



Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 06:58 AM EDT

PDB ID : 7S1I / pdb_00007s1i
EMDB ID : EMD-24802
Title : Wild-type Escherichia coli stalled ribosome with antibiotic radezolid
Authors : Young, I.D.; Stojkovic, V.; Tsai, K.; Lee, D.J.; Fraser, J.S.; Galonic Fujimori, D.
Deposited on : 2021-09-02
Resolution : 2.48 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:

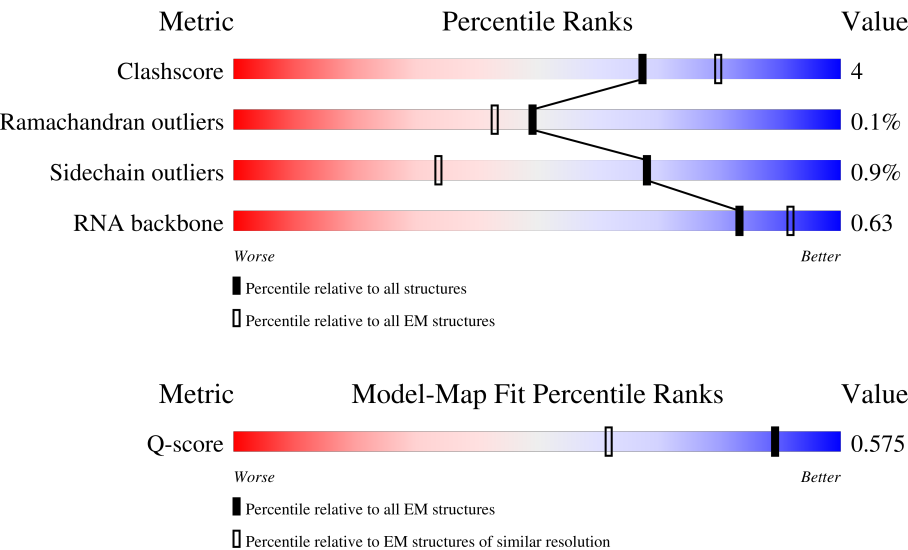
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 2.48 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.



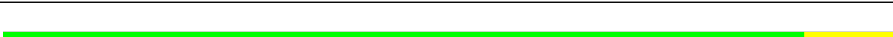
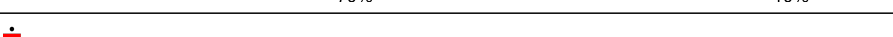
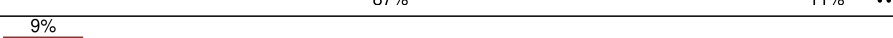
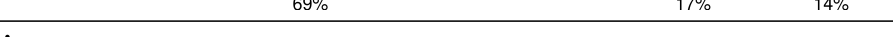
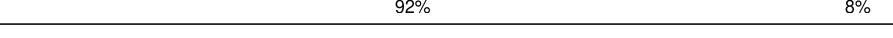
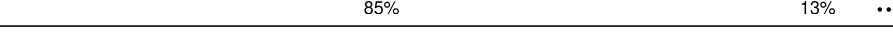
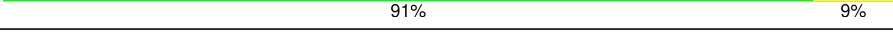
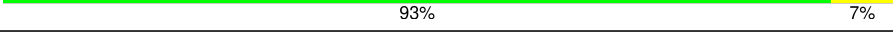
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	6178 (1.98 - 2.98)

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	71%15%14%
2	2	87	78%18%..
3	3	71	15%89%10%.

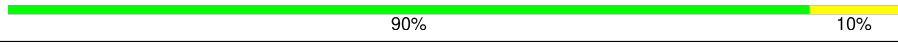
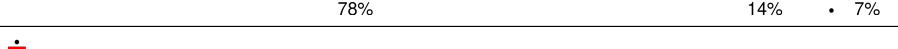
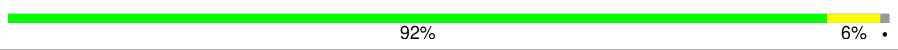
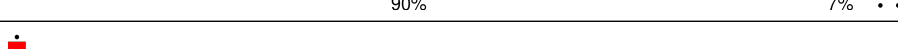
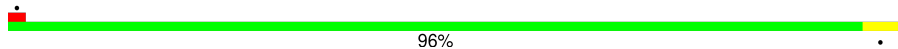
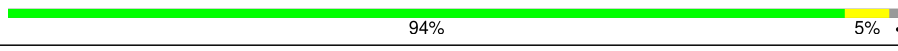
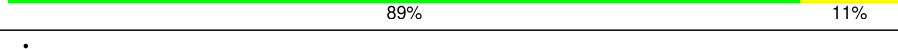
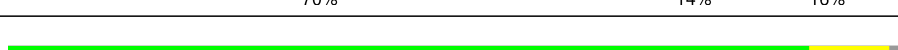
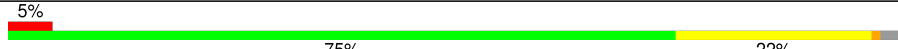
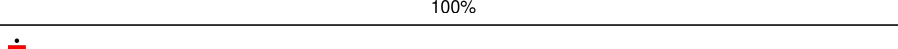
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Mol	Chain	Length	Quality of chain
4	4	15	
5	A	76	
6	C	1540	
7	D	241	
8	E	233	
9	F	206	
10	G	167	
11	H	135	
12	I	2904	
13	J	120	
14	K	273	
15	L	209	
16	M	201	
17	N	179	
18	O	177	
19	P	149	
20	Q	70	
21	R	142	
22	S	123	
23	T	144	
24	U	136	
25	V	127	
26	W	117	
27	X	115	
28	Y	118	

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Mol	Chain	Length	Quality of chain
29	Z	103	
30	a	110	
31	b	100	
32	c	104	
33	d	94	
34	e	85	
35	f	78	
36	g	63	
37	h	59	
38	i	57	
39	j	55	
40	k	46	
41	l	65	
42	m	38	
43	n	179	
44	o	130	
45	p	130	
46	q	103	
47	r	129	
48	s	5	
49	t	124	
50	u	118	
51	v	101	
52	w	89	
53	x	82	

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Mol	Chain	Length	Quality of chain
54	y	84	
55	z	75	

2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 240853 atoms, of which 96700 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 mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	4	6	Total	C	H	N	O	P	0	0
			190	56	65	20	43	6		

- Molecule 5 is a RNA chain called tRNA(PHE).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	A	76	Total	C	H	N	O	P	0	0
			2444	724	820	292	532	76		

- Molecule 6 is a RNA chain called 16S rRNA.

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

- Molecule 7 is a protein called 30S ribosomal protein S2.

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

- Molecule 8 is a protein called 30S ribosomal protein S3.

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

- Molecule 9 is a protein called 30S ribosomal protein S4.

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

- Molecule 10 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	G	150	Total	C	H	N	O	S	0	0
			2254	687	1149	211	201	6		

- Molecule 11 is a protein called 30S ribosomal protein S6.

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

- Molecule 12 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	I	2898	Total	C	H	N	O	P	0	0
			93548	27768	31319	11448	20115	2898		

- Molecule 13 is a RNA chain called 5S rRNA.

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

- Molecule 14 is a protein called 50S ribosomal protein L2.

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

- Molecule 15 is a protein called 50S ribosomal protein L3.

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

- Molecule 16 is a protein called 50S ribosomal protein L4.

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

- Molecule 17 is a protein called 50S ribosomal protein L5.

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

- Molecule 18 is a protein called 50S ribosomal protein L6.

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

- Molecule 19 is a protein called 50S ribosomal protein L9.

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

- Molecule 20 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	Q	60	Total	C	H	N	O	S	0	0
			964	299	484	90	85	6		

- Molecule 21 is a protein called 50S ribosomal protein L13.

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

- Molecule 22 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	S	122	Total	C	H	N	O	S	0	0
			1950	587	1012	180	165	6		

- Molecule 23 is a protein called 50S ribosomal protein L15.

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

- Molecule 24 is a protein called 50S ribosomal protein L16.

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

- Molecule 25 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	V	120	Total	C	H	N	O	S	0	0
			1960	593	1000	196	166	5		

- Molecule 26 is a protein called 50S ribosomal protein L18.

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

- Molecule 27 is a protein called 50S ribosomal protein L19.

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

- Molecule 28 is a protein called 50S ribosomal protein L20.

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

- Molecule 29 is a protein called Ribosomal protein L21.

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

- Molecule 30 is a protein called 50S ribosomal protein L22.

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

- Molecule 31 is a protein called 50S ribosomal protein L23.

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

- Molecule 32 is a protein called 50S ribosomal protein L24.

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

- Molecule 33 is a protein called 50S ribosomal protein L25.

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

- Molecule 34 is a protein called 50S ribosomal protein L27.

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

- Molecule 35 is a protein called 50S ribosomal protein L28.

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

- Molecule 36 is a protein called 50S ribosomal protein L29.

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

- Molecule 37 is a protein called 50S ribosomal protein L30.

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

- Molecule 38 is a protein called 50S ribosomal protein L32.

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

- Molecule 39 is a protein called 50S ribosomal protein L33.

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

- Molecule 40 is a protein called 50S ribosomal protein L34.

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

- Molecule 41 is a protein called 50S ribosomal protein L35.

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

- Molecule 42 is a protein called 50S ribosomal protein L36.

