3	27:C:186:ALA:HB1	2.01	0.42
45:V:43:LYS:HE2	45:V:54:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:8:30:GLU:OE2	57:8:32:ARG:HD3	2.20	0.42
1:a:266:C:C2	1:a:267:A:C8	3.08	0.42
1:a:494:G:H2'	1:a:495:C:C6	2.55	0.42
2:b:153:ASP:O	2:b:154:MET:HG3	2.20	0.42
5:e:16:LEU:HD12	5:e:38:THR:HG22	2.02	0.42
6:f:38:ARG:NH2	6:f:63:ASN:HD21	2.17	0.42
17:q:15:VAL:HG12	17:q:58:ILE:HA	2.01	0.42
25:A:155:U:H2'	25:A:156:A:H8	1.84	0.42
25:A:917:G:H2'	25:A:918:U:C6	2.55	0.42
25:A:1395:U:H2'	25:A:1396:G:H8	1.85	0.42
25:A:2130:C:H2'	25:A:2131:G:O4'	2.18	0.42
25:A:2182:U:H2'	25:A:2183:C:H6	1.85	0.42
25:A:2230:U:H2'	25:A:2231:U:H6	1.85	0.42
26:B:20:G:H2'	26:B:21:U:C6	2.54	0.42
30:F:65:PRO:HB3	30:F:89:VAL:HG23	2.02	0.42
1:a:162:G:H2'	1:a:163:C:C6	2.55	0.42
1:a:191:A:N1	1:a:214:G:O2'	2.52	0.42
1:a:773:C:H2'	1:a:774:A:O4'	2.20	0.42
1:a:916:G:H2'	1:a:917:A:H8	1.82	0.42
1:a:1011:U:H2'	1:a:1012:G:H8	1.85	0.42
1:a:1032:U:H2'	1:a:1033:C:C6	2.54	0.42
10:j:85:ASP:O	10:j:88:MET:HE1	2.20	0.42
13:m:22:ILE:HG22	13:m:25:VAL:HG12	2.02	0.42
16:p:42:VAL:O	16:p:44:THR:HG23	2.19	0.42
25:A:1926:5MU:OP1	25:A:2591:U:O2'	2.37	0.42
25:A:2171:A:H2'	25:A:2172:U:C6	2.54	0.42
25:A:2332:G:N3	25:A:2368:A:H2'	2.35	0.42
30:F:54:VAL:HG23	30:F:65:PRO:HG2	2.02	0.42
34:J:98:VAL:N	34:J:137:GLY:O	2.51	0.42
37:N:122:LEU:HD22	37:N:142:PHE:CE2	2.55	0.42
55:6:35:ARG:HG3	55:6:42:LEU:HD11	2.01	0.42
1:a:216:U:H2'	1:a:217:A:H8	1.84	0.42
1:a:701:U:H4'	11:k:22:HIS:ND1	2.35	0.42
1:a:1115:U:H2'	1:a:1116:U:C6	2.55	0.42
1:a:1314:C:H42	19:s:36:ARG:HB2	1.84	0.42
2:b:74:ARG:HE	2:b:75:SER:H	1.67	0.42
5:e:42:ASP:OD1	5:e:42:ASP:N	2.48	0.42
7:g:150:ALA:HB1	11:k:59:THR:HG21	2.02	0.42
8:h:18:GLN:OE1	8:h:72:ILE:HB	2.20	0.42
8:h:106:THR:HG22	8:h:122:GLY:O	2.20	0.42
11:k:58:SER:O	11:k:91:PRO:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:u:24:GLU:OE2	21:u:25:LYS:HE3	2.20	0.42
24:x:475:TRP:N	24:x:475:TRP:CD1	2.88	0.42
25:A:181:A:C2	25:A:426:A:C8	3.08	0.42
25:A:512:U:H2'	25:A:513:G:H8	1.85	0.42
25:A:1251:G:OP1	53:4:16:ARG:NH2	2.33	0.42
25:A:1404:C:O2'	25:A:1577:G:O2'	2.37	0.42
25:A:1495:A:H4'	25:A:1496:A:H5'	2.01	0.42
25:A:1519:G:C6	25:A:1520:U:C4	3.08	0.42
27:C:164:LEU:HD11	27:C:172:VAL:CG2	2.50	0.42
35:L:13:ARG:HD3	35:L:51:GLY:O	2.20	0.42
40:Q:56:ASP:OD1	40:Q:56:ASP:N	2.53	0.42
1:a:208:C:C2	1:a:209:C:C5	3.08	0.41
1:a:216:U:H2'	1:a:217:A:C8	2.55	0.41
1:a:678:U:C4	1:a:679:G:C6	3.08	0.41
1:a:1112:U:H2'	1:a:1113:C:C6	2.55	0.41
1:a:1287:G:O6	1:a:1288:A:N6	2.53	0.41
1:a:1324:U:H2'	1:a:1325:G:O4'	2.19	0.41
12:l:30:ARG:NH2	12:l:58:THR:OG1	2.30	0.41
25:A:634:A:H2'	25:A:636:A:N7	2.34	0.41
25:A:1708:U:H2'	25:A:1709:G:O4'	2.20	0.41
25:A:2193:U:O2'	25:A:2194:C:H6	2.03	0.41
25:A:2265:A:OP2	48:Y:12:ASN:ND2	2.46	0.41
25:A:2761:C:H2'	25:A:2762:A:O4'	2.20	0.41
26:B:48:U:P	40:Q:31:ARG:HH22	2.41	0.41
30:F:46:ASP:O	30:F:48:LYS:HG2	2.20	0.41
38:O:74:VAL:HG21	38:O:92:TYR:CZ	2.54	0.41
38:O:76:LYS:HB3	38:O:91:GLU:HG3	2.02	0.41
1:a:196:G:H21	1:a:460:A:N6	2.18	0.41
1:a:331:G:H2'	1:a:332:A:H8	1.83	0.41
1:a:1127:A:H2'	1:a:1128:C:H6	1.85	0.41
1:a:1311:C:H2'	1:a:1312:A:O4'	2.20	0.41
1:a:1336:C:H4'	9:i:126:GLN:O	2.20	0.41
1:a:1365:G:O3'	9:i:71:GLY:HA3	2.20	0.41
1:a:1366:U:H2'	1:a:1367:G:O4'	2.21	0.41
7:g:38:VAL:O	7:g:42:ILE:HG12	2.20	0.41
17:q:14:ARG:CZ	17:q:61:LEU:HD12	2.50	0.41
24:x:781:VAL:HG22	24:x:828:ILE:HG12	2.01	0.41
24:x:782:LEU:HD13	24:x:785:ASP:HA	2.02	0.41
25:A:1253:G:OP2	53:4:17:ARG:NE	2.53	0.41
25:A:1739:C:H2'	25:A:1740:G:C8	2.54	0.41
39:P:32:GLU:OE1	39:P:115:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1114:C:H2'	1:a:1115:U:C6	2.55	0.41
6:f:101:GLU:OE2	18:r:24:LYS:HB3	2.20	0.41
9:i:4:THR:O	9:i:5:GLN:HG2	2.21	0.41
18:r:59:ILE:CG2	18:r:63:ARG:HH21	2.34	0.41
22:v:52:G:C2	22:v:63:G:C2	3.09	0.41
24:x:719:TYR:OH	24:x:728:ASP:OD1	2.32	0.41
25:A:208:C:H2'	25:A:209:C:C6	2.56	0.41
25:A:456:G:OP2	25:A:456:G:H8	2.03	0.41
25:A:1262:A:C8	39:P:16:HIS:HD2	2.38	0.41
25:A:1431:A:H2'	25:A:1432:G:C8	2.55	0.41
25:A:2172:U:C2'	25:A:2173:G:H5'	2.49	0.41
25:A:2176:U:C6	25:A:2176:U:O5'	2.73	0.41
25:A:2544:G:H2'	25:A:2545:C:C6	2.55	0.41
37:N:87:GLY:O	37:N:89:VAL:N	2.54	0.41
40:Q:30:TYR:HB3	40:Q:37:TYR:HB2	2.02	0.41
47:X:83:HIS:HA	47:X:90:MET:HE2	2.01	0.41
1:a:1151:A:N7	1:a:1174:A:N6	2.68	0.41
1:a:1310:G:N1	1:a:1313:A:OP2	2.49	0.41
2:b:203:ASN:OD1	2:b:204:ASP:N	2.53	0.41
3:c:22:TRP:CB	3:c:59:ARG:HB2	2.51	0.41
6:f:84:VAL:O	6:f:85:ILE:HG22	2.20	0.41
10:j:88:MET:O	10:j:92:LEU:HG	2.21	0.41
13:m:9:ILE:HG13	13:m:10:PRO:HD2	2.01	0.41
16:p:5:ARG:HA	16:p:71:VAL:HG21	2.02	0.41
24:x:427:MET:HE3	24:x:427:MET:HB3	1.93	0.41
25:A:24:G:O2'	44:U:78:GLU:O	2.38	0.41
25:A:350:G:H2'	25:A:351:A:H8	1.85	0.41
25:A:872:G:H2'	25:A:873:U:O4'	2.20	0.41
25:A:1627:A:HO2'	25:A:1628:C:P	2.42	0.41
25:A:2134:A:H4'	25:A:2135:G:C8	2.54	0.41
25:A:2273:G:N3	25:A:2273:G:H2'	2.35	0.41
36:M:93:PRO:HG3	36:M:114:ILE:HG22	2.02	0.41
1:a:408:A:O2'	1:a:409:A:OP1	2.36	0.41
1:a:607:C:H2'	1:a:608:C:H6	1.84	0.41
1:a:1007:G:O2'	1:a:1009:G:O6	2.25	0.41
1:a:1143:C:H2'	1:a:1144:U:C6	2.55	0.41
4:d:164:GLN:OE1	4:d:164:GLN:N	2.52	0.41
22:v:57:A:C2'	22:v:58:A:H5'	2.50	0.41
25:A:567:G:H2'	25:A:568:G:C8	2.56	0.41
25:A:1011:A:O2'	25:A:1113:C:OP1	2.38	0.41
25:A:1381:U:H2'	25:A:1382:A:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1519:G:N2	25:A:1529:U:O2	2.41	0.41
25:A:1998:U:H2'	25:A:1999:G:O4'	2.21	0.41
25:A:2454:C:O2	38:O:124:LYS:NZ	2.48	0.41
30:F:57:LEU:HD12	30:F:60:ILE:HD11	2.02	0.41
1:a:991:U:C2	1:a:992:G:C8	3.09	0.41
1:a:1434:U:O2'	1:a:1435:A:H8	2.03	0.41
4:d:146:ARG:HE	4:d:148:LYS:HE3	1.85	0.41
24:x:413:THR:O	24:x:414:ASP:HB2	2.21	0.41
25:A:208:C:H2'	25:A:209:C:H6	1.85	0.41
25:A:733:C:OP1	28:D:135:GLY:HA2	2.20	0.41
25:A:1460:U:H2'	25:A:1461:G:O4'	2.20	0.41
25:A:2026:U:H2'	25:A:2027:G:C8	2.55	0.41
25:A:2791:C:H2'	25:A:2792:C:H6	1.85	0.41
29:E:28:HIS:HD2	37:N:6:LEU:HD12	1.85	0.41
30:F:121:SER:OG	30:F:128:TYR:HE1	2.04	0.41
52:3:17:SER:N	52:3:34:LEU:O	2.43	0.41
1:a:75:G:H2'	1:a:76:G:H8	1.84	0.41
1:a:915:U:O2'	5:e:25:THR:O	2.35	0.41
1:a:961:5MC:OP2	1:a:962:A:O2'	2.36	0.41
1:a:990:A:H2'	1:a:991:U:H6	1.86	0.41
3:c:36:ASP:O	3:c:39:VAL:HG12	2.20	0.41
9:i:12:ARG:O	9:i:15:ALA:HB3	2.20	0.41
12:l:114:ARG:O	12:l:114:ARG:HG2	2.21	0.41
13:m:23:TYR:CE1	13:m:70:ARG:HD2	2.55	0.41
13:m:53:ILE:HD12	13:m:57:ARG:HH22	1.85	0.41
19:s:52:HIS:HB2	19:s:57:HIS:CE1	2.55	0.41
19:s:63:ASN:H	19:s:66:MET:HE3	1.86	0.41
22:v:52:G:H1	22:v:62:C:H42	1.68	0.41
22:v:72:A:C5	22:v:73:A:H1'	2.55	0.41
24:x:662:LEU:HD11	24:x:726:ILE:HG23	2.02	0.41
25:A:585:C:H2'	25:A:586:A:H8	1.86	0.41
25:A:2302:G:H2'	25:A:2303:U:C6	2.55	0.41
25:A:2796:A:H2'	25:A:2797:A:C8	2.56	0.41
25:A:2807:A:H2'	25:A:2807:A:N3	2.36	0.41
30:F:6:GLU:HA	30:F:9:ARG:NH1	2.36	0.41
47:X:4:PHE:HB3	47:X:64:ILE:HG12	2.03	0.41
55:6:3:ARG:HA	55:6:3:ARG:HD3	1.90	0.41
1:a:574:C:H2'	1:a:575:G:O4'	2.21	0.41
1:a:975:U:OP2	1:a:976:U:O2'	2.31	0.41
19:s:11:ILE:HG23	19:s:15:LEU:HD23	2.02	0.41
24:x:517:ARG:HH21	24:x:539:ASP:CG	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:155:U:H2'	25:A:156:A:C8	2.56	0.41
25:A:275:C:H2'	25:A:276:U:H6	1.86	0.41
25:A:382:A:H1'	25:A:402:G:O4'	2.21	0.41
25:A:583:U:H2'	25:A:584:U:C6	2.55	0.41
25:A:2260:A:H2'	25:A:2261:A:C8	2.55	0.41
44:U:47:MET:HE3	44:U:47:MET:HB2	1.83	0.41
47:X:8:ALA:HB3	47:X:68:VAL:HG12	2.02	0.41
51:2:6:VAL:HG12	51:2:28:LEU:HD11	2.02	0.41
52:3:10:GLU:OE2	52:3:28:LEU:N	2.53	0.41
1:a:184:G:H2'	1:a:185:G:O4'	2.20	0.41
1:a:249:G:OP1	17:q:74:LYS:NZ	2.54	0.41
1:a:556:U:H5''	1:a:557:A:C5	2.56	0.41
1:a:709:A:O2'	1:a:710:A:OP1	2.37	0.41
1:a:739:U:H5'	1:a:829:G:N2	2.36	0.41
2:b:27:MET:O	2:b:31:ILE:HG12	2.21	0.41
6:f:29:ILE:HD12	6:f:64:VAL:HG13	2.03	0.41
7:g:25:LYS:HB3	7:g:101:MET:HE1	2.03	0.41
7:g:75:VAL:HG22	7:g:86:GLN:HB3	2.01	0.41
24:x:465:LEU:HD23	24:x:465:LEU:HA	1.92	0.41
24:x:739:SER:O	24:x:740:ASP:HB2	2.21	0.41
25:A:17:G:H2'	25:A:18:C:C6	2.55	0.41
25:A:977:C:H2'	25:A:978:A:O4'	2.21	0.41
25:A:1081:G:H1	25:A:1090:C:H42	1.67	0.41
25:A:1262:A:C4	39:P:16:HIS:CD2	3.08	0.41
25:A:1430:C:H2'	25:A:1431:A:H8	1.85	0.41
25:A:1672:G:H2'	25:A:1673:C:H6	1.84	0.41
25:A:1777:C:H2'	25:A:1778:A:C5	2.56	0.41
25:A:2087:G:N1	25:A:2177:G:C5	2.88	0.41
25:A:2602:U:H1'	53:4:4:GLN:HB3	2.02	0.41
28:D:151:THR:O	28:D:153:GLY:N	2.54	0.41
31:G:28:GLY:O	31:G:32:ALA:HB2	2.21	0.41
31:G:121:ILE:HG22	31:G:135:GLY:HA3	2.03	0.41
36:M:7:MET:SD	36:M:20:MET:HG3	2.61	0.41
38:O:43:THR:HG22	38:O:46:GLN:CD	2.46	0.41
44:U:11:ARG:NH1	44:U:99:ARG:O	2.54	0.41
1:a:154:A:H1'	1:a:338:A:C5	2.56	0.41
1:a:224:G:H5'	16:p:23:ASN:HD22	1.85	0.41
1:a:456:G:O2'	1:a:457:U:O5'	2.37	0.41
1:a:1004:C:H2'	1:a:1005:C:H6	1.86	0.41
7:g:44:TYR:HD1	7:g:44:TYR:HA	1.78	0.41
11:k:110:ILE:O	11:k:110:ILE:HG13	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:22:ILE:HG22	13:m:25:VAL:CG1	2.51	0.41
25:A:572:A:H2'	25:A:573:G:C8	2.56	0.41
25:A:665:A:H4'	29:E:61:GLN:NE2	2.35	0.41
25:A:817:U:H5'	25:A:818:U:C4	2.56	0.41
25:A:1742:A:N6	25:A:2681:G:O2'	2.54	0.41
25:A:2177:G:H2'	25:A:2178:A:H8	1.86	0.41
1:a:50:A:O2'	1:a:354:G:N2	2.54	0.40
1:a:354:G:H5''	24:x:680:THR:HG21	2.03	0.40
1:a:677:G:H2'	1:a:678:U:C6	2.56	0.40
1:a:701:U:C2	1:a:702:A:N7	2.89	0.40
1:a:978:C:C4	1:a:1216:G:N2	2.89	0.40
1:a:1222:C:OP1	13:m:114:LYS:HG3	2.21	0.40
7:g:57:ASP:HB3	7:g:59:LEU:HD23	2.02	0.40
9:i:88:ILE:O	9:i:92:GLU:HG3	2.20	0.40
25:A:276:U:H2'	25:A:277:U:C6	2.56	0.40
25:A:578:U:H2'	25:A:579:U:C6	2.56	0.40
25:A:764:C:O2'	25:A:767:A:N3	2.50	0.40
25:A:1098:U:HO2'	25:A:1099:C:P	2.43	0.40
25:A:1446:G:O2'	25:A:1447:U:H5'	2.21	0.40
25:A:2018:A:C6	25:A:2485:OMC:H1'	2.56	0.40
29:E:47:THR:O	29:E:51:VAL:HG23	2.20	0.40
30:F:4:LEU:HD13	30:F:100:LEU:HD23	2.03	0.40
30:F:31:VAL:HG12	30:F:96:MET:HE1	2.03	0.40
36:M:69:VAL:HG11	36:M:105:GLU:OE2	2.21	0.40
40:Q:16:ARG:NH2	40:Q:94:SER:OG	2.53	0.40
44:U:55:VAL:O	44:U:59:GLU:HG3	2.21	0.40
45:V:12:GLY:HA2	50:1:30:MET:HE1	2.02	0.40
1:a:418:G:H2'	1:a:419:A:H8	1.86	0.40
1:a:511:G:OP2	1:a:511:G:H8	2.03	0.40
1:a:827:U:H2'	1:a:828:U:H6	1.86	0.40
1:a:1025:C:H4'	1:a:1026:G:C4	2.56	0.40
1:a:1507:A:H2'	1:a:1508:G:H8	1.86	0.40
2:b:114:LEU:HD11	2:b:145:GLU:OE2	2.22	0.40
6:f:43:GLY:HA3	6:f:58:HIS:CD2	2.57	0.40
9:i:55:THR:O	9:i:57:THR:HG23	2.21	0.40
10:j:53:ILE:HD11	10:j:61:ALA:HB1	2.02	0.40
11:k:100:LEU:HA	11:k:100:LEU:HD23	1.85	0.40
13:m:81:MET:O	13:m:92:ARG:NH2	2.55	0.40
20:t:48:GLN:OE1	20:t:48:GLN:N	2.55	0.40
21:u:27:GLY:O	21:u:31:GLU:HG2	2.22	0.40
25:A:406:A:H2'	25:A:407:U:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:872:G:H3'	25:A:873:U:C6	2.57	0.40
25:A:1298:G:OP2	25:A:1298:G:N2	2.36	0.40
25:A:2279:G:H2'	25:A:2280:C:C6	2.56	0.40
25:A:2796:A:OP2	25:A:2877:G:N1	2.33	0.40
42:S:66:ASN:O	42:S:70:ARG:HG3	2.22	0.40
1:a:148:G:C6	1:a:162:G:C6	3.10	0.40
1:a:730:C:H2'	1:a:731:A:C8	2.55	0.40
1:a:1034:A:H2'	1:a:1035:G:C8	2.56	0.40
1:a:1404:A:H2'	1:a:1405:C:C6	2.55	0.40
3:c:14:ILE:HG22	3:c:15:VAL:HG13	2.02	0.40
3:c:28:ASN:OD1	3:c:28:ASN:N	2.53	0.40
4:d:157:GLN:HA	4:d:160:GLU:HG3	2.03	0.40
11:k:85:ASN:HD22	11:k:111:THR:HG1	1.64	0.40
21:u:41:PRO:O	21:u:45:ARG:NE	2.51	0.40
25:A:1161:C:H2'	25:A:1162:G:O4'	2.21	0.40
25:A:1238:C:O2'	25:A:1239:G:H3'	2.22	0.40
25:A:1870:U:H2'	25:A:1871:G:O4'	2.20	0.40
25:A:2172:U:H2'	25:A:2173:G:C8	2.31	0.40
25:A:2889:C:N4	25:A:2890:A:H62	2.18	0.40
29:E:153:ASP:OD1	29:E:154:GLU:N	2.55	0.40
30:F:127:ASN:ND2	30:F:157:THR:HA	2.34	0.40
31:G:2:SER:O	31:G:2:SER:OG	2.32	0.40
40:Q:82:LYS:HZ3	40:Q:113:GLY:HA3	1.86	0.40
1:a:678:U:C4	1:a:679:G:C5	3.10	0.40
1:a:1020:G:N1	1:a:1029:A:N6	2.35	0.40
2:b:60:LEU:HD23	2:b:67:ILE:HD11	2.02	0.40
9:i:81:HIS:CE1	9:i:85:ARG:HD2	2.57	0.40
14:n:42:TRP:O	14:n:46:VAL:HG23	2.22	0.40
16:p:39:PHE:HD1	16:p:50:LEU:HB3	1.87	0.40
19:s:12:ASP:OD2	19:s:14:HIS:NE2	2.55	0.40
20:t:35:VAL:HG22	20:t:50:ALA:HB1	2.04	0.40
20:t:44:LEU:O	20:t:47:ALA:N	2.54	0.40
25:A:247:G:H4'	25:A:377:G:C5	2.57	0.40
25:A:344:A:H2'	25:A:345:U:C6	2.56	0.40
25:A:576:A:N1	25:A:799:G:O2'	2.48	0.40
25:A:803:U:H2'	25:A:804:C:H6	1.86	0.40
25:A:1520:U:H6	25:A:1520:U:O5'	2.05	0.40
25:A:2836:U:H4'	25:A:2855:A:C2	2.56	0.40
26:B:51:G:H4'	26:B:52:A:OP1	2.21	0.40
27:C:175:ARG:HG3	27:C:181:MET:SD	2.62	0.40
28:D:149:CYS:O	28:D:151:THR:O	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:E:58:PRO:HB2	29:E:59:TRP:CE3	2.56	0.40
35:L:73:MET:HE3	35:L:73:MET:HB3	1.85	0.40
39:P:79:LEU:HD23	39:P:83:LEU:HB2	2.03	0.40
47:X:33:VAL:HG22	47:X:94:PHE:HB2	2.04	0.40
47:X:112:ILE:HD11	47:X:150:ASP:HB3	2.04	0.40
50:1:10:SER:O	50:1:14:LEU:N	2.50	0.40
1:a:202:U:N3	1:a:204:C:H5''	2.36	0.40
1:a:260:G:H1'	1:a:262:C:OP2	2.22	0.40
1:a:1431:A:H2'	1:a:1432:G:H8	1.87	0.40
1:a:1491:G:H1'	1:a:1512:MA6:H2	2.04	0.40
3:c:120:VAL:O	3:c:124:LEU:HD23	2.21	0.40
4:d:99:ASP:N	4:d:99:ASP:OD1	2.54	0.40
24:x:607:PHE:CE2	24:x:611:LYS:HD2	2.57	0.40
25:A:293:A:H2'	25:A:294:A:C8	2.57	0.40
25:A:803:U:H2'	25:A:804:C:C6	2.56	0.40
25:A:1098:U:O2'	25:A:1099:C:P	2.80	0.40
25:A:1214:A:P	42:S:12:ARG:HH12	2.45	0.40
25:A:1492:U:H2'	25:A:1493:U:H6	1.85	0.40
25:A:2087:G:O6	25:A:2177:G:O6	2.39	0.40
25:A:2220:U:H2'	25:A:2221:G:H8	1.85	0.40
25:A:2670:C:O2	36:M:70:ARG:NH2	2.55	0.40
46:W:9:GLU:OE1	46:W:21:ARG:NH2	2.49	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	222/246 (90%)	205 (92%)	16 (7%)	1 (0%)	24	48
3	c	206/228 (90%)	194 (94%)	12 (6%)	0	100	100
4	d	203/206 (98%)	175 (86%)	28 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	152/166 (92%)	139 (91%)	13 (9%)	0	100	100
6	f	104/139 (75%)	92 (88%)	10 (10%)	2 (2%)	6	17
7	g	150/156 (96%)	140 (93%)	9 (6%)	1 (1%)	18	41
8	h	127/130 (98%)	116 (91%)	10 (8%)	1 (1%)	16	37
9	i	125/130 (96%)	113 (90%)	11 (9%)	1 (1%)	16	37
10	j	97/103 (94%)	90 (93%)	7 (7%)	0	100	100
11	k	117/129 (91%)	112 (96%)	5 (4%)	0	100	100
12	l	120/123 (98%)	112 (93%)	8 (7%)	0	100	100
13	m	112/118 (95%)	99 (88%)	12 (11%)	1 (1%)	14	35
14	n	98/101 (97%)	87 (89%)	11 (11%)	0	100	100
15	o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	p	79/83 (95%)	77 (98%)	2 (2%)	0	100	100
17	q	78/88 (89%)	78 (100%)	0	0	100	100
18	r	60/76 (79%)	54 (90%)	5 (8%)	1 (2%)	7	19
19	s	81/91 (89%)	72 (89%)	9 (11%)	0	100	100
20	t	85/91 (93%)	84 (99%)	1 (1%)	0	100	100
21	u	60/71 (84%)	58 (97%)	2 (3%)	0	100	100
24	x	591/840 (70%)	544 (92%)	43 (7%)	4 (1%)	18	41
27	C	270/273 (99%)	255 (94%)	15 (6%)	0	100	100
28	D	209/211 (99%)	183 (88%)	24 (12%)	2 (1%)	12	32
29	E	198/200 (99%)	190 (96%)	6 (3%)	2 (1%)	12	32
30	F	174/179 (97%)	151 (87%)	20 (12%)	3 (2%)	7	19
31	G	173/177 (98%)	160 (92%)	13 (8%)	0	100	100
32	H	70/148 (47%)	65 (93%)	5 (7%)	0	100	100
33	I	116/166 (70%)	97 (84%)	16 (14%)	3 (3%)	4	11
34	J	132/143 (92%)	110 (83%)	21 (16%)	1 (1%)	16	37
35	L	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
36	M	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
37	N	142/144 (99%)	126 (89%)	16 (11%)	0	100	100
38	O	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
39	P	118/129 (92%)	110 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	Q	113/116 (97%)	102 (90%)	11 (10%)	0	100	100
41	R	112/116 (97%)	106 (95%)	6 (5%)	0	100	100
42	S	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
43	T	101/103 (98%)	99 (98%)	1 (1%)	1 (1%)	12	32
44	U	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
45	V	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
46	W	101/104 (97%)	93 (92%)	7 (7%)	1 (1%)	12	32
47	X	188/204 (92%)	180 (96%)	8 (4%)	0	100	100
48	Y	74/85 (87%)	71 (96%)	2 (3%)	1 (1%)	9	23
49	Z	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
50	1	59/63 (94%)	59 (100%)	0	0	100	100
51	2	55/58 (95%)	55 (100%)	0	0	100	100
52	3	45/71 (63%)	41 (91%)	3 (7%)	1 (2%)	5	14
53	4	53/60 (88%)	51 (96%)	2 (4%)	0	100	100
54	5	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
55	6	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
56	7	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
57	8	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
All	All	6429/7157 (90%)	5976 (93%)	426 (7%)	27 (0%)	31	54

