



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 04:59 PM EDT

PDB ID : 7S1H / pdb_00007s1h
EMDB ID : EMD-24801
Title : Wild-type Escherichia coli ribosome with antibiotic linezolid
Authors : Young, I.D.; Stojkovic, V.; Tsai, K.; Lee, D.J.; Fraser, J.S.; Galonic Fujimori, D.
Deposited on : 2021-09-02
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

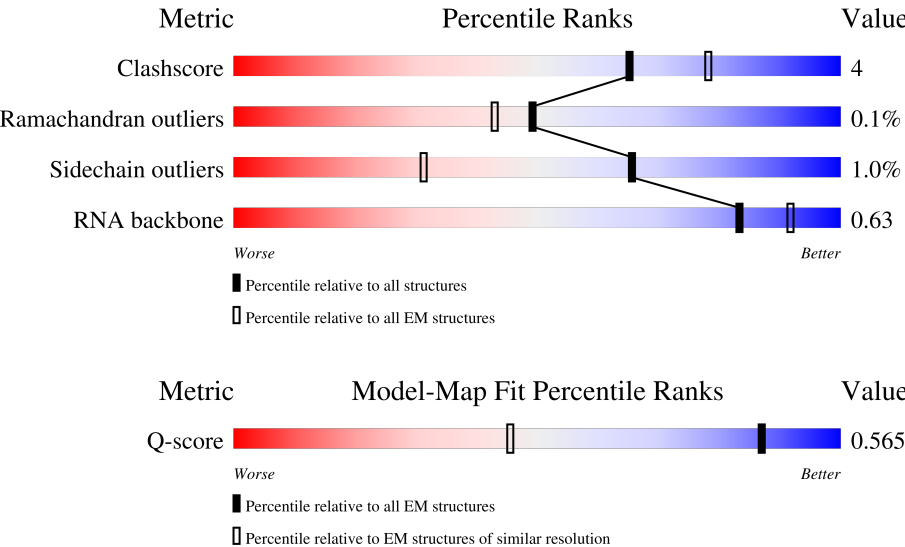
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.35 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.



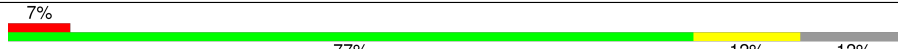
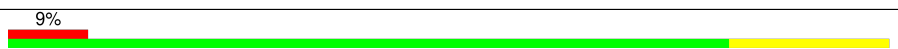
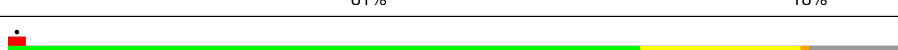
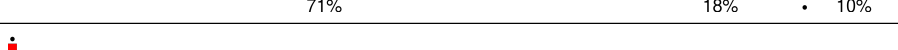
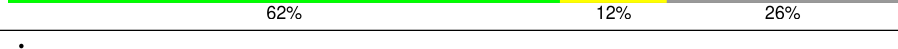
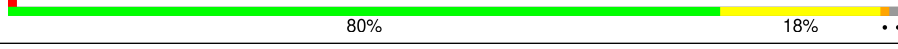
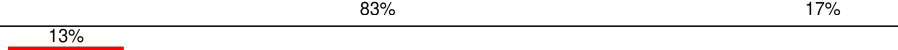
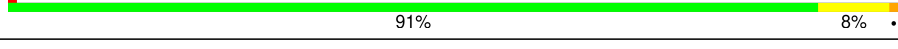
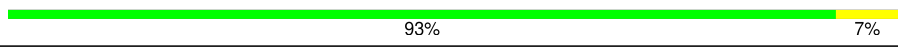
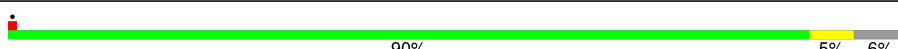
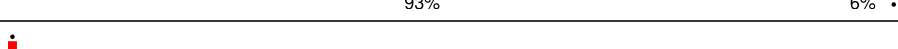
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	4607 (1.85 - 2.85)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	92	11% 76% 10% 14%
2	2	87	5% 84% 14% •
3	3	71	72% 80% 18% •

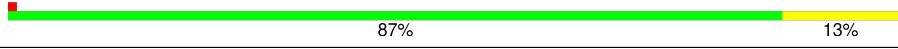
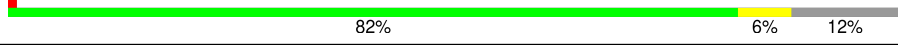
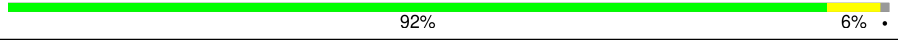
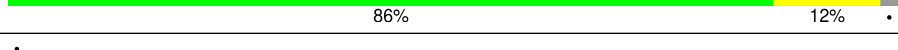
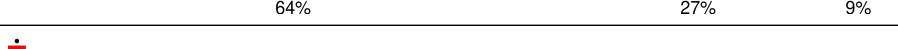
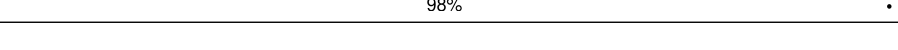
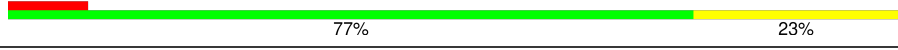
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Mol	Chain	Length	Quality of chain
4	C	1540	
5	D	240	
6	E	233	
7	F	206	
8	G	167	
9	H	135	
10	I	2904	
11	J	120	
12	K	273	
13	L	209	
14	M	201	
15	N	179	
16	O	177	
17	P	149	
18	Q	70	
19	R	142	
20	S	123	
21	T	144	
22	U	136	
23	V	127	
24	W	117	
25	X	115	
26	Y	118	
27	Z	103	
28	a	110	

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Mol	Chain	Length	Quality of chain
29	b	100	
30	c	104	
31	d	94	
32	e	85	
33	f	78	
34	g	63	
35	h	59	
36	i	57	
37	j	55	
38	k	46	
39	l	65	
40	m	38	
41	n	179	
42	o	130	
43	p	130	
44	q	103	
45	r	129	
46	t	124	
47	u	118	
48	v	101	
49	w	89	
50	x	82	
51	y	84	
52	z	75	

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 238184 atoms, of which 95792 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1	79	Total	C	H	N	O	S	0	0
			1303	408	666	120	107	2		

- Molecule 2 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	2	85	Total	C	H	N	O	S	0	0
			1380	411	715	137	114	3		

- Molecule 3 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	3	70	Total	C	H	N	O	S	0	0
			1219	366	629	125	98	1		

- Molecule 4 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	C	1540	Total	C	H	N	O	P	0	0
			49665	14735	16628	6057	10705	1540		

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	D	218	Total	C	H	N	O	S	0	0
			3438	1081	1734	305	311	7		

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	E	206	Total	C	H	N	O	S	0	0
			3321	1028	1697	305	288	3		

- Molecule 7 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	F	205	Total	C	H	N	O	S	0	0
			3352	1026	1709	315	298	4		

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	G	150	Total	C	H	N	O	S	0	0
			2255	687	1150	211	201	6		

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	H	100	Total	C	H	N	O	S	0	0
			1625	515	808	148	148	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	I	2898	Total	C	H	N	O	P	2	0
			93613	27787	31342	11455	20129	2900		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	J	118	Total	C	H	N	O	P	0	0
			3809	1126	1280	464	821	118		

- Molecule 12 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	K	271	Total	C	H	N	O	S	2	0
			4263	1294	2170	427	365	7		

- Molecule 13 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	L	209	Total	C	H	N	O	S	0	0
			3184	979	1619	288	294	4		

- Molecule 14 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	M	201	Total	C	H	N	O	S	0	0
			3172	974	1620	283	290	5		

- Molecule 15 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	N	177	Total	C	H	N	O	S	0	0
			2855	899	1445	249	256	6		

- Molecule 16 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	O	176	Total	C	H	N	O	S	0	0
			2696	832	1373	243	246	2		

- Molecule 17 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	P	149	Total	C	H	N	O	S	0	0
			2259	699	1148	197	214	1		

- Molecule 18 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	Q	60	Total	C	H	N	O	S	0	0
			963	299	483	90	85	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
19	R	142	Total	C	H	N	O	S	0	0
			2291	714	1162	212	199	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
20	S	122	Total	C	H	N	O	S	0	0
			1951	587	1013	180	165	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
21	T	144	Total	C	H	N	O	S	0	0
			2182	654	1129	207	190	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
22	U	136	Total	C	H	N	O	S	0	0
			2231	686	1156	205	178	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
23	V	120	Total	C	H	N	O	S	0	0
			1961	593	1001	196	166	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	116	Total	C	H	N	O	0	0
			1817	552	925	178	162		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
25	X	114	Total	C	H	N	O	S	0	0
			1880	574	963	179	163	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	117	Total	C	H	N	O	0	0
			1968	604	1021	192	151		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
27	Z	103	Total	C	H	N	O	S	0	0
			1657	516	841	153	145	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
28	a	110	Total	C	H	N	O	S	0	0
			1780	532	923	166	156	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
29	b	93	Total	C	H	N	O	S	0	0
			1546	466	808	139	131	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
30	c	102	Total	C	H	N	O	S	0	0
			1611	492	832	146	141			

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

Mol	Chain	Residues	Atoms						AltConf	Trace
31	d	94	Total	C	H	N	O	S	0	0
			1534	479	781	137	134	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
32	e	75	Total	C	H	N	O	S	0	0
			1168	356	593	116	102	1		

- Molecule 33 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	f	77	Total	C	H	N	O	S	0	0
			1278	388	653	129	106	2		

- Molecule 34 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	g	62	Total	C	H	N	O	S	0	0
			1033	308	532	98	94	1		

- Molecule 35 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	h	58	Total	C	H	N	O	S	0	0
			938	281	489	87	79	2		

- Molecule 36 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	i	56	Total	C	H	N	O	S	0	0
			904	269	460	94	80	1		

- Molecule 37 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	j	50	Total	C	H	N	O		0	0
			851	263	442	75	71			

- Molecule 38 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	k	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

- Molecule 39 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	l	64	Total	C	H	N	O	S	0	0
			1077	323	573	105	74	2		

- Molecule 40 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	m	38	Total	C	H	N	O	S	0	0
			645	185	343	65	48	4		

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	n	151	Total	C	H	N	O	S	0	0
			2419	735	1238	227	215	4		

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	o	129	Total	C	H	N	O	S	0	0
			2011	616	1032	173	184	6		

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	p	127	Total	C	H	N	O	S	0	0
			2093	634	1071	206	179	3		

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	q	98	Total	C	H	N	O	S	0	0
			1615	493	829	150	142	1		

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	r	117	Total	C	H	N	O	S	0	0
			1765	540	888	174	160	3		

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	t	123	Total	C	H	N	O	S	0	0
			1972	590	1017	196	165	4		

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	u	115	Total	C	H	N	O	S	0	0
			1845	552	954	179	157	3		

- Molecule 48 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	v	96	Total	C	H	N	O	S	0	0
			1600	483	826	160	128	3		

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	w	88	Total	C	H	N	O	S	0	0
			1441	437	731	143	129	1		

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	x	82	Total	C	H	N	O	S	0	0
			1315	406	666	128	114	1		

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	y	80	Total	C	H	N	O	S	0	0
			1341	411	693	121	113	3		

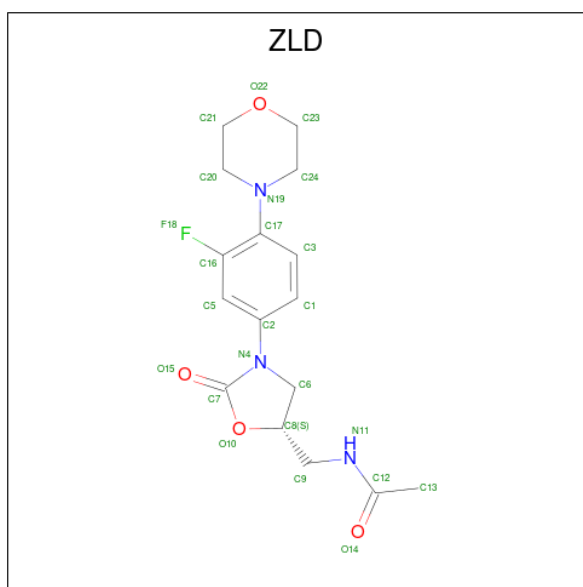
- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	z	55	Total	C	H	N	O	0	0
			934	288	479	86	81		

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	C	89	Total	Mg	0
			89	89	
53	I	113	Total	Mg	0
			113	113	
53	K	1	Total	Mg	0
			1	1	
53	L	1	Total	Mg	0
			1	1	
53	V	1	Total	Mg	0
			1	1	
53	q	1	Total	Mg	0
			1	1	

- Molecule 54 is N-{[(5S)-3-(3-fluoro-4-morpholin-4-ylphenyl)-2-oxo-1,3-oxazolidin-5-yl]methyl}acetamide (CCD ID: ZLD) (formula: C₁₆H₂₀FN₃O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
54	I	1	Total	C	F	H	N	O	0
			44	16	1	20	3	4	

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	Q	1	Total	Zn	0
			1	1	
55	m	1	Total	Zn	0
			1	1	

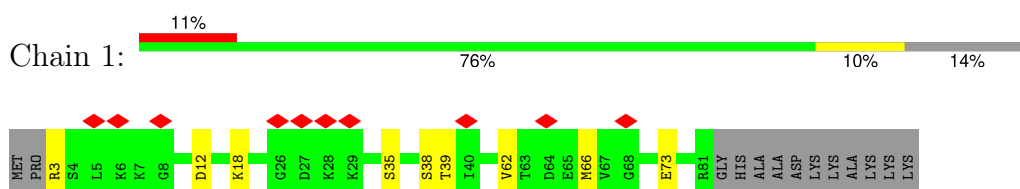
- Molecule 56 is water.

Mol	Chain	Residues	Atoms			AltConf
56	C	4	Total	H	O	0
			12	8	4	
56	I	32	Total	H	O	0
			96	64	32	
56	c	1	Total	H	O	0
			3	2	1	

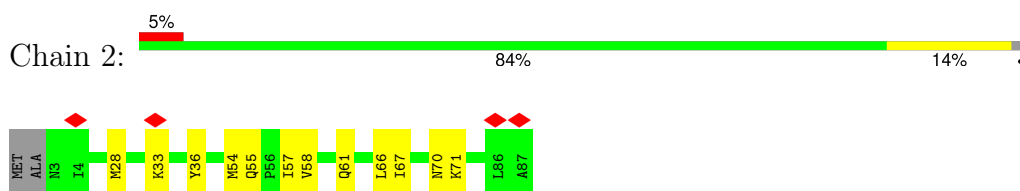
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

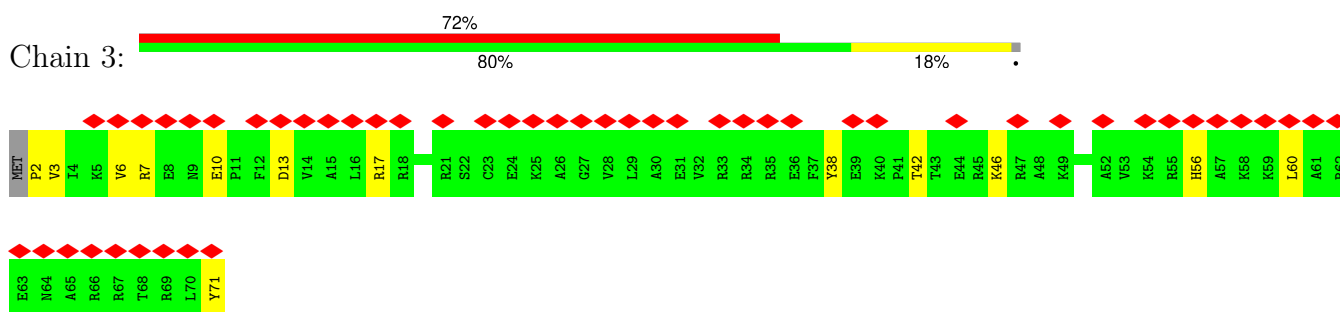
- Molecule 1: 30S ribosomal protein S19



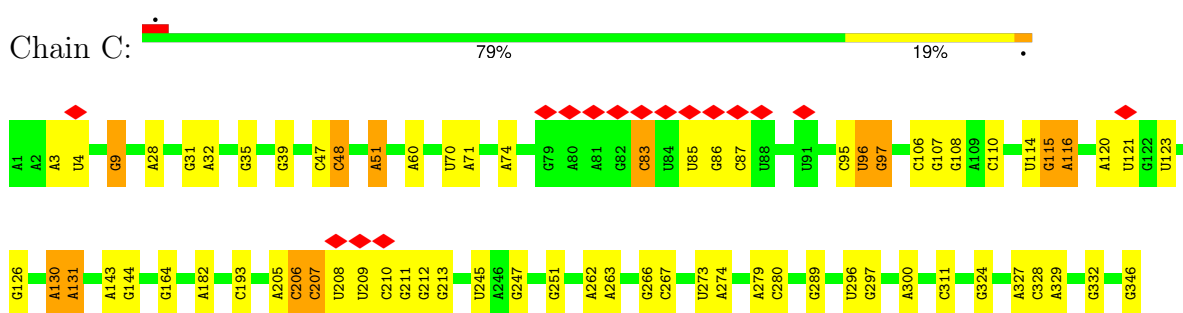
- Molecule 2: 30S ribosomal protein S20

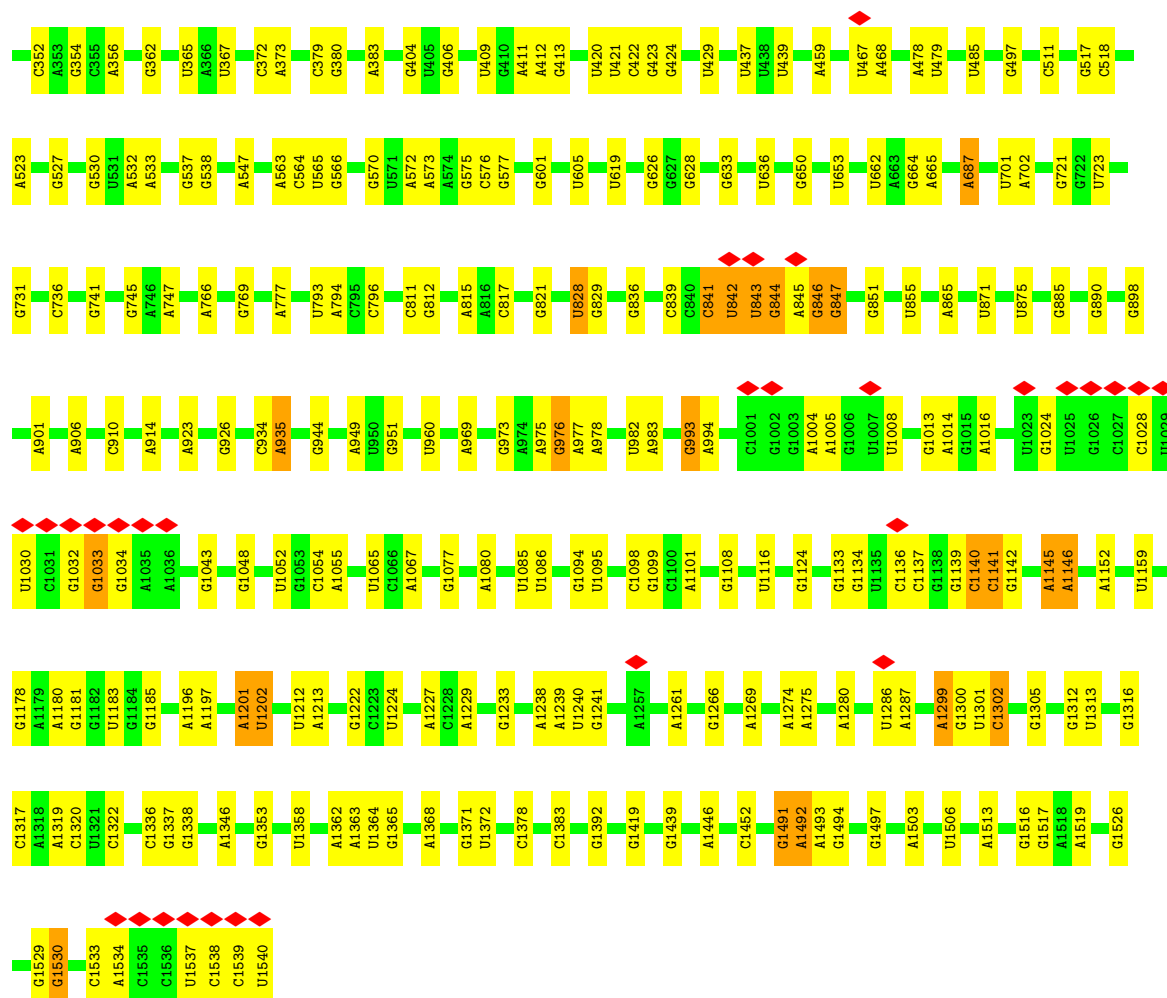


- Molecule 3: 30S ribosomal protein S21

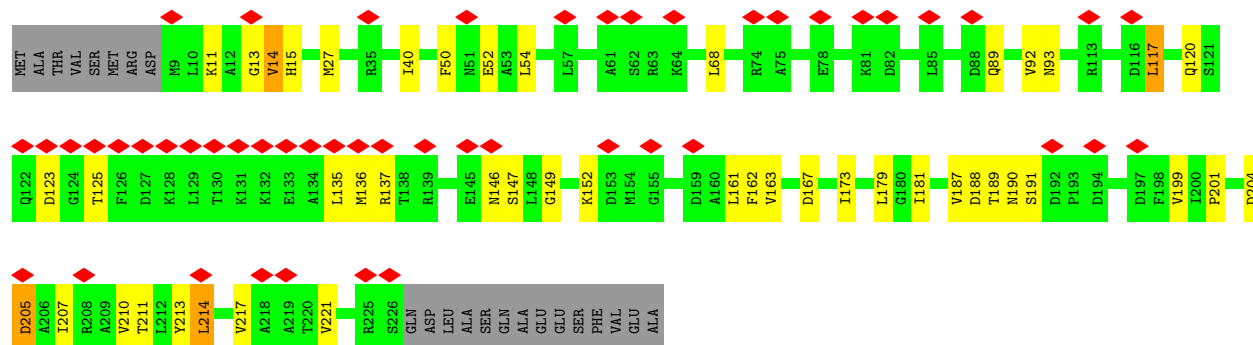


- Molecule 4: 16S rRNA

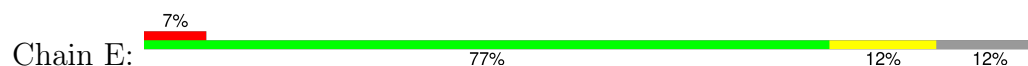


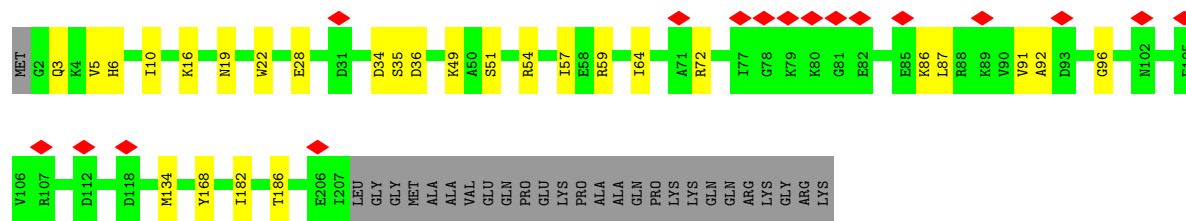


• Molecule 5: 30S ribosomal protein S2

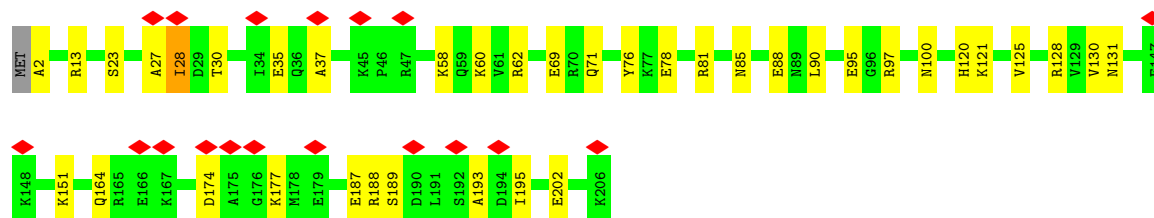
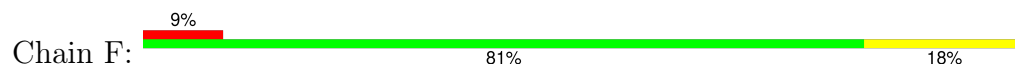