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

- Molecule 43 is a protein called 30S ribosomal protein S7.

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

- Molecule 44 is a protein called 30S ribosomal protein S8.

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

- Molecule 45 is a protein called 30S ribosomal protein S9.

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

- Molecule 46 is a protein called 30S ribosomal protein S10.

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

- Molecule 47 is a protein called 30S ribosomal protein S11.

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

- Molecule 48 is a protein called nascent peptide chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	s	5	Total	C	H	N	O	S	0	0
			91	32	47	6	5	1		

- Molecule 49 is a protein called 30S ribosomal protein S12.

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

- Molecule 50 is a protein called 30S ribosomal protein S13.

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

- Molecule 51 is a protein called 30S ribosomal protein S14.

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

- Molecule 52 is a protein called 30S ribosomal protein S15.

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

- Molecule 53 is a protein called 30S ribosomal protein S16.

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

- Molecule 54 is a protein called 30S ribosomal protein S17.

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

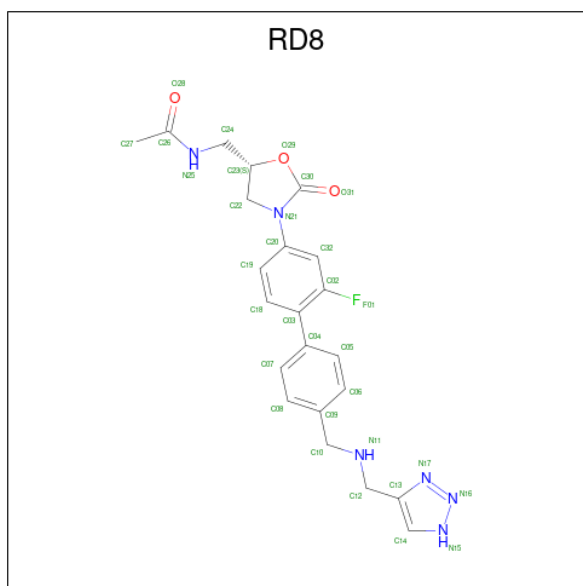
- Molecule 55 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	z	55	Total	C	H	N	O		0	0
			935	288	480	86	81			

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	C	93	Total	Mg	0
			93	93	
56	I	113	Total	Mg	0
			113	113	
56	K	1	Total	Mg	0
			1	1	
56	L	1	Total	Mg	0
			1	1	
56	V	1	Total	Mg	0
			1	1	

- Molecule 57 is Radezolid (CCD ID: RD8) (formula: $C_{22}H_{23}FN_6O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
57	I	1	Total	C	F	H	N	O	0
			54	22	1	22	6	3	

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

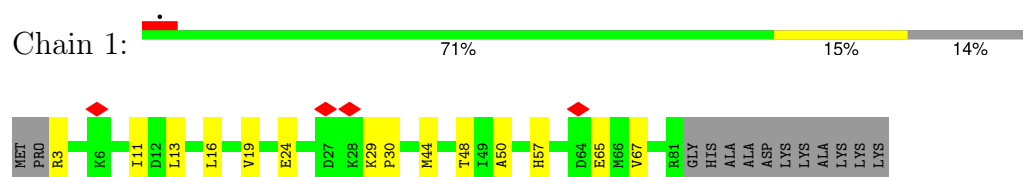
- Molecule 59 is water.

Mol	Chain	Residues	Atoms			AltConf
59	C	3	Total 9	H 6	O 3	0
59	I	32	Total 96	H 64	O 32	0
59	k	1	Total 3	H 2	O 1	0

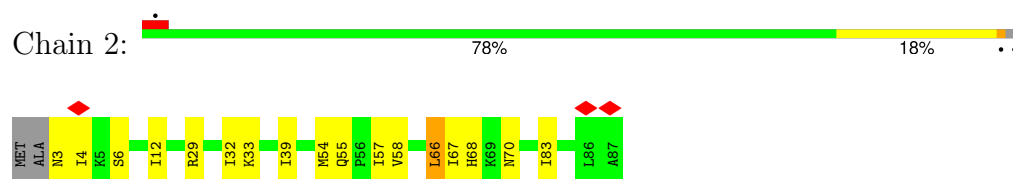
3 Residue-property plots [i](#)