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	f	84	VAL
7	g	152	SER
8	h	55	VAL
13	m	117	ARG
24	x	635	GLU
28	D	152	PRO
29	E	122	ASP
30	F	74	ILE
43	T	52	PRO
52	3	12	ILE
6	f	85	ILE
24	x	486	ALA
30	F	37	ASN

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Mol	Chain	Res	Type
30	F	114	PHE
33	I	52	VAL
24	x	554	TYR
34	J	71	THR
46	W	14	ALA
48	Y	69	PHE
33	I	106	PHE
9	i	28	ILE
18	r	18	VAL
33	I	108	ILE
24	x	371	GLU
28	D	210	ARG
2	b	89	MET
29	E	127	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	184/202 (91%)	184 (100%)	0	100	100
3	c	170/187 (91%)	169 (99%)	1 (1%)	78	91
4	d	171/174 (98%)	171 (100%)	0	100	100
5	e	113/124 (91%)	113 (100%)	0	100	100
6	f	88/119 (74%)	88 (100%)	0	100	100
7	g	118/122 (97%)	118 (100%)	0	100	100
8	h	108/109 (99%)	108 (100%)	0	100	100
9	i	104/106 (98%)	104 (100%)	0	100	100
10	j	87/92 (95%)	87 (100%)	0	100	100
11	k	90/98 (92%)	90 (100%)	0	100	100
12	l	106/107 (99%)	106 (100%)	0	100	100
13	m	95/99 (96%)	95 (100%)	0	100	100
14	n	80/82 (98%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	o	74/75 (99%)	73 (99%)	1 (1%)	59	82
16	p	64/65 (98%)	64 (100%)	0	100	100
17	q	73/79 (92%)	73 (100%)	0	100	100
18	r	48/64 (75%)	48 (100%)	0	100	100
19	s	72/78 (92%)	72 (100%)	0	100	100
20	t	69/70 (99%)	69 (100%)	0	100	100
21	u	51/60 (85%)	51 (100%)	0	100	100
24	x	417/668 (62%)	417 (100%)	0	100	100
27	C	212/213 (100%)	212 (100%)	0	100	100
28	D	162/162 (100%)	162 (100%)	0	100	100
29	E	157/158 (99%)	155 (99%)	2 (1%)	61	83
30	F	149/153 (97%)	149 (100%)	0	100	100
31	G	138/141 (98%)	138 (100%)	0	100	100
32	H	44/107 (41%)	44 (100%)	0	100	100
33	I	2/122 (2%)	2 (100%)	0	100	100
34	J	13/110 (12%)	13 (100%)	0	100	100
35	L	119/119 (100%)	119 (100%)	0	100	100
36	M	102/102 (100%)	102 (100%)	0	100	100
37	N	106/106 (100%)	106 (100%)	0	100	100
38	O	110/110 (100%)	110 (100%)	0	100	100
39	P	99/104 (95%)	99 (100%)	0	100	100
40	Q	86/87 (99%)	86 (100%)	0	100	100
41	R	96/98 (98%)	94 (98%)	2 (2%)	47	75
42	S	86/88 (98%)	86 (100%)	0	100	100
43	T	86/86 (100%)	86 (100%)	0	100	100
44	U	87/87 (100%)	87 (100%)	0	100	100
45	V	79/82 (96%)	79 (100%)	0	100	100
46	W	84/88 (96%)	84 (100%)	0	100	100
47	X	154/164 (94%)	154 (100%)	0	100	100
48	Y	56/61 (92%)	55 (98%)	1 (2%)	51	78
49	Z	66/67 (98%)	65 (98%)	1 (2%)	57	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	1	54/55 (98%)	54 (100%)	0	100	100
51	2	48/49 (98%)	48 (100%)	0	100	100
52	3	41/61 (67%)	41 (100%)	0	100	100
53	4	48/52 (92%)	48 (100%)	0	100	100
54	5	47/47 (100%)	47 (100%)	0	100	100
55	6	37/37 (100%)	37 (100%)	0	100	100
56	7	54/55 (98%)	54 (100%)	0	100	100
57	8	34/34 (100%)	34 (100%)	0	100	100
All	All	5038/5785 (87%)	5030 (100%)	8 (0%)	85	95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	86	LYS
15	o	88	ARG
29	E	73	ARG
29	E	74	SER
41	R	34	LYS
41	R	37	ASP
48	Y	70	GLU
49	Z	2	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	42	ASN
2	b	109	GLN
2	b	177	ASN
3	c	139	GLN
4	d	41	HIS
4	d	43	GLN
5	e	20	ASN
5	e	74	GLN
6	f	63	ASN
7	g	28	ASN
8	h	85	GLN
11	k	24	HIS
11	k	28	ASN