• Molecule 6: 30S ribosomal protein S3





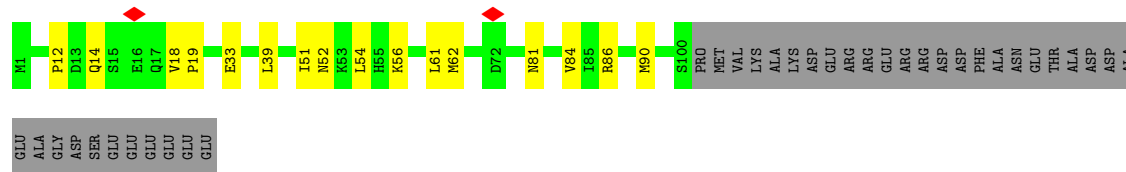
• Molecule 7: 30S ribosomal protein S4



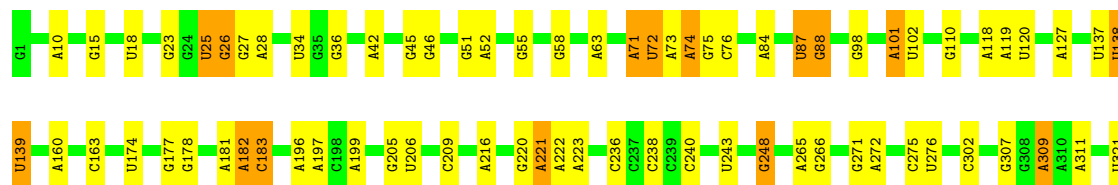
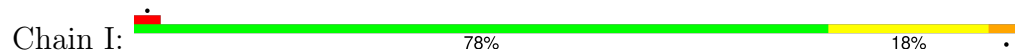
• Molecule 8: 30S ribosomal protein S5



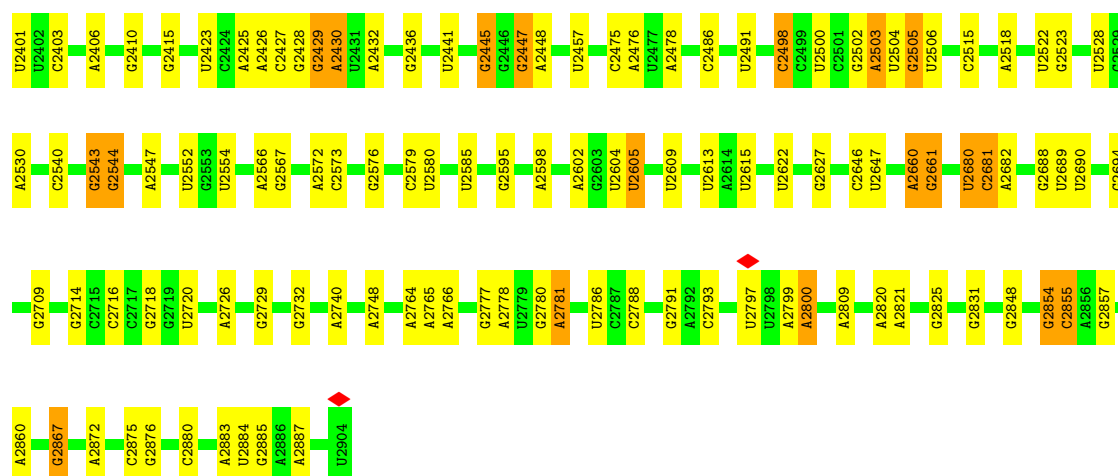
• Molecule 9: 30S ribosomal protein S6



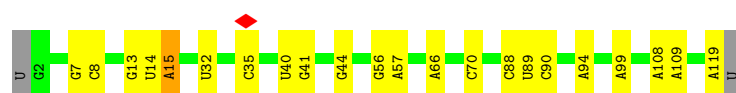
• Molecule 10: 23S rRNA







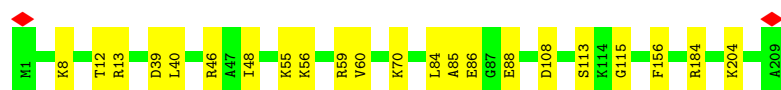
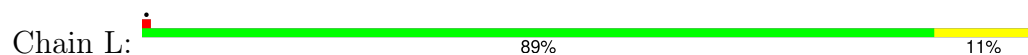
• Molecule 11: 5S rRNA



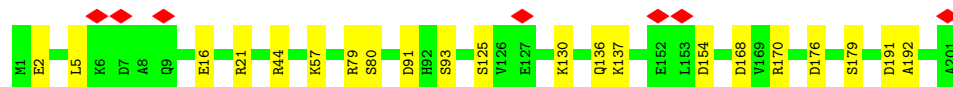
• Molecule 12: 50S ribosomal protein L2



• Molecule 13: 50S ribosomal protein L3

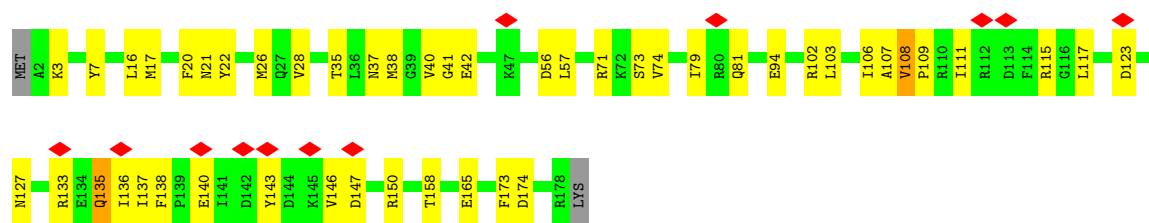


• Molecule 14: 50S ribosomal protein L4

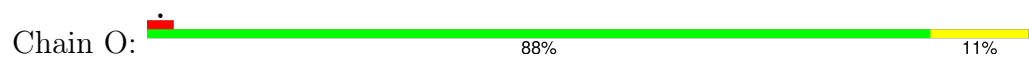


• Molecule 15: 50S ribosomal protein L5

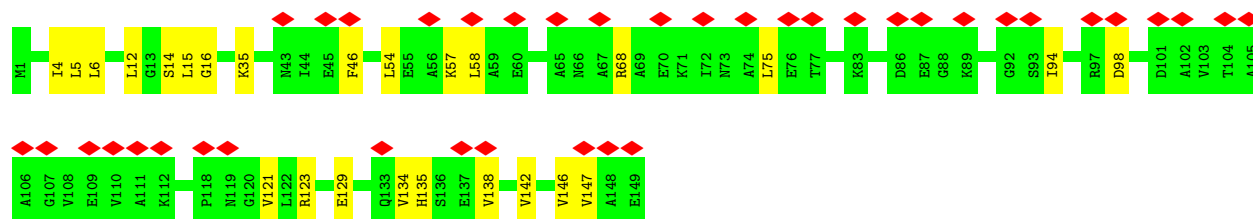
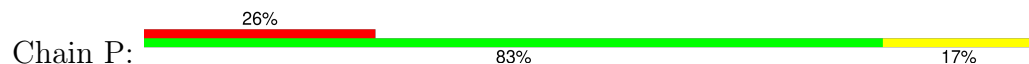




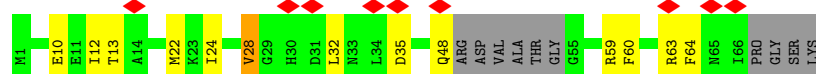
- Molecule 16: 50S ribosomal protein L6



- Molecule 17: 50S ribosomal protein L9



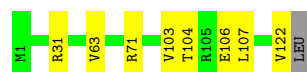
- Molecule 18: 50S ribosomal protein L31



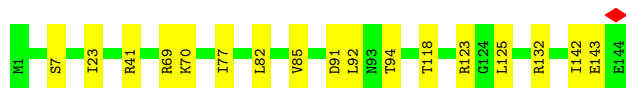
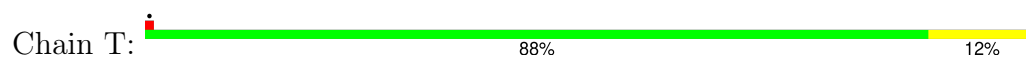
- Molecule 19: 50S ribosomal protein L13



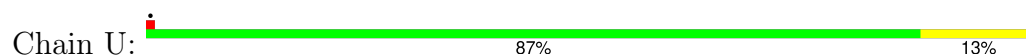
- Molecule 20: 50S ribosomal protein L14



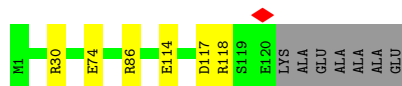
- Molecule 21: 50S ribosomal protein L15



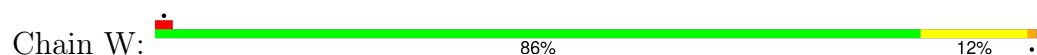
- Molecule 22: 50S ribosomal protein L16



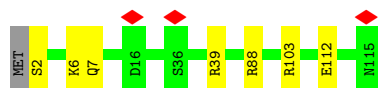
- Molecule 23: 50S ribosomal protein L17



- Molecule 24: 50S ribosomal protein L18



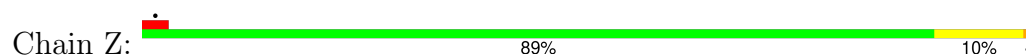
- Molecule 25: 50S ribosomal protein L19



- Molecule 26: 50S ribosomal protein L20



- Molecule 27: 50S ribosomal protein L21

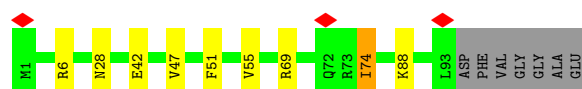
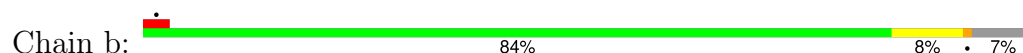




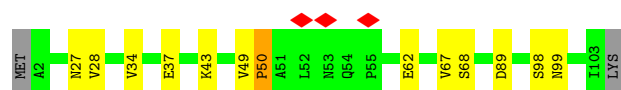
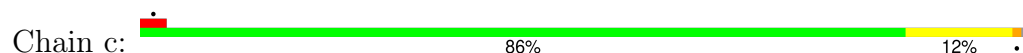
- Molecule 28: 50S ribosomal protein L22



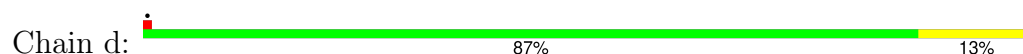
- Molecule 29: 50S ribosomal protein L23



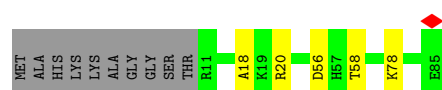
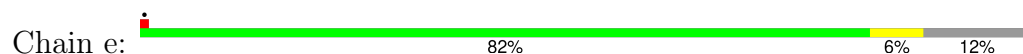
- Molecule 30: 50S ribosomal protein L24



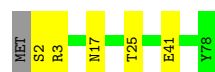
- Molecule 31: 50S ribosomal protein L25



- Molecule 32: 50S ribosomal protein L27

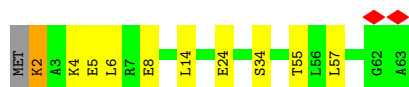


- Molecule 33: 50S ribosomal protein L28



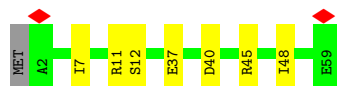
- Molecule 34: 50S ribosomal protein L29

Chain g:  83% 14%



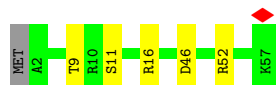
- Molecule 35: 50S ribosomal protein L30

Chain h:  86% 12%



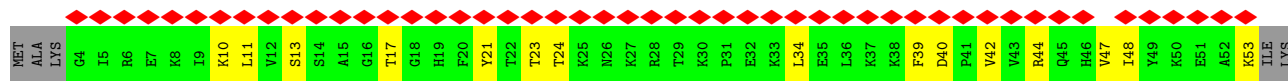
- Molecule 36: 50S ribosomal protein L32

Chain i:  89% 9%

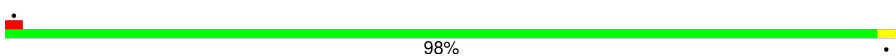


- Molecule 37: 50S ribosomal protein L33

Chain j:  89% 64% 27% 9%



- Molecule 38: 50S ribosomal protein L34

Chain k:  98%

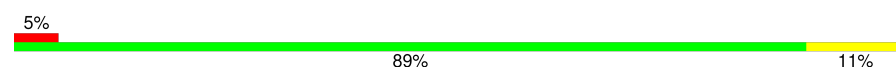


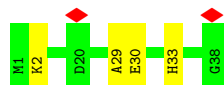
- Molecule 39: 50S ribosomal protein L35

Chain l:  89% 9%

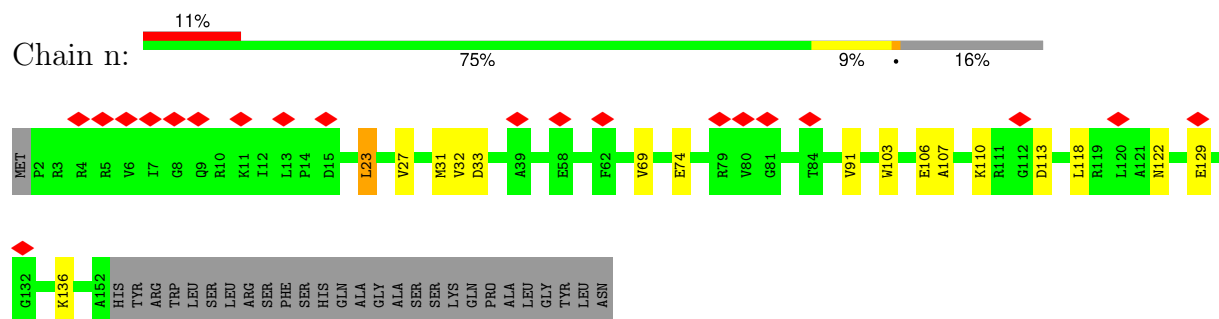


- Molecule 40: 50S ribosomal protein L36

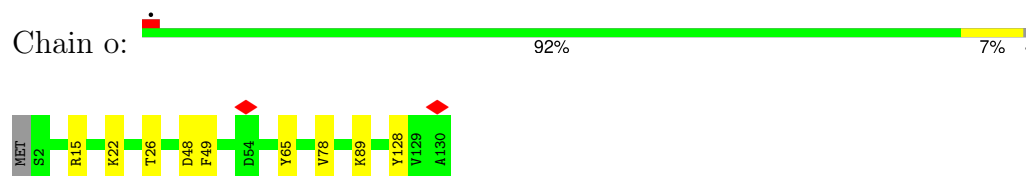
Chain m:  5% 89% 11%



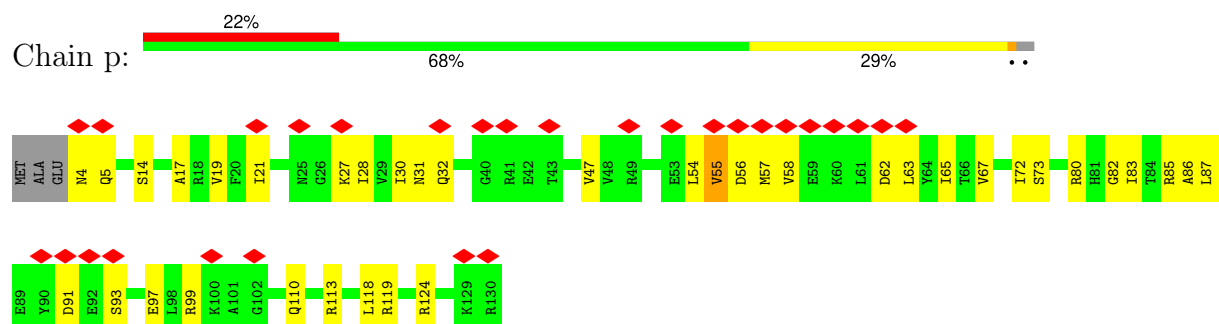
- Molecule 41: 30S ribosomal protein S7



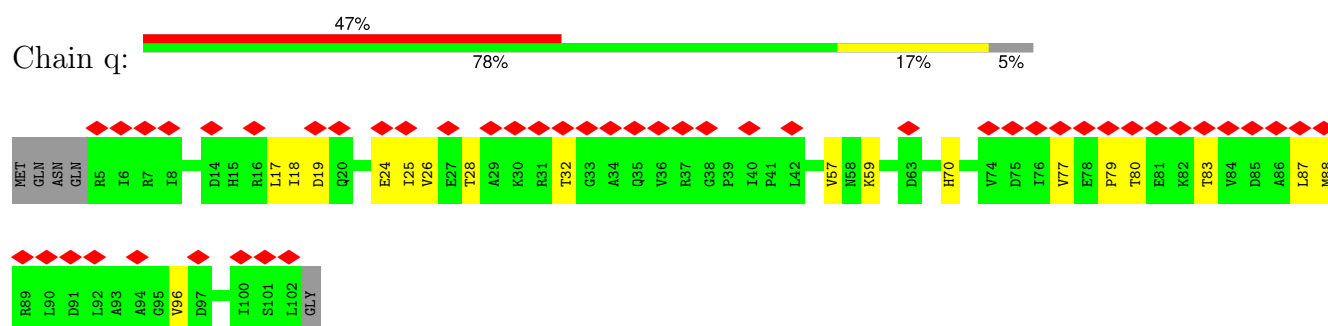
- Molecule 42: 30S ribosomal protein S8



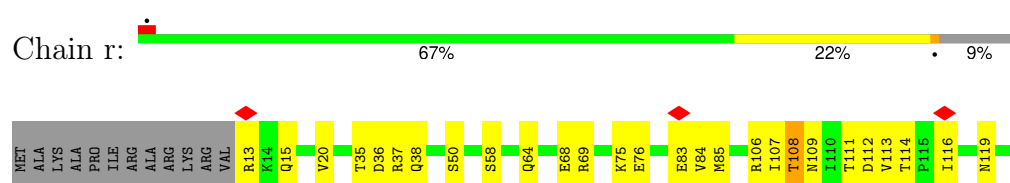
- Molecule 43: 30S ribosomal protein S9



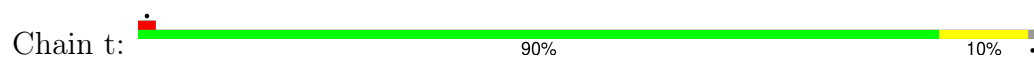
- Molecule 44: 30S ribosomal protein S10



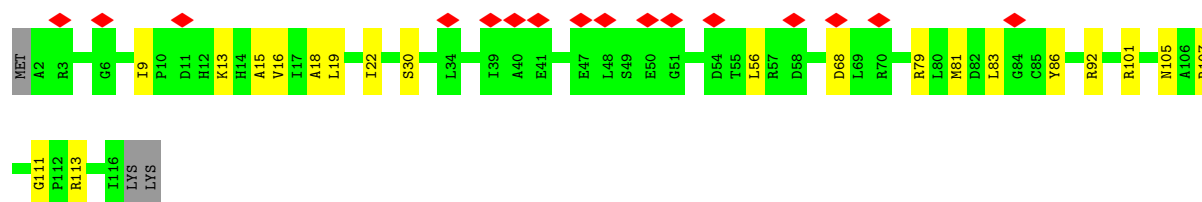
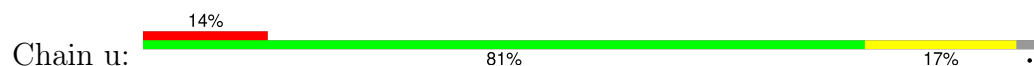
- Molecule 45: 30S ribosomal protein S11



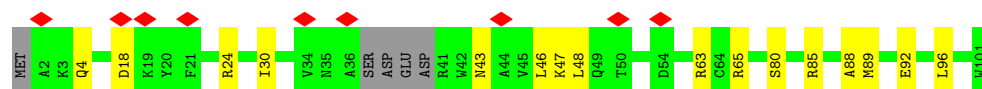
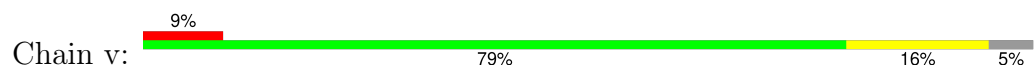
- Molecule 46: 30S ribosomal protein S12



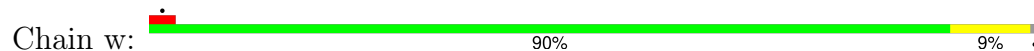
- Molecule 47: 30S ribosomal protein S13



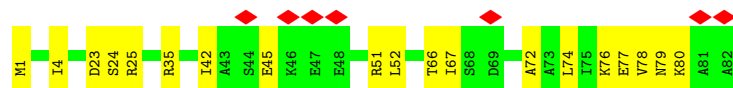
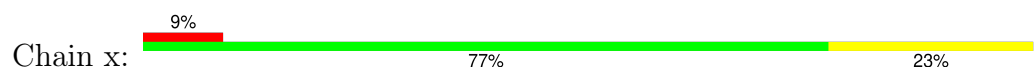
- Molecule 48: 30S ribosomal protein S14



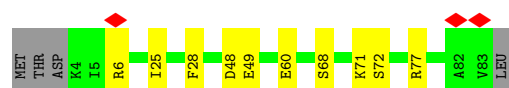
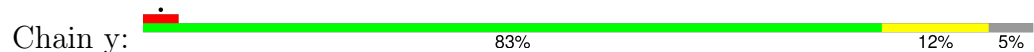
- Molecule 49: 30S ribosomal protein S15



- Molecule 50: 30S ribosomal protein S16



- Molecule 51: 30S ribosomal protein S17



- Molecule 52: 30S ribosomal protein S18



MET	ALA	ARG	TYR	PHE	ARG	ARG	ARG	LYS	PHE	CYS	ARG	PHE	THR	ALA	GLU	GLY	VAL	GLN	E20	K24	D25	I26	G37	R61	A62	R63	Y64	L65	S66	L67	L68	R73	H74	GLN
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	360239	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	24.695	Depositor
Minimum map value	-10.110	Depositor
Average map value	-0.018	Depositor
Map value standard deviation	0.748	Depositor
Recommended contour level	2	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8125, 0.8125, 0.8125	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, MG, ZLD, 6MZ, H2U, 5MU, 2MG, OMU, 5MC, G7M, 1MG, OMG, ZN, OMC, 2MA, 3TD, 4D4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.09	0/652	0.24	0/877
2	2	0.09	0/671	0.24	0/888
3	3	0.15	0/598	0.33	1/792 (0.1%)
4	C	0.08	0/36991	0.15	0/57705
5	D	0.10	0/1735	0.28	0/2338
6	E	0.08	0/1651	0.23	0/2225
7	F	0.09	0/1665	0.27	0/2227
8	G	0.11	0/1118	0.29	0/1504
9	H	0.11	0/835	0.31	0/1128
10	I	0.10	0/69168	0.17	0/107901
11	J	0.07	0/2828	0.14	0/4410
12	K	0.10	0/2139	0.25	0/2876
13	L	0.09	0/1586	0.22	0/2134
14	M	0.10	0/1571	0.26	0/2113
15	N	0.11	0/1434	0.32	0/1926
16	O	0.09	0/1343	0.24	0/1816
17	P	0.10	0/1122	0.28	0/1515
18	Q	0.11	0/488	0.28	0/649
19	R	0.09	0/1152	0.23	0/1551
20	S	0.11	0/947	0.28	0/1268
21	T	0.09	0/1062	0.23	0/1413
22	U	0.11	0/1081	0.29	0/1443
23	V	0.08	0/973	0.21	0/1301
24	W	0.09	0/902	0.24	0/1209
25	X	0.09	0/929	0.22	0/1242
26	Y	0.09	0/960	0.21	0/1278
27	Z	0.11	0/829	0.32	0/1107
28	a	0.08	0/864	0.21	0/1156
29	b	0.09	0/744	0.23	0/994
30	c	0.15	0/787	0.40	1/1051 (0.1%)
31	d	0.10	0/766	0.26	0/1025