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

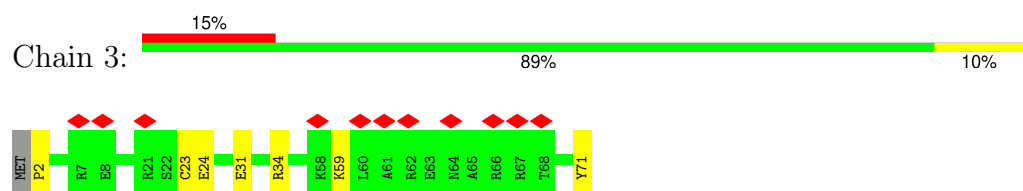
- Molecule 1: 30S ribosomal protein S19



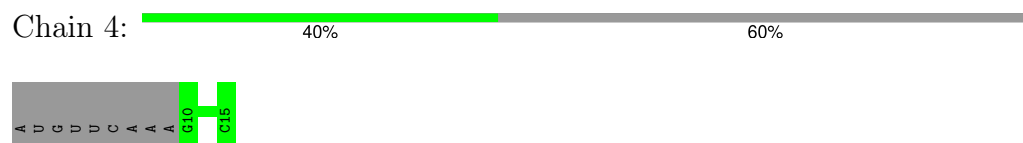
- Molecule 2: 30S ribosomal protein S20



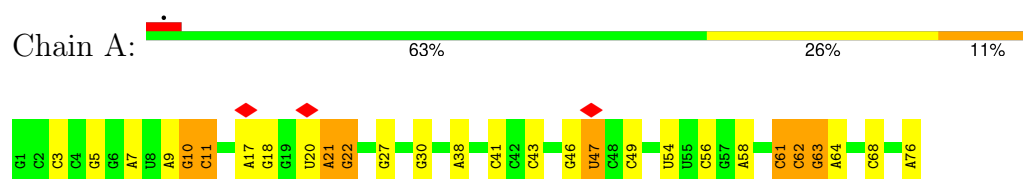
- Molecule 3: 30S ribosomal protein S21



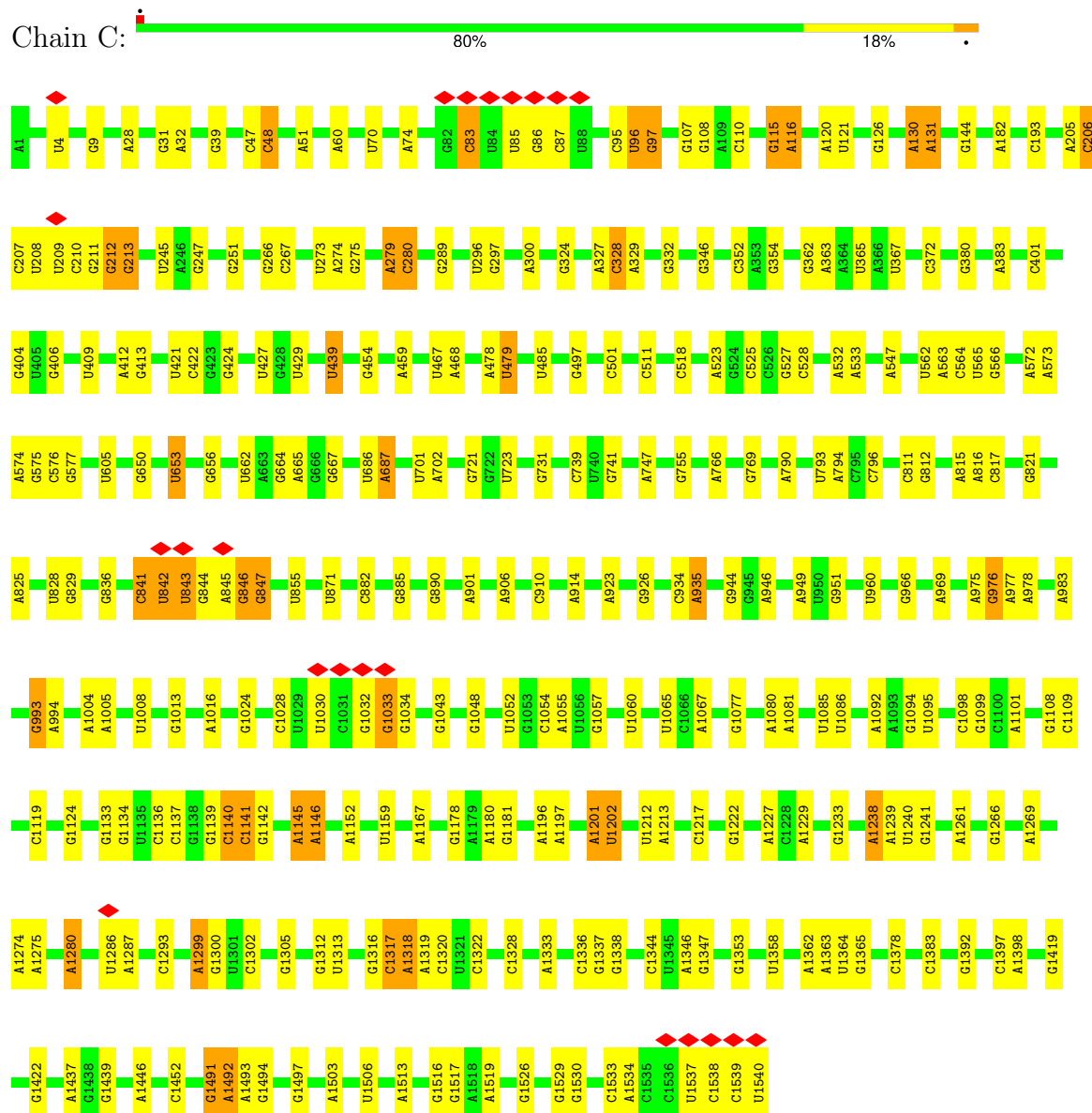
- Molecule 4: mRNA



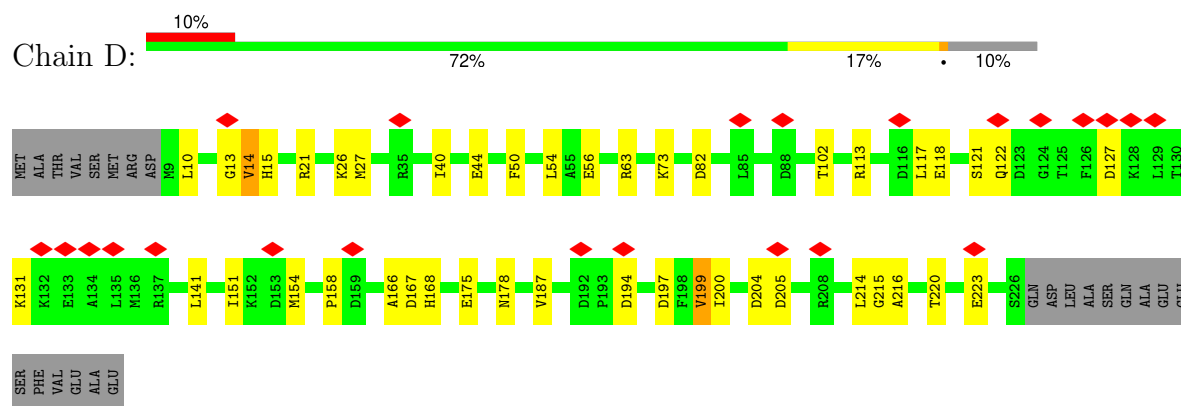
- Molecule 5: tRNA(PHE)



- Molecule 6: 16S rRNA

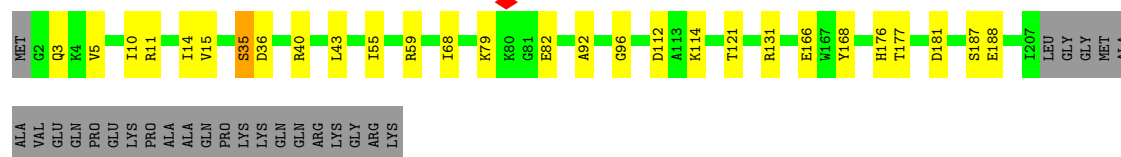


- Molecule 7: 30S ribosomal protein S2



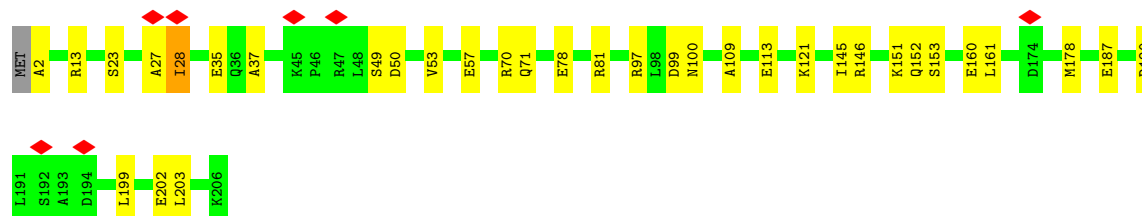
- Molecule 8: 30S ribosomal protein S3

Chain E: 



- Molecule 9: 30S ribosomal protein S4

Chain F: 



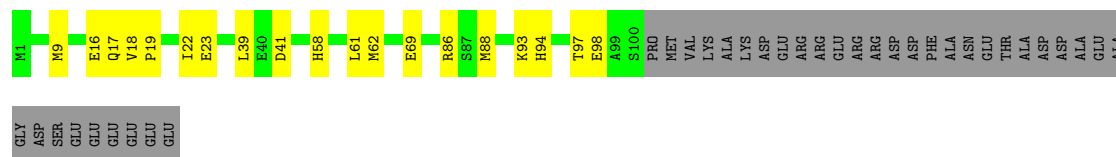
- Molecule 10: 30S ribosomal protein S5

Chain G: 



- Molecule 11: 30S ribosomal protein S6

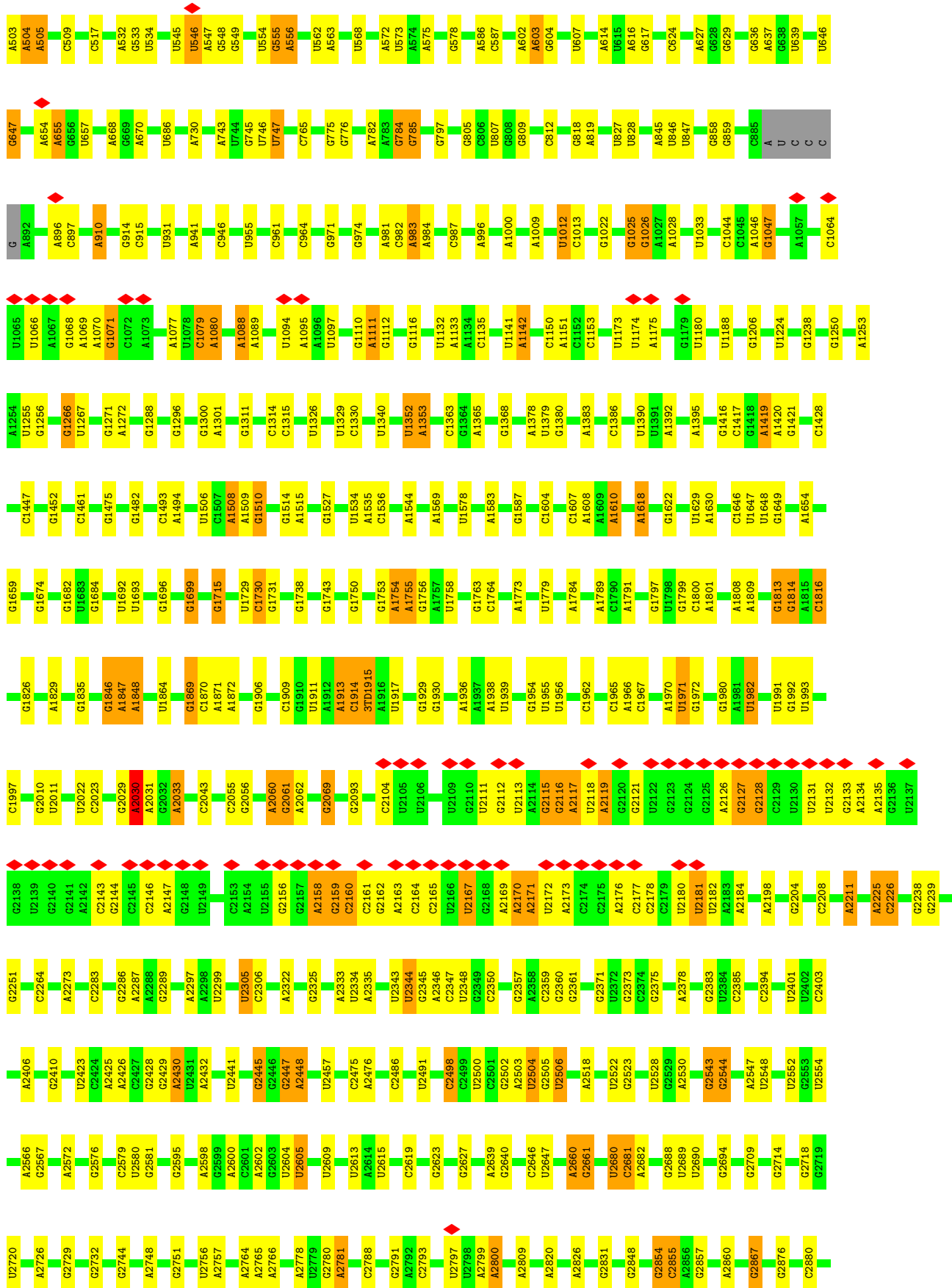
Chain H: 

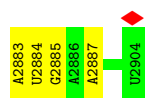


- Molecule 12: 23S rRNA

Chain I: 