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Mol	Chain	Res	Type
11	k	38	GLN
11	k	64	GLN
11	k	118	HIS
12	l	46	ASN
12	l	73	ASN
13	m	14	HIS
13	m	55	GLN
13	m	74	ASN
14	n	71	HIS
15	o	17	GLN
15	o	37	ASN
20	t	3	ASN
20	t	13	GLN
20	t	82	HIS
24	x	383	HIS
24	x	463	ASN
24	x	668	GLN
27	C	22	GLN
27	C	61	HIS
27	C	134	ASN
27	C	153	GLN
27	C	261	ASN
28	D	126	ASN
28	D	136	ASN
28	D	173	GLN
29	E	61	GLN
30	F	37	ASN
30	F	127	ASN
31	G	23	GLN
31	G	56	ASN
32	H	20	ASN
35	L	23	GLN
36	M	56	GLN
37	N	58	HIS
38	O	57	HIS
38	O	98	GLN
39	P	16	HIS
39	P	62	ASN
40	Q	39	GLN
41	R	7	GLN
41	R	8	GLN
41	R	15	ASN

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Mol	Chain	Res	Type
41	R	39	GLN
44	U	61	ASN
45	V	28	GLN
45	V	90	GLN
46	W	99	GLN
47	X	25	ASN
47	X	113	ASN
48	Y	40	GLN
48	Y	57	HIS
49	Z	16	ASN
49	Z	35	HIS
49	Z	36	HIS
50	1	13	GLN
50	1	31	GLN
50	1	39	GLN
51	2	32	ASN
52	3	33	HIS
55	6	29	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1520/1536 (98%)	268 (17%)	0
22	v	75/77 (97%)	16 (21%)	0
23	w	5/24 (20%)	0	0
25	A	2881/2891 (99%)	548 (19%)	47 (1%)
26	B	116/120 (96%)	14 (12%)	2 (1%)
All	All	4597/4648 (98%)	846 (18%)	49 (1%)

All (846) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	C
1	a	6	G
1	a	7	A
1	a	9	G
1	a	30	U
1	a	31	G
1	a	32	A
1	a	39	G
1	a	47	C

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Mol	Chain	Res	Type
1	a	48	C
1	a	50	A
1	a	51	A
1	a	54	C
1	a	60	A
1	a	61	G
1	a	71	U
1	a	72	G
1	a	77	G
1	a	82	U
1	a	83	G
1	a	88	U
1	a	91	A
1	a	95	A
1	a	116	G
1	a	121	G
1	a	123	A
1	a	124	A
1	a	125	U
1	a	138	G
1	a	140	G
1	a	151	C
1	a	157	C
1	a	177	G
1	a	182	G
1	a	184	G
1	a	191	A
1	a	192	G
1	a	202	U
1	a	204	C
1	a	206	G
1	a	217	A
1	a	239	U
1	a	241	G
1	a	245	G
1	a	260	G
1	a	261	C
1	a	283	A
1	a	287	G
1	a	315	A
1	a	322	C
1	a	323	A

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Mol	Chain	Res	Type
1	a	334	U
1	a	338	A
1	a	341	G
1	a	345	G
1	a	346	C
1	a	348	G
1	a	361	U
1	a	363	G
1	a	366	C
1	a	376	A
1	a	378	G
1	a	386	C
1	a	391	A
1	a	400	G
1	a	406	A
1	a	407	G
1	a	408	A
1	a	409	A
1	a	418	G
1	a	423	U
1	a	433	U
1	a	443	G
1	a	446	A
1	a	447	G
1	a	455	A
1	a	457	U
1	a	460	A
1	a	461	U
1	a	462	A
1	a	475	G
1	a	478	G
1	a	490	A
1	a	491	U
1	a	492	A
1	a	503	A
1	a	505	C
1	a	507	U
1	a	509	G
1	a	511	G
1	a	512	C
1	a	513	C
1	a	521	7MG

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Mol	Chain	Res	Type
1	a	526	A
1	a	527	A
1	a	534	G
1	a	539	C
1	a	541	A
1	a	553	A
1	a	556	U
1	a	558	C
1	a	562	G
1	a	566	A
1	a	567	A
1	a	570	C
1	a	571	G
1	a	573	G
1	a	582	G
1	a	584	U
1	a	585	C
1	a	627	G
1	a	647	A
1	a	659	A
1	a	680	U
1	a	681	A
1	a	682	G
1	a	687	G
1	a	688	A
1	a	689	A
1	a	696	A
1	a	710	A
1	a	712	A
1	a	716	G
1	a	718	G
1	a	725	G
1	a	749	A
1	a	754	G
1	a	756	U
1	a	757	G
1	a	758	C
1	a	771	A
1	a	781	A
1	a	787	U
1	a	788	A
1	a	806	G

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Mol	Chain	Res	Type
1	a	807	U
1	a	809	A
1	a	811	C
1	a	815	G
1	a	822	A
1	a	861	G
1	a	866	A
1	a	870	C
1	a	884	G
1	a	894	A
1	a	896	G
1	a	908	A
1	a	920	G
1	a	921	G
1	a	928	C
1	a	952	A
1	a	954	U
1	a	955	U
1	a	962	A
1	a	963	A
1	a	964	C
1	a	965	G
1	a	969	A
1	a	970	G
1	a	971	A
1	a	975	U
1	a	977	A
1	a	987	G
1	a	988	A
1	a	990	A
1	a	997	G
1	a	998	A
1	a	1003	U
1	a	1004	C
1	a	1009	G
1	a	1015	U
1	a	1016	U
1	a	1018	G
1	a	1020	G
1	a	1021	C
1	a	1023	U
1	a	1025	C

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Mol	Chain	Res	Type
1	a	1026	G
1	a	1031	C
1	a	1039	C
1	a	1044	G
1	a	1059	U
1	a	1073	G
1	a	1077	U
1	a	1078	G
1	a	1079	U
1	a	1088	G
1	a	1089	U
1	a	1095	A
1	a	1102	G
1	a	1118	G
1	a	1119	U
1	a	1124	A
1	a	1130	U
1	a	1132	G
1	a	1133	G
1	a	1152	C
1	a	1153	U
1	a	1162	C
1	a	1175	G
1	a	1178	G
1	a	1190	A
1	a	1191	A
1	a	1196	U
1	a	1201	2MG
1	a	1206	U
1	a	1207	A
1	a	1213	A
1	a	1214	G
1	a	1218	U
1	a	1219	A
1	a	1221	A
1	a	1222	C
1	a	1230	A
1	a	1232	A
1	a	1234	U
1	a	1235	G
1	a	1242	A
1	a	1248	G

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Mol	Chain	Res	Type
1	a	1251	U
1	a	1252	G
1	a	1264	G
1	a	1266	U
1	a	1273	A
1	a	1274	A
1	a	1279	A
1	a	1280	U
1	a	1281	A
1	a	1293	A
1	a	1294	G
1	a	1295	U
1	a	1296	C
1	a	1299	G
1	a	1314	C
1	a	1316	C
1	a	1332	G
1	a	1340	A
1	a	1341	G
1	a	1342	U
1	a	1347	G
1	a	1357	A
1	a	1358	U
1	a	1373	G
1	a	1375	U
1	a	1388	A
1	a	1391	C
1	a	1392	A
1	a	1400	U
1	a	1413	G
1	a	1420	G
1	a	1422	U
1	a	1426	G
1	a	1435	A
1	a	1440	A
1	a	1446	A
1	a	1448	G
1	a	1469	G
1	a	1487	A
1	a	1491	G
1	a	1493	A
1	a	1497	A

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Mol	Chain	Res	Type
1	a	1500	U
1	a	1501	A
1	a	1502	G
1	a	1511	G
1	a	1514	C
1	a	1523	G
1	a	1524	G
22	v	6	G
22	v	8	4SU
22	v	16	C
22	v	17	C
22	v	18	G
22	v	21	A
22	v	46	G
22	v	47	U
22	v	48	C
22	v	61	C
22	v	69	C
22	v	70	G
22	v	71	C
22	v	72	A
22	v	75	C
22	v	76	A
25	A	2	G
25	A	15	G
25	A	28	A
25	A	34	U
25	A	35	G
25	A	44	A
25	A	46	G
25	A	50	U
25	A	58	G
25	A	70	G
25	A	71	A
25	A	74	A
25	A	75	G
25	A	79	C
25	A	82	G
25	A	83	G
25	A	84	A
25	A	85	G
25	A	92	A

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Mol	Chain	Res	Type
25	A	95	A
25	A	96	G
25	A	97	A
25	A	100	U
25	A	102	G
25	A	110	G
25	A	114	U
25	A	115	C
25	A	118	A
25	A	119	A
25	A	120	U
25	A	124	G
25	A	125	G
25	A	131	A
25	A	142	C
25	A	160	A
25	A	163	C
25	A	166	U
25	A	181	A
25	A	196	A
25	A	199	A
25	A	205	G
25	A	206	U
25	A	215	G
25	A	216	A
25	A	220	G
25	A	221	A
25	A	222	A
25	A	224	U
25	A	230	G
25	A	233	A
25	A	240	U
25	A	242	G
25	A	243	U
25	A	244	A
25	A	248	G
25	A	249	C
25	A	250	G
25	A	252	G
25	A	255	A
25	A	261	G
25	A	265	A

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Mol	Chain	Res	Type
25	A	266	G
25	A	271	U
25	A	273	A
25	A	289	G
25	A	293	A
25	A	294	A
25	A	296	G
25	A	305	A
25	A	315	U
25	A	316	A
25	A	318	U
25	A	319	G
25	A	322	U
25	A	323	G
25	A	324	A
25	A	337	C
25	A	348	U
25	A	349	U
25	A	356	A
25	A	358	A
25	A	359	U
25	A	376	C
25	A	377	G
25	A	380	A
25	A	387	G
25	A	396	U
25	A	397	G
25	A	400	G
25	A	403	A
25	A	435	C
25	A	445	A
25	A	447	C
25	A	456	G
25	A	461	A
25	A	464	G
25	A	471	A
25	A	472	G
25	A	482	G
25	A	485	G
25	A	487	G
25	A	495	U
25	A	496	A

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Mol	Chain	Res	Type
25	A	499	A
25	A	519	A
25	A	520	A
25	A	521	G
25	A	522	C
25	A	523	A
25	A	536	U
25	A	537	U
25	A	538	G
25	A	544	U
25	A	553	A
25	A	558	U
25	A	563	U
25	A	565	A
25	A	576	A
25	A	582	A
25	A	583	U
25	A	593	A
25	A	594	G
25	A	599	A
25	A	601	C
25	A	603	U
25	A	604	A
25	A	605	U
25	A	608	G
25	A	622	A
25	A	627	A
25	A	635	U
25	A	636	A
25	A	637	G
25	A	644	U
25	A	645	A
25	A	647	U
25	A	649	G
25	A	659	G
25	A	660	A
25	A	667	A
25	A	675	A
25	A	676	U
25	A	687	G
25	A	720	A
25	A	728	C

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Mol	Chain	Res	Type
25	A	730	C
25	A	737	U
25	A	738	G
25	A	743	G
25	A	747	G
25	A	754	A
25	A	755	C
25	A	765	G
25	A	766	G
25	A	772	A
25	A	774	G
25	A	775	G
25	A	779	A
25	A	793	U
25	A	795	G
25	A	802	C
25	A	820	G
25	A	835	A
25	A	836	U
25	A	841	C
25	A	848	G
25	A	855	A
25	A	866	U
25	A	870	G
25	A	871	G
25	A	875	A
25	A	876	U
25	A	877	C
25	A	878	C
25	A	880	G
25	A	884	U
25	A	886	C
25	A	889	A
25	A	899	A
25	A	903	C
25	A	904	C
25	A	908	U
25	A	911	C
25	A	921	C
25	A	922	G
25	A	931	A
25	A	935	A

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Mol	Chain	Res	Type
25	A	936	C
25	A	949	A
25	A	951	C
25	A	952	G
25	A	964	A
25	A	972	C
25	A	973	A
25	A	986	A
25	A	993	G
25	A	995	C
25	A	999	A
25	A	1002	U
25	A	1003	U
25	A	1007	G
25	A	1012	G
25	A	1016	U
25	A	1017	A
25	A	1023	U
25	A	1030	A
25	A	1037	G
25	A	1041	G
25	A	1043	U
25	A	1044	A
25	A	1047	A
25	A	1051	U
25	A	1060	A
25	A	1063	A
25	A	1074	A
25	A	1075	A
25	A	1078	A
25	A	1080	A
25	A	1091	U
25	A	1099	C
25	A	1100	G
25	A	1102	G
25	A	1112	G
25	A	1117	A
25	A	1119	A
25	A	1120	U
25	A	1122	U
25	A	1124	A
25	A	1125	C

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Mol	Chain	Res	Type
25	A	1129	G
25	A	1133	A
25	A	1148	G
25	A	1162	G
25	A	1169	A
25	A	1170	C
25	A	1193	G
25	A	1199	G
25	A	1211	A
25	A	1214	A
25	A	1225	G
25	A	1234	A
25	A	1237	G
25	A	1238	C
25	A	1240	A
25	A	1243	G
25	A	1249	A
25	A	1253	G
25	A	1255	A
25	A	1258	G
25	A	1259	A
25	A	1261	A
25	A	1263	U
25	A	1276	C
25	A	1287	A
25	A	1288	A
25	A	1307	C
25	A	1308	A
25	A	1316	U
25	A	1334	G
25	A	1339	U
25	A	1347	G
25	A	1352	A
25	A	1354	A
25	A	1355	A
25	A	1366	U
25	A	1370	A
25	A	1372	A
25	A	1373	C
25	A	1382	A
25	A	1403	G
25	A	1404	C

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Mol	Chain	Res	Type
25	A	1406	A
25	A	1407	U
25	A	1408	G
25	A	1414	A
25	A	1415	C
25	A	1420	A
25	A	1421	A
25	A	1439	G
25	A	1447	U
25	A	1448	C
25	A	1449	C
25	A	1454	U
25	A	1469	G
25	A	1475	U
25	A	1477	A
25	A	1480	U
25	A	1497	G
25	A	1498	G
25	A	1502	A
25	A	1509	A
25	A	1511	G
25	A	1512	A
25	A	1537	U
25	A	1556	A
25	A	1558	G
25	A	1559	A
25	A	1560	A
25	A	1568	U
25	A	1573	U
25	A	1574	U
25	A	1575	C
25	A	1576	A
25	A	1593	A
25	A	1597	C
25	A	1628	C
25	A	1629	C
25	A	1634	C
25	A	1637	U
25	A	1638	U
25	A	1639	G
25	A	1641	G
25	A	1643	G