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	e	0.10	0/582	0.26	0/769
33	f	0.09	0/635	0.24	0/848
34	g	0.11	0/502	0.30	0/667
35	h	0.10	0/453	0.25	0/605
36	i	0.11	0/450	0.27	0/599
37	j	0.09	0/416	0.25	0/554
38	k	0.08	0/380	0.20	0/498
39	l	0.08	0/513	0.21	0/676
40	m	0.11	0/303	0.26	0/397
41	n	0.10	0/1195	0.28	0/1602
42	o	0.09	0/989	0.23	0/1326
43	p	0.12	0/1034	0.34	0/1375
44	q	0.11	0/796	0.31	0/1077
45	r	0.12	0/893	0.34	0/1205
46	t	0.09	0/969	0.25	0/1300
47	u	0.10	0/900	0.27	0/1204
48	v	0.11	0/785	0.29	0/1043
49	w	0.10	0/718	0.24	0/959
50	x	0.11	0/659	0.26	0/884
51	y	0.10	0/657	0.26	0/881
52	z	0.09	0/462	0.23	0/621
All	All	0.09	0/153882	0.20	2/230152 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	50	PRO	CA-N-CD	-7.38	101.66	112.00
3	3	2	PRO	CA-N-CD	-5.38	104.46	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	637	666	665	7	0
2	2	665	715	714	11	0
3	3	590	629	629	11	0
4	C	33037	16628	16626	127	0
5	D	1704	1734	1732	38	0
6	E	1624	1697	1696	18	0
7	F	1643	1709	1707	29	0
8	G	1105	1150	1148	21	0
9	H	817	808	808	14	0
10	I	62271	31342	31340	252	0
11	J	2529	1280	1281	10	0
12	K	2093	2170	2157	17	0
13	L	1565	1619	1616	15	0
14	M	1552	1620	1619	17	0
15	N	1410	1445	1444	41	0
16	O	1323	1373	1371	14	0
17	P	1111	1148	1148	18	0
18	Q	480	483	478	13	0
19	R	1129	1162	1162	11	0
20	S	938	1013	1012	7	0
21	T	1053	1129	1128	10	0
22	U	1075	1156	1155	13	0
23	V	960	1001	1000	3	0
24	W	892	925	923	13	0
25	X	917	963	962	6	0
26	Y	947	1021	1019	8	0
27	Z	816	841	839	14	0
28	a	857	923	922	6	0
29	b	738	808	807	5	0
30	c	779	832	831	12	0
31	d	753	781	780	8	0
32	e	575	593	592	3	0
33	f	625	653	652	4	0
34	g	501	532	531	8	0
35	h	449	489	488	5	0
36	i	444	460	458	4	0
37	j	409	442	440	11	0
38	k	377	418	418	1	0
39	l	504	573	572	5	0
40	m	302	343	340	3	0
41	n	1181	1238	1238	13	0
42	o	979	1032	1031	6	0
43	p	1022	1071	1070	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	q	786	829	827	18	0
45	r	877	888	887	27	0
46	t	955	1017	1016	12	0
47	u	891	954	952	19	0
48	v	774	826	824	14	0
49	w	710	731	728	5	0
50	x	649	666	666	15	0
51	y	648	693	691	7	0
52	z	455	479	478	7	0
53	C	89	0	0	0	0
53	I	113	0	0	0	0
53	K	1	0	0	0	0
53	L	1	0	0	0	0
53	V	1	0	0	0	0
53	q	1	0	0	0	0
54	I	24	20	20	0	0
55	Q	1	0	0	0	0
55	m	1	0	0	0	0
56	C	4	8	0	1	0
56	I	32	64	0	0	0
56	c	1	2	0	0	0
All	All	142392	95792	95638	890	0