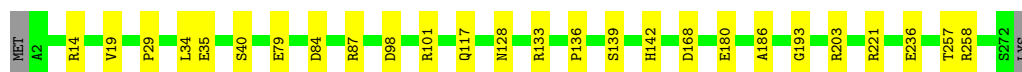
• Molecule 13: 5S rRNA

Chain J: 83% 15%



• Molecule 14: 50S ribosomal protein L2

Chain K: 90% 10%



• Molecule 15: 50S ribosomal protein L3

Chain L: 89% 11%



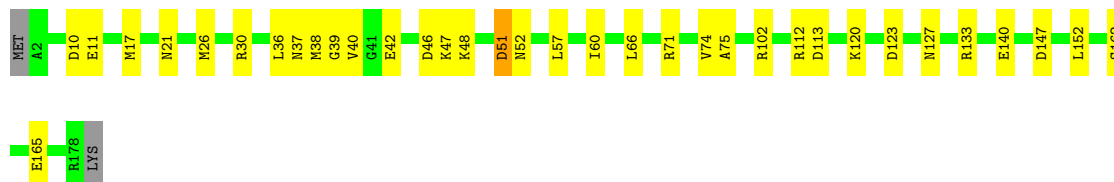
• Molecule 16: 50S ribosomal protein L4

Chain M: 88% 11%



• Molecule 17: 50S ribosomal protein L5

Chain N: 79% 19%

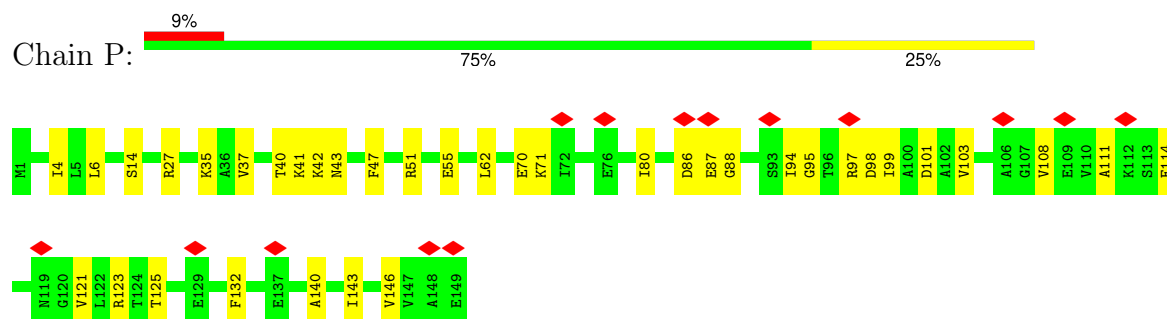


• Molecule 18: 50S ribosomal protein L6

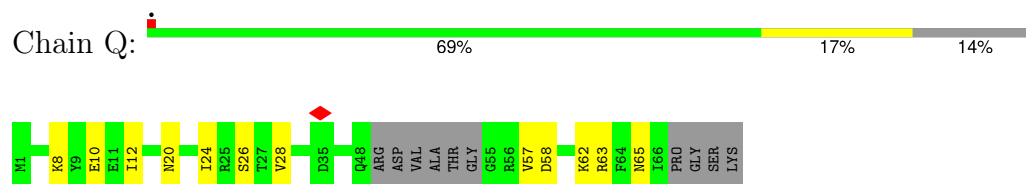
Chain O: 87% 11%



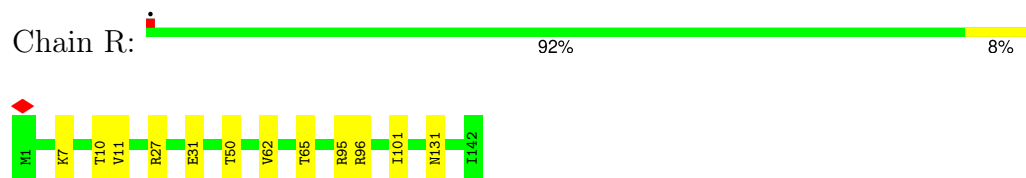
- Molecule 19: 50S ribosomal protein L9



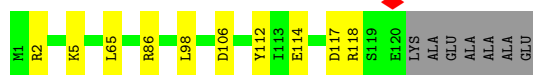
- Molecule 20: 50S ribosomal protein L31



- Molecule 21: 50S ribosomal protein L13



Chain V:  87% 8% 6%



- Molecule 26: 50S ribosomal protein L18

Chain W:  88% 11%

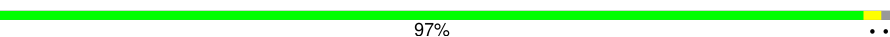


- Molecule 27: 50S ribosomal protein L19

Chain X:  90% 10%



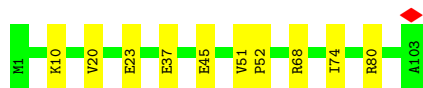
- Molecule 28: 50S ribosomal protein L20

Chain Y:  97%



- Molecule 29: Ribosomal protein L21

Chain Z:  90% 10%



- Molecule 30: 50S ribosomal protein L22

Chain a:  90% 10%

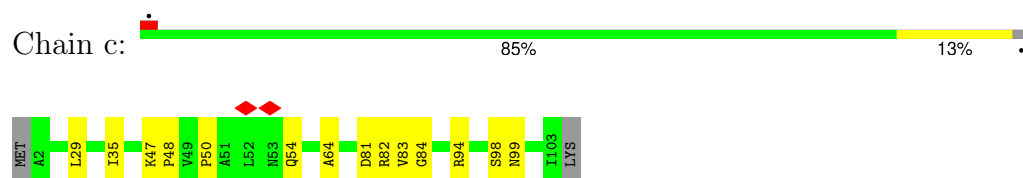


- Molecule 31: 50S ribosomal protein L23

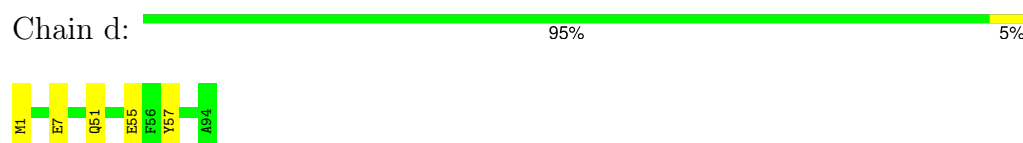
Chain b:  78% 14% 7%



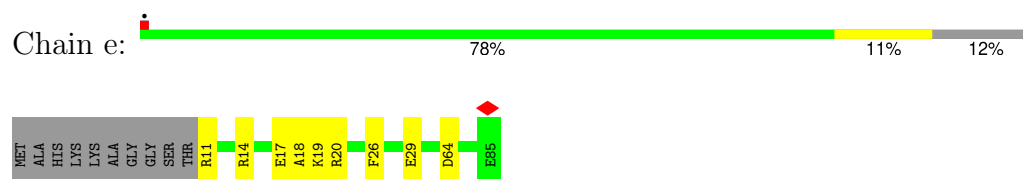
- Molecule 32: 50S ribosomal protein L24



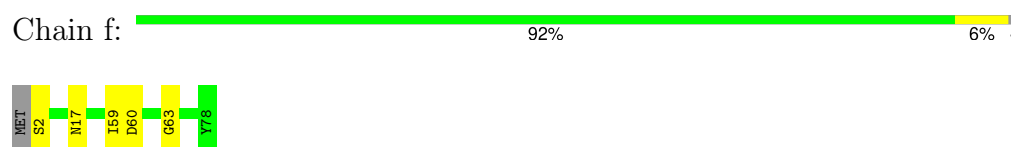
- Molecule 33: 50S ribosomal protein L25



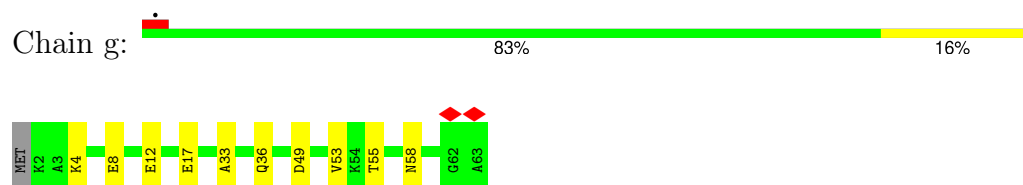
- Molecule 34: 50S ribosomal protein L27



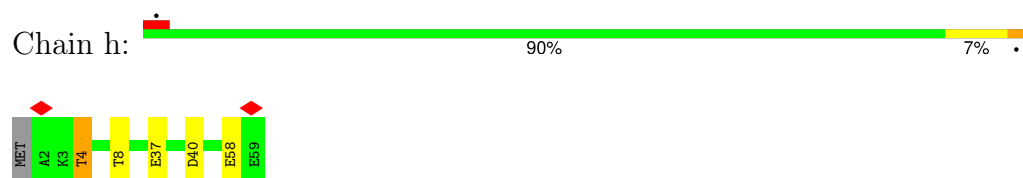
- Molecule 35: 50S ribosomal protein L28



- Molecule 36: 50S ribosomal protein L29



- Molecule 37: 50S ribosomal protein L30

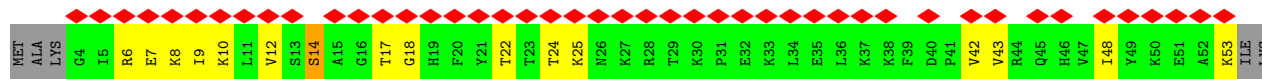
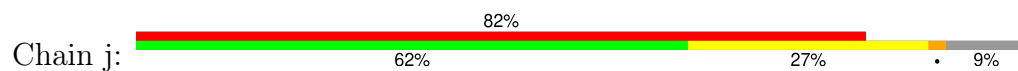


- Molecule 38: 50S ribosomal protein L32

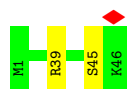




- Molecule 39: 50S ribosomal protein L33



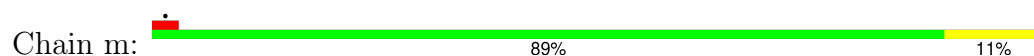
- Molecule 40: 50S ribosomal protein L34