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Mol	Chain	Res	Type
25	A	1650	G
25	A	1654	A
25	A	1657	G
25	A	1664	G
25	A	1673	C
25	A	1685	G
25	A	1686	G
25	A	1690	A
25	A	1705	G
25	A	1712	G
25	A	1716	U
25	A	1717	U
25	A	1720	U
25	A	1721	C
25	A	1725	A
25	A	1735	U
25	A	1736	G
25	A	1742	A
25	A	1745	U
25	A	1750	G
25	A	1751	G
25	A	1760	A
25	A	1763	G
25	A	1771	A
25	A	1773	A
25	A	1787	C
25	A	1788	A
25	A	1789	A
25	A	1795	A
25	A	1797	A
25	A	1798	G
25	A	1803	C
25	A	1816	A
25	A	1829	G
25	A	1835	A
25	A	1837	G
25	A	1841	A
25	A	1851	U
25	A	1853	A
25	A	1865	G
25	A	1890	G
25	A	1892	C

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Mol	Chain	Res	Type
25	A	1893	G
25	A	1894	G
25	A	1897	G
25	A	1900	A
25	A	1906	A
25	A	1909	G
25	A	1916	G
25	A	1917	G
25	A	1918	U
25	A	1923	A
25	A	1942	U
25	A	1954	C
25	A	1957	A
25	A	1958	U
25	A	1959	G
25	A	1974	G
25	A	1978	U
25	A	1980	U
25	A	1984	C
25	A	2008	A
25	A	2010	C
25	A	2018	A
25	A	2020	A
25	A	2023	C
25	A	2030	U
25	A	2042	C
25	A	2043	G
25	A	2047	A
25	A	2048	G
25	A	2049	A
25	A	2055	U
25	A	2056	7MG
25	A	2058	A
25	A	2067	G
25	A	2094	C
25	A	2096	U
25	A	2097	G
25	A	2098	U
25	A	2099	G
25	A	2100	U
25	A	2101	A
25	A	2103	G

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Mol	Chain	Res	Type
25	A	2105	U
25	A	2106	A
25	A	2110	G
25	A	2112	G
25	A	2114	G
25	A	2115	G
25	A	2116	C
25	A	2117	U
25	A	2118	U
25	A	2119	U
25	A	2120	G
25	A	2121	A
25	A	2122	A
25	A	2127	G
25	A	2129	A
25	A	2132	C
25	A	2133	C
25	A	2135	G
25	A	2140	C
25	A	2143	G
25	A	2145	A
25	A	2146	G
25	A	2147	C
25	A	2148	C
25	A	2150	U
25	A	2151	C
25	A	2158	A
25	A	2160	A
25	A	2161	C
25	A	2171	A
25	A	2174	C
25	A	2175	U
25	A	2177	G
25	A	2185	A
25	A	2187	C
25	A	2191	G
25	A	2194	C
25	A	2199	A
25	A	2200	U
25	A	2201	C
25	A	2212	A
25	A	2225	G

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Mol	Chain	Res	Type
25	A	2226	G
25	A	2229	G
25	A	2238	OMG
25	A	2239	G
25	A	2265	A
25	A	2270	U
25	A	2274	A
25	A	2275	A
25	A	2292	U
25	A	2294	G
25	A	2296	A
25	A	2297	A
25	A	2306	C
25	A	2309	A
25	A	2312	A
25	A	2313	U
25	A	2314	A
25	A	2323	A
25	A	2330	U
25	A	2332	G
25	A	2334	C
25	A	2337	C
25	A	2348	C
25	A	2358	G
25	A	2359	U
25	A	2361	C
25	A	2366	G
25	A	2370	G
25	A	2372	C
25	A	2389	U
25	A	2393	U
25	A	2398	A
25	A	2407	C
25	A	2409	C
25	A	2410	U
25	A	2412	A
25	A	2414	C
25	A	2416	G
25	A	2417	A
25	A	2422	A
25	A	2428	U
25	A	2434	G

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Mol	Chain	Res	Type
25	A	2435	A
25	A	2446	A
25	A	2462	C
25	A	2467	C
25	A	2474	G
25	A	2478	U
25	A	2485	OMC
25	A	2489	G
25	A	2492	G
25	A	2493	U
25	A	2505	A
25	A	2506	U
25	A	2516	G
25	A	2534	A
25	A	2537	G
25	A	2553	A
25	A	2554	G
25	A	2560	C
25	A	2565	G
25	A	2569	G
25	A	2572	U
25	A	2586	G
25	A	2589	A
25	A	2596	U
25	A	2600	U
25	A	2602	U
25	A	2616	U
25	A	2617	U
25	A	2640	U
25	A	2641	A
25	A	2650	G
25	A	2672	G
25	A	2676	U
25	A	2677	U
25	A	2689	G
25	A	2692	A
25	A	2701	G
25	A	2705	G
25	A	2713	U
25	A	2720	A
25	A	2735	A
25	A	2744	A

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Mol	Chain	Res	Type
25	A	2752	A
25	A	2763	A
25	A	2765	A
25	A	2766	U
25	A	2783	C
25	A	2784	U
25	A	2785	U
25	A	2786	G
25	A	2787	A
25	A	2794	U
25	A	2795	G
25	A	2807	A
25	A	2808	A
25	A	2812	U
25	A	2820	U
25	A	2836	U
25	A	2846	G
25	A	2852	U
25	A	2854	G
25	A	2860	A
25	A	2867	C
25	A	2871	U
25	A	2873	G
25	A	2889	C
25	A	2890	A
26	B	9	G
26	B	24	G
26	B	35	U
26	B	37	C
26	B	41	C
26	B	52	A
26	B	53	A
26	B	67	U
26	B	73	A
26	B	89	U
26	B	90	C
26	B	91	C
26	B	109	A
26	B	117	G

All (49) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	27	G
25	A	81	G
25	A	83	G
25	A	87	C
25	A	114	U
25	A	243	U
25	A	265	A
25	A	314	A
25	A	434	A
25	A	444	A
25	A	470	A
25	A	687	G
25	A	774	G
25	A	792	A
25	A	840	U
25	A	920	C
25	A	963	A
25	A	1016	U
25	A	1042	C
25	A	1098	U
25	A	1099	C
25	A	1169	A
25	A	1233	A
25	A	1340	A
25	A	1407	U
25	A	1448	C
25	A	1497	G
25	A	1574	U
25	A	1627	A
25	A	1642	A
25	A	1672	G
25	A	1741	A
25	A	1834	A
25	A	1891	G
25	A	1917	G
25	A	2029	A
25	A	2149	A
25	A	2228	A
25	A	2273	G
25	A	2274	A
25	A	2392	G
25	A	2461	U
25	A	2536	G

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Mol	Chain	Res	Type
25	A	2743	U
25	A	2783	C
25	A	2793	C
25	A	2851	G
26	B	51	G
26	B	66	A

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

26 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	$\# Z > 2$
25	6MZ	A	2017	25	22,25,26	1.85	6 (27%)	29,36,39	3.51	10 (34%)
25	OMC	A	2485	58,25	19,22,23	0.81	0	25,31,34	0.91	1 (4%)
1	2MG	a	1510	1	23,26,27	1.22	3 (13%)	33,38,41	2.25	9 (27%)
1	2MG	a	960	1	23,26,27	1.25	4 (17%)	33,38,41	2.20	8 (24%)
1	7MG	a	521	1	23,26,27	1.30	3 (13%)	27,39,42	2.67	7 (25%)
25	5MC	A	1949	25	19,22,23	1.52	3 (15%)	26,32,35	1.08	2 (7%)
22	5MU	v	54	22	19,22,23	1.42	6 (31%)	27,32,35	2.09	5 (18%)
25	2MA	A	2490	58,25	22,25,26	1.45	4 (18%)	32,37,40	2.28	9 (28%)
22	4SU	v	8	22	18,21,22	1.95	5 (27%)	25,30,33	1.90	5 (20%)
22	5MC	v	32	22	19,22,23	1.45	3 (15%)	26,32,35	1.30	3 (11%)
1	MA6	a	1513	1	23,26,27	1.47	5 (21%)	33,38,41	2.42	15 (45%)
25	2MG	A	2432	58,25	23,26,27	1.26	3 (13%)	33,38,41	2.27	9 (27%)
25	OMU	A	2539	25	19,22,23	1.26	3 (15%)	25,31,34	1.85	5 (20%)
25	7MG	A	2056	58,25	23,26,27	1.30	3 (13%)	27,39,42	2.65	7 (25%)
1	MA6	a	1512	1	23,26,27	1.48	4 (17%)	33,38,41	2.42	13 (39%)
25	OMG	A	2238	25	23,26,27	1.21	3 (13%)	32,38,41	1.96	6 (18%)
22	PSU	v	55	22	18,21,22	1.37	2 (11%)	21,30,33	2.05	4 (19%)
25	6MZ	A	1608	25	22,25,26	1.86	5 (22%)	29,36,39	3.41	9 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	2MG	A	1822	25	23,26,27	1.24	3 (13%)	33,38,41	2.19	6 (18%)
1	4OC	a	1396	1	20,23,24	0.73	0	25,32,35	1.00	2 (8%)
1	5MC	a	961	1	19,22,23	1.53	3 (15%)	26,32,35	1.11	2 (7%)
25	1MG	A	735	25	23,26,27	1.16	3 (13%)	33,39,42	1.70	5 (15%)
25	5MU	A	1926	25	19,22,23	1.39	5 (26%)	27,32,35	2.16	6 (22%)
1	2MG	a	1201	1	23,26,27	1.28	4 (17%)	33,38,41	2.20	7 (21%)
1	UR3	a	1492	1	19,22,23	0.98	1 (5%)	26,32,35	1.78	2 (7%)
25	UR3	A	1902	25	19,22,23	1.03	1 (5%)	26,32,35	1.75	4 (15%)

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
25	6MZ	A	2017	25	-	2/9/27/28	0/3/3/3
25	OMC	A	2485	58,25	-	1/9/27/28	0/2/2/2
1	2MG	a	1510	1	-	0/9/27/28	0/3/3/3
1	2MG	a	960	1	-	0/9/27/28	0/3/3/3
1	7MG	a	521	1	-	2/7/37/38	0/3/3/3
25	5MC	A	1949	25	-	0/7/25/26	0/2/2/2
22	5MU	v	54	22	-	0/7/25/26	0/2/2/2
25	2MA	A	2490	58,25	-	1/7/25/26	0/3/3/3
22	4SU	v	8	22	-	1/7/25/26	0/2/2/2
22	5MC	v	32	22	-	0/7/25/26	0/2/2/2
1	MA6	a	1513	1	-	4/11/29/30	0/3/3/3
25	2MG	A	2432	58,25	-	0/9/27/28	0/3/3/3
25	OMU	A	2539	25	-	0/9/27/28	0/2/2/2
25	7MG	A	2056	58,25	-	2/7/37/38	0/3/3/3
1	MA6	a	1512	1	-	1/11/29/30	0/3/3/3
25	OMG	A	2238	25	-	2/9/27/28	0/3/3/3
22	PSU	v	55	22	-	0/7/25/26	0/2/2/2
25	6MZ	A	1608	25	-	0/9/27/28	0/3/3/3
25	2MG	A	1822	25	-	0/9/27/28	0/3/3/3
1	4OC	a	1396	1	-	2/9/29/30	0/2/2/2
1	5MC	a	961	1	-	0/7/25/26	0/2/2/2
25	1MG	A	735	25	-	0/7/25/26	0/3/3/3
25	5MU	A	1926	25	-	0/7/25/26	0/2/2/2
1	2MG	a	1201	1	-	3/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	a	1492	1	-	0/7/25/26	0/2/2/2
25	UR3	A	1902	25	-	0/7/25/26	0/2/2/2

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1608	6MZ	C6-N6	5.51	1.40	1.34
25	A	1949	5MC	C5-C4	5.44	1.48	1.44
1	a	961	5MC	C5-C4	5.42	1.48	1.44
25	A	2017	6MZ	C6-N6	5.40	1.40	1.34
22	v	8	4SU	C4-S4	-4.97	1.59	1.68
22	v	32	5MC	C5-C4	4.88	1.47	1.44
1	a	1512	MA6	C5-C4	4.49	1.47	1.39
1	a	1513	MA6	C5-C4	4.46	1.47	1.39
25	A	1608	6MZ	C5-C4	4.34	1.46	1.39
25	A	2490	2MA	C5-C4	4.28	1.46	1.39
25	A	2017	6MZ	C5-C4	4.25	1.46	1.39
22	v	8	4SU	C4-N3	-3.74	1.33	1.37
22	v	55	PSU	C6-C5	3.41	1.39	1.35
25	A	2056	7MG	C4-N9	-3.31	1.33	1.37
1	a	521	7MG	C5-C4	3.20	1.47	1.37
22	v	8	4SU	C5-C4	-3.20	1.38	1.42
1	a	1201	2MG	C5-C4	3.19	1.47	1.38
25	A	735	1MG	C5-C4	3.10	1.47	1.38
1	a	960	2MG	C5-C4	3.07	1.47	1.38
25	A	2056	7MG	C5-C4	3.04	1.47	1.37
25	A	2238	OMG	C5-C4	3.02	1.47	1.38
25	A	1822	2MG	C5-C4	2.99	1.47	1.38
1	a	1510	2MG	C5-C4	2.93	1.46	1.38
1	a	521	7MG	C4-N9	-2.91	1.34	1.37
25	A	1926	5MU	C4-N3	-2.90	1.33	1.38
25	A	2539	OMU	C4-N3	-2.90	1.33	1.38
25	A	2432	2MG	C5-C4	2.88	1.46	1.38
1	a	1513	MA6	C5-C6	2.86	1.48	1.41
25	A	2238	OMG	C6-N1	-2.75	1.33	1.38
25	A	2432	2MG	C6-N1	-2.75	1.33	1.38
25	A	1822	2MG	C6-N1	-2.71	1.33	1.38
25	A	2056	7MG	C6-N1	-2.69	1.33	1.38
22	v	54	5MU	C6-C5	2.69	1.39	1.34
1	a	1512	MA6	C5-C6	2.68	1.48	1.41
25	A	2017	6MZ	C5-C6	2.68	1.48	1.41
22	v	8	4SU	C2-N3	-2.65	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	v	55	PSU	C4-N3	-2.63	1.33	1.38
1	a	961	5MC	C6-C5	2.62	1.38	1.34
22	v	54	5MU	C4-N3	-2.61	1.34	1.38
1	a	1201	2MG	C6-N1	-2.60	1.34	1.38
25	A	1608	6MZ	C5-C6	2.59	1.48	1.41
25	A	2539	OMU	C2-N3	-2.58	1.33	1.38
25	A	1926	5MU	C6-C5	2.57	1.38	1.34
25	A	2490	2MA	C5-C6	2.57	1.48	1.41
22	v	32	5MC	C6-C5	2.57	1.38	1.34
1	a	1512	MA6	C5-N7	-2.55	1.34	1.39
1	a	1510	2MG	C6-N1	-2.55	1.34	1.38
25	A	1949	5MC	C6-C5	2.54	1.38	1.34
1	a	521	7MG	C6-N1	-2.52	1.34	1.38
25	A	1608	6MZ	C5-N7	-2.52	1.34	1.39
25	A	1926	5MU	C6-N1	-2.49	1.33	1.38
1	a	960	2MG	C6-N1	-2.49	1.34	1.38
22	v	54	5MU	C2-N1	2.48	1.42	1.38
25	A	1926	5MU	C2-N3	-2.44	1.33	1.38
25	A	1949	5MC	C6-N1	-2.42	1.33	1.38
22	v	32	5MC	C6-N1	-2.42	1.33	1.38
25	A	2490	2MA	C5-N7	-2.40	1.34	1.39
25	A	2017	6MZ	C5-N7	-2.39	1.34	1.39
1	a	961	5MC	C6-N1	-2.37	1.34	1.38
22	v	54	5MU	C4-C5	2.33	1.48	1.44
25	A	2238	OMG	C5-N7	-2.32	1.34	1.39
25	A	735	1MG	C5-N7	-2.32	1.34	1.39
1	a	1201	2MG	C2-N3	2.30	1.36	1.32
25	A	1902	UR3	C2-N1	2.29	1.41	1.38
1	a	1513	MA6	C5-N7	-2.27	1.34	1.39
25	A	2432	2MG	C5-N7	-2.27	1.34	1.39
25	A	2539	OMU	C5-C4	-2.26	1.38	1.43
22	v	54	5MU	C6-N1	-2.25	1.34	1.38
25	A	735	1MG	C2-N1	2.25	1.41	1.37
25	A	2490	2MA	C8-N7	2.24	1.36	1.31
1	a	1513	MA6	C8-N7	2.23	1.36	1.31
1	a	1201	2MG	C5-N7	-2.19	1.34	1.39
1	a	960	2MG	C5-N7	-2.16	1.34	1.39
1	a	960	2MG	C2-N3	2.16	1.36	1.32
25	A	1822	2MG	C5-N7	-2.15	1.34	1.39
1	a	1513	MA6	C4-N9	-2.14	1.33	1.37
25	A	2017	6MZ	C8-N7	2.14	1.35	1.31
25	A	2017	6MZ	C4-N9	-2.12	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1492	UR3	C2-N1	2.11	1.41	1.38
25	A	1926	5MU	C4-C5	2.09	1.48	1.44
25	A	1608	6MZ	C8-N7	2.08	1.35	1.31
22	v	8	4SU	C2-N1	2.03	1.41	1.38
1	a	1512	MA6	C8-N7	2.02	1.35	1.31
1	a	1510	2MG	C5-N7	-2.01	1.35	1.39
22	v	54	5MU	C2-N3	-2.01	1.34	1.38