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

All (890) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:1755:A:OP1	25:X:103:ARG:NH2	2.02	0.91
10:I:938:G:OP2	39:l:52:LYS:NZ	2.05	0.90
27:Z:51:VAL:HG23	27:Z:52:PRO:CD	2.02	0.90
16:O:124:GLU:OE1	16:O:125:CYS:N	2.07	0.88
11:J:7:G:OP1	24:W:4:LYS:NZ	2.10	0.84
4:C:736:C:OP1	52:z:61:ARG:NH1	2.10	0.84
37:j:13:SER:OG	37:j:40:ASP:OD2	1.96	0.84
37:j:44:ARG:O	39:l:38:THR:OG1	1.95	0.84
5:D:167:ASP:OD1	5:D:191:SER:OG	1.96	0.83
14:M:170:ARG:NH2	14:M:176:ASP:OD2	2.12	0.82
4:C:1116:U:O2'	43:p:110:GLN:OE1	1.95	0.82
4:C:910:C:OP2	46:t:18:LYS:NZ	2.11	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:p:27:LYS:NZ	43:p:62:ASP:OD2	2.14	0.81
49:w:26:GLU:N	49:w:26:GLU:OE1	2.13	0.80
10:I:910:A:N3	10:I:2264:C:O2'	2.16	0.79
10:I:602:A:HO2'	10:I:604:G:HO2'	1.13	0.79
27:Z:51:VAL:HG23	27:Z:52:PRO:HD2	1.64	0.79
10:I:138:U:O2'	10:I:139:U:OP1	2.00	0.79
10:I:248:G:O2'	10:I:2432:A:OP1	2.01	0.79
10:I:2831:G:OP2	13:L:59:ARG:NH1	2.15	0.79
4:C:1491:G:O2'	4:C:1492:A:OP1	2.00	0.78
18:Q:10:GLU:N	18:Q:10:GLU:OE1	2.17	0.77
4:C:207:C:O2	4:C:212:G:N2	2.18	0.77
10:I:1826:G:O2'	10:I:1971:U:OP2	2.01	0.77
10:I:2298:A:OP1	15:N:71:ARG:NH1	2.16	0.77
41:n:113:ASP:OD2	41:n:122:ASN:ND2	2.16	0.77
10:I:1296:G:OP1	10:I:2709:G:O2'	2.01	0.77
7:F:13:ARG:NH2	7:F:37:ALA:O	2.18	0.76
10:I:1846:G:O2'	10:I:1847:A:OP1	2.02	0.76
4:C:537:G:OP1	46:t:110:ARG:NH2	2.18	0.76
4:C:1124:G:O2'	4:C:1145:A:N6	2.19	0.76
4:C:842:U:O2'	4:C:843:U:O4'	2.03	0.76
10:I:275:C:O2	10:I:362:A:N6	2.19	0.76
10:I:1390:U:O2	10:I:1395:A:N6	2.18	0.76
4:C:949:A:N7	47:u:105:ASN:ND2	2.33	0.75
22:U:26:VAL:HG13	22:U:104:GLU:OE2	1.85	0.75
10:I:1066:U:O2'	10:I:1068:G:N7	2.18	0.75
1:1:35:SER:OG	1:1:38:SER:OG	2.04	0.75
10:I:2135:A:N6	10:I:2156:G:O2'	2.19	0.75
4:C:1028:C:O2	4:C:1033:G:N2	2.20	0.74
10:I:160:A:N3	10:I:2208:C:O2'	2.20	0.74
4:C:636:U:OP1	51:y:6:ARG:NH1	2.19	0.74
24:W:114:GLY:O	24:W:116:GLN:NE2	2.20	0.74
10:I:2180:U:O2'	10:I:2181:U:O4'	2.05	0.74
10:I:1715:G:O2'	10:I:1743:G:O6	2.04	0.74
23:V:30:ARG:NH1	23:V:74:GLU:OE1	2.21	0.73
45:r:20:VAL:HG13	45:r:83:GLU:HB3	1.71	0.73
10:I:2119:A:N6	10:I:2167:U:O2'	2.22	0.73
5:D:188:ASP:OD2	5:D:190:ASN:ND2	2.21	0.73
3:3:71:TYR:O	4:C:1098:C:O2'	2.07	0.73
4:C:1261:A:N6	4:C:1274:A:O2'	2.22	0.73
10:I:309:A:N3	10:I:329:G:O2'	2.22	0.73
10:I:2786:U:OP1	13:L:70:LYS:NZ	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:213:TYR:O	5:D:217:VAL:HG23	1.90	0.72
10:I:2543:G:O2'	10:I:2544:G:OP1	2.05	0.72
10:I:1754:A:O2'	10:I:1755:A:OP1	2.06	0.72
23:V:86:ARG:NE	23:V:117:ASP:OD2	2.23	0.72
10:I:197:A:N6	10:I:2430:A:O2'	2.23	0.71
4:C:1371:G:OP1	43:p:14:SER:OG	2.09	0.71
4:C:1067:A:N1	4:C:1108:G:O2'	2.22	0.71
33:f:17:ASN:OD1	33:f:25:THR:OG1	2.08	0.71
6:E:34:ASP:OD1	48:v:65:ARG:NE	2.23	0.71
50:x:77:GLU:OE1	50:x:80:LYS:NZ	2.24	0.71
4:C:626:G:OP1	50:x:35:ARG:NH1	2.24	0.71
4:C:409:U:OP1	7:F:23:SER:OG	2.06	0.70
27:Z:51:VAL:HG23	27:Z:52:PRO:HD3	1.73	0.70
44:q:24:GLU:N	44:q:24:GLU:OE1	2.23	0.70
3:3:13:ASP:OD2	3:3:17:ARG:NH2	2.25	0.70
27:Z:43:ASN:ND2	27:Z:43:ASN:O	2.24	0.70
4:C:1152:A:OP1	44:q:70:HIS:ND1	2.25	0.70
13:L:46:ARG:NH1	13:L:85:ALA:O	2.23	0.70
4:C:362:G:N2	4:C:365:U:OP2	2.20	0.69
10:I:1779:U:OP2	10:I:1784:A:N6	2.22	0.69
10:I:2680:U:O2'	10:I:2681:C:O5'	2.11	0.69
10:I:1508:A:O2'	10:I:1509:A:O4'	2.10	0.69
10:I:1419:A:O2'	10:I:1421:G:N7	2.21	0.69
4:C:701:U:OP1	4:C:702:A:O2'	2.08	0.69
4:C:1140:C:O2'	4:C:1141:C:O5'	2.11	0.69
16:O:38:ASN:ND2	16:O:64:GLN:OE1	2.26	0.69
16:O:170:ARG:NH2	40:m:29:ALA:O	2.25	0.69
16:O:173:GLU:OE2	16:O:174:ALA:N	2.25	0.69
4:C:1266:G:N2	4:C:1269:A:OP2	2.26	0.69
10:I:1864:U:OP1	10:I:2410:G:O2'	2.10	0.69
4:C:841:C:O2'	4:C:843:U:OP2	2.05	0.68
4:C:28:A:O2'	4:C:296:U:OP1	2.11	0.68
42:o:48:ASP:OD1	42:o:49:PHE:N	2.26	0.68
10:I:58:G:O2'	10:I:73:A:N1	2.24	0.68
10:I:2799:A:O2'	10:I:2800:A:O5'	2.11	0.68
2:2:55:GLN:NE2	4:C:193:C:O4'	2.27	0.68
10:I:2595:G:N2	10:I:2598:A:OP2	2.26	0.68
17:P:4:ILE:O	17:P:4:ILE:HD12	1.93	0.68
43:p:30:ILE:HG12	43:p:65:ILE:HD11	1.76	0.68
4:C:126:G:OP1	4:C:605:U:O2'	2.08	0.68
5:D:117:LEU:HD11	5:D:137:ARG:HG2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:2528:U:O2'	10:I:2530:A:OP1	2.09	0.68
29:b:28:ASN:ND2	29:b:88:LYS:O	2.27	0.68
10:I:1799:G:O2'	12:K:180:GLU:OE2	2.09	0.68
10:I:1607:C:N4	10:I:1622:G:OP2	2.21	0.68
8:G:14:LYS:NZ	8:G:116:GLU:OE2	2.26	0.67
10:I:1417:C:HO2'	10:I:1587:G:HO2'	1.40	0.67
4:C:944:G:N1	4:C:1338:G:OP2	2.27	0.67
10:I:1798:U:OP2	12:K:271:ARG:NH2	2.27	0.67
10:I:2121:G:O6	10:I:2176:A:N6	2.27	0.67
52:z:37:GLY:O	52:z:63:ARG:NH2	2.26	0.67
4:C:1222:G:OP2	4:C:1322:C:N4	2.27	0.67
44:q:18:ILE:HD12	44:q:19:ASP:N	2.09	0.67
45:r:108:THR:OG1	45:r:109:ASN:OD1	2.13	0.67
4:C:575:G:O2'	4:C:821:G:OP2	2.08	0.67
6:E:35:SER:OG	6:E:59:ARG:NH2	2.28	0.67
10:I:1682:G:OP2	10:I:1699:G:N2	2.28	0.66
44:q:32:THR:HG23	44:q:83:THR:HG22	1.77	0.66
45:r:13:ARG:N	45:r:76:GLU:OE2	2.29	0.66
5:D:40:ILE:O	5:D:40:ILE:HD12	1.95	0.66
4:C:116:A:OP2	56:C:3101:HOH:O	2.13	0.66
10:I:1079:C:O2'	10:I:1080:A:OP1	2.13	0.66
15:N:79:ILE:HD12	15:N:79:ILE:O	1.95	0.66
10:I:2340:A:O5'	11:J:41:G:N2	2.24	0.66
10:I:2646:C:OP2	10:I:2732:G:O2'	2.13	0.66
43:p:54:LEU:O	43:p:56:ASP:N	2.28	0.66
43:p:56:ASP:OD1	43:p:57:MET:N	2.28	0.66
3:3:3:VAL:HG23	45:r:111:THR:HG22	1.76	0.66
10:I:1071:G:N2	10:I:1089:A:O2'	2.29	0.66
4:C:380:G:N2	4:C:383:A:OP2	2.28	0.66
27:Z:45:GLU:OE1	27:Z:45:GLU:N	2.29	0.66
4:C:83:C:O2	4:C:86:G:N2	2.28	0.65
4:C:1233:G:OP1	43:p:119:ARG:NH1	2.29	0.65
4:C:1316:G:N1	4:C:1319:A:OP2	2.28	0.65
27:Z:43:ASN:C	27:Z:43:ASN:HD22	2.02	0.65
4:C:662:U:O2'	4:C:836:G:OP1	2.14	0.65
10:I:1693:U:OP2	10:I:1694:C:N4	2.30	0.65
10:I:1754:A:N1	10:I:2716:C:O2'	2.27	0.65
16:O:80:THR:OG1	16:O:81:GLU:OE1	2.07	0.65
46:t:30:LYS:NZ	46:t:59:ASN:OD1	2.26	0.65
4:C:1052:U:O2'	4:C:1055:A:OP2	2.06	0.65
10:I:788:A:OP1	10:I:791:C:N4	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:1078:U:O2'	10:I:1088:A:OP1	2.14	0.65
17:P:57:LYS:HA	17:P:57:LYS:HE2	1.77	0.65
30:c:37:GLU:OE1	30:c:37:GLU:N	2.30	0.65
44:q:24:GLU:O	44:q:28:THR:OG1	2.11	0.65
10:I:807:U:OP2	21:T:41:ARG:NH2	2.30	0.64
43:p:55:VAL:HG13	43:p:56:ASP:H	1.60	0.64
4:C:1178:G:N2	4:C:1181:G:OP2	2.29	0.64
4:C:811:C:O2'	4:C:901:A:N1	2.29	0.64
10:I:2627:G:O2'	10:I:2781:A:N1	2.23	0.64
15:N:115:ARG:NE	18:Q:48:GLN:OE1	2.30	0.64
43:p:88:MET:HA	43:p:88:MET:HE2	1.77	0.64
47:u:81:MET:HE3	47:u:92:ARG:HG3	1.80	0.64
10:I:265:A:N1	10:I:427:U:O2'	2.30	0.64
21:T:91:ASP:OD1	21:T:92:LEU:N	2.31	0.64
44:q:28:THR:O	44:q:32:THR:HG22	1.97	0.64
10:I:1753:G:N2	10:I:1756:G:OP2	2.29	0.64
4:C:843:U:OP1	4:C:844:G:N2	2.31	0.64
10:I:2344:U:O2'	37:j:21:TYR:OH	2.14	0.64
7:F:151:LYS:HE3	7:F:151:LYS:HA	1.79	0.64
4:C:1140:C:HO2'	4:C:1141:C:P	2.21	0.64
4:C:1145:A:O2'	4:C:1146:A:O5'	2.15	0.64
10:I:1447:C:O2'	10:I:1544:A:N3	2.28	0.64
3:3:46:LYS:NZ	4:C:1530:G:N7	2.36	0.64
6:E:22:TRP:NE1	6:E:36:ASP:OD2	2.31	0.64
4:C:1312:G:OP2	18:Q:63:ARG:NH2	2.30	0.63
16:O:47:ASP:OD1	16:O:48:ASN:N	2.29	0.63
7:F:62:ARG:NE	7:F:69:GLU:OE1	2.31	0.63
10:I:1693:U:O2'	12:K:14:ARG:NH2	2.30	0.63
15:N:137:ILE:HD12	15:N:138:PHE:N	2.13	0.63
10:I:2170:A:O2'	10:I:2171:A:OP2	2.15	0.63
15:N:108:VAL:HG12	15:N:109:PRO:HD3	1.79	0.63
10:I:2116:G:O6	10:I:2171:A:N6	2.32	0.63
3:3:7:ARG:O	45:r:106:ARG:NH2	2.31	0.63
4:C:1005:A:OP2	4:C:1024:G:N2	2.30	0.63
10:I:411:G:OP2	10:I:2406:A:O2'	2.16	0.63
10:I:84:A:N1	10:I:98:G:O2'	2.27	0.63
10:I:2875:C:O2'	25:X:6:LYS:NZ	2.32	0.62
23:V:114:GLU:OE1	23:V:118:ARG:NH1	2.32	0.62
24:W:40:ILE:HD13	24:W:47:VAL:HG23	1.82	0.62
9:H:51:ILE:HG22	9:H:52:ASN:OD1	2.00	0.62
5:D:13:GLY:O	5:D:14:VAL:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:71:GLN:OE1	7:F:97:ARG:NH1	2.33	0.62
10:I:1996:C:OP1	20:S:31:ARG:NH1	2.31	0.62
6:E:57:ILE:HG23	6:E:64:ILE:HD11	1.82	0.62
10:I:475:C:O2	10:I:479:A:N6	2.32	0.62
10:I:2127:G:O2'	10:I:2128:G:O5'	2.13	0.62
10:I:2146:C:OP2	10:I:2147:A:N6	2.33	0.61
4:C:601:G:OP1	42:o:89:LYS:NZ	2.33	0.61
10:I:25:U:O2'	10:I:26:G:OP1	2.19	0.61
10:I:1064:C:N4	10:I:1069:A:O2'	2.33	0.61
10:I:2159:G:O2'	10:I:2160:C:O5'	2.17	0.61
11:J:14:U:OP2	11:J:70:C:O2'	2.19	0.61
37:j:10:LYS:O	37:j:53:LYS:N	2.33	0.61
24:W:99:TYR:OH	24:W:111:ARG:NH2	2.33	0.61
7:F:85:ASN:ND2	7:F:88:GLU:OE1	2.34	0.61
10:I:2343:U:O2'	10:I:2373:G:O2'	2.15	0.61
15:N:123:ASP:OD2	15:N:127:ASN:ND2	2.33	0.61
21:T:132:ARG:HD3	21:T:142:ILE:HD13	1.83	0.60
4:C:563:A:O2'	4:C:566:G:O3'	2.19	0.60
10:I:1353:A:OP1	10:I:1570:A:O2'	2.18	0.60
1:l:3:ARG:N	4:C:1313:U:OP2	2.34	0.60
5:D:205:ASP:OD1	5:D:205:ASP:N	2.33	0.60
14:M:176:ASP:OD1	14:M:179:SER:OG	2.15	0.60
50:x:23:ASP:OD1	50:x:24:SER:N	2.34	0.60
50:x:79:ASN:OD1	50:x:80:LYS:N	2.34	0.60
10:I:2116:G:N2	10:I:2162:G:OP1	2.33	0.60
43:p:57:MET:N	43:p:57:MET:HE3	2.16	0.60
7:F:188:ARG:NH2	7:F:193:ALA:O	2.34	0.60
10:I:1007:C:OP1	19:R:37:ARG:NH1	2.33	0.60
26:Y:97:ASP:OD2	27:Z:13:ARG:NE	2.35	0.60
4:C:110:C:O2'	50:x:25:ARG:O	2.19	0.60
45:r:85:MET:HE2	45:r:85:MET:HA	1.82	0.60
10:I:18:U:OP1	26:Y:30:ARG:NH2	2.35	0.60
4:C:1077:G:N2	4:C:1080:A:OP2	2.31	0.60
8:G:50:TYR:O	8:G:66:LYS:NZ	2.20	0.60
10:I:624:C:O2'	10:I:657:U:OP1	2.18	0.60
10:I:1288:G:OP2	10:I:1288:G:N2	2.27	0.59
19:R:128:ASN:O	19:R:128:ASN:ND2	2.34	0.59
45:r:36:ASP:OD1	45:r:38:GLN:N	2.32	0.59
10:I:2543:G:HO2'	10:I:2544:G:P	2.26	0.59
4:C:982:U:OP2	48:v:63:ARG:NH2	2.34	0.59
32:e:18:ALA:O	32:e:20:ARG:NH1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:568:U:H1'	10:I:2030:6MZ:H9C1	1.85	0.59
10:I:2848:G:O2'	10:I:2867:G:N2	2.22	0.59
15:N:102:ARG:HG3	18:Q:24:ILE:HD11	1.84	0.59
43:p:4:ASN:OD1	43:p:5:GLN:N	2.35	0.59
51:y:60:GLU:OE1	51:y:77:ARG:NH1	2.36	0.59
10:I:2092:U:N3	10:I:2226:C:OP2	2.36	0.59
15:N:17:MET:O	15:N:21:ASN:N	2.36	0.59
39:l:32:ILE:O	39:l:36:LYS:NZ	2.34	0.59
4:C:846:G:O2'	4:C:847:G:OP1	2.20	0.59
22:U:12:MET:HE2	22:U:12:MET:HA	1.84	0.59
30:c:89:ASP:OD1	30:c:89:ASP:N	2.36	0.59
5:D:188:ASP:OD1	5:D:189:THR:N	2.36	0.58
45:r:13:ARG:N	45:r:15:GLN:OE1	2.36	0.58
3:3:6:VAL:HG23	3:3:10:GLU:OE1	2.03	0.58
7:F:28:ILE:HD12	7:F:30:THR:OG1	2.02	0.58
7:F:187:GLU:OE1	7:F:187:GLU:N	2.34	0.58
7:F:78:GLU:OE2	7:F:81:ARG:NH1	2.36	0.58
15:N:173:PHE:O	15:N:174:ASP:OD1	2.22	0.58
10:I:476:G:N1	10:I:479:A:OP2	2.37	0.58
10:I:1813:G:O2'	10:I:1814:G:OP1	2.21	0.58
10:I:1079:C:HO2'	10:I:1080:A:P	2.26	0.58
4:C:297:G:N2	4:C:300:A:OP2	2.37	0.58
4:C:106:C:O2'	4:C:379:C:OP1	2.20	0.57
29:b:6:ARG:NE	29:b:42:GLU:OE1	2.37	0.57
4:C:31:G:O2'	4:C:48:C:N4	2.37	0.57
10:I:2660:A:O2'	10:I:2661:G:OP1	2.20	0.57
47:u:79:ARG:O	47:u:83:LEU:HD12	2.04	0.57
10:I:987:C:O2'	10:I:1000:A:N3	2.36	0.57
4:C:890:G:O2'	4:C:906:A:N6	2.38	0.57
5:D:163:VAL:HG21	5:D:173:ILE:CD1	2.34	0.57
10:I:514:A:N3	10:I:581:C:O2'	2.36	0.57
13:L:48:ILE:HG23	13:L:84:LEU:HD11	1.85	0.57
5:D:163:VAL:HG21	5:D:173:ILE:HD11	1.87	0.57
10:I:2204:G:OP2	12:K:147:LYS:NZ	2.36	0.57
10:I:2447:G:O2'	10:I:2500:U:OP2	2.12	0.57
14:M:2:GLU:HA	14:M:2:GLU:OE1	2.05	0.57
44:q:87:LEU:C	44:q:87:LEU:HD13	2.30	0.57
10:I:586:A:N1	10:I:809:G:O2'	2.34	0.57
10:I:2158:A:O2'	10:I:2159:G:OP2	2.16	0.57
50:x:74:LEU:O	50:x:78:VAL:HG12	2.05	0.57
10:I:1047:G:HO2'	10:I:1110:G:H1	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:1028:A:N3	10:I:2486:C:O2'	2.28	0.57
10:I:1421:G:N2	10:I:1495:A:N1	2.53	0.57
16:O:16:ASP:OD1	16:O:16:ASP:N	2.38	0.57
10:I:223:A:O2'	10:I:420:C:O2'	2.21	0.56
51:y:25:ILE:HD12	51:y:25:ILE:N	2.19	0.56
10:I:500:G:N1	10:I:503:A:OP2	2.37	0.56
10:I:2334:U:O3'	24:W:13:ARG:NH1	2.38	0.56
15:N:56:ASP:OD2	15:N:135:GLN:NE2	2.37	0.56
24:W:14:ALA:O	24:W:18:LEU:HD23	2.04	0.56
27:Z:43:ASN:ND2	27:Z:43:ASN:C	2.63	0.56
10:I:1527:G:N1	10:I:1544:A:OP2	2.36	0.56
10:I:1009:A:N3	10:I:1153:C:O2'	2.38	0.56
43:p:118:LEU:HD22	43:p:124:ARG:HG2	1.86	0.56
4:C:993:G:O2'	4:C:994:A:N7	2.39	0.56
10:I:1315:C:O2'	10:I:1392:A:N3	2.39	0.56
10:I:1365:A:OP1	33:f:3:ARG:NH1	2.38	0.56
35:h:11:ARG:NH1	35:h:11:ARG:HB2	2.21	0.56
43:p:83:ILE:HG22	43:p:87:LEU:HD13	1.88	0.56
47:u:19:LEU:HD12	47:u:19:LEU:H	1.70	0.56
10:I:25:U:HO2'	10:I:26:G:P	2.29	0.56
4:C:205:A:N1	4:C:206:C:N4	2.53	0.56
4:C:664:G:H22	4:C:741:G:H1	1.52	0.56
46:t:68:GLY:O	46:t:99:ARG:NH1	2.36	0.56
48:v:85:ARG:O	48:v:89:MET:N	2.38	0.56
5:D:13:GLY:O	5:D:15:HIS:N	2.35	0.55
10:I:2159:G:O2'	10:I:2160:C:O4'	2.23	0.55
41:n:106:GLU:O	41:n:110:LYS:NZ	2.33	0.55
15:N:16:LEU:HD23	15:N:28:VAL:CG2	2.37	0.55
10:I:2375:G:N2	10:I:2378:A:OP2	2.34	0.55
16:O:24:ILE:HD12	16:O:24:ILE:O	2.06	0.55
10:I:1755:A:N6	10:I:2694:G:O2'	2.40	0.55
10:I:2522:U:O2'	10:I:2647:U:OP1	2.16	0.55
22:U:33:LEU:HD13	22:U:117:PHE:HB3	1.89	0.55
4:C:346:G:OP1	25:X:39:ARG:NH1	2.39	0.55
15:N:140:GLU:OE1	18:Q:28:VAL:N	2.40	0.55
48:v:46:LEU:HD13	48:v:46:LEU:O	2.07	0.55
4:C:517:G:N2	4:C:530:G:OP1	2.40	0.55
10:I:2115:G:O2'	10:I:2117:A:N7	2.36	0.55
44:q:19:ASP:N	44:q:19:ASP:OD1	2.35	0.55
4:C:130:A:N3	4:C:263:A:O2'	2.38	0.55
6:E:3:GLN:N	6:E:3:GLN:OE1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:743:A:O2'	10:I:1659:G:OP1	2.21	0.55
43:p:91:ASP:OD1	43:p:93:SER:OG	2.24	0.55
10:I:177:G:OP2	10:I:177:G:N2	2.34	0.55
10:I:578:G:OP1	10:I:1255:U:O2'	2.22	0.54
10:I:1055:G:O2'	10:I:1084:A:N6	2.40	0.54
10:I:2128:G:N3	10:I:2173:A:O2'	2.40	0.54
16:O:24:ILE:HD12	16:O:24:ILE:C	2.33	0.54
20:S:103:VAL:O	20:S:122:VAL:HG23	2.07	0.54
4:C:839:C:O2	4:C:847:G:N2	2.39	0.54
6:E:16:LYS:NZ	6:E:182:ILE:O	2.37	0.54
17:P:135:HIS:HB3	17:P:138:VAL:HG22	1.89	0.54
47:u:68:ASP:N	47:u:68:ASP:OD1	2.40	0.54
50:x:42:ILE:O	50:x:42:ILE:HG22	2.07	0.54
10:I:1068:G:N2	10:I:1095:A:O2'	2.41	0.54
10:I:2681:C:OP1	13:L:8:LYS:NZ	2.21	0.54
45:r:20:VAL:HG13	45:r:83:GLU:CB	2.38	0.54
47:u:9:ILE:HD12	47:u:9:ILE:C	2.32	0.54
31:d:77:VAL:HG23	31:d:89:ILE:HD13	1.90	0.54
44:q:18:ILE:HD12	44:q:18:ILE:C	2.32	0.54
20:S:63:VAL:HG12	20:S:107:LEU:HD11	1.88	0.54
41:n:23:LEU:HD13	41:n:23:LEU:O	2.08	0.54
43:p:19:VAL:HG13	43:p:65:ILE:HG21	1.89	0.54
8:G:12:GLN:N	8:G:40:GLY:O	2.39	0.54
10:I:182:A:O2'	10:I:183:C:OP1	2.25	0.54
17:P:6:LEU:N	17:P:35:LYS:O	2.40	0.54
1:l:66:MET:HG2	47:u:83:LEU:HD23	1.89	0.53
42:o:78:VAL:HG21	42:o:128:TYR:CE2	2.43	0.53
4:C:115:G:H4'	4:C:116:A:O5'	2.08	0.53
10:I:23:G:OP1	10:I:504:A:N6	2.42	0.53
10:I:1475:G:O2'	10:I:1514:G:O6	2.22	0.53
45:r:109:ASN:OD1	45:r:109:ASN:N	2.39	0.53
10:I:221:A:N1	10:I:265:A:O2'	2.41	0.53
10:I:1141:U:OP2	19:R:65:THR:OG1	2.24	0.53
7:F:58:LYS:NZ	7:F:69:GLU:OE2	2.39	0.53
10:I:1311:G:OP2	10:I:1311:G:N2	2.33	0.53
15:N:73:SER:OG	15:N:81:GLN:N	2.41	0.53
4:C:404:G:O6	7:F:2:ALA:N	2.41	0.53
4:C:439:U:O3'	7:F:121:LYS:NZ	2.42	0.53
47:u:15:ALA:O	47:u:19:LEU:HD12	2.09	0.53
6:E:28:GLU:N	6:E:28:GLU:OE1	2.40	0.53
9:H:14:GLN:N	9:H:14:GLN:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:39:LEU:HD13	9:H:39:LEU:C	2.34	0.53
12:K:6:CYS:SG	12:K:13:ARG:NH2	2.82	0.53
15:N:102:ARG:CG	18:Q:24:ILE:HD11	2.38	0.53
43:p:63:LEU:O	43:p:63:LEU:HD12	2.08	0.53
43:p:21:ILE:HG12	43:p:86:ALA:HB1	1.89	0.53
10:I:1846:G:O2'	10:I:1847:A:P	2.67	0.52
5:D:207:ILE:N	5:D:207:ILE:HD12	2.24	0.52
15:N:38:MET:HE3	15:N:57:LEU:HD21	1.91	0.52
33:f:2:SER:O	33:f:2:SER:OG	2.21	0.52
4:C:828:U:OP1	42:o:22:LYS:NZ	2.42	0.52
7:F:60:LYS:HE2	7:F:195:ILE:HG22	1.91	0.52
7:F:128:ARG:NH1	7:F:128:ARG:HB3	2.24	0.52
4:C:875:U:O2'	42:o:15:ARG:NH1	2.41	0.52
4:C:1229:A:OP2	47:u:113:ARG:NH2	2.42	0.52
6:E:87:LEU:O	6:E:91:VAL:HG12	2.10	0.52
10:I:631:A:N3	10:I:2415:G:O2'	2.37	0.52
3:3:3:VAL:HG23	45:r:111:THR:CG2	2.40	0.52
10:I:1509:A:O2'	10:I:1510:G:OP2	2.21	0.52
8:G:15:LEU:HD21	8:G:18:VAL:HG23	1.91	0.52
4:C:324:G:N1	4:C:327:A:OP2	2.42	0.52
10:I:964:C:O2'	10:I:2273:A:N3	2.41	0.52
10:I:2688:G:N1	10:I:2720:U:OP2	2.38	0.52
4:C:846:G:O2'	4:C:847:G:P	2.67	0.52
5:D:120:GLN:OE1	5:D:137:ARG:NH1	2.43	0.52
10:I:2104:C:H42	10:I:2184:A:H61	1.57	0.52
16:O:81:GLU:OE1	16:O:81:GLU:N	2.43	0.52
41:n:136:LYS:HE3	41:n:136:LYS:HA	1.92	0.52
43:p:65:ILE:C	43:p:65:ILE:HD12	2.34	0.52
17:P:121:VAL:O	17:P:121:VAL:HG12	2.10	0.51
10:I:1846:G:HO2'	10:I:1847:A:P	2.33	0.51
10:I:2788:C:O2'	10:I:2809:A:N3	2.41	0.51
19:R:140:LEU:HD21	19:R:142:ILE:HD11	1.93	0.51
45:r:107:ILE:HD12	45:r:107:ILE:O	2.10	0.51
9:H:12:PRO:HD2	9:H:54:LEU:HD11	1.92	0.51
21:T:77:ILE:HD12	21:T:77:ILE:N	2.25	0.51
4:C:1145:A:HO2'	4:C:1146:A:P	2.34	0.51
10:I:1332:G:N7	10:I:1609:A:O2'	2.38	0.51
12:K:168:ASP:OD1	12:K:168:ASP:C	2.54	0.51
41:n:113:ASP:HB3	41:n:118:LEU:HD23	1.92	0.51
47:u:9:ILE:HD12	47:u:9:ILE:O	2.11	0.51
10:I:572:A:OP2	27:Z:80:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:71:ARG:NH1	20:S:106:GLU:OE2	2.42	0.51
10:I:2503:2MA:O2'	10:I:2505:G:OP2	2.28	0.51
6:E:51:SER:O	6:E:51:SER:OG	2.27	0.51
5:D:89:GLN:OE1	5:D:89:GLN:HA	2.09	0.51
10:I:1954:G:O2'	10:I:1956:U:O4	2.19	0.51
10:I:2854:G:O2'	10:I:2855:C:OP1	2.28	0.51
4:C:855:U:OP2	4:C:871:U:N3	2.43	0.50
10:I:2478:A:OP2	40:m:2:LYS:NZ	2.42	0.50
2:2:70:ASN:OD1	2:2:71:LYS:N	2.44	0.50
10:I:1827:U:O2'	10:I:1970:A:N3	2.38	0.50
50:x:23:ASP:OD1	50:x:23:ASP:C	2.53	0.50
43:p:56:ASP:OD1	43:p:58:VAL:N	2.41	0.50
4:C:1300:G:N2	4:C:1301:U:O4	2.44	0.50
10:I:1266:G:OP1	36:i:16:ARG:NE	2.40	0.50
10:I:2029:G:N1	10:I:2033:A:OP2	2.41	0.50
15:N:74:VAL:HG22	15:N:79:ILE:HD11	1.92	0.50
19:R:62:VAL:HG11	19:R:101:ILE:HD11	1.94	0.50
4:C:273:U:O4	4:C:274:A:N6	2.45	0.50
4:C:1368:A:OP1	43:p:113:ARG:NH2	2.45	0.50
10:I:1715:G:O2'	10:I:1716:U:OP2	2.30	0.50
10:I:328:U:O2'	30:c:68:SER:OG	2.28	0.50
3:3:38:TYR:N	45:r:124:PRO:O	2.41	0.50
10:I:1094:U:N3	10:I:1097:U:OP2	2.45	0.50
4:C:35:G:O2'	46:t:115:SER:O	2.20	0.50
6:E:5:VAL:HG21	6:E:10:ILE:HD11	1.94	0.50
10:I:2260:C:O2'	10:I:2388:A:O2'	2.22	0.50
11:J:8:C:OP1	24:W:15:ARG:NH2	2.39	0.50
47:u:56:LEU:H	47:u:56:LEU:HD22	1.77	0.50
4:C:766:A:OP2	4:C:812:G:N2	2.45	0.49
24:W:18:LEU:O	24:W:22:GLY:N	2.45	0.49
41:n:129:GLU:HA	41:n:129:GLU:OE1	2.11	0.49
4:C:51:A:N7	4:C:114:U:O2'	2.41	0.49
11:J:57:A:C4	15:N:26:MET:HE1	2.47	0.49
4:C:923:A:N6	4:C:1392:G:O6	2.45	0.49
8:G:151:GLU:OE1	8:G:151:GLU:N	2.37	0.49
16:O:42:GLU:OE1	16:O:43:VAL:N	2.46	0.49
31:d:43:ASP:C	31:d:43:ASP:OD1	2.56	0.49
44:q:17:LEU:O	44:q:17:LEU:HD23	2.12	0.49
4:C:1516:G:N2	4:C:1519:A:OP2	2.45	0.49
10:I:818:G:N1	10:I:1188:U:OP2	2.36	0.49
10:I:910:A:C8	22:U:13:HIS:NE2	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:1025:G:O2'	10:I:1026:G:P	2.70	0.49
10:I:2430:A:N3	10:I:2430:A:H2'	2.27	0.49
12:K:33:LEU:HD23	12:K:103:TYR:CD2	2.47	0.49
13:L:108:ASP:N	13:L:204:LYS:O	2.30	0.49
4:C:1201:A:H1'	4:C:1202:U:OP2	2.12	0.49
4:C:1238:A:H5'	4:C:1336:C:H41	1.77	0.49
6:E:92:ALA:O	6:E:96:GLY:N	2.42	0.49
10:I:1813:G:HO2'	10:I:1814:G:P	2.35	0.49
31:d:35:GLU:OE1	31:d:35:GLU:N	2.36	0.49
14:M:191:ASP:OD1	14:M:192:ALA:N	2.46	0.49
22:U:2:LEU:H	22:U:2:LEU:HD23	1.77	0.49
22:U:34:LYS:HE3	22:U:131:VAL:HG11	1.94	0.49
34:g:2:LYS:O	34:g:6:LEU:HD22	2.13	0.49
48:v:43:ASN:OD1	48:v:47:LYS:NZ	2.31	0.49
4:C:769:G:H4'	4:C:1513:A:H4'	1.95	0.49
7:F:202:GLU:OE1	8:G:112:ARG:NH2	2.38	0.49
5:D:50:PHE:O	5:D:54:LEU:HD12	2.12	0.49
10:I:182:A:O2'	10:I:183:C:P	2.71	0.49
10:I:1378:A:O2'	10:I:1380:G:OP2	2.31	0.49
10:I:2225:A:H1'	10:I:2226:C:OP2	2.13	0.49
15:N:106:ILE:HD11	18:Q:22:MET:HE2	1.93	0.49
17:P:123:ARG:HG3	17:P:123:ARG:HH11	1.78	0.49
44:q:88:MET:SD	44:q:88:MET:N	2.78	0.49
8:G:61:GLN:OE1	8:G:61:GLN:HA	2.12	0.49
22:U:47:GLU:OE1	22:U:47:GLU:HA	2.13	0.49
2:2:54:MET:HE3	2:2:58:VAL:HG21	1.94	0.48
6:E:5:VAL:HG11	6:E:10:ILE:HD11	1.94	0.48
10:I:1750:G:O2'	10:I:2860:A:N1	2.44	0.48
10:I:1754:A:O2'	10:I:1755:A:P	2.71	0.48
43:p:32:GLN:N	43:p:32:GLN:OE1	2.46	0.48
4:C:1013:G:N2	4:C:1016:A:OP2	2.41	0.48
10:I:1352:U:O2'	10:I:1353:A:P	2.72	0.48
10:I:1754:A:HO2'	10:I:1755:A:P	2.34	0.48
17:P:146:VAL:O	17:P:147:VAL:HG13	2.12	0.48
8:G:105:ILE:O	8:G:112:ARG:NH1	2.46	0.48
9:H:33:GLU:OE2	9:H:33:GLU:HA	2.12	0.48
10:I:1631:G:N2	10:I:1634:A:OP2	2.38	0.48
13:L:55:LYS:HD2	13:L:60:VAL:HG22	1.95	0.48
40:m:30:GLU:OE1	40:m:33:HIS:NE2	2.46	0.48
4:C:3:A:N1	4:C:628:G:O2'	2.45	0.48
10:I:2854:G:O2'	10:I:2855:C:P	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:18:LYS:NZ	4:C:1014:A:OP2	2.46	0.48
4:C:60:A:N1	4:C:107:G:O2'	2.39	0.48
6:E:19:ASN:OD1	6:E:54:ARG:NH1	2.46	0.48
4:C:846:G:HO2'	4:C:847:G:P	2.36	0.48
44:q:80:THR:O	44:q:83:THR:OG1	2.24	0.48
10:I:463:G:N2	10:I:466:A:OP2	2.44	0.48
10:I:537:G:H22	10:I:555:G:H2'	1.77	0.48
10:I:1266:G:O2'	10:I:1267:U:OP2	2.31	0.48
13:L:184:ARG:HH21	25:X:7:GLN:HE22	1.62	0.48
4:C:96:U:O2'	4:C:97:G:P	2.71	0.48
10:I:2134:A:O2'	10:I:2159:G:N2	2.41	0.48
35:h:7:ILE:HG21	35:h:48:ILE:HD11	1.94	0.48
4:C:1491:G:O2'	4:C:1492:A:P	2.72	0.48
5:D:199:VAL:HG12	5:D:201:PRO:HD3	1.96	0.48
2:2:33:LYS:NZ	4:C:1439:G:OP2	2.47	0.47
9:H:54:LEU:HD21	9:H:56:LYS:O	2.14	0.47
10:I:243:U:OP2	39:l:8:ARG:NH1	2.47	0.47
10:I:1071:G:O2'	10:I:1089:A:OP2	2.26	0.47
15:N:16:LEU:HD23	15:N:28:VAL:HG23	1.95	0.47
18:Q:35:ASP:OD1	18:Q:35:ASP:C	2.57	0.47
36:i:52:ARG:HB3	36:i:52:ARG:NH1	2.29	0.47
50:x:72:ALA:O	50:x:76:LYS:NZ	2.47	0.47
5:D:179:LEU:HB2	5:D:181:ILE:HD12	1.96	0.47
20:S:104:THR:HG22	20:S:106:GLU:OE1	2.14	0.47
4:C:951:G:OP2	47:u:101:ARG:NH2	2.47	0.47
5:D:11:LYS:HE2	5:D:11:LYS:HA	1.95	0.47
10:I:784:G:H5'	10:I:785:G:OP1	2.13	0.47
15:N:16:LEU:HD11	15:N:20:PHE:HE2	1.79	0.47
43:p:88:MET:HE2	43:p:88:MET:CA	2.44	0.47
37:j:34:LEU:HD23	37:j:34:LEU:H	1.79	0.47
5:D:187:VAL:HG23	5:D:191:SER:HB2	1.96	0.47
5:D:207:ILE:HD12	5:D:207:ILE:H	1.78	0.47
10:I:52:A:H8	10:I:178:G:H21	1.60	0.47
18:Q:59:ARG:HA	18:Q:59:ARG:NE	2.29	0.47
19:R:43:GLU:OE1	19:R:43:GLU:N	2.46	0.47
21:T:82:LEU:HD23	21:T:82:LEU:C	2.39	0.47
34:g:8:GLU:C	34:g:8:GLU:OE2	2.58	0.47
34:g:24:GLU:O	34:g:24:GLU:OE2	2.33	0.47
48:v:4:GLN:HA	48:v:4:GLN:OE1	2.14	0.47
41:n:110:LYS:HD3	41:n:110:LYS:N	2.29	0.47