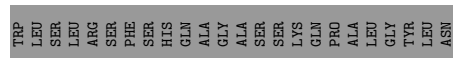
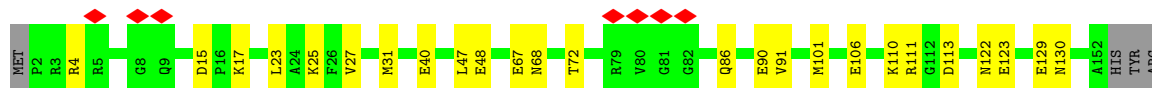
- Molecule 41: 50S ribosomal protein L35



- Molecule 42: 50S ribosomal protein L36



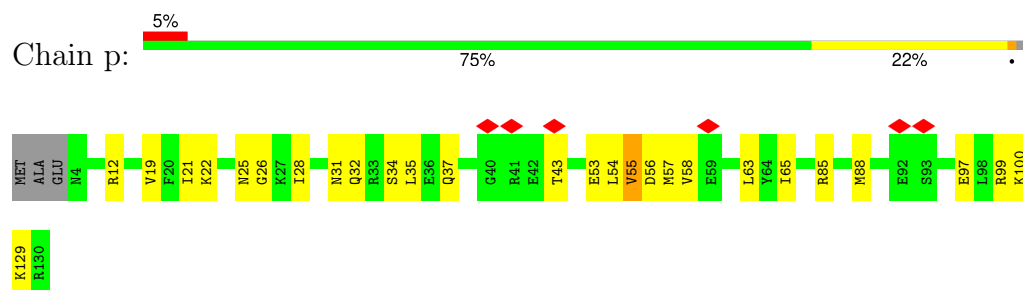
- Molecule 43: 30S ribosomal protein S7



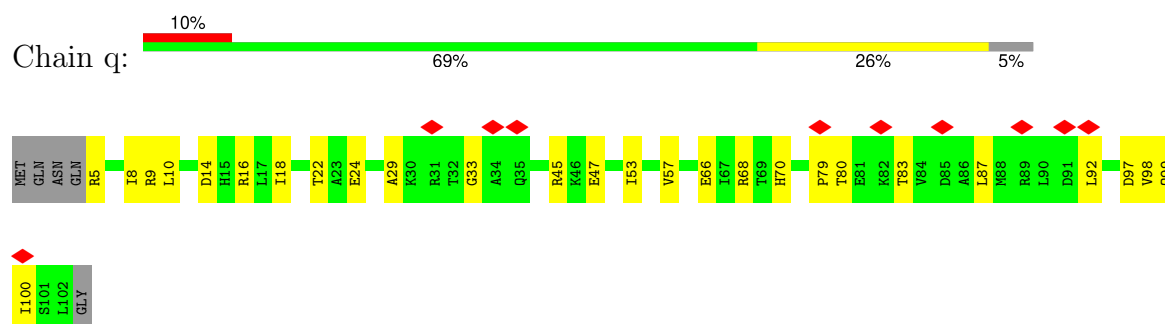
- Molecule 44: 30S ribosomal protein S8



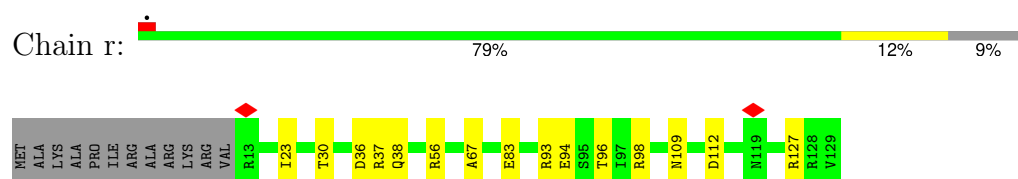
- Molecule 45: 30S ribosomal protein S9



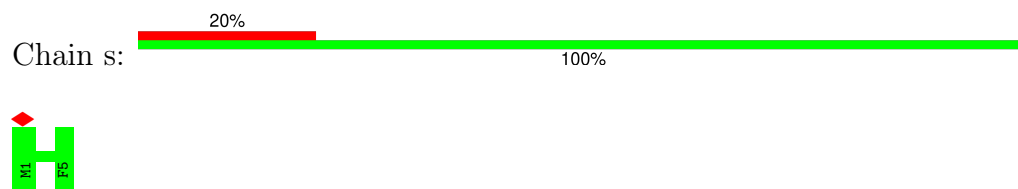
- Molecule 46: 30S ribosomal protein S10



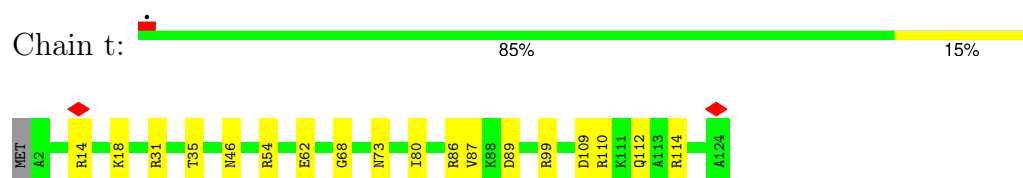
- Molecule 47: 30S ribosomal protein S11



- Molecule 48: nascent peptide chain



- Molecule 49: 30S ribosomal protein S12

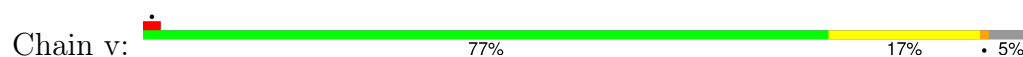


- Molecule 50: 30S ribosomal protein S13

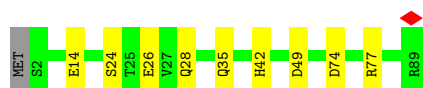
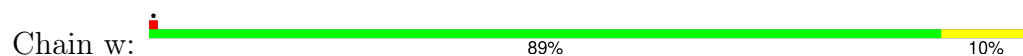




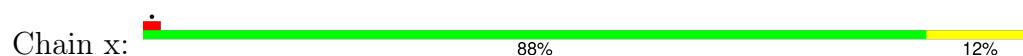
- Molecule 51: 30S ribosomal protein S14



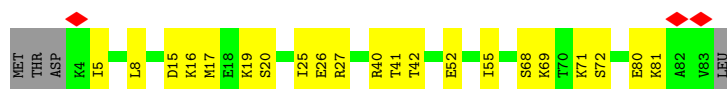
- Molecule 52: 30S ribosomal protein S15



- Molecule 53: 30S ribosomal protein S16



- Molecule 54: 30S ribosomal protein S17



- Molecule 55: 30S ribosomal protein S18



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	240596	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 ($e^-/\text{\AA}^2$)	52.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	25.561	Depositor
Minimum map value	-9.732	Depositor
Average map value	-0.014	Depositor
Map value standard deviation	0.828	Depositor
Recommended contour level	2	Depositor
Map size (Å)	422.4, 422.4, 422.4	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, OMG, 2MG, 3TD, RD8, PSU, 4D4, MG, 5MU, 5MC, 6MZ, 2MA, OMU, ZN, H2U, 1MG, G7M

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	0.10	0/652	0.28	0/877
2	2	0.11	0/671	0.32	0/888
3	3	0.13	0/598	0.35	0/792
4	4	0.07	0/138	0.14	0/212
5	A	0.08	0/1815	0.20	0/2828
6	C	0.08	0/36991	0.15	0/57705
7	D	0.12	0/1735	0.32	0/2338
8	E	0.09	0/1651	0.25	0/2225
9	F	0.10	0/1665	0.28	0/2227
10	G	0.10	0/1118	0.29	0/1504
11	H	0.13	0/835	0.34	0/1128
12	I	0.10	0/69121	0.17	1/107828 (0.0%)
13	J	0.07	0/2828	0.14	0/4410
14	K	0.10	0/2139	0.25	0/2876
15	L	0.09	0/1586	0.24	0/2134
16	M	0.10	0/1571	0.27	0/2113
17	N	0.11	0/1434	0.28	0/1926
18	O	0.09	0/1343	0.24	0/1816
19	P	0.11	0/1122	0.29	0/1515
20	Q	0.12	0/488	0.33	0/649
21	R	0.09	0/1152	0.23	0/1551
22	S	0.11	0/947	0.29	0/1268
23	T	0.09	0/1062	0.24	0/1413
24	U	0.10	0/1081	0.26	0/1443
25	V	0.08	0/973	0.21	0/1301
26	W	0.10	0/902	0.28	0/1209
27	X	0.09	0/929	0.22	0/1242
28	Y	0.08	0/960	0.20	0/1278
29	Z	0.10	0/829	0.26	0/1107
30	a	0.08	0/864	0.22	0/1156
31	b	0.11	0/744	0.29	0/994