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2017	6MZ	C9-N6-C6	-14.98	108.95	122.85
25	A	1608	6MZ	C9-N6-C6	-14.33	109.56	122.85
1	a	521	7MG	N9-C4-N3	9.32	139.12	125.46
25	A	2056	7MG	N9-C4-N3	9.03	138.70	125.46
25	A	2490	2MA	C5-C4-N3	-8.01	118.75	127.18
25	A	2432	2MG	C2-N3-C4	7.40	121.25	112.00
1	a	1510	2MG	C2-N3-C4	7.23	121.04	112.00
1	a	1201	2MG	C2-N3-C4	7.18	120.98	112.00
25	A	1822	2MG	C2-N3-C4	7.14	120.93	112.00
1	a	960	2MG	C2-N3-C4	7.09	120.86	112.00
1	a	1492	UR3	C4-N3-C2	-7.04	118.91	124.58
25	A	1902	UR3	C4-N3-C2	-6.56	119.30	124.58
1	a	1201	2MG	C5-C4-N3	-6.38	118.23	128.39
22	v	55	PSU	N1-C2-N3	6.37	121.89	115.17
25	A	2238	OMG	C5-C4-N3	-6.27	118.42	128.39
25	A	2432	2MG	C5-C4-N3	-6.22	118.49	128.39
25	A	2490	2MA	N3-C4-N9	6.18	134.84	126.99
25	A	1822	2MG	C5-C4-N3	-6.17	118.58	128.39
1	a	960	2MG	C5-C4-N3	-6.14	118.62	128.39
25	A	1608	6MZ	C5-C4-N3	-6.04	118.40	126.72
1	a	1510	2MG	C5-C4-N3	-5.93	118.95	128.39
1	a	1512	MA6	C5-C4-N3	-5.78	118.76	126.72
25	A	2017	6MZ	C5-C4-N3	-5.69	118.89	126.72
1	a	521	7MG	C5-C4-N3	-5.64	117.55	128.13
25	A	2056	7MG	N9-C8-N7	-5.63	95.40	103.37
1	a	1513	MA6	C5-C4-N3	-5.46	119.20	126.72
25	A	1926	5MU	C4-N3-C2	-5.37	120.29	127.34
25	A	2056	7MG	C5-C4-N3	-5.35	118.08	128.13
22	v	8	4SU	C5-C4-N3	5.31	119.69	114.75
25	A	1926	5MU	N3-C2-N1	5.31	121.80	114.89
25	A	735	1MG	C5-C4-N3	-5.25	120.03	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	521	7MG	N9-C8-N7	-5.25	95.94	103.37
22	v	54	5MU	C4-N3-C2	-5.08	120.69	127.34
22	v	54	5MU	N3-C2-N1	5.01	121.42	114.89
25	A	2238	OMG	C2-N3-C4	4.98	120.88	112.30
25	A	2539	OMU	C4-N3-C2	-4.94	120.48	126.61
1	a	1201	2MG	N9-C4-N3	4.89	135.72	125.95
25	A	1608	6MZ	N3-C4-N9	4.77	135.28	127.17
22	v	8	4SU	C4-N3-C2	-4.68	122.83	127.31
1	a	1512	MA6	N3-C4-N9	4.68	135.12	127.17
1	a	1513	MA6	C10-N6-C6	-4.67	108.64	120.52
25	A	2238	OMG	N9-C4-N3	4.67	135.28	125.95
25	A	1822	2MG	N9-C4-N3	4.62	135.19	125.95
1	a	960	2MG	N9-C4-N3	4.61	135.16	125.95
25	A	2432	2MG	N9-C4-N3	4.60	135.16	125.95
1	a	1512	MA6	C10-N6-C6	-4.52	109.03	120.52
25	A	1926	5MU	C5-C4-N3	4.49	119.23	115.32
1	a	521	7MG	C2-N3-C4	4.43	119.93	112.30
25	A	735	1MG	C2-N3-C4	4.37	121.80	111.98
22	v	54	5MU	C5-C4-N3	4.35	119.10	115.32
25	A	2539	OMU	N3-C2-N1	4.30	120.49	114.89
25	A	2056	7MG	C2-N3-C4	4.29	119.69	112.30
1	a	1513	MA6	C9-N6-C6	-4.27	109.67	120.52
1	a	1513	MA6	C2-N1-C6	4.23	122.15	111.83
25	A	2017	6MZ	N3-C4-N9	4.20	134.31	127.17
1	a	1510	2MG	N9-C4-N3	4.17	134.30	125.95
1	a	1513	MA6	N3-C4-N9	4.17	134.26	127.17
1	a	1512	MA6	C2-N1-C6	4.15	121.97	111.83
22	v	55	PSU	C4-N3-C2	-4.14	120.67	126.37
25	A	2539	OMU	C5-C4-N3	4.09	120.53	114.80
25	A	2017	6MZ	C6-C5-N7	4.02	136.81	132.43
22	v	54	5MU	O4-C4-C5	-3.98	120.37	124.92
25	A	735	1MG	N9-C4-N3	3.94	133.83	125.95
25	A	1926	5MU	C5-C6-N1	-3.91	119.06	123.31
25	A	1926	5MU	O4-C4-C5	-3.90	120.45	124.92
25	A	1608	6MZ	C2-N3-C4	3.81	121.13	111.83
25	A	2017	6MZ	C4-C5-N7	-3.81	106.23	110.58
25	A	2017	6MZ	C2-N3-C4	3.76	121.01	111.83
1	a	1512	MA6	N1-C6-N6	3.74	121.42	116.86
1	a	1513	MA6	C4-C5-N7	-3.73	106.32	110.58
1	a	1513	MA6	C2-N3-C4	3.72	120.91	111.83
1	a	1512	MA6	C2-N3-C4	3.67	120.78	111.83
1	a	1512	MA6	C9-N6-C6	-3.66	111.20	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1510	2MG	C6-C5-N7	3.64	136.91	130.29
22	v	55	PSU	O2-C2-N1	-3.62	119.06	122.79
22	v	8	4SU	C5-C4-S4	-3.57	120.23	124.31
25	A	2490	2MA	C4-C5-N7	-3.49	106.59	110.58
1	a	1512	MA6	C4-C5-N7	-3.44	106.65	110.58
1	a	1492	UR3	C5-C4-N3	3.43	119.56	115.04
25	A	1608	6MZ	C4-C5-N7	-3.42	106.67	110.58
1	a	1513	MA6	N1-C2-N3	-3.42	123.41	128.58
25	A	2017	6MZ	N1-C2-N3	-3.36	123.50	128.58
25	A	2432	2MG	C6-C5-N7	3.32	136.33	130.29
25	A	1902	UR3	C5-C4-N3	3.29	119.37	115.04
22	v	54	5MU	C5-C6-N1	-3.29	119.74	123.31
25	A	1608	6MZ	N1-C2-N3	-3.26	123.64	128.58
25	A	1608	6MZ	C6-C5-N7	3.25	135.97	132.43
1	a	1512	MA6	N1-C2-N3	-3.22	123.71	128.58
25	A	1822	2MG	C6-C5-N7	3.19	136.09	130.29
22	v	32	5MC	C5-C6-N1	-3.18	119.86	123.31
25	A	2539	OMU	O4-C4-C5	-3.18	119.68	125.16
1	a	961	5MC	C5-C6-N1	-3.15	119.90	123.31
25	A	1949	5MC	C5-C6-N1	-3.15	119.90	123.31
1	a	960	2MG	C6-C5-N7	3.14	136.00	130.29
22	v	8	4SU	N3-C2-N1	3.10	118.93	114.89
22	v	32	5MC	C5-C4-N3	-3.09	118.59	121.75
25	A	2238	OMG	C6-C5-N7	3.00	135.75	130.29
1	a	1201	2MG	C6-C5-N7	2.92	135.61	130.29
22	v	32	5MC	O2-C2-N3	-2.92	117.73	122.33
25	A	2490	2MA	N6-C6-N1	2.86	120.89	117.03
25	A	1926	5MU	O2-C2-N1	-2.84	119.09	122.80
1	a	1513	MA6	C4-N9-C8	2.80	108.68	105.74
1	a	1513	MA6	N1-C6-N6	2.76	120.22	116.86
1	a	1510	2MG	C4-C5-N7	-2.76	106.30	110.67
25	A	2490	2MA	C4-N9-C8	2.70	108.57	105.74
1	a	521	7MG	C5-C6-N1	2.69	115.68	110.94
25	A	735	1MG	C6-C5-N7	2.69	135.34	129.36
25	A	1949	5MC	C5-C4-N3	-2.68	119.00	121.75
1	a	1513	MA6	C10-N6-C9	-2.68	107.57	116.18
1	a	961	5MC	C5-C4-N3	-2.67	119.02	121.75
1	a	1513	MA6	C5-N7-C8	2.67	107.65	103.45
1	a	1512	MA6	C4-N9-C8	2.67	108.54	105.74
25	A	2490	2MA	C2-N1-C6	2.67	122.20	118.10
25	A	2056	7MG	C5-C6-N1	2.66	115.61	110.94
25	A	2017	6MZ	C5-N7-C8	2.62	107.57	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1510	2MG	N1-C2-N2	2.59	119.21	116.56
1	a	1512	MA6	C5-C6-N6	-2.59	121.24	125.33
25	A	2490	2MA	C5-N7-C8	2.57	107.50	103.45
25	A	735	1MG	C4-C5-N7	-2.57	106.59	110.67
1	a	1512	MA6	C5-N7-C8	2.56	107.48	103.45
25	A	2432	2MG	C4-C5-N7	-2.54	106.64	110.67
25	A	1902	UR3	C1'-N1-C2	2.53	121.18	117.04
25	A	1608	6MZ	C5-N7-C8	2.51	107.39	103.45
1	a	960	2MG	C4-C5-N7	-2.51	106.70	110.67
25	A	1822	2MG	C4-C5-N7	-2.50	106.71	110.67
25	A	1608	6MZ	C4-N9-C8	2.49	108.35	105.74
25	A	2432	2MG	N1-C2-N2	2.49	119.10	116.56
25	A	2238	OMG	C4-C5-N7	-2.45	106.78	110.67
25	A	2056	7MG	C5-C4-N9	-2.44	103.21	106.33
25	A	2017	6MZ	C4-N9-C8	2.43	108.29	105.74
22	v	8	4SU	C1'-N1-C2	2.43	121.95	117.59
1	a	1201	2MG	C4-C5-N7	-2.41	106.86	110.67
1	a	1396	4OC	C6-C5-C4	2.40	119.89	117.00
25	A	2485	OMC	O2-C2-N3	-2.35	118.63	122.33
1	a	521	7MG	C5-C4-N9	-2.35	103.33	106.33
25	A	2490	2MA	C6-C5-N7	2.28	136.49	132.09
1	a	1396	4OC	O2-C2-N3	-2.28	118.73	122.33
1	a	1513	MA6	C6-C5-N7	2.27	137.06	133.43
25	A	2432	2MG	O6-C6-C5	-2.24	120.61	126.53
1	a	1512	MA6	C10-N6-C9	-2.23	109.02	116.18
1	a	960	2MG	O6-C6-C5	-2.22	120.68	126.53
25	A	1902	UR3	C6-N1-C2	-2.20	120.00	121.80
1	a	1513	MA6	N9-C8-N7	-2.20	110.82	113.94
22	v	55	PSU	C5-C6-N1	-2.16	119.14	122.14
1	a	1201	2MG	O6-C6-C5	-2.16	120.83	126.53
25	A	2539	OMU	O2-C2-N1	-2.15	120.00	122.80
25	A	2238	OMG	O6-C6-C5	-2.13	120.91	126.53
25	A	2490	2MA	N9-C8-N7	-2.12	110.92	113.94
1	a	1510	2MG	O6-C6-C5	-2.12	120.93	126.53
1	a	521	7MG	O6-C6-C5	-2.10	122.46	127.62
25	A	1822	2MG	O6-C6-C5	-2.09	121.01	126.53
25	A	2056	7MG	O6-C6-C5	-2.07	122.54	127.62
1	a	1513	MA6	C5-C6-N6	-2.06	122.07	125.33
25	A	2432	2MG	C2-N1-C6	-2.05	122.07	124.55
1	a	960	2MG	N1-C2-N2	2.05	118.65	116.56
1	a	1510	2MG	C2-N1-C6	-2.04	122.08	124.55
1	a	1510	2MG	N2-C2-N3	-2.04	117.91	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2432	2MG	C5-C6-N1	2.02	118.39	113.25
25	A	2017	6MZ	C2-N1-C6	2.01	121.91	115.24
1	a	1201	2MG	C2-N1-C6	-2.01	122.12	124.55
1	a	960	2MG	C2-N1-C6	-2.00	122.13	124.55

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1201	2MG	O4'-C4'-C5'-O5'
25	A	2238	OMG	O4'-C4'-C5'-O5'
1	a	521	7MG	C3'-C4'-C5'-O5'
1	a	1201	2MG	C3'-C4'-C5'-O5'
1	a	1396	4OC	O4'-C4'-C5'-O5'
1	a	1513	MA6	O4'-C4'-C5'-O5'
1	a	521	7MG	O4'-C4'-C5'-O5'
25	A	2056	7MG	O4'-C4'-C5'-O5'
25	A	2056	7MG	C3'-C4'-C5'-O5'
25	A	2017	6MZ	O4'-C4'-C5'-O5'
25	A	2238	OMG	C3'-C4'-C5'-O5'
25	A	2017	6MZ	C3'-C4'-C5'-O5'
1	a	1396	4OC	C3'-C4'-C5'-O5'
1	a	1513	MA6	C3'-C4'-C5'-O5'
1	a	1512	MA6	C5-C6-N6-C9
1	a	1513	MA6	C5-C6-N6-C9
25	A	2485	OMC	O4'-C4'-C5'-O5'
1	a	1513	MA6	N1-C6-N6-C9
22	v	8	4SU	O4'-C4'-C5'-O5'
1	a	1201	2MG	C4'-C5'-O5'-P
25	A	2490	2MA	C4'-C5'-O5'-P

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	2017	6MZ	1	0
25	A	2485	OMC	2	0
1	a	1510	2MG	1	0
22	v	54	5MU	2	0
22	v	8	4SU	3	0
1	a	1513	MA6	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	a	1512	MA6	2	0
1	a	1396	4OC	2	0
1	a	961	5MC	2	0
25	A	1926	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 599 ligands modelled in this entry, 597 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
60	GCP	x	902	58	32,34,34	1.38	5 (15%)	49,54,54	1.75	7 (14%)
59	FME	v	102	22	8,9,10	0.40	0	8,9,11	1.23	1 (12%)

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
60	GCP	x	902	58	-	1/19/38/38	0/3/3/3
59	FME	v	102	22	-	1/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	x	902	GCP	C5-C4	3.06	1.47	1.38
60	x	902	GCP	PG-O3G	2.72	1.61	1.55
60	x	902	GCP	PG-O2G	2.62	1.60	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	x	902	GCP	C6-N1	-2.55	1.34	1.38
60	x	902	GCP	C5-N7	-2.09	1.34	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	x	902	GCP	C5-C4-N3	-5.93	118.95	128.39
60	x	902	GCP	C2-N3-C4	4.95	120.82	112.30
60	x	902	GCP	N9-C4-N3	4.38	134.71	125.95
60	x	902	GCP	C6-C5-N7	3.37	136.43	130.29
60	x	902	GCP	PB-O3A-PA	-2.94	122.76	132.37
60	x	902	GCP	C4-C5-N7	-2.55	106.62	110.67
60	x	902	GCP	O6-C6-C5	-2.10	120.99	126.53
59	v	102	FME	O1-CN-N	-2.02	120.09	125.32

There are no chirality outliers.