44:q:17:LEU:HD22	44:q:96:VAL:CG1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:v:24:ARG:C	48:v:24:ARG:HD3	2.39	0.47
5:D:135:LEU:HD13	5:D:135:LEU:C	2.40	0.47
10:I:321:U:OP1	14:M:130:LYS:NZ	2.46	0.47
10:I:652:U:OP1	10:I:654:A:N6	2.48	0.47
10:I:2159:G:HO2'	10:I:2160:C:C5'	2.26	0.47
15:N:103:LEU:HA	15:N:107:ALA:HB3	1.96	0.47
17:P:68:ARG:CD	17:P:134:VAL:HG21	2.45	0.47
21:T:85:VAL:HG13	21:T:94:THR:HG22	1.97	0.47
28:a:96:ILE:HD12	28:a:96:ILE:C	2.39	0.47
48:v:46:LEU:HD13	48:v:46:LEU:C	2.40	0.47
8:G:109:GLY:O	8:G:110:ALA:HB3	2.15	0.47
10:I:534:U:HO2'	26:Y:49:ASP:CG	2.23	0.47
43:p:72:ILE:HD12	43:p:73:SER:N	2.29	0.47
46:t:56:ARG:HG3	46:t:56:ARG:HH11	1.79	0.47
10:I:52:A:H2	10:I:119:A:H62	1.61	0.47
10:I:2127:G:O2'	10:I:2128:G:P	2.72	0.47
30:c:99:ASN:C	30:c:99:ASN:OD1	2.58	0.47
8:G:83:HIS:NE2	8:G:148:ASN:OD1	2.42	0.47
10:I:555:G:H4'	10:I:556:A:OP1	2.14	0.47
10:I:2505:G:N2	10:I:2506[B]:U:O4	2.41	0.47
14:M:136:GLN:OE1	14:M:136:GLN:HA	2.15	0.47
21:T:69:ARG:HH11	21:T:69:ARG:HG2	1.80	0.47
10:I:1789:A:OP2	12:K:221:ARG:NH1	2.48	0.46
10:I:2020:A:H5'	36:i:9:THR:HG21	1.97	0.46
34:g:5:GLU:OE2	34:g:5:GLU:N	2.47	0.46
36:i:46:ASP:OD1	36:i:46:ASP:N	2.36	0.46
45:r:84:VAL:O	45:r:85:MET:HE2	2.15	0.46
45:r:126:LYS:HA	45:r:126:LYS:HE2	1.97	0.46
10:I:1313:U:O2'	10:I:1314:C:OP1	2.26	0.46
11:J:13:G:O2'	11:J:15:A:OP2	2.32	0.46
11:J:57:A:C5	15:N:26:MET:HE1	2.50	0.46
42:o:22:LYS:O	42:o:65:TYR:OH	2.28	0.46
9:H:18:VAL:N	9:H:19:PRO:HD2	2.30	0.46
10:I:182:A:HO2'	10:I:183:C:P	2.37	0.46
6:E:6:HIS:HB3	48:v:89:MET:HE2	1.97	0.46
10:I:2523:G:O2'	10:I:2764:A:O2'	2.32	0.46
15:N:143:TYR:O	15:N:146:VAL:HG22	2.15	0.46
34:g:14:LEU:HB3	34:g:57:LEU:HD21	1.96	0.46
4:C:96:U:O2'	4:C:97:G:OP1	2.31	0.46
7:F:174:ASP:OD2	7:F:177:LYS:NZ	2.40	0.46
8:G:34:THR:HG22	8:G:52:LYS:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:138:U:HO2'	10:I:139:U:P	2.33	0.46
10:I:499:U:OP1	30:c:43:LYS:NZ	2.48	0.46
10:I:2334:U:C6	24:W:12:THR:HG21	2.50	0.46
20:S:103:VAL:HG13	20:S:107:LEU:HD12	1.97	0.46
26:Y:111:GLU:HA	26:Y:111:GLU:OE1	2.16	0.46
34:g:2:LYS:HE3	34:g:6:LEU:HD21	1.97	0.46
43:p:57:MET:HE3	43:p:57:MET:H	1.80	0.46
10:I:205:G:O2'	10:I:206:U:OP2	2.31	0.46
10:I:1847:A:O2'	10:I:1848:A:P	2.74	0.46
13:L:86:GLU:OE1	13:L:86:GLU:HA	2.16	0.46
5:D:68:LEU:HD23	5:D:161:LEU:HD13	1.97	0.46
22:U:82:MET:HE2	22:U:82:MET:HA	1.98	0.46
50:x:4:ILE:HD13	50:x:67:ILE:HD13	1.98	0.46
8:G:16:ILE:HD11	8:G:38:VAL:HG22	1.98	0.46
10:I:2306:C:OP2	10:I:2307:G:O2'	2.32	0.46
10:I:2854:G:HO2'	10:I:2855:C:P	2.39	0.46
45:r:64:GLN:NE2	45:r:68:GLU:OE2	2.46	0.46
2:2:57:ILE:HD12	2:2:57:ILE:C	2.41	0.46
6:E:134:MET:HE2	6:E:168:TYR:CE1	2.51	0.46
10:I:2334:U:O3'	24:W:13:ARG:NH2	2.49	0.46
11:J:66:A:OP2	11:J:108:A:N6	2.48	0.46
12:K:69:ARG:O	12:K:189:ARG:NH1	2.49	0.46
15:N:111:ILE:HA	15:N:137:ILE:HG21	1.98	0.46
4:C:420:U:O2'	4:C:423:G:O6	2.33	0.45
9:H:61:LEU:HD23	9:H:62:MET:N	2.31	0.45
10:I:971:G:O2'	10:I:983:A:N3	2.45	0.45
10:I:2331:G:O2'	10:I:2336:A:N1	2.40	0.45
18:Q:60:PHE:CD1	18:Q:60:PHE:C	2.92	0.45
8:G:36:LEU:HD13	8:G:134:ILE:HD13	1.97	0.45
31:d:55:GLU:OE1	31:d:55:GLU:N	2.45	0.45
45:r:36:ASP:OD1	45:r:36:ASP:C	2.58	0.45
5:D:204:ASP:OD1	5:D:204:ASP:N	2.49	0.45
10:I:1629:U:O4	10:I:1630:A:N6	2.49	0.45
10:I:1833:C:O2'	10:I:1969:A:N1	2.47	0.45
17:P:15:LEU:HD22	17:P:58:LEU:HD12	1.98	0.45
45:r:112:ASP:OD1	45:r:114:THR:HG22	2.16	0.45
45:r:116:ILE:HG22	45:r:116:ILE:O	2.15	0.45
11:J:94:A:OP1	31:d:19:ARG:NH1	2.47	0.45
12:K:71:LYS:NZ	12:K:100:GLU:OE2	2.49	0.45
13:L:39:ASP:OD1	13:L:40:LEU:N	2.50	0.45
47:u:83:LEU:HD12	47:u:83:LEU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1183:U:O2'	4:C:1185:G:OP2	2.35	0.45
19:R:4:PHE:O	26:Y:64:ARG:NH2	2.46	0.45
4:C:1239:A:H62	4:C:1299:A:N6	2.14	0.45
8:G:25:VAL:HG22	8:G:26:LYS:N	2.32	0.45
10:I:603:A:H5''	10:I:655:A:H61	1.80	0.45
10:I:2799:A:HO2'	10:I:2800:A:P	2.38	0.45
2:2:70:ASN:OD1	2:2:70:ASN:C	2.59	0.45
30:c:98:SER:O	30:c:99:ASN:OD1	2.35	0.45
35:h:37:GLU:OE1	35:h:37:GLU:HA	2.16	0.45
41:n:110:LYS:HD3	41:n:110:LYS:H	1.82	0.45
43:p:30:ILE:CG1	43:p:65:ILE:HD11	2.45	0.45
4:C:565:U:OP2	4:C:566:G:O2'	2.33	0.45
10:I:629:G:N3	10:I:639:U:O2'	2.50	0.45
10:I:1869:G:N2	10:I:1871:A:O2'	2.49	0.45
15:N:74:VAL:CG2	15:N:79:ILE:HD11	2.47	0.45
30:c:49:VAL:HG22	30:c:50:PRO:CD	2.47	0.45
4:C:123:U:OP1	4:C:311:C:O2'	2.30	0.45
12:K:261:LYS:HA	12:K:264:ASP:OD2	2.17	0.45
15:N:133:ARG:HA	15:N:133:ARG:NE	2.32	0.45
17:P:46:PHE:CD1	17:P:46:PHE:C	2.95	0.45
27:Z:26:ASP:CG	27:Z:26:ASP:O	2.60	0.45
31:d:7:GLU:OE1	31:d:8:VAL:O	2.35	0.45
44:q:25:ILE:HD12	44:q:26:VAL:N	2.31	0.45
45:r:113:VAL:O	45:r:113:VAL:CG1	2.65	0.45
47:u:16:VAL:HG23	47:u:30:SER:OG	2.17	0.45
5:D:187:VAL:HG11	5:D:199:VAL:HG13	1.98	0.45
17:P:5:LEU:HD21	17:P:12:LEU:HD23	1.99	0.45
43:p:28:ILE:CD1	43:p:63:LEU:HD11	2.47	0.45
48:v:92:GLU:HA	48:v:92:GLU:OE2	2.17	0.45
4:C:1372:U:P	43:p:73:SER:HG	2.37	0.44
10:I:2359:C:O2'	39:l:54:ASP:OD2	2.29	0.44
10:I:2436:G:O2'	10:I:2598:A:N1	2.48	0.44
10:I:2680:U:O2'	10:I:2681:C:P	2.75	0.44
15:N:94:GLU:OE2	15:N:94:GLU:HA	2.17	0.44
25:X:88:ARG:NE	25:X:112:GLU:OE1	2.50	0.44
43:p:5:GLN:HA	43:p:5:GLN:OE1	2.17	0.44
50:x:42:ILE:HD13	50:x:42:ILE:N	2.32	0.44
51:y:48:ASP:C	51:y:48:ASP:OD1	2.60	0.44
10:I:534:U:O2'	26:Y:49:ASP:OD1	2.28	0.44
10:I:858:G:OP1	32:e:78:LYS:NZ	2.37	0.44
17:P:94:ILE:O	17:P:94:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:u:107:ARG:O	47:u:111:GLY:N	2.49	0.44
4:C:898:G:N2	4:C:901:A:OP2	2.44	0.44
4:C:935:A:O2'	4:C:1383:C:N3	2.47	0.44
10:I:55:G:O2'	10:I:127:A:N1	2.47	0.44
10:I:2335:A:P	24:W:13:ARG:HH12	2.40	0.44
22:U:1:MET:HE1	22:U:44:ARG:NE	2.32	0.44
22:U:34:LYS:CE	22:U:131:VAL:HG11	2.46	0.44
29:b:47:VAL:HG23	29:b:51:PHE:HD2	1.80	0.44
29:b:69:ARG:NH1	29:b:74:ILE:HD13	2.33	0.44
18:Q:63:ARG:HG3	18:Q:64:PHE:HB2	1.99	0.44
34:g:4:LYS:H	34:g:4:LYS:HD2	1.81	0.44
48:v:89:MET:HE3	48:v:89:MET:HA	2.00	0.44
2:2:66:LEU:HG	2:2:67:ILE:HG23	1.98	0.44
10:I:2576:G:O2'	10:I:2579:C:OP2	2.26	0.44
14:M:21:ARG:HG3	14:M:21:ARG:HH11	1.81	0.44
30:c:62:GLU:H	30:c:62:GLU:CD	2.24	0.44
44:q:25:ILE:HD12	44:q:25:ILE:C	2.42	0.44
45:r:75:LYS:HZ2	45:r:75:LYS:HB3	1.83	0.44
50:x:1:MET:CE	50:x:66:THR:HG21	2.47	0.44
51:y:72:SER:O	51:y:72:SER:OG	2.33	0.44
4:C:619:U:N3	7:F:131:ASN:OD1	2.50	0.44
11:J:40:U:N3	11:J:44:G:OP2	2.39	0.44
15:N:38:MET:HE3	15:N:57:LEU:CD2	2.47	0.44
29:b:47:VAL:HG13	29:b:55:VAL:HG21	1.99	0.44
2:2:36:TYR:CD1	2:2:36:TYR:C	2.96	0.44
10:I:989:G:OP2	35:h:12:SER:OG	2.21	0.44
10:I:1019:U:OP1	10:I:1035:U:O2'	2.28	0.44
10:I:2391:G:N2	10:I:2429:G:O4'	2.51	0.44
17:P:129:GLU:HA	17:P:129:GLU:OE2	2.17	0.44
28:a:4:ILE:HD11	28:a:104:THR:HG23	1.99	0.44
5:D:52:GLU:C	5:D:52:GLU:CD	2.86	0.44
5:D:146:ASN:C	5:D:146:ASN:OD1	2.60	0.44
10:I:74:A:O2'	10:I:88:G:OP1	2.36	0.44
21:T:69:ARG:HG2	21:T:69:ARG:NH1	2.33	0.44
43:p:65:ILE:HD12	43:p:65:ILE:O	2.18	0.44
44:q:17:LEU:HD22	44:q:96:VAL:HG13	1.99	0.44
45:r:20:VAL:N	45:r:35:THR:O	2.42	0.44
1:1:62:VAL:HA	1:1:66:MET:HE2	2.00	0.44
4:C:1372:U:OP1	43:p:73:SER:OG	2.19	0.44
10:I:1141:U:H4'	10:I:1142:A:O4'	2.18	0.44
10:I:2627:G:N2	10:I:2777:G:OP2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T:123:ARG:NH2	21:T:143:GLU:OE1	2.51	0.44
5:D:68:LEU:HD11	5:D:92:VAL:HG23	2.00	0.43
14:M:91:ASP:OD1	14:M:91:ASP:C	2.60	0.43
4:C:130:A:O2'	4:C:131:A:O5'	2.36	0.43
4:C:1302:C:OP1	47:u:13:LYS:NZ	2.41	0.43
10:I:1248:G:OP1	14:M:44:ARG:NH1	2.41	0.43
10:I:2821:A:OP2	13:L:115:GLY:N	2.45	0.43
19:R:43:GLU:N	19:R:43:GLU:CD	2.76	0.43
46:t:56:ARG:HG3	46:t:56:ARG:NH1	2.31	0.43
49:w:67:LEU:HD11	49:w:87:LEU:HD11	2.00	0.43
3:3:42:THR:HG23	4:C:1526:G:OP2	2.18	0.43
4:C:745:G:OP1	4:C:851:G:O2'	2.33	0.43
7:F:76:TYR:HA	7:F:90:LEU:HD13	2.00	0.43
8:G:90:THR:HG22	8:G:91:GLY:N	2.33	0.43
4:C:687:A:O2'	4:C:701:U:O4	2.14	0.43
4:C:1086:U:H3	4:C:1099:G:H22	1.65	0.43
7:F:125:VAL:O	7:F:125:VAL:HG13	2.18	0.43
10:I:764:A:N3	12:K:212:ARG:NH1	2.66	0.43
15:N:173:PHE:O	15:N:174:ASP:CG	2.60	0.43
22:U:42:THR:HG22	22:U:43:ALA:N	2.33	0.43
24:W:112:GLU:CD	24:W:112:GLU:H	2.27	0.43
10:I:71:A:H4'	10:I:72:U:H5'	1.99	0.43
10:I:1420:A:N1	10:I:2211:A:N6	2.66	0.43
10:I:479:A:H4'	10:I:480:A:OP1	2.18	0.43
10:I:1224:U:OP2	27:Z:68:ARG:NH2	2.51	0.43
28:a:1:MET:HE3	28:a:2:GLU:O	2.19	0.43
4:C:1491:G:O3'	46:t:44:LYS:NZ	2.52	0.43
37:j:17:THR:HB	37:j:42:VAL:HG11	2.00	0.43
43:p:19:VAL:HG13	43:p:65:ILE:CG2	2.48	0.43
52:z:26:ILE:HG23	52:z:68:LEU:HD21	2.00	0.43
4:C:1180:A:OP2	43:p:99:ARG:NH2	2.48	0.43
15:N:42:GLU:H	15:N:42:GLU:CD	2.26	0.43
15:N:136:ILE:HD13	15:N:136:ILE:N	2.34	0.43
37:j:11:LEU:HD21	37:j:34:LEU:HD21	2.01	0.43
45:r:126:LYS:HE2	45:r:126:LYS:CA	2.49	0.43
51:y:49:GLU:OE2	51:y:49:GLU:HA	2.18	0.43
10:I:1800:C:H3'	12:K:146:MET:HE1	2.01	0.43
14:M:79:ARG:O	14:M:80:SER:OG	2.25	0.43
21:T:23:ILE:HD13	27:Z:82:HIS:CD2	2.54	0.43
22:U:57:VAL:O	22:U:57:VAL:HG23	2.19	0.43
33:f:41:GLU:OE2	33:f:41:GLU:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:n:74:GLU:HG2	41:n:91:VAL:HG12	2.00	0.43
43:p:28:ILE:HD12	43:p:63:LEU:HD11	2.01	0.43
4:C:131:A:O2'	4:C:262:A:N3	2.41	0.43
5:D:210:VAL:HG12	5:D:214:LEU:HD21	2.01	0.43
17:P:98:ASP:OD1	17:P:98:ASP:N	2.51	0.43
18:Q:12:ILE:HG13	18:Q:24:ILE:HG23	2.01	0.43
30:c:34:VAL:HG13	30:c:67:VAL:HG12	1.99	0.43
4:C:796:C:O3'	45:r:127:ARG:NH1	2.52	0.42
4:C:1224:U:O2'	4:C:1322:C:OP1	2.33	0.42
5:D:162:PHE:CZ	5:D:217:VAL:HG21	2.53	0.42
8:G:151:GLU:H	8:G:151:GLU:CD	2.25	0.42
10:I:27:G:O2'	10:I:28:A:OP2	2.33	0.42
10:I:1326:U:O2'	10:I:2010:G:O2'	2.36	0.42
16:O:103:ILE:CD1	16:O:117:LEU:HD21	2.49	0.42
43:p:17:ALA:CB	43:p:67:VAL:HG12	2.49	0.42
47:u:9:ILE:HD13	47:u:18:ALA:HB1	2.01	0.42
49:w:82:ILE:HG13	49:w:83:GLU:N	2.34	0.42
7:F:13:ARG:HG3	7:F:13:ARG:HH11	1.84	0.42
10:I:2540:C:O2'	10:I:2740:A:N3	2.46	0.42
15:N:135:GLN:HE22	15:N:150:ARG:HE	1.67	0.42
28:a:3:THR:OG1	28:a:62:ASP:OD2	2.33	0.42
45:r:119:ASN:OD1	45:r:119:ASN:N	2.52	0.42
2:2:61:GLN:HB3	2:2:66:LEU:HD21	2.01	0.42
4:C:437:U:O2'	7:F:120:HIS:ND1	2.44	0.42
4:C:523:A:H61	46:t:89:ASP:HB2	1.84	0.42
10:I:87:U:H5''	10:I:88:G:OP2	2.19	0.42
10:I:1980:G:O2'	10:I:1982:U:OP2	2.35	0.42
10:I:2126:A:O2'	10:I:2162:G:N2	2.52	0.42
10:I:2831:G:OP1	13:L:56:LYS:NZ	2.42	0.42
32:e:56:ASP:OD1	32:e:58:THR:OG1	2.35	0.42
47:u:19:LEU:O	47:u:22:ILE:HD12	2.19	0.42
5:D:136:MET:HE3	5:D:137:ARG:N	2.34	0.42
10:I:2660:A:HO2'	10:I:2661:G:P	2.39	0.42
12:K:79:GLU:N	12:K:93:LEU:O	2.48	0.42
28:a:73:LYS:NZ	28:a:73:LYS:HB3	2.34	0.42
50:x:51:ARG:C	50:x:52:LEU:HD22	2.44	0.42
1:1:35:SER:HG	1:1:38:SER:HG	1.38	0.42
4:C:976:G:OP2	4:C:1358:U:O2'	2.37	0.42
5:D:135:LEU:HD13	5:D:135:LEU:O	2.19	0.42
9:H:81:ASN:HB3	9:H:84:VAL:HG12	2.01	0.42
10:I:1077:A:H61	10:I:1088:A:H2'	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:1129:A:HO2'	10:I:2515:C:HO2'	1.63	0.42
13:L:85:ALA:HB3	13:L:88:GLU:OE1	2.19	0.42
15:N:147:ASP:OD1	15:N:147:ASP:N	2.52	0.42
41:n:27:VAL:O	41:n:31:MET:N	2.48	0.42
43:p:19:VAL:HA	43:p:65:ILE:HG22	2.02	0.42
45:r:50:SER:OG	45:r:69:ARG:NH2	2.53	0.42
6:E:49:LYS:O	6:E:72:ARG:NH2	2.52	0.42
10:I:1474:U:O4	10:I:1475:G:N1	2.53	0.42
10:I:1477:A:N6	10:I:1514:G:O2'	2.53	0.42
12:K:152:GLY:O	12:K:156:ARG:NH1	2.52	0.42
15:N:40:VAL:HG23	15:N:41:GLY:N	2.35	0.42
17:P:5:LEU:O	17:P:15:LEU:HD12	2.18	0.42
1:l:73:GLU:O	47:u:86:TYR:N	2.51	0.42
12:K:108:LYS:N	12:K:194:GLU:O	2.53	0.42
15:N:3:LYS:O	15:N:7:TYR:N	2.45	0.42
16:O:129:THR:OG1	16:O:130:GLU:OE2	2.35	0.42
37:j:47:VAL:HG12	37:j:48:ILE:N	2.35	0.42
3:3:60:LEU:H	3:3:60:LEU:HD22	1.85	0.42
9:H:86:ARG:HE	9:H:86:ARG:HB2	1.77	0.42
9:H:90:MET:HE1	52:z:61:ARG:HD3	2.02	0.42
10:I:993:G:OP2	26:Y:51:ARG:NH2	2.48	0.42
15:N:22:TYR:OH	15:N:165:GLU:OE1	2.29	0.42
41:n:103:TRP:O	41:n:107:ALA:N	2.49	0.42
4:C:9:G:OP2	8:G:126:LYS:NZ	2.47	0.42
7:F:131:ASN:OD1	7:F:131:ASN:N	2.51	0.42
9:H:61:LEU:HD11	52:z:24:LYS:HE3	2.02	0.42
10:I:491:G:O6	28:a:49:LYS:NZ	2.50	0.42
10:I:2346:A:HO2'	37:j:39:PHE:HZ	1.64	0.42
43:p:19:VAL:HG11	43:p:83:ILE:HG12	2.01	0.42
4:C:538:G:P	46:t:112:GLN:HE21	2.43	0.42
4:C:1363:A:O2'	4:C:1365:G:N7	2.40	0.42
10:I:1730:C:O2	10:I:1731:G:N1	2.53	0.42
10:I:2333:A:H4'	10:I:2334:U:H2'	2.01	0.42
14:M:125:SER:O	14:M:137:LYS:NZ	2.53	0.42
14:M:154:ASP:OD1	14:M:154:ASP:C	2.63	0.42
30:c:27:ASN:OD1	30:c:28:VAL:N	2.53	0.42
35:h:40:ASP:OD1	35:h:45:ARG:NE	2.50	0.42
50:x:45:GLU:H	50:x:45:GLU:CD	2.27	0.42
8:G:132:ASN:OD1	8:G:134:ILE:HG22	2.20	0.41
10:I:1025:G:O2'	10:I:1026:G:OP2	2.35	0.41
10:I:2258:C:O2'	10:I:2427:C:OP2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:12:THR:CG2	13:L:13:ARG:N	2.83	0.41
14:M:5:LEU:HD22	14:M:5:LEU:H	1.85	0.41
14:M:168:ASP:OD2	14:M:170:ARG:NH1	2.44	0.41
20:S:103:VAL:CG1	20:S:107:LEU:HD12	2.50	0.41
4:C:973:G:OP1	44:q:59:LYS:NZ	2.53	0.41
5:D:207:ILE:O	5:D:211:THR:HG23	2.20	0.41
10:I:548:G:C4'	10:I:549:G:OP1	2.68	0.41
10:I:603:A:N1	10:I:625:G:O2'	2.50	0.41
22:U:64:TRP:HB2	22:U:104:GLU:HB2	2.01	0.41
37:j:17:THR:HG21	37:j:42:VAL:HB	2.01	0.41
49:w:33:THR:O	49:w:37:ASN:ND2	2.53	0.41
5:D:27:MET:SD	5:D:187:VAL:HG22	2.60	0.41
10:I:1422:G:O3'	10:I:1492:G:O2'	2.33	0.41
10:I:2159:G:HO2'	10:I:2160:C:C4'	2.33	0.41
10:I:2876:G:OP1	25:X:2:SER:N	2.52	0.41
15:N:108:VAL:N	15:N:109:PRO:CD	2.83	0.41
16:O:81:GLU:N	16:O:81:GLU:CD	2.77	0.41
27:Z:49:ILE:HD13	27:Z:49:ILE:N	2.36	0.41
48:v:18:ASP:O	48:v:18:ASP:OD2	2.38	0.41
19:R:31:GLU:OE1	19:R:34:ARG:NH1	2.53	0.41
4:C:1492:A:OP2	46:t:44:LYS:NZ	2.52	0.41
5:D:123:ASP:OD2	5:D:125:THR:HG23	2.21	0.41
7:F:35:GLU:OE1	7:F:35:GLU:N	2.40	0.41
10:I:1028:A:OP2	10:I:1126:A:N6	2.52	0.41
10:I:1688:U:O2'	10:I:1700:A:N7	2.40	0.41
10:I:1913:A:H1'	10:I:1914:C:P	2.60	0.41
10:I:2038:G:H2'	10:I:2039:U:O4'	2.20	0.41
10:I:2857:G:N2	10:I:2860:A:OP2	2.44	0.41
48:v:88:ALA:HB1	48:v:96:LEU:HD23	2.01	0.41
50:x:45:GLU:CD	50:x:45:GLU:N	2.79	0.41
7:F:27:ALA:O	7:F:28:ILE:O	2.39	0.41
10:I:984:A:N3	10:I:984:A:H2'	2.34	0.41
14:M:91:ASP:OD1	14:M:93:SER:N	2.47	0.41
31:d:51:GLN:OE1	31:d:57:TYR:OH	2.37	0.41
41:n:69:VAL:O	41:n:69:VAL:HG12	2.21	0.41
4:C:115:G:H1'	4:C:116:A:OP2	2.21	0.41
10:I:101:A:N3	10:I:101:A:H2'	2.35	0.41
46:t:110:ARG:NH1	46:t:112:GLN:O	2.53	0.41
49:w:17:ARG:NH1	49:w:17:ARG:HB2	2.36	0.41
2:2:33:LYS:NZ	4:C:1439:G:P	2.93	0.41
3:3:56:HIS:O	3:3:60:LEU:HD22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:76:C:O2'	34:g:55:THR:HG21	2.20	0.41
10:I:2622:U:O2'	10:I:2825:G:N7	2.54	0.41
17:P:146:VAL:O	17:P:146:VAL:HG23	2.21	0.41
31:d:73:LYS:HE3	31:d:73:LYS:HB3	1.92	0.41
51:y:68:SER:OG	51:y:71:LYS:HB2	2.20	0.41
5:D:146:ASN:OD1	5:D:147:SER:N	2.54	0.41
6:E:86:LYS:HD2	6:E:86:LYS:C	2.46	0.41
8:G:83:HIS:O	8:G:85:VAL:HG13	2.20	0.41
10:I:18:U:O2'	10:I:554:U:OP1	2.34	0.41
10:I:36:G:N3	10:I:450:G:O2'	2.53	0.41
10:I:2225:A:H4'	10:I:2226:C:O5'	2.20	0.41
10:I:2314:A:H5'	15:N:35:THR:HG21	2.03	0.41
10:I:2335:A:H5'	24:W:13:ARG:HH22	1.86	0.41
10:I:2401:U:O2	10:I:2401:U:O5'	2.37	0.41
14:M:16:GLU:OE2	14:M:16:GLU:HA	2.20	0.41
15:N:137:ILE:HD12	15:N:138:PHE:H	1.85	0.41
30:c:27:ASN:OD1	30:c:27:ASN:C	2.64	0.41
43:p:47:VAL:HG12	43:p:80:ARG:HG3	2.02	0.41
43:p:85:ARG:HG2	43:p:85:ARG:HH11	1.86	0.41
45:r:37:ARG:HG3	45:r:37:ARG:HH11	1.85	0.41
4:C:570:G:O6	4:C:865:A:N6	2.54	0.41
5:D:217:VAL:O	5:D:221:VAL:HG23	2.21	0.41
13:L:156:PHE:CE1	19:R:81:ILE:HD13	2.56	0.41
15:N:106:ILE:HD11	18:Q:22:MET:CE	2.51	0.41
30:c:98:SER:O	30:c:99:ASN:CG	2.64	0.41
2:2:28:MET:HE1	2:2:67:ILE:HG21	2.03	0.40
4:C:212:G:H4'	4:C:213:G:OP1	2.20	0.40
5:D:93:ASN:OD1	5:D:93:ASN:N	2.45	0.40
7:F:95:GLU:OE1	7:F:100:ASN:ND2	2.52	0.40
9:H:52:ASN:OD1	9:H:52:ASN:N	2.54	0.40
19:R:90:GLU:OE2	19:R:90:GLU:HA	2.20	0.40
44:q:79:PRO:O	44:q:80:THR:C	2.63	0.40
6:E:5:VAL:HG22	6:E:6:HIS:N	2.36	0.40
7:F:128:ARG:HB3	7:F:128:ARG:CZ	2.51	0.40
7:F:164:GLN:OE1	7:F:164:GLN:N	2.54	0.40
10:I:796:C:OP1	14:M:57:LYS:HE2	2.21	0.40
10:I:1636:U:HO2'	10:I:1760:C:HO2'	1.64	0.40
10:I:1847:A:C2'	10:I:1848:A:OP2	2.69	0.40
12:K:133:ARG:NH1	12:K:133:ARG:HB2	2.36	0.40
17:P:75:LEU:O	17:P:142:VAL:HG23	2.21	0.40
4:C:978:A:HO2'	4:C:1322:C:H5	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:37:THR:HG21	8:G:64:MET:HE2	2.03	0.40
9:H:86:ARG:HD3	52:z:64:TYR:O	2.22	0.40
15:N:174:ASP:OD1	15:N:174:ASP:C	2.64	0.40
17:P:15:LEU:HD12	17:P:16:GLY:N	2.37	0.40
27:Z:73:LYS:HE2	27:Z:73:LYS:HB3	1.91	0.40
41:n:32:VAL:HG13	41:n:33:ASP:OD1	2.21	0.40
43:p:19:VAL:HG21	43:p:82:GLY:HA3	2.03	0.40
43:p:85:ARG:HG2	43:p:85:ARG:NH1	2.37	0.40
5:D:149:GLY:O	5:D:152:LYS:NZ	2.54	0.40
8:G:151:GLU:N	8:G:151:GLU:CD	2.80	0.40
26:Y:91:ASP:OD1	26:Y:91:ASP:C	2.63	0.40
38:k:1:MET:SD	38:k:1:MET:N	2.94	0.40
43:p:97:GLU:OE1	43:p:97:GLU:N	2.47	0.40
48:v:24:ARG:NH2	48:v:48:LEU:HD13	2.36	0.40
52:z:65:LEU:O	52:z:66:SER:OG	2.35	0.40
7:F:125:VAL:HG12	7:F:130:VAL:CG2	2.52	0.40
37:j:23:THR:HG22	37:j:24:THR:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
2	2	83/87 (95%)	83 (100%)	0	0	100	100
3	3	68/71 (96%)	68 (100%)	0	0	100	100
5	D	216/240 (90%)	209 (97%)	6 (3%)	1 (0%)	24	27
6	E	204/233 (88%)	200 (98%)	4 (2%)	0	100	100
7	F	203/206 (98%)	193 (95%)	9 (4%)	1 (0%)	24	27
8	G	148/167 (89%)	140 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	H	98/135 (73%)	97 (99%)	1 (1%)	0	100	100
12	K	271/273 (99%)	261 (96%)	10 (4%)	0	100	100
13	L	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
14	M	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
15	N	175/179 (98%)	171 (98%)	4 (2%)	0	100	100
16	O	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
17	P	147/149 (99%)	144 (98%)	3 (2%)	0	100	100
18	Q	56/70 (80%)	54 (96%)	2 (4%)	0	100	100
19	R	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
20	S	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
21	T	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
22	U	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
23	V	118/127 (93%)	118 (100%)	0	0	100	100
24	W	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
25	X	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
26	Y	115/118 (98%)	115 (100%)	0	0	100	100
27	Z	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
28	a	108/110 (98%)	108 (100%)	0	0	100	100
29	b	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
30	c	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
31	d	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
32	e	73/85 (86%)	73 (100%)	0	0	100	100
33	f	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
34	g	60/63 (95%)	60 (100%)	0	0	100	100
35	h	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
36	i	54/57 (95%)	54 (100%)	0	0	100	100
37	j	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
38	k	44/46 (96%)	44 (100%)	0	0	100	100
39	l	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
40	m	36/38 (95%)	36 (100%)	0	0	100	100
41	n	149/179 (83%)	147 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	o	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
43	p	125/130 (96%)	117 (94%)	7 (6%)	1 (1%)	16	17
44	q	96/103 (93%)	90 (94%)	5 (5%)	1 (1%)	12	12
45	r	115/129 (89%)	111 (96%)	4 (4%)	0	100	100
46	t	121/124 (98%)	117 (97%)	4 (3%)	0	100	100
47	u	113/118 (96%)	106 (94%)	7 (6%)	0	100	100
48	v	92/101 (91%)	90 (98%)	2 (2%)	0	100	100
49	w	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
50	x	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
51	y	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
52	z	53/75 (71%)	53 (100%)	0	0	100	100
All	All	5555/5912 (94%)	5424 (98%)	127 (2%)	4 (0%)	49	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	F	28	ILE
43	p	55	VAL
44	q	57	VAL
5	D	14	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	70/79 (89%)	68 (97%)	2 (3%)	37	49
2	2	65/66 (98%)	65 (100%)	0	100	100
3	3	60/61 (98%)	60 (100%)	0	100	100
5	D	180/198 (91%)	177 (98%)	3 (2%)	53	68
6	E	170/190 (90%)	169 (99%)	1 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	F	172/173 (99%)	171 (99%)	1 (1%)	78	87
8	G	113/126 (90%)	112 (99%)	1 (1%)	70	82
9	H	87/116 (75%)	87 (100%)	0	100	100
12	K	218/218 (100%)	217 (100%)	1 (0%)	81	89
13	L	164/164 (100%)	163 (99%)	1 (1%)	78	87
14	M	165/165 (100%)	165 (100%)	0	100	100
15	N	148/150 (99%)	143 (97%)	5 (3%)	32	43
16	O	137/138 (99%)	136 (99%)	1 (1%)	76	86
17	P	114/114 (100%)	112 (98%)	2 (2%)	51	66
18	Q	55/62 (89%)	52 (94%)	3 (6%)	19	24
19	R	116/116 (100%)	115 (99%)	1 (1%)	70	82
20	S	103/104 (99%)	103 (100%)	0	100	100
21	T	103/103 (100%)	99 (96%)	4 (4%)	28	39
22	U	108/108 (100%)	108 (100%)	0	100	100
23	V	100/103 (97%)	100 (100%)	0	100	100
24	W	86/87 (99%)	84 (98%)	2 (2%)	44	58
25	X	99/100 (99%)	99 (100%)	0	100	100
26	Y	89/90 (99%)	88 (99%)	1 (1%)	65	79
27	Z	84/84 (100%)	83 (99%)	1 (1%)	63	77
28	a	93/93 (100%)	92 (99%)	1 (1%)	65	79
29	b	80/84 (95%)	79 (99%)	1 (1%)	61	76
30	c	83/85 (98%)	83 (100%)	0	100	100
31	d	78/78 (100%)	77 (99%)	1 (1%)	61	76
32	e	57/63 (90%)	57 (100%)	0	100	100
33	f	67/68 (98%)	67 (100%)	0	100	100
34	g	54/55 (98%)	52 (96%)	2 (4%)	30	40
35	h	48/49 (98%)	48 (100%)	0	100	100
36	i	47/48 (98%)	46 (98%)	1 (2%)	47	61
37	j	45/49 (92%)	45 (100%)	0	100	100
38	k	38/38 (100%)	38 (100%)	0	100	100
39	l	51/52 (98%)	51 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	m	34/34 (100%)	34 (100%)	0	100	100
41	n	124/147 (84%)	123 (99%)	1 (1%)	73	84
42	o	104/105 (99%)	103 (99%)	1 (1%)	68	81
43	p	105/107 (98%)	104 (99%)	1 (1%)	68	81
44	q	86/90 (96%)	85 (99%)	1 (1%)	63	77
45	r	90/99 (91%)	88 (98%)	2 (2%)	45	59
46	t	103/104 (99%)	102 (99%)	1 (1%)	68	81
47	u	93/96 (97%)	93 (100%)	0	100	100
48	v	79/84 (94%)	77 (98%)	2 (2%)	42	55
49	w	75/77 (97%)	75 (100%)	0	100	100
50	x	65/65 (100%)	65 (100%)	0	100	100
51	y	74/78 (95%)	73 (99%)	1 (1%)	59	73
52	z	48/65 (74%)	48 (100%)	0	100	100
All	All	4627/4828 (96%)	4581 (99%)	46 (1%)	65	81