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.08	0/787	0.24	0/1051
33	d	0.09	0/766	0.25	0/1025
34	e	0.09	0/582	0.25	0/769
35	f	0.10	0/635	0.23	0/848
36	g	0.11	0/502	0.28	0/667
37	h	0.11	0/453	0.24	0/605
38	i	0.11	0/450	0.27	0/599
39	j	0.08	0/416	0.31	0/554
40	k	0.08	0/380	0.19	0/498
41	l	0.09	0/513	0.21	0/676
42	m	0.12	0/303	0.31	0/397
43	n	0.10	0/1195	0.26	0/1602
44	o	0.09	0/989	0.24	0/1326
45	p	0.11	0/1034	0.33	0/1375
46	q	0.10	0/796	0.27	0/1077
47	r	0.12	0/893	0.30	0/1205
48	s	0.06	0/45	0.14	0/57
49	t	0.09	0/969	0.26	0/1300
50	u	0.09	0/900	0.25	0/1204
51	v	0.11	0/785	0.27	0/1043
52	w	0.11	0/718	0.26	0/959
53	x	0.09	0/659	0.25	0/884
54	y	0.12	0/657	0.33	0/881
55	z	0.09	0/462	0.22	0/621
All	All	0.09	0/155833	0.20	1/233176 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
24	U	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	I	2506	U	C5'-C4'-C3'	5.83	123.94	115.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	U	6	ARG	Sidechain