All (2) torsion outliers are listed below:

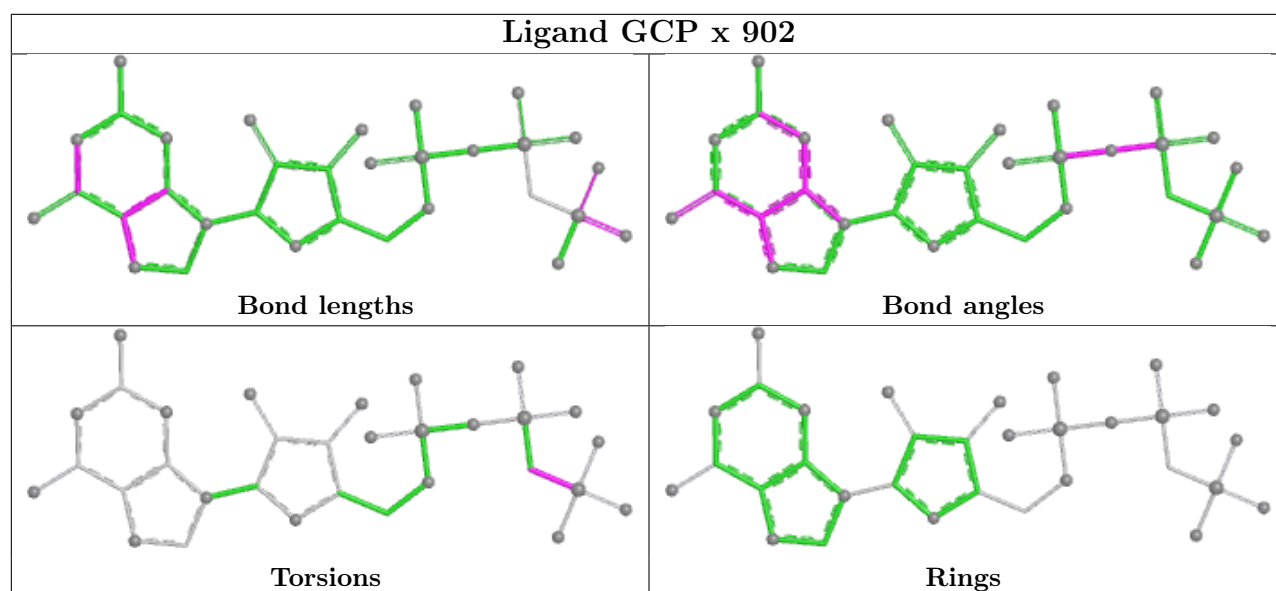
Mol	Chain	Res	Type	Atoms
59	v	102	FME	CB-CG-SD-CE
60	x	902	GCP	PB-C3B-PG-O1G

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	x	902	GCP	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

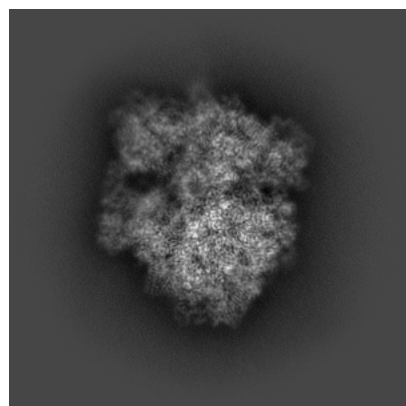
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26634. These allow visual inspection of the internal detail of the map and identification of artifacts.

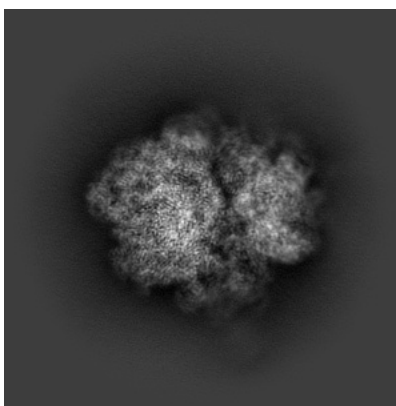
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

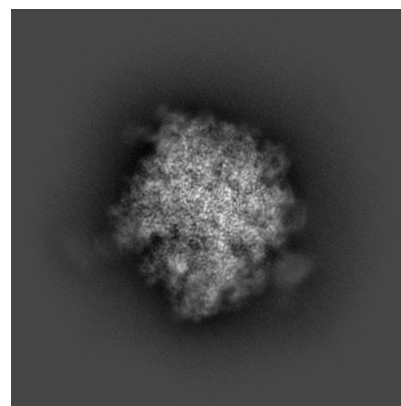
6.1.1 Primary map



X

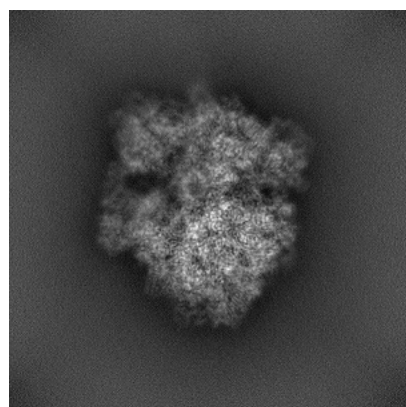


Y

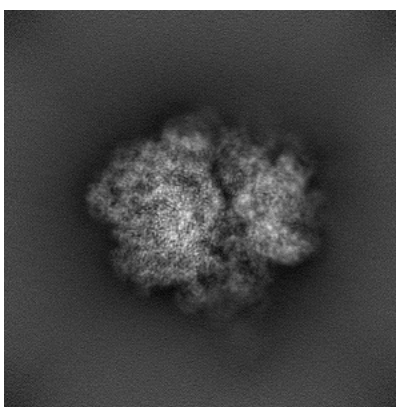


Z

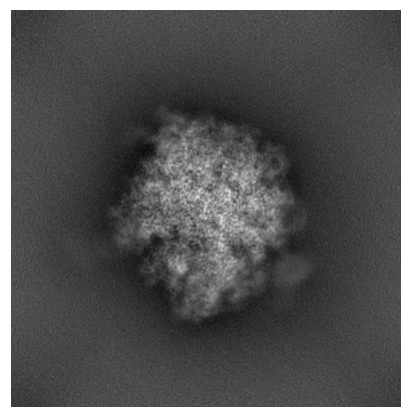
6.1.2 Raw map



X



Y

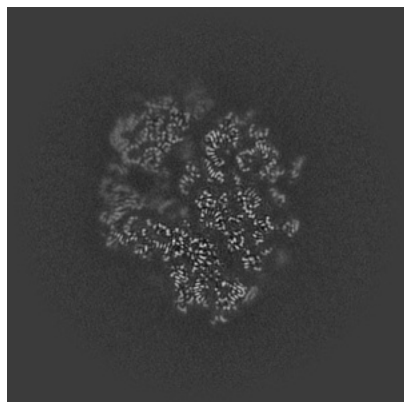


Z

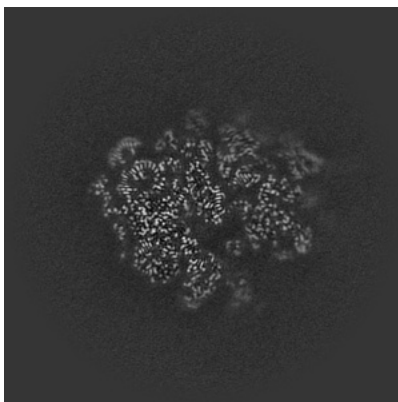
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

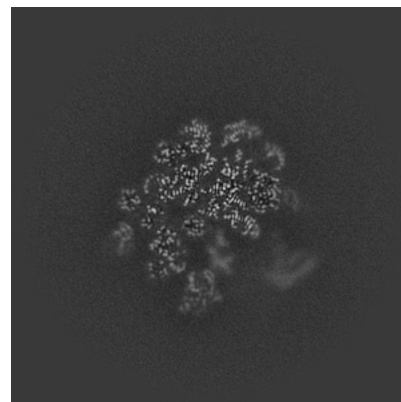
6.2.1 Primary map



X Index: 256

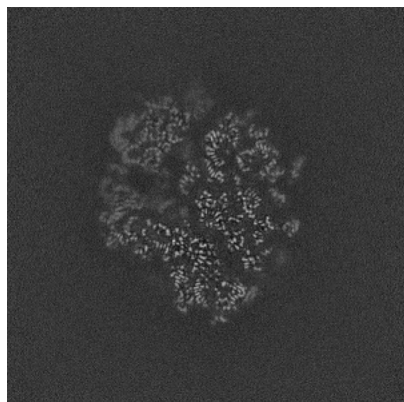


Y Index: 256

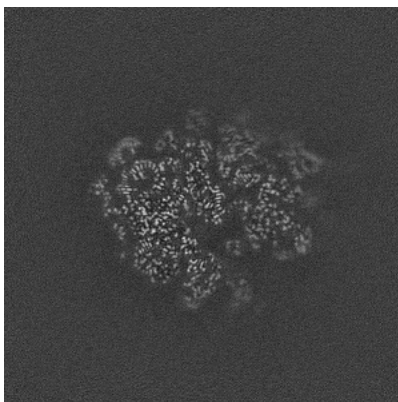


Z Index: 256

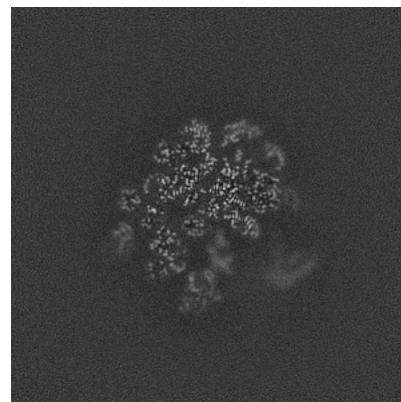
6.2.2 Raw map



X Index: 256



Y Index: 256

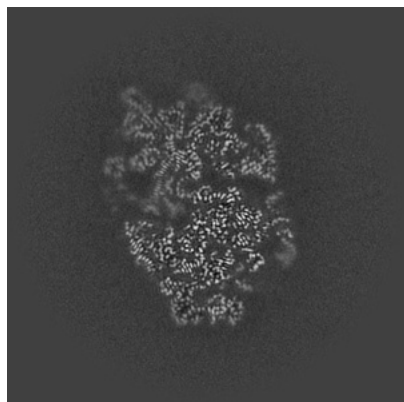


Z Index: 256

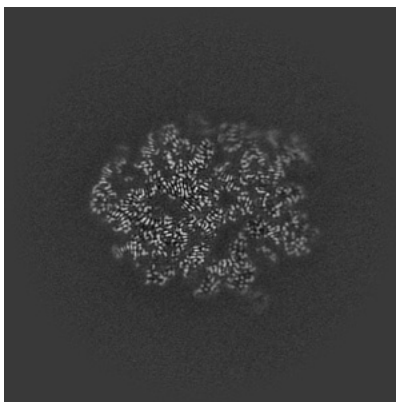
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

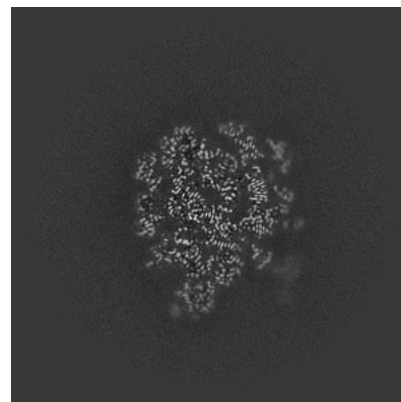
6.3.1 Primary map



X Index: 270

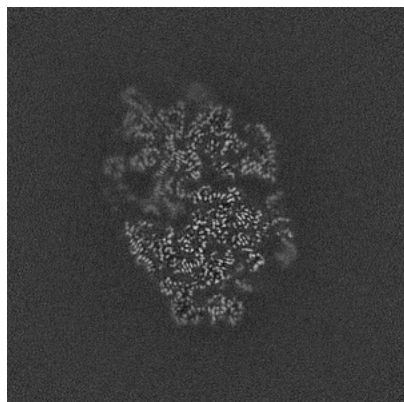


Y Index: 270

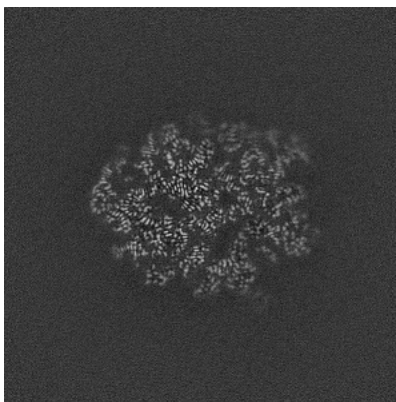


Z Index: 211

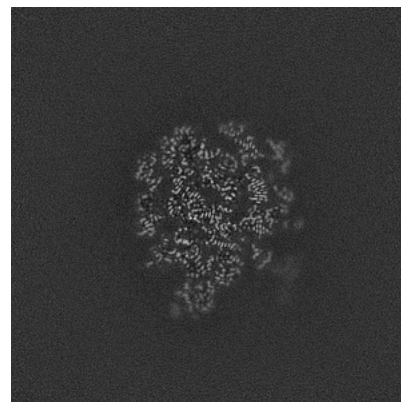
6.3.2 Raw map



X Index: 270



Y Index: 270

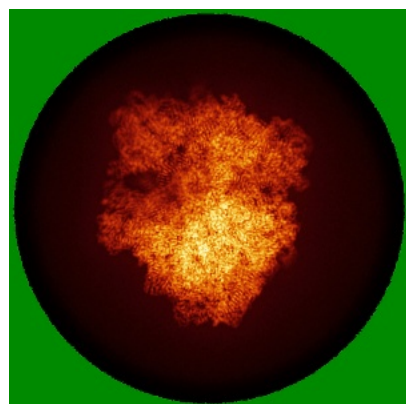


Z Index: 211

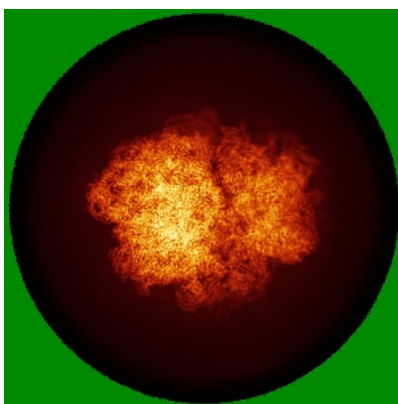
The images above show the largest variance slices of the map in three orthogonal directions.