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	12	ASP
1	1	39	THR
5	D	117	LEU
5	D	205	ASP
5	D	214	LEU
6	E	186	THR
7	F	189	SER
8	G	64	MET
12	K	118	SER
13	L	113	SER
15	N	37	ASN
15	N	108	VAL
15	N	117	LEU
15	N	135	GLN
15	N	158	THR
16	O	168	VAL
17	P	14	SER
17	P	54	LEU
18	Q	13	THR

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Mol	Chain	Res	Type
18	Q	28	VAL
18	Q	32	LEU
19	R	128	ASN
21	T	7	SER
21	T	70	LYS
21	T	118	THR
21	T	125	LEU
24	W	18	LEU
24	W	100	HIS
26	Y	88	VAL
27	Z	43	ASN
28	a	53	SER
29	b	74	ILE
31	d	61	LEU
34	g	2	LYS
34	g	34	SER
36	i	11	SER
41	n	23	LEU
42	o	26	THR
43	p	31	ASN
44	q	77	VAL
45	r	58	SER
45	r	108	THR
46	t	5	ASN
48	v	30	ILE
48	v	80	SER
51	y	28	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	20	HIS
5	D	19	GLN
5	D	190	ASN
6	E	8	ASN
7	F	196	ASN
8	G	73	ASN
8	G	78	ASN
12	K	90	ASN
12	K	134	ASN
12	K	243	HIS
14	M	90	GLN

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Mol	Chain	Res	Type
14	M	165	HIS
16	O	30	ASN
16	O	48	ASN
16	O	128	GLN
16	O	139	GLN
18	Q	65	ASN
19	R	132	HIS
23	V	18	GLN
23	V	62	ASN
23	V	73	ASN
24	W	104	GLN
25	X	15	GLN
25	X	56	HIS
26	Y	20	GLN
27	Z	12	HIS
27	Z	86	GLN
29	b	15	HIS
30	c	45	HIS
30	c	46	GLN
33	f	36	HIS
34	g	31	GLN
34	g	41	HIS
37	j	46	HIS
44	q	56	HIS
44	q	58	ASN
45	r	40	ASN
45	r	101	ASN
46	t	112	GLN
47	u	52	GLN
49	w	40	GLN
50	x	9	HIS
52	z	74	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	I	2894/2904 (99%)	359 (12%)	29 (1%)
11	J	117/120 (97%)	10 (8%)	0
4	C	1539/1540 (99%)	174 (11%)	7 (0%)
All	All	4550/4564 (99%)	543 (11%)	36 (0%)

All (543) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	C	4	U
4	C	9	G
4	C	32	A
4	C	39	G
4	C	47	C
4	C	48	C
4	C	51	A
4	C	70	U
4	C	71	A
4	C	74	A
4	C	83	C
4	C	85	U
4	C	87	C
4	C	95	C
4	C	97	G
4	C	108	G
4	C	116	A
4	C	120	A
4	C	121	U
4	C	130	A
4	C	131	A
4	C	143	A
4	C	144	G
4	C	164	G
4	C	182	A
4	C	207	C
4	C	208	U
4	C	209	U
4	C	210	C
4	C	211	G
4	C	245	U
4	C	247	G
4	C	251	G
4	C	266	G
4	C	267	C
4	C	279	A
4	C	280	C
4	C	289	G
4	C	328	C
4	C	329	A
4	C	332	G
4	C	352	C
4	C	354	G

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Mol	Chain	Res	Type
4	C	356	A
4	C	367	U
4	C	372	C
4	C	373	A
4	C	406	G
4	C	411	A
4	C	412	A
4	C	413	G
4	C	421	U
4	C	422	C
4	C	424	G
4	C	429	U
4	C	459	A
4	C	467	U
4	C	468	A
4	C	478	A
4	C	479	U
4	C	485	U
4	C	497	G
4	C	511	C
4	C	518	C
4	C	527	G
4	C	532	A
4	C	533	A
4	C	547	A
4	C	564	C
4	C	572	A
4	C	573	A
4	C	576	C
4	C	577	G
4	C	633	G
4	C	650	G
4	C	653	U
4	C	665	A
4	C	687	A
4	C	721	G
4	C	723	U
4	C	731	G
4	C	747	A
4	C	777	A
4	C	793	U
4	C	794	A

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Mol	Chain	Res	Type
4	C	815	A
4	C	817	C
4	C	828	U
4	C	829	G
4	C	841	C
4	C	842	U
4	C	843	U
4	C	844	G
4	C	845	A
4	C	846	G
4	C	847	G
4	C	885	G
4	C	914	A
4	C	926	G
4	C	934	C
4	C	935	A
4	C	960	U
4	C	969	A
4	C	975	A
4	C	976	G
4	C	977	A
4	C	983	A
4	C	993	G
4	C	1004	A
4	C	1008	U
4	C	1030	U
4	C	1032	G
4	C	1033	G
4	C	1034	G
4	C	1043	G
4	C	1048	G
4	C	1054	C
4	C	1065	U
4	C	1085	U
4	C	1094	G
4	C	1095	U
4	C	1101	A
4	C	1133	G
4	C	1134	G
4	C	1136	C
4	C	1137	C
4	C	1139	G

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Mol	Chain	Res	Type
4	C	1140	C
4	C	1141	C
4	C	1142	G
4	C	1145	A
4	C	1146	A
4	C	1159	U
4	C	1196	A
4	C	1197	A
4	C	1202	U
4	C	1212	U
4	C	1213	A
4	C	1227	A
4	C	1240	U
4	C	1241	G
4	C	1275	A
4	C	1280	A
4	C	1286	U
4	C	1287	A
4	C	1299	A
4	C	1302	C
4	C	1305	G
4	C	1317	C
4	C	1320	C
4	C	1337	G
4	C	1346	A
4	C	1353	G
4	C	1362	A
4	C	1364	U
4	C	1378	C
4	C	1419	G
4	C	1446	A
4	C	1452	C
4	C	1492	A
4	C	1493	A
4	C	1494	G
4	C	1497	G
4	C	1503	A
4	C	1506	U
4	C	1517	G
4	C	1529	G
4	C	1530	G
4	C	1533	C

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Mol	Chain	Res	Type
4	C	1534	A
4	C	1537	U
4	C	1538	C
4	C	1539	C
4	C	1540	U
10	I	10	A
10	I	15	G
10	I	26	G
10	I	34	U
10	I	42	A
10	I	45	G
10	I	46	G
10	I	51	G
10	I	63	A
10	I	71	A
10	I	72	U
10	I	74	A
10	I	75	G
10	I	88	G
10	I	101	A
10	I	102	U
10	I	110	G
10	I	118	A
10	I	120	U
10	I	137	U
10	I	139	U
10	I	163	C
10	I	174	U
10	I	181	A
10	I	183	C
10	I	196	A
10	I	199	A
10	I	209	C
10	I	216	A
10	I	220	G
10	I	221	A
10	I	222	A
10	I	236	C
10	I	238	C
10	I	240	C
10	I	248	G
10	I	266	G

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Mol	Chain	Res	Type
10	I	272	A
10	I	276	U
10	I	302	C
10	I	307	G
10	I	309	A
10	I	311	A
10	I	329	G
10	I	330	A
10	I	345	A
10	I	353	C
10	I	361	G
10	I	362	A
10	I	371	A
10	I	372	G
10	I	376	G
10	I	379	G
10	I	386	G
10	I	391	A
10	I	396	G
10	I	404	A
10	I	405	U
10	I	411	G
10	I	437	U
10	I	456	C
10	I	457	A
10	I	475	C
10	I	481	G
10	I	491	G
10	I	504	A
10	I	505	A
10	I	507	A
10	I	509	C
10	I	532	A
10	I	546	U
10	I	548	G
10	I	549	G
10	I	556	A
10	I	562	U
10	I	563	A
10	I	572	A
10	I	573	U
10	I	575	A

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Mol	Chain	Res	Type
10	I	587	C
10	I	603	A
10	I	607	U
10	I	614	A
10	I	616	A
10	I	627	A
10	I	632	A
10	I	637	A
10	I	646	U
10	I	647	G
10	I	654	A
10	I	655	A
10	I	668	A
10	I	686	U
10	I	730	A
10	I	747	5MU
10	I	765	C
10	I	775	G
10	I	776	G
10	I	782	A
10	I	784	G
10	I	785	G
10	I	805	G
10	I	812	C
10	I	819	A
10	I	827	U
10	I	828	U
10	I	845	A
10	I	846	U
10	I	847	U
10	I	858	G
10	I	896	A
10	I	897	C
10	I	910	A
10	I	914	G
10	I	915	C
10	I	931	U
10	I	941	A
10	I	946	C
10	I	961	C
10	I	974	G
10	I	983	A

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Mol	Chain	Res	Type
10	I	996	A
10	I	1012	U
10	I	1013	C
10	I	1022	G
10	I	1025	G
10	I	1026	G
10	I	1033	U
10	I	1046	A
10	I	1047	G
10	I	1061	U
10	I	1070	A
10	I	1071	G
10	I	1080	A
10	I	1088	A
10	I	1111	A
10	I	1112	G
10	I	1116	G
10	I	1132	U
10	I	1133	A
10	I	1135	C
10	I	1142	A
10	I	1150	C
10	I	1151	A
10	I	1173	U
10	I	1174	U
10	I	1175	A
10	I	1179	G
10	I	1180	U
10	I	1206	G
10	I	1236	G
10	I	1238	G
10	I	1250	G
10	I	1253	A
10	I	1256	G
10	I	1266	G
10	I	1271	G
10	I	1272	A
10	I	1300	G
10	I	1301	A
10	I	1314	C
10	I	1340	U
10	I	1352	U

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Mol	Chain	Res	Type
10	I	1353	A
10	I	1365	A
10	I	1368	G
10	I	1378	A
10	I	1379	U
10	I	1383	A
10	I	1416	G
10	I	1428	C
10	I	1452	G
10	I	1482	G
10	I	1493	C
10	I	1494	A
10	I	1506	U
10	I	1508	A
10	I	1510	G
10	I	1515	A
10	I	1534	U
10	I	1535	A
10	I	1536	C
10	I	1566	A
10	I	1569	A
10	I	1578	U
10	I	1583	A
10	I	1608	A
10	I	1610	A
10	I	1618	6MZ
10	I	1646	C
10	I	1647	U
10	I	1648	U
10	I	1649	G
10	I	1674	G
10	I	1684	G
10	I	1692	U
10	I	1696	G
10	I	1699	G
10	I	1715	G
10	I	1729	U
10	I	1730	C
10	I	1738	G
10	I	1755	A
10	I	1758	U
10	I	1763	G

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Mol	Chain	Res	Type
10	I	1764	C
10	I	1773	A
10	I	1791	A
10	I	1800	C
10	I	1801	A
10	I	1808	A
10	I	1814	G
10	I	1816	C
10	I	1829	A
10	I	1847	A
10	I	1848	A
10	I	1869	G
10	I	1870	C
10	I	1872	A
10	I	1906	G
10	I	1909	C
10	I	1913	A
10	I	1914	C
10	I	1915	3TD
10	I	1929	G
10	I	1930	G
10	I	1936	A
10	I	1938	A
10	I	1955	U
10	I	1967	C
10	I	1970	A
10	I	1971	U
10	I	1972	G
10	I	1982	U
10	I	1991	U
10	I	1993	U
10	I	1997	C
10	I	2021	C
10	I	2022	U
10	I	2023	C
10	I	2030	6MZ
10	I	2031	A
10	I	2033	A
10	I	2043	C
10	I	2055	C
10	I	2056	G
10	I	2060	A

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Mol	Chain	Res	Type
10	I	2061	G
10	I	2069	G7M
10	I	2093	G
10	I	2111	U
10	I	2112	G
10	I	2113	U
10	I	2115	G
10	I	2116	G
10	I	2117	A
10	I	2118	U
10	I	2119	A
10	I	2128	G
10	I	2131	U
10	I	2132	U
10	I	2133	G
10	I	2134	A
10	I	2146	C
10	I	2159	G
10	I	2160	C
10	I	2163	A
10	I	2164	C
10	I	2165	C
10	I	2167	U
10	I	2169	A
10	I	2170	A
10	I	2171	A
10	I	2172	U
10	I	2177	C
10	I	2178	C
10	I	2181	U
10	I	2198	A
10	I	2204	G
10	I	2211	A
10	I	2225	A
10	I	2226	C
10	I	2238	G
10	I	2239	G
10	I	2278	A
10	I	2283	C
10	I	2287	A
10	I	2297	A
10	I	2305	U

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Mol	Chain	Res	Type
10	I	2322	A
10	I	2325	G
10	I	2333	A
10	I	2335	A
10	I	2345	G
10	I	2347	C
10	I	2350	C
10	I	2361	G
10	I	2371	G
10	I	2383	G
10	I	2385	C
10	I	2403	C
10	I	2423	U
10	I	2425	A
10	I	2426	A
10	I	2428	G
10	I	2429	G
10	I	2430	A
10	I	2441	U
10	I	2445	2MG
10	I	2448	A
10	I	2475	C
10	I	2476	A
10	I	2491	U
10	I	2498	OMC
10	I	2502	G
10	I	2505	G
10	I	2518	A
10	I	2543	G
10	I	2544	G
10	I	2547	A
10	I	2554	U
10	I	2566	A
10	I	2567	G
10	I	2572	A
10	I	2573	C
10	I	2585	U
10	I	2602	A
10	I	2605	PSU
10	I	2609	U
10	I	2613	U
10	I	2615	U

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Mol	Chain	Res	Type
10	I	2661	G
10	I	2681	C
10	I	2682	A
10	I	2689	U
10	I	2690	U
10	I	2714	G
10	I	2718	G
10	I	2726	A
10	I	2729	G
10	I	2748	A
10	I	2765	A
10	I	2766	A
10	I	2778	A
10	I	2780	G
10	I	2781	A
10	I	2791	G
10	I	2793	C
10	I	2797	U
10	I	2800	A
10	I	2820	A
10	I	2855	C
10	I	2867	G
10	I	2872	A
10	I	2880	C
10	I	2883	A
10	I	2884	U
10	I	2885	G
10	I	2887	A
11	J	15	A
11	J	32	U
11	J	35	C
11	J	56	G
11	J	88	C
11	J	89	U
11	J	90	C
11	J	99	A
11	J	109	A
11	J	119	A

All (36) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
4	C	96	U
4	C	115	G
4	C	206	C
4	C	846	G
4	C	1145	A
4	C	1201	A
4	C	1491	G
10	I	25	U
10	I	87	U
10	I	138	U
10	I	182	A
10	I	271	G
10	I	404	A
10	I	504	A
10	I	548	G
10	I	555	G
10	I	784	G
10	I	1025	G
10	I	1079	C
10	I	1313	U
10	I	1352	U
10	I	1754	A
10	I	1813	G
10	I	1846	G
10	I	1847	A
10	I	1913	A
10	I	2127	G
10	I	2158	A
10	I	2159	G
10	I	2225	A
10	I	2425	A
10	I	2447	G
10	I	2543	G
10	I	2660	A
10	I	2680	U
10	I	2854	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	4D4	U	81	22	9,11,12	2.26	2 (22%)	7,13,15	2.18	3 (42%)
10	PSU	I	2457	10	18,21,22	0.93	1 (5%)	21,30,33	2.01	4 (19%)
10	PSU	I	2580	10,53	18,21,22	0.97	2 (11%)	21,30,33	1.97	5 (23%)
10	PSU	I	1917	10	18,21,22	0.89	0	21,30,33	1.97	4 (19%)
10	PSU	I	2604	10	18,21,22	0.90	1 (5%)	21,30,33	2.00	4 (19%)
10	5MC	I	1962	10	19,22,23	1.23	2 (10%)	26,32,35	1.10	3 (11%)
10	6MZ	I	2030	10	22,25,26	1.08	1 (4%)	29,36,39	2.25	9 (31%)
10	1MG	I	745	10	23,26,27	0.91	2 (8%)	33,39,42	1.78	6 (18%)
10	3TD	I	1915	10	19,22,23	1.08	2 (10%)	23,32,35	1.88	2 (8%)
10	G7M	I	2069	10	23,26,27	0.54	0	34,39,42	0.91	2 (5%)
10	PSU	I	955	10	18,21,22	0.94	0	21,30,33	2.00	4 (19%)
10	PSU	I	2605	10	18,21,22	0.93	1 (5%)	21,30,33	1.96	4 (19%)
10	OMU	I	2552	10	19,22,23	0.97	2 (10%)	25,31,34	1.94	6 (24%)
10	PSU	I	746	10,53	18,21,22	0.99	1 (5%)	21,30,33	1.88	4 (19%)
10	5MU	I	747	10	19,22,23	1.03	2 (10%)	27,32,35	2.13	6 (22%)
10	2MG	I	2445	10	23,26,27	0.77	0	33,38,41	2.21	11 (33%)
10	2MG	I	1835	10	23,26,27	0.77	0	33,38,41	2.17	10 (30%)
10	6MZ	I	1618	10	22,25,26	1.09	1 (4%)	29,36,39	2.19	9 (31%)
10	2MA	I	2503	10,53	22,25,26	1.33	3 (13%)	32,37,40	2.05	7 (21%)
10	H2U	I	2449	10	18,21,22	0.43	0	19,30,33	0.67	0
10	PSU	I	1911	10	18,21,22	0.89	0	21,30,33	2.00	4 (19%)
10	PSU	I	2504	10	18,21,22	0.91	1 (5%)	21,30,33	1.99	4 (19%)
10	OMC	I	2498	10,53	19,22,23	0.89	1 (5%)	25,31,34	0.96	1 (4%)
10	OMG	I	2251	10	23,26,27	0.73	0	32,38,41	1.94	9 (28%)
10	5MU	I	1939	10	19,22,23	1.02	2 (10%)	27,32,35	2.12	6 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	4D4	U	81	22	-	1/11/12/14	-
10	PSU	I	2457	10	-	0/7/25/26	0/2/2/2
10	PSU	I	2580	10,53	-	0/7/25/26	0/2/2/2
10	PSU	I	1917	10	-	0/7/25/26	0/2/2/2
10	PSU	I	2604	10	-	0/7/25/26	0/2/2/2
10	5MC	I	1962	10	-	0/7/25/26	0/2/2/2
10	6MZ	I	2030	10	-	2/9/27/28	0/3/3/3
10	1MG	I	745	10	-	0/7/25/26	0/3/3/3
10	3TD	I	1915	10	-	2/7/25/26	0/2/2/2
10	G7M	I	2069	10	-	0/7/25/26	0/3/3/3
10	PSU	I	955	10	-	0/7/25/26	0/2/2/2
10	PSU	I	2605	10	-	2/7/25/26	0/2/2/2
10	OMU	I	2552	10	-	0/9/27/28	0/2/2/2
10	PSU	I	746	10,53	-	1/7/25/26	0/2/2/2
10	5MU	I	747	10	-	0/7/25/26	0/2/2/2
10	2MG	I	2445	10	-	2/9/27/28	0/3/3/3
10	2MG	I	1835	10	-	0/9/27/28	0/3/3/3
10	6MZ	I	1618	10	-	2/9/27/28	0/3/3/3
10	2MA	I	2503	10,53	-	2/7/25/26	0/3/3/3
10	H2U	I	2449	10	-	0/7/38/39	0/2/2/2
10	PSU	I	1911	10	-	0/7/25/26	0/2/2/2
10	PSU	I	2504	10	-	2/7/25/26	0/2/2/2
10	OMC	I	2498	10,53	-	1/9/27/28	0/2/2/2
10	OMG	I	2251	10	-	0/9/27/28	0/3/3/3
10	5MU	I	1939	10	-	0/7/25/26	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	U	81	4D4	CZ-NE	5.38	1.43	1.33
10	I	2503	2MA	C6-N1	3.96	1.40	1.35
10	I	1962	5MC	C5-C4	-3.93	1.41	1.44
10	I	1618	6MZ	C6-N6	3.85	1.38	1.34
10	I	2030	6MZ	C6-N6	3.70	1.38	1.34
22	U	81	4D4	CZ-NH2	3.50	1.44	1.32
10	I	2503	2MA	C5-N7	-2.97	1.33	1.39
10	I	2498	OMC	C2-N1	-2.58	1.34	1.40
10	I	747	5MU	C2-N1	-2.53	1.34	1.38
10	I	1915	3TD	C4-N3	-2.53	1.35	1.40
10	I	1962	5MC	C2-N1	-2.47	1.34	1.40
10	I	2552	OMU	C2-N1	-2.46	1.34	1.38
10	I	1915	3TD	C4-C5	-2.43	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	2503	2MA	C5-C6	2.43	1.47	1.41
10	I	745	1MG	C6-N1	-2.37	1.35	1.40
10	I	1939	5MU	C2-N1	-2.34	1.34	1.38
10	I	746	PSU	O4'-C1'	-2.12	1.40	1.43
10	I	1939	5MU	C4-N3	-2.11	1.34	1.38
10	I	2552	OMU	C4-N3	-2.10	1.35	1.38
10	I	2580	PSU	O4'-C1'	-2.08	1.41	1.43
10	I	747	5MU	C4-N3	-2.06	1.35	1.38
10	I	2457	PSU	C4-N3	-2.04	1.35	1.38
10	I	2580	PSU	C4-N3	-2.03	1.35	1.38
10	I	2604	PSU	C4-N3	-2.02	1.35	1.38
10	I	2605	PSU	C4-N3	-2.01	1.35	1.38
10	I	2504	PSU	C4-N3	-2.01	1.35	1.38
10	I	745	1MG	C2-N2	2.01	1.37	1.34