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	12	0
2	2	665	715	714	14	0
3	3	590	629	629	6	0
4	4	125	65	65	0	0
5	A	1624	820	820	18	0
6	C	33037	16628	16626	123	0
7	D	1704	1734	1732	39	0
8	E	1624	1697	1696	20	0
9	F	1643	1709	1707	26	0
10	G	1105	1149	1148	20	0
11	H	817	808	808	14	0
12	I	62229	31319	31319	234	0
13	J	2529	1280	1281	5	0
14	K	2093	2170	2157	20	0
15	L	1565	1619	1616	17	0
16	M	1552	1620	1619	18	0
17	N	1410	1445	1444	30	0
18	O	1323	1373	1371	19	0
19	P	1111	1148	1148	29	0
20	Q	480	484	478	10	0
21	R	1129	1162	1162	11	0
22	S	938	1012	1012	18	0
23	T	1053	1129	1128	10	0
24	U	1075	1156	1154	5	0
25	V	960	1000	1000	5	0
26	W	892	925	923	12	0
27	X	917	963	962	9	0
28	Y	947	1021	1019	2	0
29	Z	816	841	839	8	0
30	a	857	923	922	7	0
31	b	738	808	807	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	c	779	832	831	8	0
33	d	753	781	780	4	0
34	e	575	593	592	5	0
35	f	625	653	652	4	0
36	g	501	532	531	9	0
37	h	449	489	488	3	0
38	i	444	460	458	4	0
39	j	409	442	440	17	0
40	k	377	418	418	2	0
41	l	504	573	572	3	0
42	m	302	343	340	3	0
43	n	1181	1238	1238	18	0
44	o	979	1032	1031	7	0
45	p	1022	1071	1070	26	0
46	q	786	829	828	17	0
47	r	877	888	887	11	0
48	s	44	47	47	0	0
49	t	955	1017	1016	14	0
50	u	891	954	952	9	0
51	v	774	826	824	13	0
52	w	710	731	728	9	0
53	x	649	666	666	9	0
54	y	648	693	691	18	0
55	z	455	480	478	7	0
56	C	93	0	0	0	0
56	I	113	0	0	0	0
56	K	1	0	0	0	0
56	L	1	0	0	0	0
56	V	1	0	0	0	0
57	I	32	22	0	0	0
58	Q	1	0	0	0	0
58	m	1	0	0	0	0
59	C	3	6	0	0	0
59	I	32	64	0	0	0
59	k	1	2	0	0	0
All	All	144153	96700	96529	864	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 (864) 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)
12:I:2344:U:O4	39:j:22:THR:OG1	1.92	0.87
33:d:51:GLN:OE1	33:d:57:TYR:OH	1.94	0.85
9:F:13:ARG:NH1	9:F:37:ALA:O	2.10	0.84
45:p:34:SER:OG	45:p:37:GLN:OE1	1.95	0.84
6:C:1057:G:O2'	8:E:188:GLU:OE2	1.96	0.84
52:w:26:GLU:OE2	52:w:77:ARG:NH1	2.11	0.83
18:O:104:ASN:ND2	18:O:114:ASP:OD1	2.11	0.82
12:I:2640:G:OP1	21:R:95:ARG:NH2	2.13	0.82
12:I:138:U:O2'	12:I:139:U:OP1	1.98	0.81
9:F:99:ASP:OD2	9:F:100:ASN:N	2.13	0.81
12:I:2619:C:OP1	15:L:157:LYS:NZ	2.13	0.81
13:J:113:C:O2'	26:W:46:GLU:OE1	1.98	0.81
6:C:275:G:O5'	54:y:16:LYS:NZ	2.13	0.81
8:E:168:TYR:OH	10:G:55:GLU:OE2	1.98	0.81
12:I:1846:G:O2'	12:I:1847:A:OP1	1.99	0.80
2:2:33:LYS:NZ	6:C:1439:G:OP1	2.14	0.80
6:C:501:C:OP1	49:t:114:ARG:NH2	2.15	0.80
6:C:842:U:O2'	6:C:843:U:O4'	2.00	0.79
12:I:2116:G:N2	12:I:2162:G:OP1	2.15	0.79
12:I:126:A:OP1	40:k:45:SER:OG	2.00	0.78
6:C:1119:C:OP1	45:p:85:ARG:NH2	2.17	0.78
27:X:89:ARG:NH2	27:X:115:ASN:OD1	2.16	0.78
5:A:21:A:O2'	5:A:22:G:OP1	2.01	0.78
44:o:48:ASP:OD1	44:o:49:PHE:N	2.16	0.77
1:1:24:GLU:N	1:1:24:GLU:OE1	2.17	0.77
12:I:1753:G:N2	12:I:1756:G:OP2	2.17	0.77
17:N:140:GLU:OE1	20:Q:26:SER:OG	2.03	0.77
18:O:47:ASP:OD1	18:O:48:ASN:N	2.17	0.77
12:I:1826:G:O2'	12:I:1971:U:OP2	2.03	0.77
45:p:88:MET:HA	45:p:88:MET:HE2	1.65	0.77
10:G:105:ILE:O	10:G:112:ARG:NH2	2.19	0.76
6:C:363:A:OP2	49:t:31:ARG:NH1	2.19	0.76
5:A:30:G:OP1	6:C:1229:A:O2'	2.04	0.76
12:I:1390:U:O2	12:I:1395:A:N6	2.18	0.76
12:I:1754:A:O2'	27:X:103:ARG:NH2	2.18	0.76
7:D:73:LYS:NZ	7:D:204:ASP:OD1	2.19	0.76
6:C:1028:C:O2	6:C:1033:G:N2	2.19	0.75
6:C:1312:G:OP2	20:Q:63:ARG:NH2	2.20	0.75
50:u:17:ILE:O	50:u:20:THR:OG1	2.04	0.75
12:I:2119:A:N6	12:I:2167:U:O2'	2.19	0.75
12:I:602:A:HO2'	12:I:604:G:HO2'	1.27	0.75
12:I:2543:G:O2'	12:I:2544:G:OP1	2.04	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:2343:U:O4	39:j:8:LYS:NZ	2.19	0.74
12:I:2135:A:N6	12:I:2156:G:O2'	2.21	0.74
12:I:534:U:O2'	28:Y:49:ASP:OD2	2.02	0.74
55:z:22:ASP:OD2	55:z:24:LYS:NZ	2.21	0.74
12:I:309:A:N3	12:I:329:G:O2'	2.21	0.73
32:c:81:ASP:OD2	32:c:98:SER:OG	2.03	0.73
12:I:2286:G:H21	39:j:10:LYS:HD2	1.53	0.73
12:I:2289:G:N2	12:I:2344:U:O2	2.21	0.73
55:z:22:ASP:OD1	55:z:24:LYS:N	2.21	0.73
12:I:1715:G:O2'	12:I:1743:G:O6	2.04	0.73
8:E:131:ARG:NH1	8:E:166:GLU:OE1	2.21	0.73
12:I:1071:G:N2	12:I:1089:A:O2'	2.22	0.72
6:C:409:U:OP1	9:F:23:SER:OG	2.07	0.72
12:I:58:G:O2'	12:I:73:A:N1	2.21	0.72
19:P:88:GLY:O	19:P:125:THR:OG1	2.04	0.72
6:C:83:C:O2	6:C:86:G:N2	2.22	0.72
12:I:2359:C:O2'	41:l:54:ASP:OD2	2.07	0.72
34:e:26:PHE:N	34:e:29:GLU:OE2	2.22	0.72
43:n:106:GLU:OE2	43:n:110:LYS:NZ	2.20	0.72
47:r:83:GLU:OE2	47:r:109:ASN:ND2	2.23	0.72
39:j:14:SER:OG	39:j:48:ILE:O	2.08	0.72
6:C:910:C:OP2	49:t:18:LYS:NZ	2.23	0.72
8:E:36:ASP:OD1	8:E:59:ARG:NH1	2.21	0.72
43:n:113:ASP:OD2	43:n:122:ASN:ND2	2.22	0.72
47:r:93:ARG:NH2	47:r:112:ASP:OD1	2.21	0.72
6:C:1124:G:O2'	6:C:1145:A:N6	2.23	0.71
12:I:2680:U:O2'	12:I:2681:C:O5'	2.08	0.71
2:2:68:HIS:ND1	2:2:70:ASN:OD1	2.22	0.71
6:C:949:A:N7	50:u:105:ASN:ND2	2.39	0.71
6:C:439:U:O3'	9:F:121:LYS:NZ	2.23	0.71
25:V:86:ARG:NE	25:V:117:ASP:OD2	2.24	0.71
32:c:81:ASP:OD1	32:c:82:ARG:N	2.24	0.70
12:I:2170:A:O2'	12:I:2171:A:OP2	2.08	0.70
2:2:57:ILE:HD12	2:2:58:VAL:N	2.06	0.70
12:I:1779:U:OP2	12:I:1784:A:N6	2.22	0.70
12:I:2334:U:O3'	26:W:13:ARG:NH1	2.25	0.70
12:I:248:G:O2'	12:I:2432:A:OP1	2.06	0.70
12:I:1079:C:O2'	12:I:1080:A:OP1	2.09	0.70
6:C:575:G:O2'	6:C:821:G:OP2	2.06	0.69
12:I:1064:C:N4	12:I:1069:A:O2'	2.25	0.69
12:I:1066:U:O2'	12:I:1068:G:N7	2.20	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:2831:G:OP2	15:L:59:ARG:NH1	2.25	0.69
47:r:23:ILE:HD12	47:r:96:THR:HG21	1.73	0.69
5:A:10:G:O2'	5:A:11:C:OP1	2.09	0.69
5:A:22:G:H22	5:A:46:G:H1	1.38	0.69
17:N:60:ILE:O	17:N:102:ARG:NH2	2.26	0.69
6:C:1222:G:OP2	6:C:1322:C:N4	2.24	0.69
19:P:94:ILE:O	19:P:121:VAL:HG22	1.92	0.69
46:q:18:ILE:O	46:q:22:THR:HG22	1.93	0.68
6:C:1140:C:O2'	6:C:1141:C:O5'	2.12	0.68
7:D:223:GLU:OE1	7:D:223:GLU:N	2.23	0.67
14:K:133:ARG:HB3	14:K:186:ALA:HB1	1.76	0.67
6:C:126:G:OP1	6:C:605:U:O2'	2.10	0.67
43:n:40:GLU:OE2	45:p:43:THR:OG1	2.08	0.67
6:C:811:C:O2'	6:C:901:A:N1	2.26	0.67
12:I:475:C:O2	12:I:479:A:N6	2.27	0.67
12:I:1797:G:HO2'	14:K:257:THR:HG1	1.40	0.67
6:C:890:G:O2'	6:C:906:A:N6	2.28	0.67
5:A:27:G:OP2	5:A:27:G:N2	2.24	0.66
12:I:197:A:N6	12:I:2430:A:O2'	2.27	0.66
12:I:1419:A:O2'	12:I:1421:G:N7	2.21	0.66
15:L:89:GLU:N	15:L:89:GLU:OE1	2.29	0.66
12:I:2646:C:OP2	12:I:2732:G:O2'	2.12	0.66
17:N:42:GLU:N	17:N:42:GLU:OE1	2.28	0.66
46:q:66:GLU:OE2	46:q:68:ARG:NE	2.29	0.66
6:C:701:U:OP1	6:C:702:A:O2'	2.05	0.66
12:I:411:G:OP2	12:I:2406:A:O2'	2.12	0.66
12:I:2660:A:O2'	12:I:2661:G:OP1	2.14	0.66
12:I:2681:C:OP1	15:L:8:LYS:NZ	2.19	0.66
12:I:320:A:N3	16:M:163:ASN:ND2	2.44	0.66
16:M:122:GLU:N	16:M:122:GLU:OE1	2.29	0.66
9:F:187:GLU:N	9:F:190:ASP:OD2	2.28	0.66
6:C:362:G:N2	6:C:365:U:OP2	2.28	0.65
16:M:176:ASP:OD1	16:M:179:SER:OG	2.14	0.65
12:I:1508:A:O2'	12:I:1509:A:O4'	2.14	0.65
46:q:14:ASP:OD1	46:q:16:ARG:N	2.28	0.65
12:I:2346:A:O2'	39:j:18:GLY:O	2.14	0.65
6:C:1052:U:O2'	6:C:1055:A:OP2	2.06	0.65
3:3:31:GLU:OE2	3:3:34:ARG:NH2	2.29	0.65
44:o:113:ASP:OD1	44:o:114:ARG:N	2.30	0.65
7:D:27:MET:HE2	7:D:187:VAL:HG12	1.79	0.65
12:I:2159:G:O2'	12:I:2160:C:O5'	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:14:ILE:HG22	8:E:15:VAL:HG13	1.78	0.64
2:2:66:LEU:HD12	2:2:67:ILE:HG23	1.79	0.64
7:D:40:ILE:O	7:D:40:ILE:HD12	1.97	0.64
7:D:102:THR:HG23	7:D:175:GLU:HB3	1.79	0.64
9:F:151:LYS:HE2	9:F:151:LYS:H	1.61	0.64
12:I:1607:C:N4	12:I:1622:G:OP2	2.27	0.64
12:I:1296:G:OP1	12:I:2709:G:O2'	2.12	0.64