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

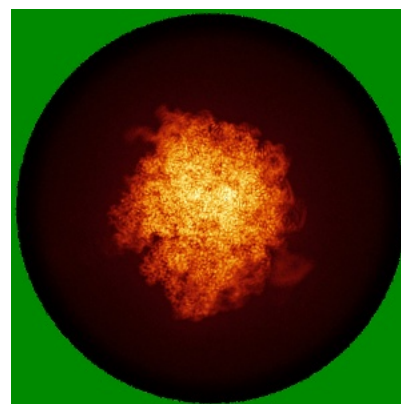
6.4.1 Primary map



X

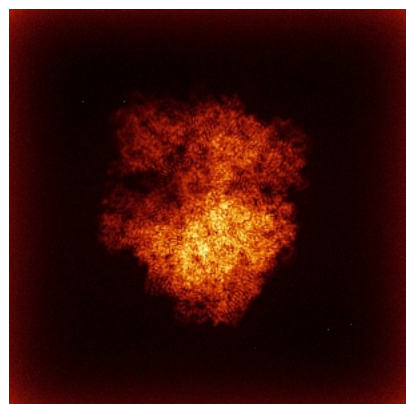


Y

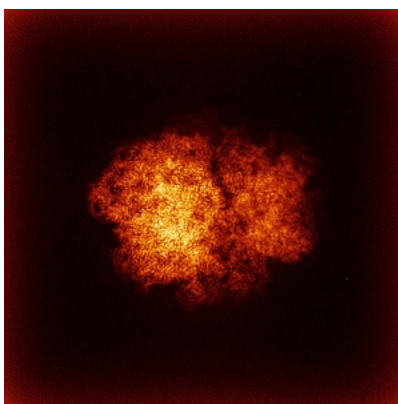


Z

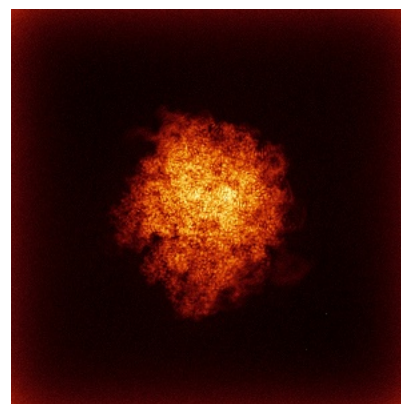
6.4.2 Raw map



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



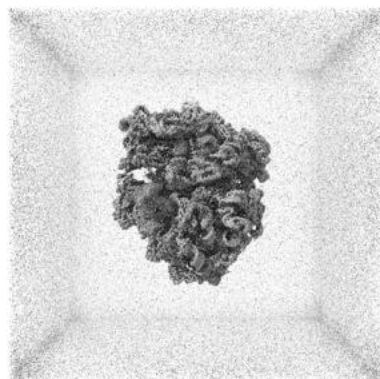
Y



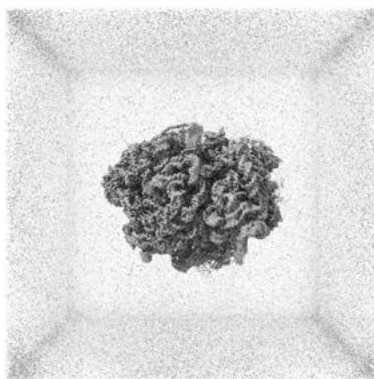
Z

The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

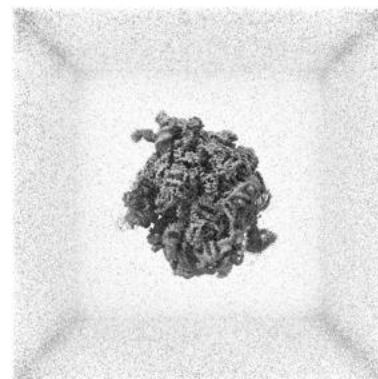
6.5.2 Raw map



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.

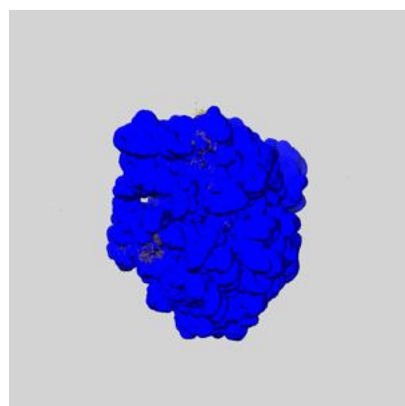
6.6 Mask visualisation [i](#)

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

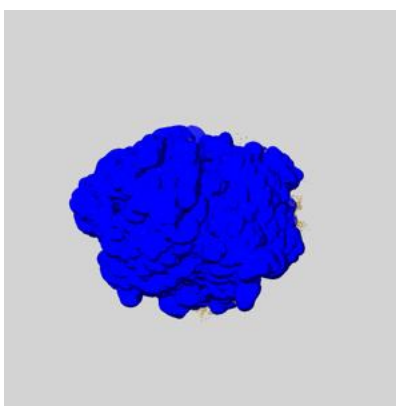
A mask typically either:

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

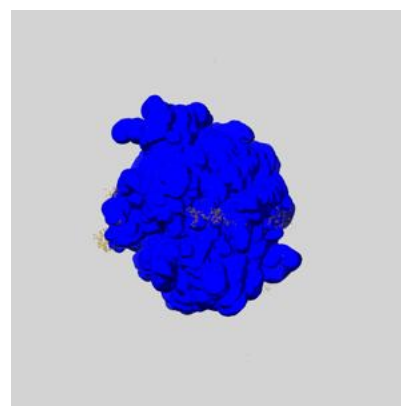
6.6.1 emd_26634_msk_1.map [i](#)



X



Y

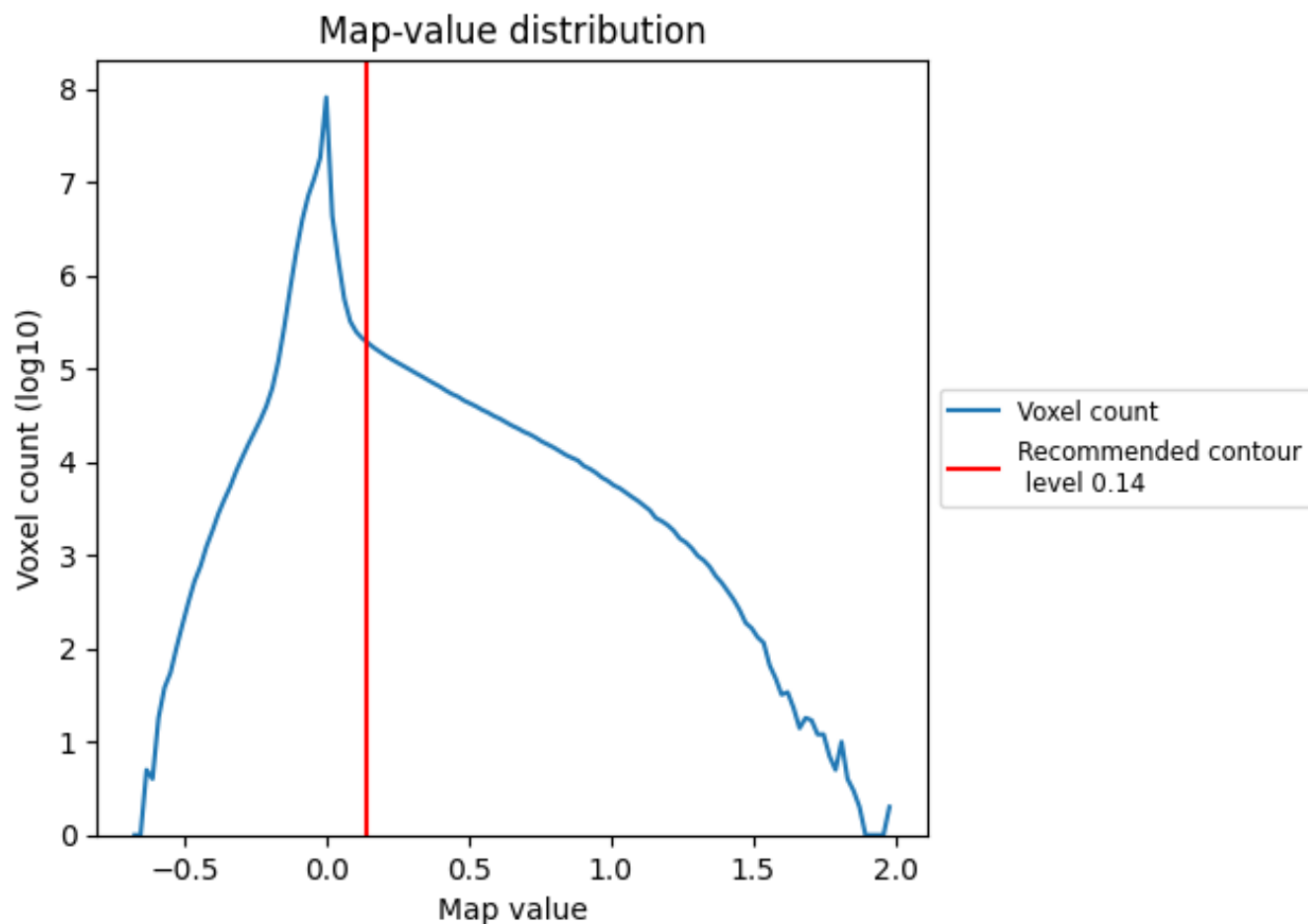


Z

7 Map analysis [i](#)

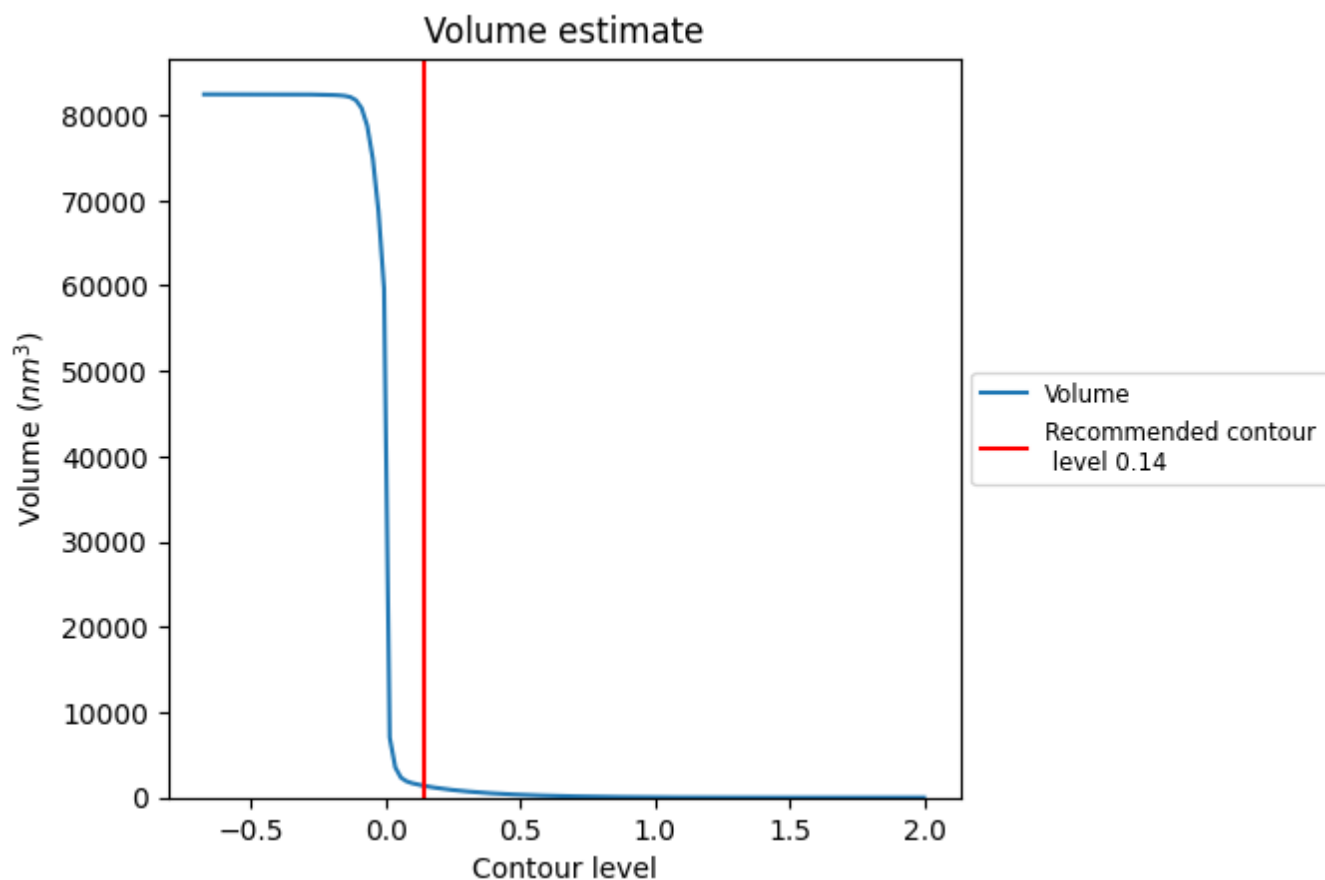
This section contains the results of statistical analysis of the map.

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.

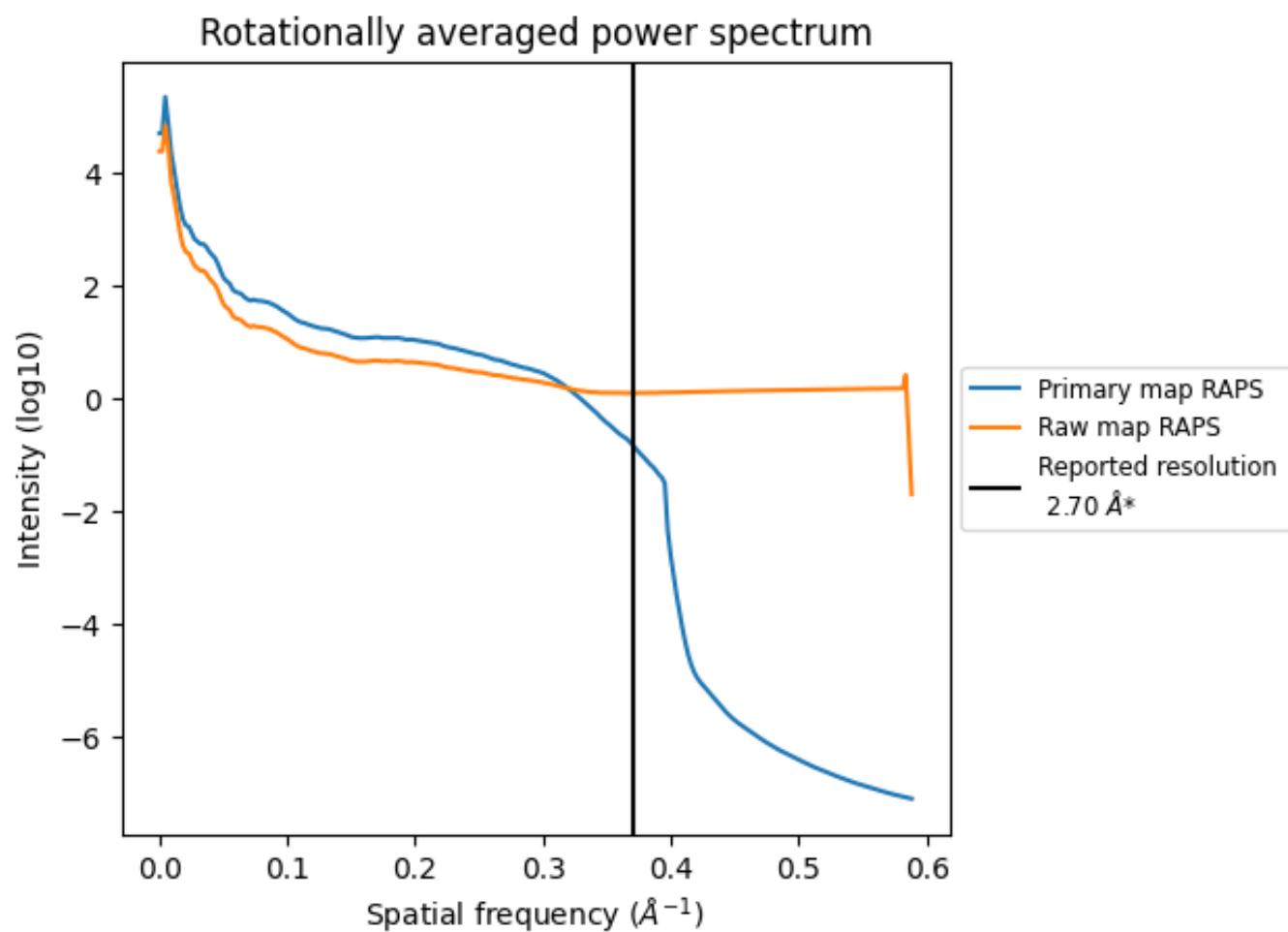
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1392 nm^3 ; this corresponds to an approximate mass of 1258 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