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	1835	2MG	C2-N3-C4	7.29	121.12	112.00
10	I	2445	2MG	C2-N3-C4	7.26	121.08	112.00
10	I	1915	3TD	N1-C2-N3	6.55	120.89	116.13
10	I	2503	2MA	C5-C4-N3	-6.23	120.62	127.18
10	I	2457	PSU	N1-C2-N3	5.65	121.13	115.17
10	I	2030	6MZ	C5-C4-N3	-5.62	118.98	126.72
10	I	955	PSU	N1-C2-N3	5.62	121.09	115.17
10	I	2604	PSU	N1-C2-N3	5.59	121.06	115.17
10	I	1911	PSU	N1-C2-N3	5.59	121.06	115.17
10	I	2504	PSU	N1-C2-N3	5.56	121.04	115.17
10	I	1835	2MG	C5-C4-N3	-5.51	119.61	128.39
10	I	745	1MG	C5-C4-N3	-5.51	119.63	128.39
10	I	1917	PSU	N1-C2-N3	5.49	120.95	115.17
10	I	1618	6MZ	C5-C4-N3	-5.48	119.17	126.72
10	I	2251	OMG	C5-C4-N3	-5.48	119.66	128.39
10	I	2605	PSU	N1-C2-N3	5.47	120.94	115.17
10	I	2580	PSU	N1-C2-N3	5.46	120.93	115.17
10	I	1939	5MU	C4-N3-C2	-5.43	120.23	127.34
10	I	746	PSU	N1-C2-N3	5.42	120.89	115.17
10	I	747	5MU	C4-N3-C2	-5.42	120.24	127.34
10	I	2445	2MG	C5-C4-N3	-5.35	119.88	128.39
10	I	2552	OMU	C4-N3-C2	-5.21	120.14	126.61
10	I	2251	OMG	C2-N3-C4	5.09	121.06	112.30
10	I	2503	2MA	N3-C4-N9	4.99	133.32	126.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	747	5MU	N3-C2-N1	4.80	121.14	114.89
10	I	1939	5MU	N3-C2-N1	4.78	121.11	114.89
10	I	2552	OMU	N3-C2-N1	4.72	121.04	114.89
10	I	1939	5MU	C5-C4-N3	4.70	119.41	115.32
10	I	747	5MU	C5-C4-N3	4.62	119.34	115.32
10	I	2604	PSU	C4-N3-C2	-4.56	120.09	126.37
10	I	2504	PSU	C4-N3-C2	-4.55	120.11	126.37
10	I	955	PSU	C4-N3-C2	-4.54	120.12	126.37
10	I	2457	PSU	C4-N3-C2	-4.53	120.13	126.37
10	I	1917	PSU	C4-N3-C2	-4.53	120.14	126.37
10	I	1911	PSU	C4-N3-C2	-4.52	120.14	126.37
10	I	2605	PSU	C4-N3-C2	-4.51	120.16	126.37
10	I	2030	6MZ	N3-C4-N9	4.51	134.84	127.17
10	I	1618	6MZ	N3-C4-N9	4.51	134.83	127.17
10	I	746	PSU	C4-N3-C2	-4.46	120.23	126.37
10	I	2580	PSU	C4-N3-C2	-4.41	120.30	126.37
10	I	1915	3TD	C4-N3-C2	-4.28	120.08	124.61
10	I	2503	2MA	N6-C6-N1	4.26	122.77	117.03
10	I	745	1MG	C2-N3-C4	4.20	121.41	111.98
10	I	1835	2MG	N9-C4-N3	4.17	134.29	125.95
10	I	2251	OMG	N9-C4-N3	4.13	134.22	125.95
10	I	745	1MG	N9-C4-N3	4.11	134.17	125.95
10	I	1618	6MZ	N1-C2-N3	-4.10	122.38	128.58
10	I	2030	6MZ	N1-C2-N3	-4.05	122.45	128.58
10	I	2030	6MZ	C5-N7-C8	4.04	109.80	103.45
10	I	1939	5MU	O4-C4-C5	-4.03	120.30	124.92
10	I	747	5MU	O4-C4-C5	-4.02	120.32	124.92
10	I	2445	2MG	N9-C4-N3	3.96	133.87	125.95
10	I	1618	6MZ	C5-N7-C8	3.84	109.48	103.45
22	U	81	4D4	NE-CZ-NH2	-3.75	114.24	120.67
10	I	2503	2MA	C5-N7-C8	3.70	109.26	103.45
10	I	2030	6MZ	C2-N3-C4	3.63	120.70	111.83
22	U	81	4D4	NH1-CZ-NE	3.62	127.50	119.27
10	I	1618	6MZ	C2-N3-C4	3.62	120.67	111.83
10	I	2445	2MG	C2-N1-C6	-3.60	120.20	124.55
10	I	1835	2MG	C2-N1-C6	-3.52	120.29	124.55
10	I	2030	6MZ	C9-N6-C6	-3.50	119.61	122.85
10	I	747	5MU	C5-C6-N1	-3.48	119.54	123.31
10	I	1939	5MU	C5-C6-N1	-3.41	119.61	123.31
10	I	2552	OMU	C5-C4-N3	3.37	119.53	114.80
10	I	2030	6MZ	C4-C5-N7	-3.24	106.88	110.58
10	I	1962	5MC	C5-C6-N1	-3.22	119.81	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	2457	PSU	O2-C2-N1	-3.22	119.47	122.79
10	I	1618	6MZ	C9-N6-C6	-3.22	119.87	122.85
10	I	2552	OMU	CM2-O2'-C2'	-3.18	106.30	114.47
10	I	955	PSU	O2-C2-N1	-3.18	119.50	122.79
10	I	2069	G7M	C8-N7-C5	-3.16	103.84	107.78
10	I	1911	PSU	O2-C2-N1	-3.15	119.54	122.79
10	I	2503	2MA	N9-C8-N7	-3.15	109.47	113.94
10	I	2604	PSU	O2-C2-N1	-3.14	119.55	122.79
10	I	2504	PSU	O2-C2-N1	-3.12	119.57	122.79
10	I	2445	2MG	N1-C2-N2	3.07	119.70	116.56
10	I	1618	6MZ	C4-C5-N7	-3.07	107.07	110.58
10	I	2580	PSU	O2-C2-N1	-3.07	119.62	122.79
10	I	2605	PSU	O2-C2-N1	-3.06	119.63	122.79
10	I	1917	PSU	O2-C2-N1	-3.06	119.64	122.79
10	I	746	PSU	O2-C2-N1	-3.02	119.68	122.79
10	I	2030	6MZ	N9-C8-N7	-2.96	109.74	113.94
10	I	2445	2MG	C8-N7-C5	2.85	109.34	104.26
10	I	2251	OMG	C8-N7-C5	2.84	109.33	104.26
10	I	1618	6MZ	N9-C8-N7	-2.84	109.91	113.94
10	I	745	1MG	C8-N7-C5	2.84	109.31	104.26
10	I	2503	2MA	C5-C6-N1	-2.83	114.50	118.90
10	I	2552	OMU	O4-C4-C5	-2.82	120.30	125.16
10	I	747	5MU	O2-C2-N1	-2.79	119.17	122.80
10	I	1835	2MG	C8-N7-C5	2.77	109.19	104.26
10	I	2251	OMG	C2-N1-C6	-2.67	120.27	125.11
10	I	2503	2MA	C4-C5-N7	-2.52	107.70	110.58
10	I	2552	OMU	O2-C2-N1	-2.45	119.61	122.80
10	I	1835	2MG	N1-C2-N2	2.37	118.98	116.56
10	I	955	PSU	C6-N1-C2	-2.36	120.50	122.69
10	I	2030	6MZ	C6-C5-N7	2.33	134.97	132.43
10	I	2498	OMC	CM2-O2'-C2'	-2.32	108.51	114.47
10	I	2457	PSU	C6-N1-C2	-2.31	120.55	122.69
10	I	2604	PSU	C6-N1-C2	-2.29	120.56	122.69
10	I	1962	5MC	C5-C4-N3	-2.29	119.41	121.75
10	I	2445	2MG	C6-C5-N7	2.27	134.42	130.29
10	I	1939	5MU	O2-C2-N1	-2.26	119.85	122.80
10	I	2504	PSU	C6-N1-C2	-2.25	120.61	122.69
10	I	1911	PSU	C6-N1-C2	-2.24	120.61	122.69
10	I	1618	6MZ	C6-C5-N7	2.24	134.87	132.43
10	I	2445	2MG	C4-C5-N7	-2.23	107.13	110.67
10	I	2580	PSU	C6-N1-C2	-2.23	120.62	122.69
10	I	1962	5MC	O2-C2-N3	-2.21	118.85	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	U	81	4D4	O-C-CA	-2.21	119.09	124.77
10	I	745	1MG	C6-C5-N7	2.18	134.20	129.36
10	I	1835	2MG	O6-C6-C5	-2.17	120.79	126.53
10	I	746	PSU	C6-N1-C2	-2.17	120.68	122.69
10	I	2251	OMG	C4-C5-N7	-2.17	107.23	110.67
10	I	2445	2MG	O6-C6-C5	-2.17	120.81	126.53
10	I	745	1MG	C4-C5-N7	-2.16	107.24	110.67
10	I	2605	PSU	C6-N1-C2	-2.15	120.70	122.69
10	I	2580	PSU	O4'-C1'-C2'	2.15	108.12	105.15
10	I	2251	OMG	CM2-O2'-C2'	-2.15	108.97	114.47
10	I	1917	PSU	C6-N1-C2	-2.13	120.72	122.69
10	I	2251	OMG	O6-C6-C5	-2.12	120.94	126.53
10	I	2251	OMG	C6-C5-N7	2.12	134.14	130.29
10	I	1835	2MG	C4-C5-N7	-2.09	107.35	110.67
10	I	2069	G7M	CN7-N7-C8	2.08	127.94	124.79
10	I	2445	2MG	C5-C6-N1	2.03	118.42	113.25
10	I	1835	2MG	C6-C5-N7	2.02	133.97	130.29
10	I	2445	2MG	N9-C8-N7	-2.02	109.65	113.40
10	I	1835	2MG	C5-C6-N1	2.01	118.38	113.25

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	I	1618	6MZ	O4'-C4'-C5'-O5'
10	I	1915	3TD	O4'-C4'-C5'-O5'
10	I	1618	6MZ	C3'-C4'-C5'-O5'
10	I	1915	3TD	C3'-C4'-C5'-O5'
10	I	2445	2MG	C3'-C4'-C5'-O5'
10	I	2504	PSU	O4'-C4'-C5'-O5'
10	I	2605	PSU	C3'-C4'-C5'-O5'
10	I	2605	PSU	O4'-C4'-C5'-O5'
10	I	2030	6MZ	O4'-C4'-C5'-O5'
10	I	2445	2MG	O4'-C4'-C5'-O5'
10	I	2030	6MZ	C3'-C4'-C5'-O5'
10	I	2503	2MA	O4'-C4'-C5'-O5'
10	I	2503	2MA	C3'-C4'-C5'-O5'
10	I	2504	PSU	C3'-C4'-C5'-O5'
10	I	2498	OMC	C4'-C5'-O5'-P
10	I	746	PSU	O4'-C1'-C5-C6
22	U	81	4D4	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	I	2030	6MZ	1	0
10	I	2503	2MA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 209 ligands modelled in this entry, 208 are monoatomic - leaving 1 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
54	ZLD	I	3114	53	26,26,26	1.33	3 (11%)	36,36,36	1.86	11 (30%)

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
54	ZLD	I	3114	53	-	0/13/33/33	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	I	3114	ZLD	C7-N4	3.61	1.40	1.36
54	I	3114	ZLD	C9-C8	3.21	1.55	1.51
54	I	3114	ZLD	O10-C8	-3.10	1.41	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	I	3114	ZLD	C8-O10-C7	4.69	113.85	110.10
54	I	3114	ZLD	C6-N4-C7	-4.03	108.19	111.17
54	I	3114	ZLD	C8-C6-N4	3.04	104.72	101.85
54	I	3114	ZLD	O10-C8-C6	-2.88	101.71	104.50
54	I	3114	ZLD	O10-C7-N4	-2.83	107.54	109.92
54	I	3114	ZLD	C5-C16-C17	-2.72	120.94	123.35
54	I	3114	ZLD	F18-C16-C17	2.69	120.93	118.37
54	I	3114	ZLD	C24-N19-C17	2.57	122.29	116.19
54	I	3114	ZLD	C6-C8-C9	2.40	116.09	113.38
54	I	3114	ZLD	O15-C7-N4	2.32	130.95	128.80
54	I	3114	ZLD	C6-N4-C2	2.03	124.89	121.36

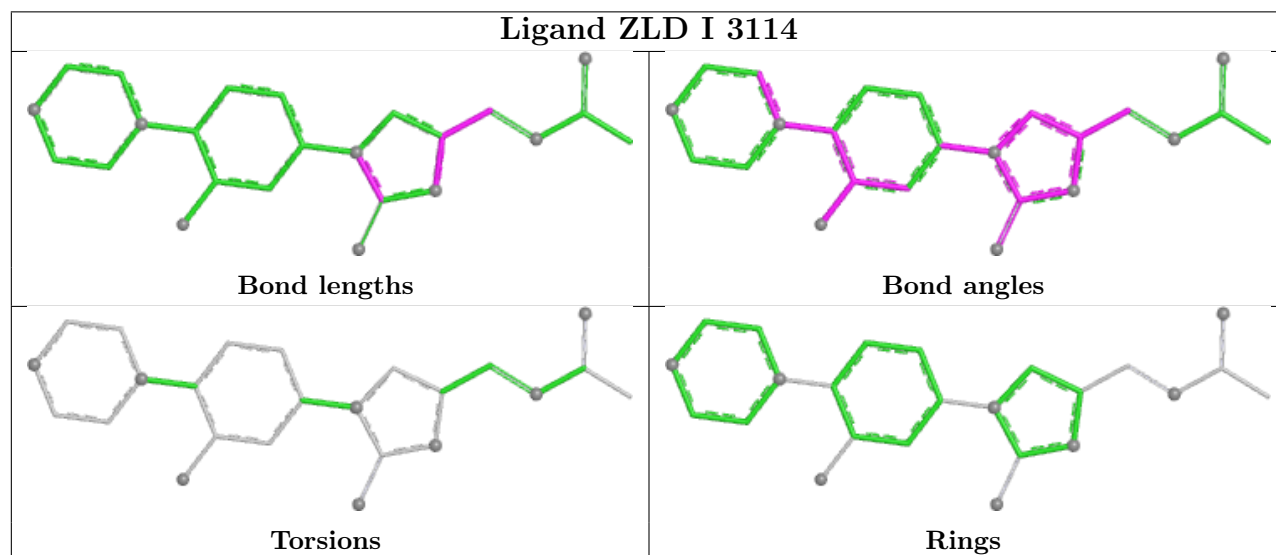
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

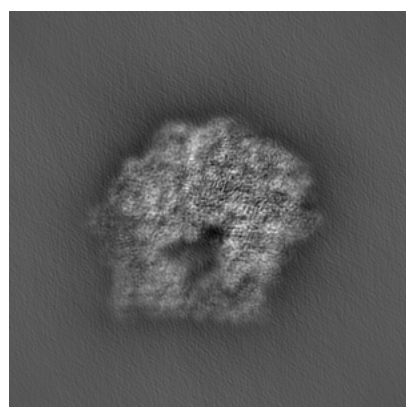
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24801. These allow visual inspection of the internal detail of the map and identification of artifacts.

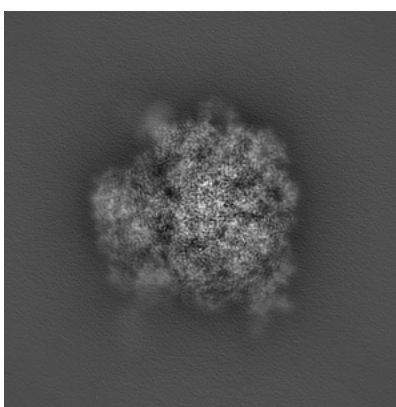
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

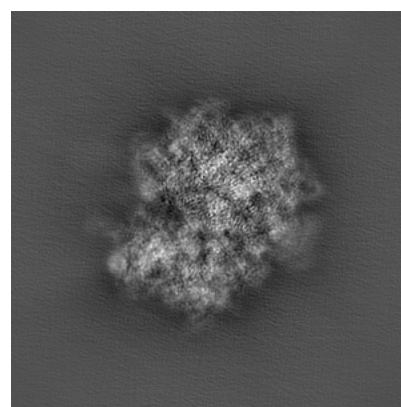
6.1.1 Primary map



X



Y

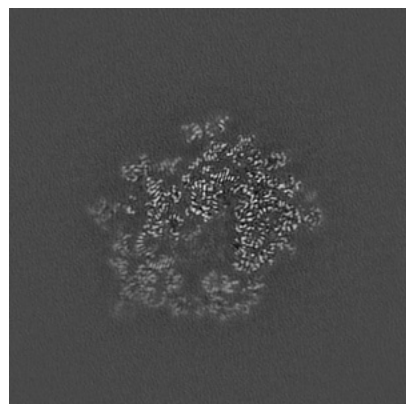


Z

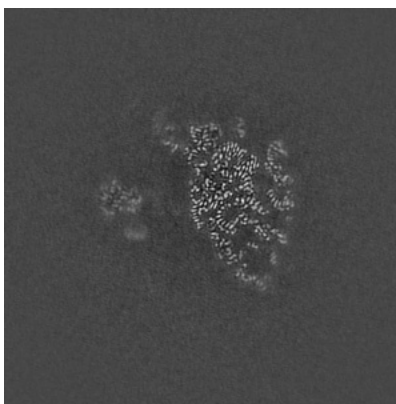
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

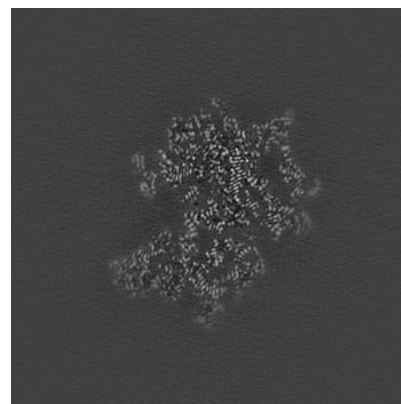
6.2.1 Primary map



X Index: 256



Y Index: 256

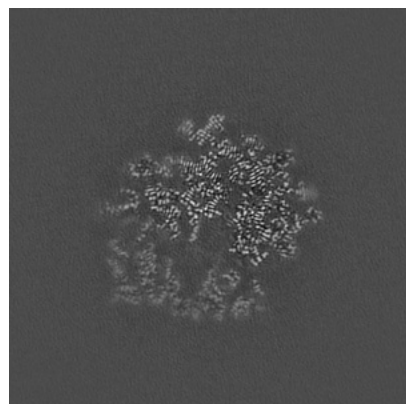


Z Index: 256

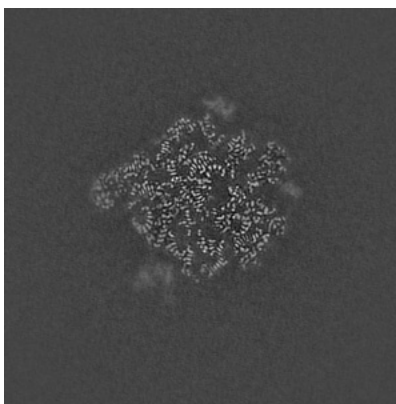
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

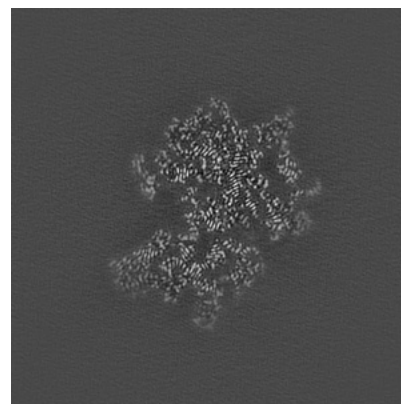
6.3.1 Primary map



X Index: 263



Y Index: 292

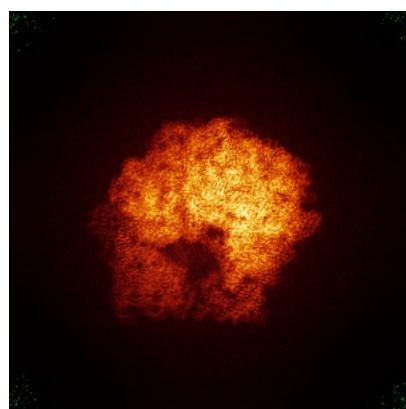


Z Index: 254

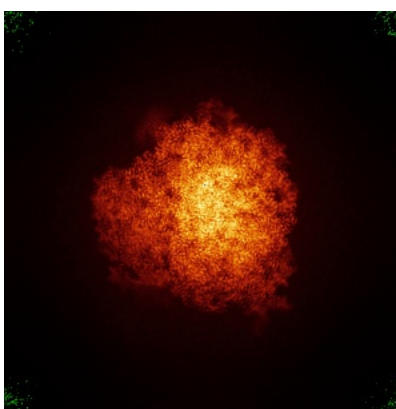
The images above show the largest variance slices of the map in three orthogonal directions.

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

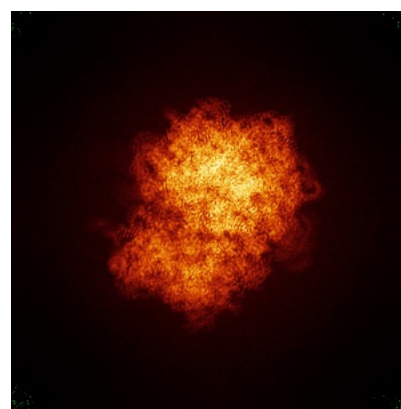
6.4.1 Primary map



X



Y

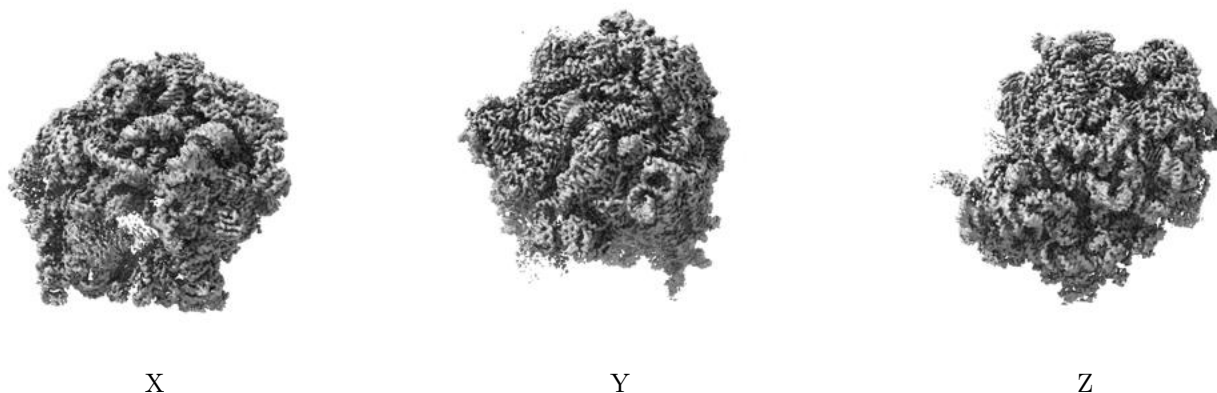


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

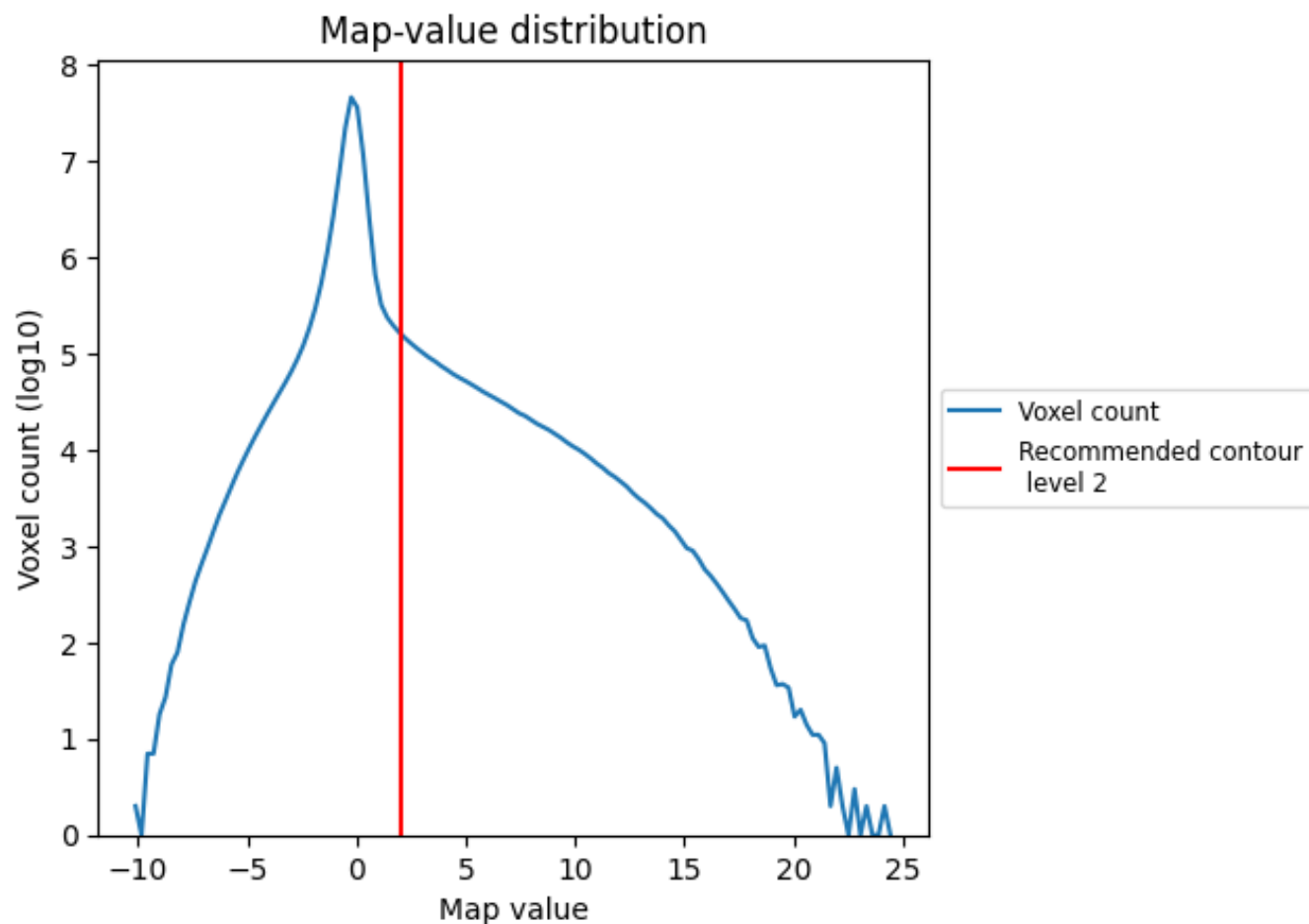
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

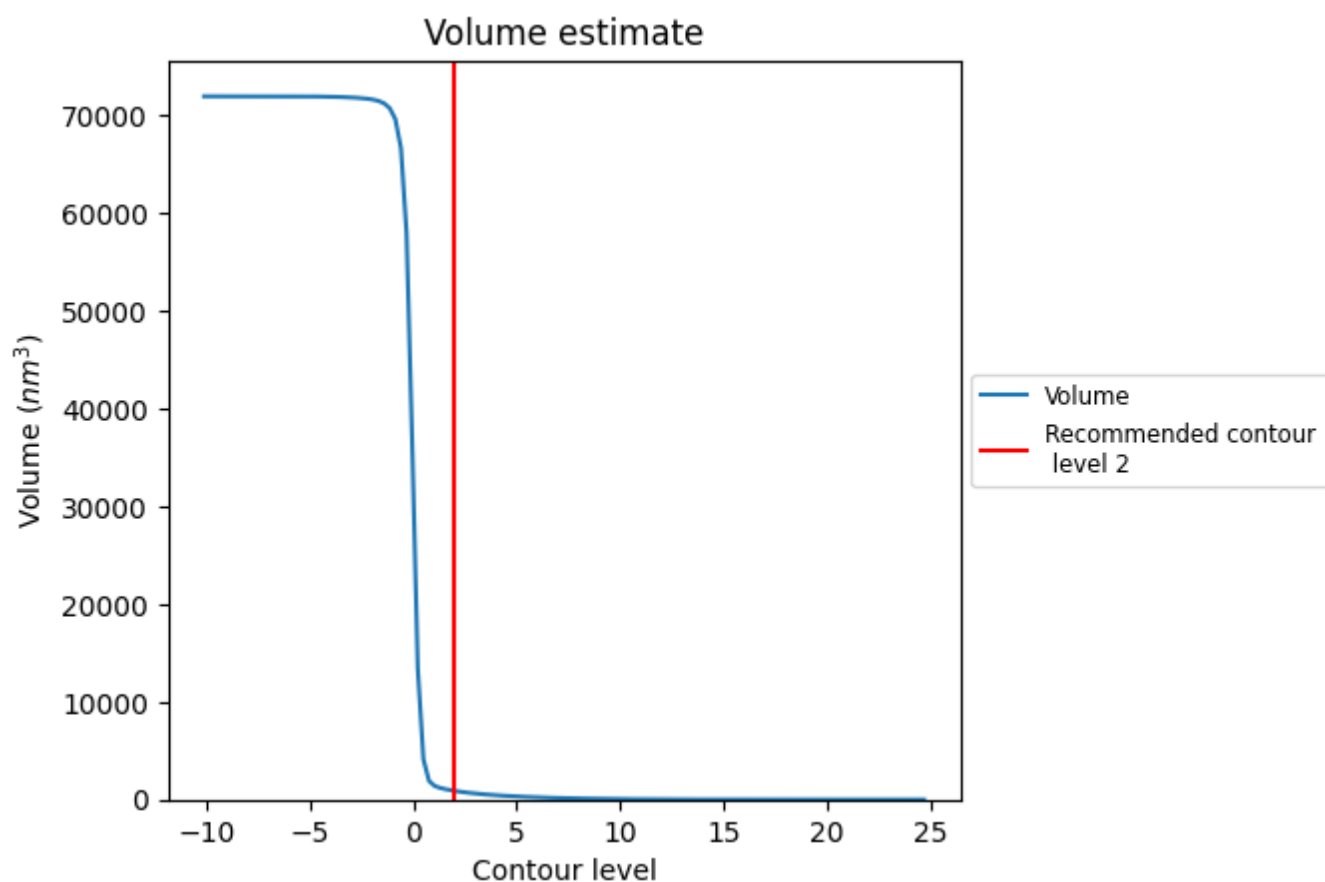
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

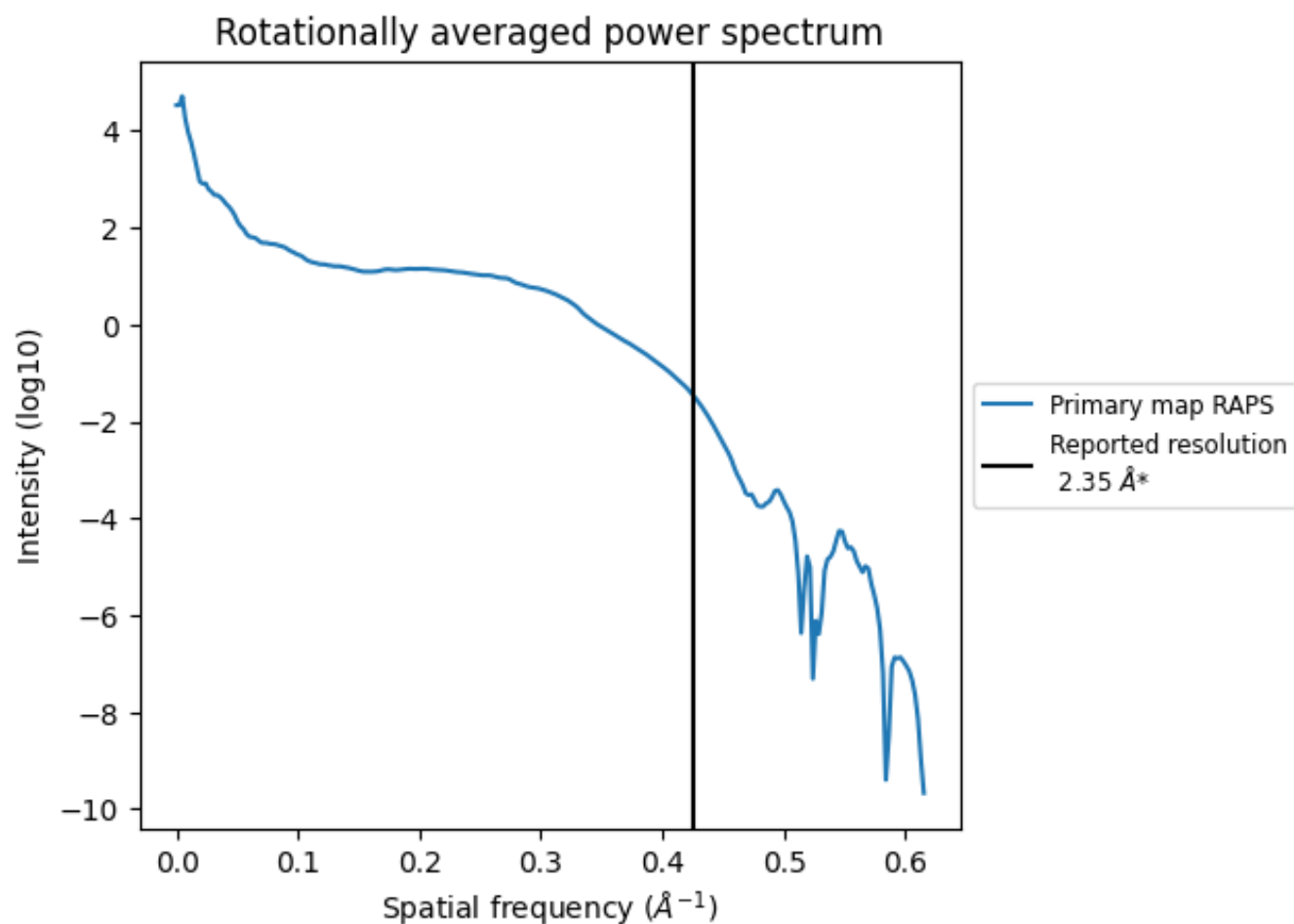
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 890 nm^3 ; this corresponds to an approximate mass of 804 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 ⓘ

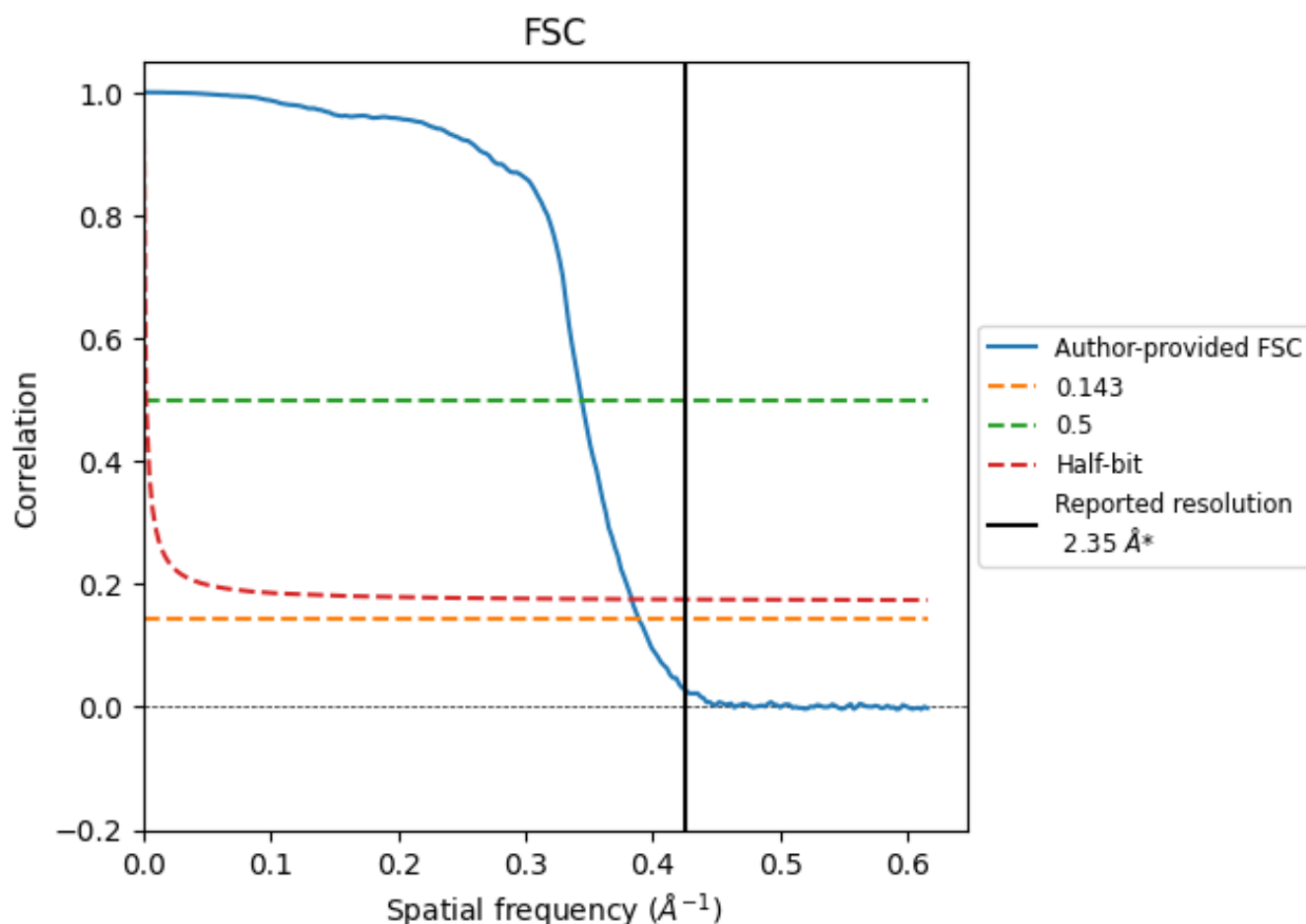


*Reported resolution corresponds to spatial frequency of 0.426 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.426 Å⁻¹

8.2 Resolution estimates [i](#)

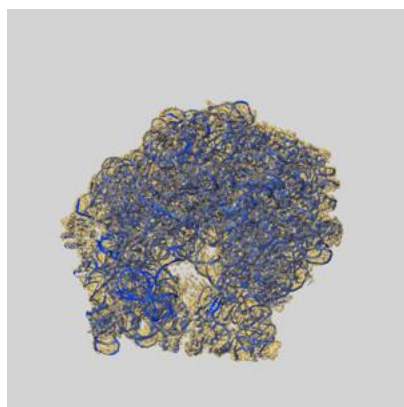
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	2.57	2.91	2.61
Unmasked-calculated*	-	-	-

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

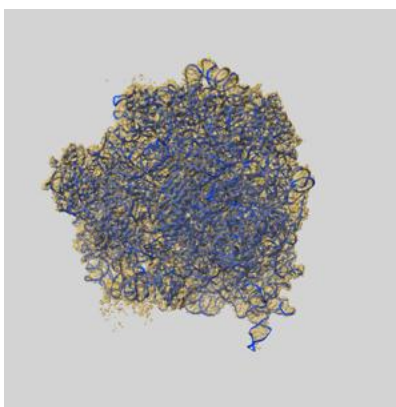
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24801 and PDB model 7S1H. Per-residue inclusion information can be found in section [3](#) on page [14](#).

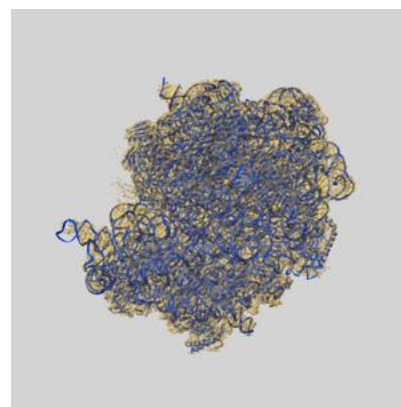
9.1 Map-model overlay [i](#)



X



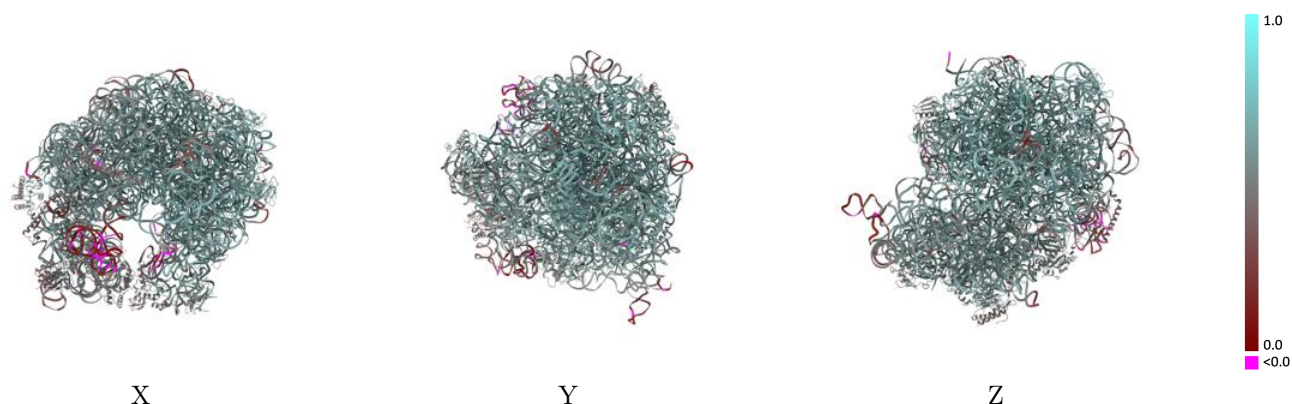
Y



Z

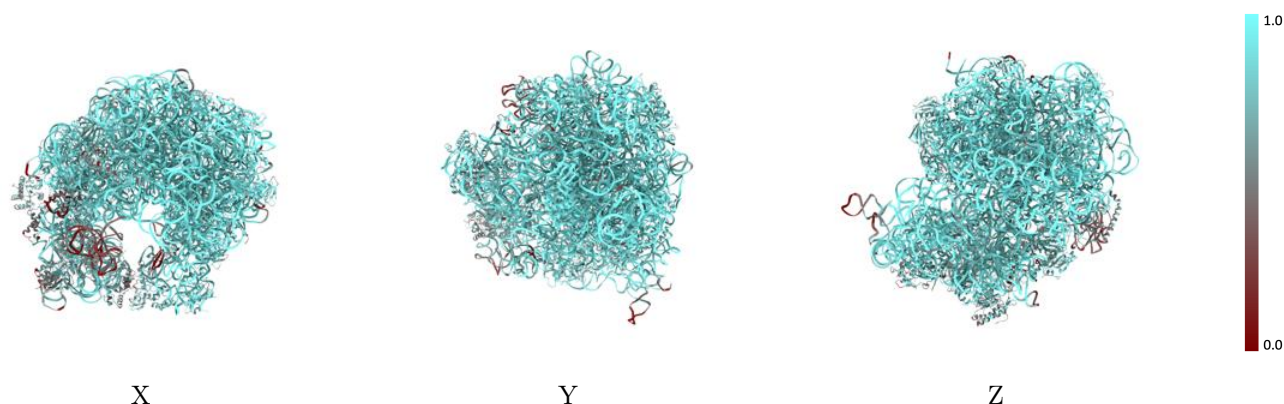
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



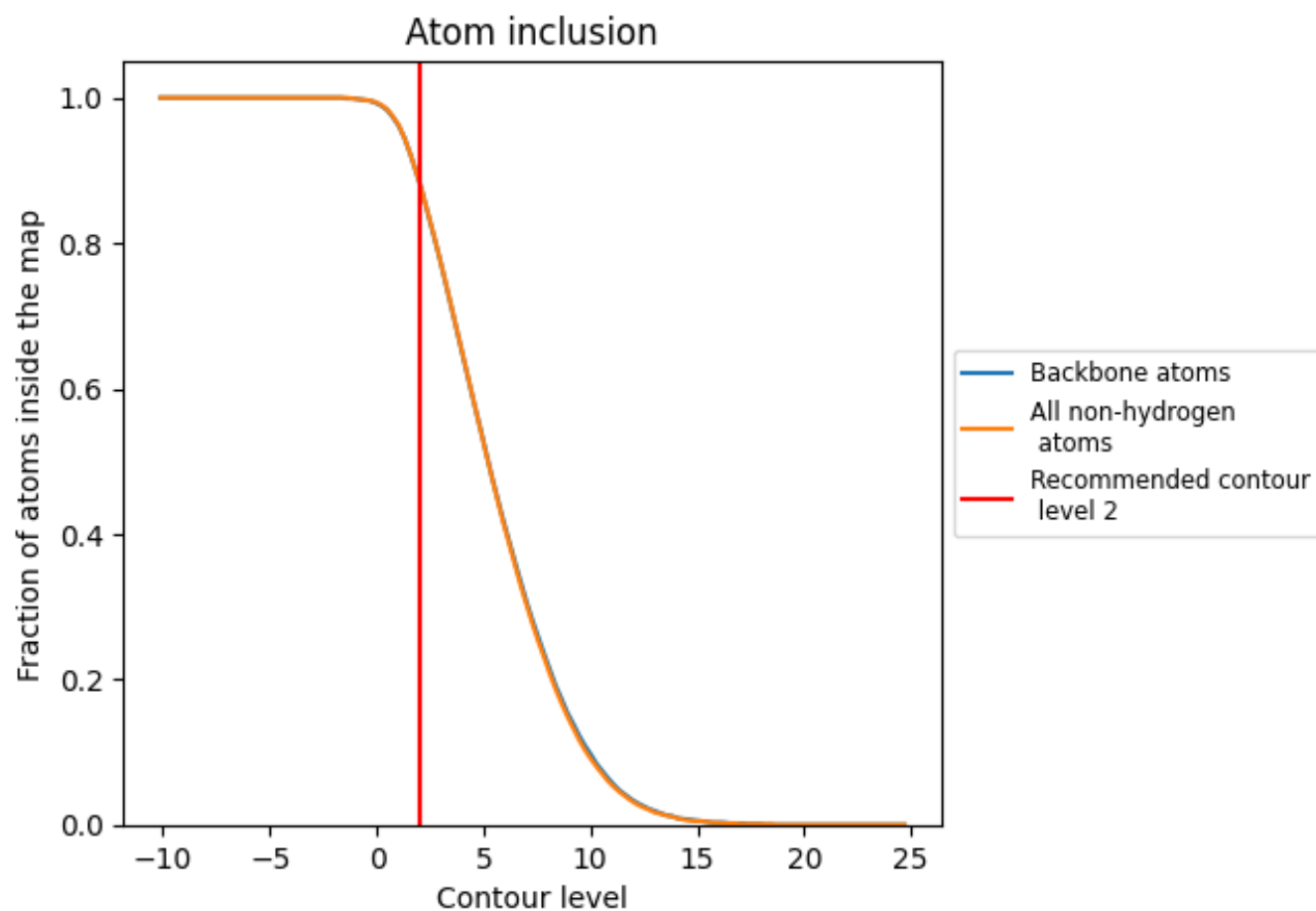
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 88% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8840	 0.5650
1	 0.6410	 0.4510
2	 0.7860	 0.5280
3	 0.2910	 0.3720
C	 0.9080	 0.5540
D	 0.5850	 0.4690
E	 0.6860	 0.5250
F	 0.7150	 0.5050
G	 0.8330	 0.5630
H	 0.7840	 0.5120
I	 0.9410	 0.5840
J	 0.9560	 0.5730
K	 0.9330	 0.6210
L	 0.9100	 0.6180
M	 0.8500	 0.5920
N	 0.7100	 0.4820
O	 0.7850	 0.5260
P	 0.5770	 0.4270
Q	 0.6380	 0.4450
R	 0.9180	 0.6170
S	 0.9010	 0.6100
T	 0.8960	 0.6110
U	 0.8830	 0.5960
V	 0.9460	 0.6300
W	 0.7960	 0.5430
X	 0.8910	 0.6070
Y	 0.9460	 0.6350
Z	 0.8870	 0.6050
a	 0.8950	 0.6210
b	 0.8280	 0.5810
c	 0.8360	 0.5690
d	 0.8360	 0.5760
e	 0.9140	 0.6230
f	 0.9030	 0.6130
g	 0.7870	 0.5410



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Chain	Atom inclusion	Q-score
h	 0.8810	 0.6000
i	 0.8900	 0.6120
j	 0.0670	 0.0100
k	 0.9440	 0.6490
l	 0.9390	 0.6410
m	 0.9040	 0.6030
n	 0.6540	 0.4710
o	 0.8420	 0.5800
p	 0.5870	 0.4510
q	 0.4380	 0.4280
r	 0.8080	 0.5360
t	 0.8660	 0.5710
u	 0.6730	 0.4900
v	 0.6900	 0.5070
w	 0.8600	 0.5660
x	 0.7780	 0.5400
y	 0.7940	 0.5450
z	 0.8670	 0.5610