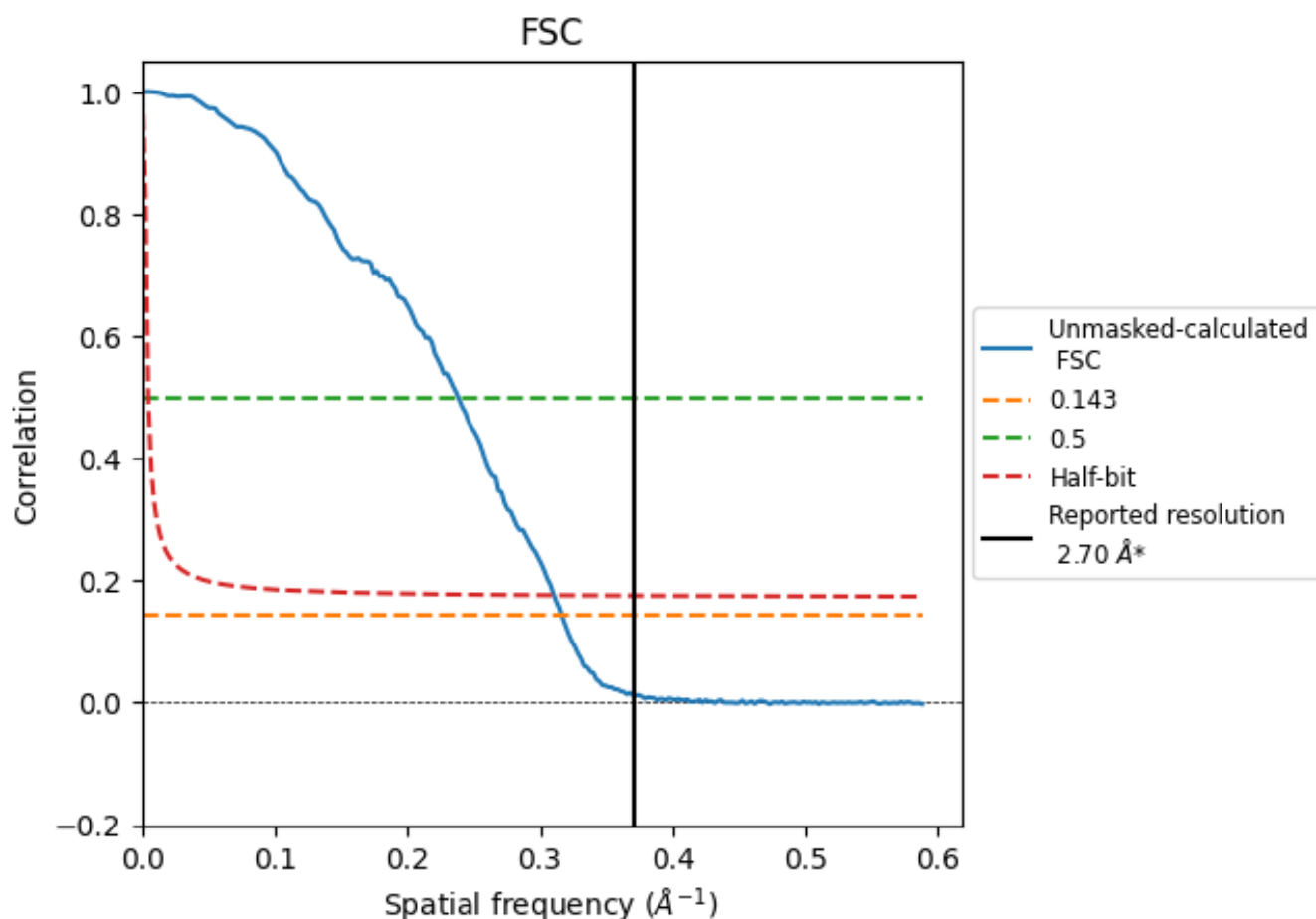


*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

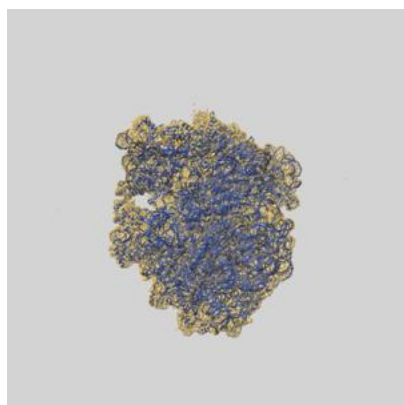
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.16	4.20	3.22

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

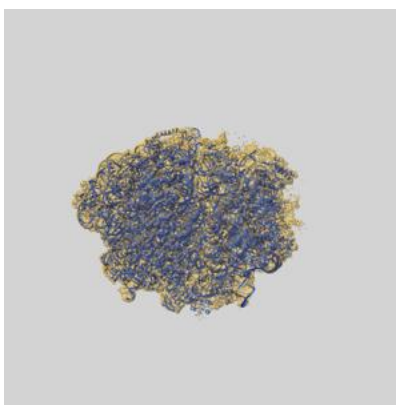
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26634 and PDB model 7UNV. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

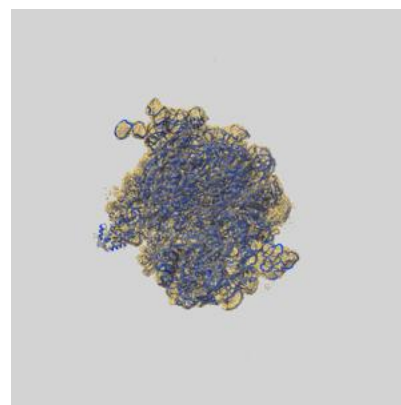
9.1 Map-model overlay [i](#)



X



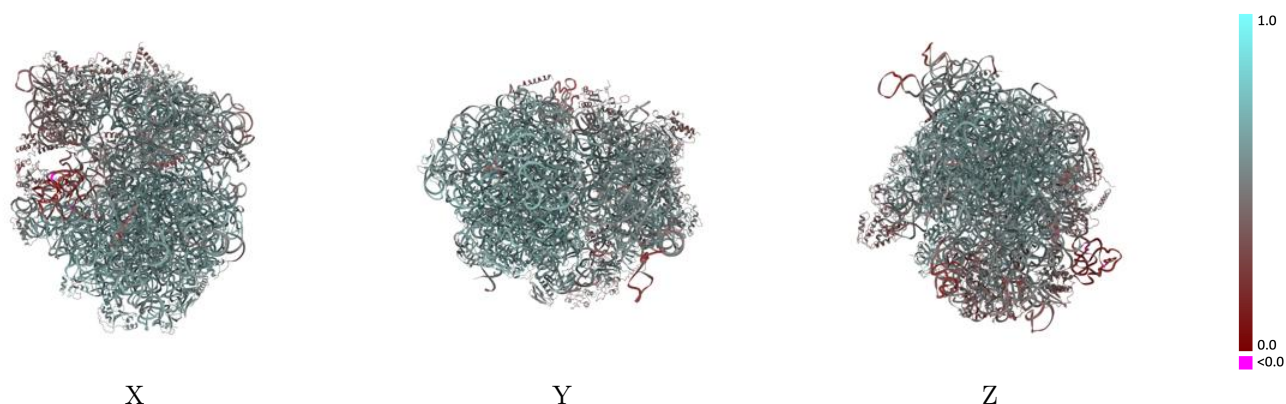
Y



Z

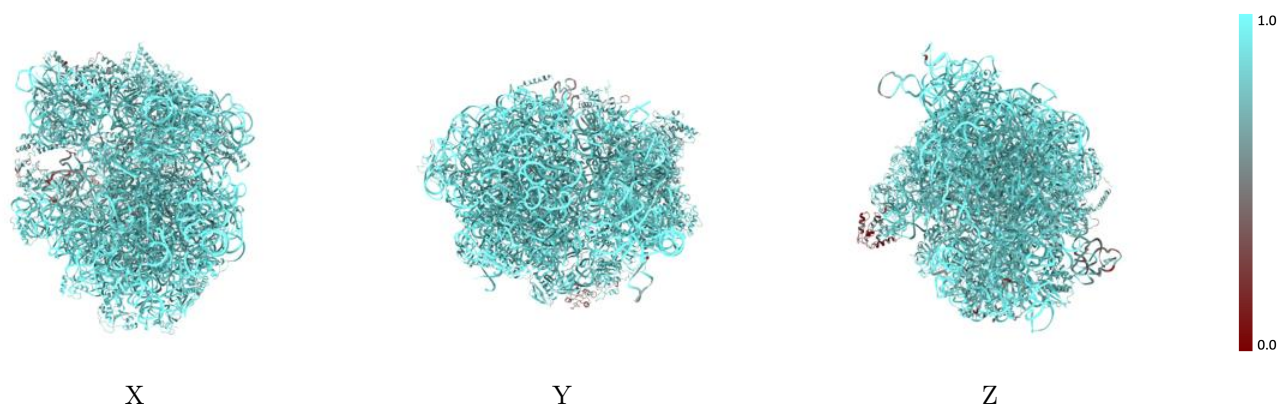
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



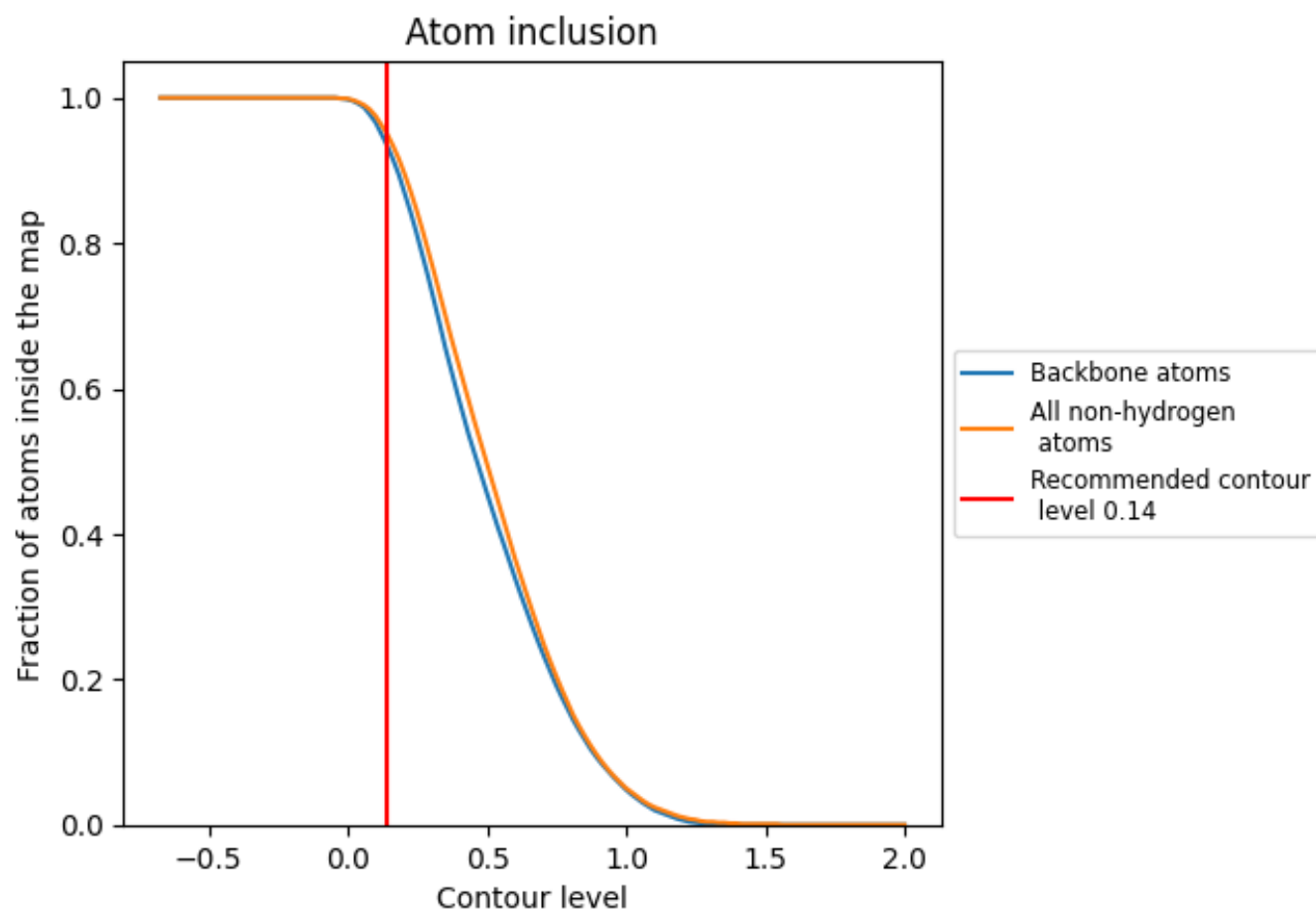
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.14).

9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9500	 0.5540
1	 0.9250	 0.5560
2	 0.9610	 0.5990
3	 0.5810	 0.3460
4	 0.9410	 0.5940
5	 0.9010	 0.5720
6	 0.9710	 0.6220
7	 0.9780	 0.6260
8	 0.9420	 0.6070
A	 0.9820	 0.5920
B	 0.9920	 0.5470
C	 0.9640	 0.6130
D	 0.9480	 0.5980
E	 0.9510	 0.5880
F	 0.8220	 0.4250
G	 0.8970	 0.5390
H	 0.8080	 0.4670
I	 0.2610	 0.3650
J	 0.7740	 0.3840
L	 0.9640	 0.6020
M	 0.9470	 0.6060
N	 0.9600	 0.5970
O	 0.9520	 0.6130
P	 0.9710	 0.6060
Q	 0.9210	 0.5310
R	 0.9420	 0.5960
S	 0.9730	 0.6120
T	 0.9470	 0.5850
U	 0.9470	 0.5970
V	 0.9440	 0.5810
W	 0.8820	 0.5380
X	 0.9250	 0.5570
Y	 0.9590	 0.6120
Z	 0.9550	 0.5980
a	 0.9850	 0.5300



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Chain	Atom inclusion	Q-score
b	 0.8080	 0.4340
c	 0.8580	 0.4940
d	 0.8960	 0.5280
e	 0.9170	 0.5460
f	 0.8440	 0.4070
g	 0.7830	 0.3990
h	 0.9120	 0.5380
i	 0.8530	 0.4210
j	 0.7850	 0.4350
k	 0.8450	 0.4570
l	 0.9300	 0.5780
m	 0.8130	 0.3890
n	 0.8630	 0.4420
o	 0.9210	 0.5200
p	 0.9450	 0.5580
q	 0.9250	 0.5380
r	 0.8010	 0.4440
s	 0.7800	 0.3840
t	 0.9240	 0.5330
u	 0.7860	 0.4480
v	 0.9410	 0.4170
w	 0.9770	 0.5630
x	 0.8900	 0.5250