1:1:3:ARG:N	6:C:1313:U:OP2	2.30	0.64
18:O:24:ILE:HG21	18:O:72:LEU:HD21	1.80	0.64
5:A:61:C:O2'	5:A:62:C:O5'	2.15	0.63
6:C:1092:A:OP2	43:n:4:ARG:NH1	2.31	0.63
6:C:380:G:N2	6:C:383:A:OP2	2.29	0.63
6:C:1145:A:O2'	6:C:1146:A:O5'	2.16	0.63
7:D:13:GLY:O	7:D:14:VAL:HG12	1.98	0.63
6:C:1005:A:OP2	6:C:1024:G:N2	2.29	0.63
7:D:10:LEU:HD12	7:D:10:LEU:O	1.99	0.63
54:y:8:LEU:HD13	54:y:25:ILE:HD13	1.80	0.63
6:C:28:A:O2'	6:C:296:U:OP1	2.16	0.62
6:C:841:C:O2'	6:C:843:U:OP2	2.05	0.62
6:C:1261:A:N6	6:C:1274:A:O2'	2.31	0.62
54:y:19:LYS:O	54:y:71:LYS:NZ	2.32	0.62
19:P:4:ILE:O	19:P:4:ILE:HD12	1.99	0.62
12:I:2375:G:N2	12:I:2378:A:OP2	2.32	0.62
12:I:2447:G:O2'	12:I:2500:U:OP2	2.12	0.62
47:r:36:ASP:OD1	47:r:38:GLN:N	2.31	0.62
12:I:2627:G:O2'	12:I:2781:A:N1	2.26	0.62
16:M:194:LYS:HE2	16:M:194:LYS:HA	1.80	0.62
17:N:36:LEU:O	17:N:36:LEU:HD12	2.00	0.62
17:N:123:ASP:OD2	17:N:127:ASN:ND2	2.32	0.62
12:I:987:C:O2'	12:I:1000:A:N3	2.32	0.62
12:I:2595:G:N2	12:I:2598:A:OP2	2.31	0.62
17:N:162:SER:OG	17:N:165:GLU:OE1	2.18	0.61
46:q:83:THR:O	46:q:87:LEU:HD23	2.00	0.61
45:p:25:ASN:OD1	45:p:26:GLY:N	2.31	0.61
12:I:1813:G:O2'	12:I:1814:G:OP1	2.17	0.61
50:u:11:ASP:OD1	50:u:46:SER:OG	2.19	0.61
12:I:807:U:OP2	23:T:41:ARG:NH2	2.33	0.61
14:K:29:PRO:HG2	14:K:34:LEU:HD11	1.82	0.61
5:A:21:A:HO2'	5:A:22:G:P	2.24	0.61
45:p:63:LEU:O	45:p:63:LEU:HD12	2.01	0.61
6:C:1266:G:N2	6:C:1269:A:OP2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:2180:U:O2'	12:I:2181:U:O4'	2.16	0.61
12:I:2799:A:O2'	12:I:2800:A:O5'	2.18	0.61
6:C:1491:G:O2'	6:C:1492:A:OP1	2.16	0.60
21:R:62:VAL:HG11	21:R:101:ILE:HD11	1.82	0.60
22:S:106:GLU:OE1	22:S:106:GLU:N	2.35	0.60
31:b:25:GLU:OE2	31:b:26:LYS:NZ	2.34	0.60
12:I:2528:U:O2'	12:I:2530:A:OP1	2.16	0.60
11:H:93:LYS:O	11:H:94:HIS:ND1	2.34	0.60
12:I:568:U:H1'	12:I:2030:6MZ:H9C1	1.84	0.60
6:C:662:U:O2'	6:C:836:G:OP1	2.19	0.60
46:q:100:ILE:HG22	46:q:100:ILE:O	2.01	0.60
9:F:71:GLN:OE1	9:F:97:ARG:NH1	2.34	0.60
10:G:25:VAL:HG13	10:G:27:GLY:H	1.66	0.60
8:E:40:ARG:NH1	8:E:55:ILE:O	2.34	0.59
12:I:797:G:OP1	16:M:55:SER:OG	2.15	0.59
17:N:40:VAL:HG22	17:N:42:GLU:OE1	2.02	0.59
6:C:846:G:HO2'	6:C:847:G:P	2.25	0.59
12:I:221:A:N1	12:I:265:A:O2'	2.35	0.59
6:C:1060:U:H5''	46:q:53:ILE:HD12	1.83	0.59
19:P:51:ARG:NE	19:P:55:GLU:OE2	2.35	0.59
12:I:500:G:N1	12:I:503:A:OP2	2.35	0.59
12:I:2121:G:O6	12:I:2176:A:N6	2.36	0.59
45:p:97:GLU:OE1	45:p:100:LYS:NZ	2.34	0.59
20:Q:24:ILE:HD12	20:Q:24:ILE:O	2.02	0.59
3:3:71:TYR:O	6:C:1098:C:O2'	2.17	0.59
6:C:1363:A:O2'	6:C:1365:G:N7	2.28	0.59
6:C:1067:A:N1	6:C:1108:G:O2'	2.32	0.59
12:I:1693:U:O2'	14:K:14:ARG:NH2	2.35	0.59
12:I:572:A:OP2	29:Z:80:ARG:NH1	2.33	0.59
12:I:2857:G:N2	12:I:2860:A:OP2	2.32	0.59
55:z:21:ILE:HD11	55:z:55:LEU:HA	1.84	0.59
47:r:94:GLU:OE2	47:r:98:ARG:NH2	2.33	0.58
12:I:1028:A:N3	12:I:2486:C:O2'	2.32	0.58
12:I:227:A:O2'	12:I:228:C:OP2	2.18	0.58
12:I:1509:A:O2'	12:I:1510:G:OP2	2.19	0.58
15:L:39:ASP:OD1	15:L:40:LEU:N	2.37	0.58
12:I:517:C:O2'	30:a:78:GLU:OE2	2.14	0.58
54:y:5:ILE:HD12	54:y:5:ILE:C	2.28	0.58
2:2:3:ASN:OD1	2:2:4:ILE:N	2.36	0.58
34:e:64:ASP:OD1	34:e:64:ASP:N	2.37	0.58
22:S:17:ARG:HD3	22:S:47:ILE:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:100:ILE:HG22	23:T:101:ILE:HG23	1.86	0.58
26:W:52:SER:OG	26:W:54:VAL:HG22	2.04	0.58
6:C:1140:C:HO2'	6:C:1141:C:P	2.27	0.57
45:p:56:ASP:OD1	45:p:57:MET:N	2.36	0.57
18:O:137:ASP:OD1	18:O:139:GLN:N	2.38	0.57
24:U:33:LEU:HD13	24:U:117:PHE:HB3	1.86	0.57
6:C:110:C:O2'	53:x:25:ARG:O	2.18	0.57
7:D:205:ASP:OD1	7:D:205:ASP:N	2.37	0.57
12:I:265:A:N1	12:I:427:U:O2'	2.35	0.57
6:C:1180:A:OP2	45:p:99:ARG:NH2	2.36	0.57
7:D:167:ASP:OD1	7:D:168:HIS:N	2.38	0.57
49:t:68:GLY:O	49:t:99:ARG:NH1	2.36	0.57
51:v:89:MET:HA	51:v:89:MET:HE2	1.85	0.57
9:F:109:ALA:N	9:F:113:GLU:OE2	2.35	0.57
2:2:29:ARG:NH2	6:C:1437:A:OP1	2.36	0.57
22:S:92:GLU:OE2	22:S:111:LYS:NZ	2.36	0.57
43:n:86:GLN:N	43:n:86:GLN:OE1	2.38	0.57
12:I:476:G:N1	12:I:479:A:OP2	2.38	0.56
6:C:297:G:N2	6:C:300:A:OP2	2.38	0.56
6:C:1344:C:OP1	45:p:124:ARG:NH1	2.37	0.56
12:I:16:C:HO2'	38:i:11:SER:HG	1.54	0.56
12:I:981:A:OP2	12:I:982:C:N4	2.37	0.56
12:I:2146:C:OP2	12:I:2147:A:N6	2.38	0.56
12:I:2522:U:O2'	12:I:2647:U:OP1	2.16	0.56
12:I:2548:U:O2	22:S:23:LYS:NZ	2.37	0.56
17:N:11:GLU:OE1	17:N:11:GLU:N	2.38	0.56
33:d:1:MET:HA	33:d:1:MET:HE2	1.87	0.56
12:I:25:U:O2'	12:I:26:G:OP1	2.19	0.56
12:I:320:A:OP1	16:M:130:LYS:NZ	2.38	0.56
14:K:19:VAL:HG23	14:K:203[B]:ARG:HB2	1.87	0.56
19:P:80:ILE:HG23	19:P:146:VAL:HG12	1.86	0.56
45:p:124:ARG:NH1	45:p:124:ARG:HB2	2.21	0.56
6:C:562:U:OP2	49:t:14:ARG:NH1	2.38	0.56
7:D:131:LYS:HE2	7:D:131:LYS:HA	1.88	0.56
17:N:17:MET:O	17:N:21:ASN:N	2.37	0.56
44:o:54:ASP:OD1	44:o:55:THR:N	2.38	0.56
1:1:67:VAL:HG21	20:Q:57:VAL:HG22	1.88	0.56
3:3:59:LYS:N	3:3:59:LYS:HE2	2.21	0.56
5:A:46:G:O2'	5:A:47:U:O4'	2.21	0.56
6:C:944:G:N1	6:C:1338:G:OP2	2.37	0.56
9:F:202:GLU:OE1	10:G:105:ILE:N	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:V:114:GLU:OE1	25:V:118:ARG:NH1	2.37	0.56
6:C:273:U:O4	6:C:274:A:N6	2.38	0.56
17:N:46:ASP:OD1	17:N:48:LYS:N	2.35	0.56
32:c:47:LYS:NZ	32:c:48:PRO:O	2.39	0.56
49:t:62:GLU:OE2	49:t:62:GLU:HA	2.05	0.56
6:C:454:G:N2	6:C:479:U:O2	2.39	0.56
12:I:23:G:OP1	12:I:504:A:N6	2.39	0.56
31:b:92:ASN:OD1	31:b:93:LEU:N	2.39	0.56
6:C:1152:A:OP1	46:q:70:HIS:ND1	2.36	0.55
19:P:71:LYS:CD	19:P:108:VAL:HG11	2.36	0.55
51:v:86:GLU:OE1	51:v:86:GLU:HA	2.07	0.55
7:D:199:VAL:C	7:D:200:ILE:HD13	2.31	0.55
9:F:152:GLN:O	9:F:153:SER:OG	2.21	0.55
12:I:471:A:OP1	16:M:79:ARG:NH2	2.38	0.55
12:I:2158:A:O2'	12:I:2159:G:OP2	2.20	0.55
6:C:324:G:N1	6:C:327:A:OP2	2.38	0.55
9:F:57:GLU:HG3	9:F:199:LEU:HD12	1.87	0.55
39:j:7:GLU:OE2	39:j:8:LYS:N	2.40	0.55
12:I:2576:G:O2'	12:I:2579:C:OP2	2.23	0.55
54:y:5:ILE:HD12	54:y:5:ILE:O	2.07	0.55
12:I:1864:U:OP1	12:I:2410:G:O2'	2.23	0.55
26:W:106:LEU:C	26:W:106:LEU:HD23	2.32	0.55
5:A:38:A:O2'	6:C:790:A:OP1	2.25	0.54
11:H:17:GLN:OE1	11:H:17:GLN:O	2.26	0.54
12:I:1079:C:HO2'	12:I:1080:A:P	2.30	0.54
12:I:2115:G:O2'	12:I:2117:A:N7	2.39	0.54
6:C:212:G:H4'	6:C:213:G:OP1	2.07	0.54
39:j:17:THR:HB	39:j:42:VAL:HG11	1.89	0.54
10:G:94:VAL:CG1	10:G:96:MET:HE2	2.37	0.54
12:I:299:A:N3	12:I:319:G:O2'	2.39	0.54
6:C:1077:G:N2	6:C:1080:A:OP2	2.37	0.54
12:I:1730:C:O2	12:I:1731:G:N1	2.40	0.54
13:J:14:U:OP2	13:J:70:C:O2'	2.25	0.54
17:N:52:ASN:ND2	17:N:147:ASP:OD2	2.37	0.54
27:X:88:ARG:NH2	27:X:110:ILE:O	2.36	0.54
6:C:846:G:O2'	6:C:847:G:OP1	2.22	0.54
12:I:2128:G:N3	12:I:2173:A:O2'	2.41	0.54
47:r:36:ASP:OD1	47:r:36:ASP:C	2.51	0.54
52:w:35:GLN:OE1	52:w:35:GLN:HA	2.08	0.54
6:C:1316:G:N1	6:C:1319:A:OP2	2.40	0.54
12:I:2127:G:O2'	12:I:2128:G:O5'	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:2143:C:N4	12:I:2144:G:O6	2.41	0.54
12:I:2848:G:O2'	12:I:2867:G:N2	2.29	0.54
6:C:1013:G:N2	6:C:1016:A:OP2	2.37	0.54
14:K:98:ASP:C	14:K:98:ASP:OD1	2.50	0.54
35:f:2:SER:O	35:f:2:SER:OG	2.22	0.54
12:I:25:U:HO2'	12:I:26:G:P	2.31	0.53
19:P:97:ARG:HE	19:P:97:ARG:HA	1.73	0.53
6:C:1145:A:HO2'	6:C:1146:A:P	2.32	0.53
12:I:2343:U:HO2'	12:I:2373:G:HO2'	1.49	0.53
17:N:120:LYS:HE2	17:N:120:LYS:HA	1.89	0.53
29:Z:51:VAL:HB	29:Z:52:PRO:CD	2.38	0.53
45:p:53:GLU:OE2	45:p:54:LEU:HD22	2.08	0.53
6:C:855:U:OP2	6:C:871:U:N3	2.39	0.53
8:E:11:ARG:NH1	8:E:177:THR:O	2.41	0.53
12:I:964:C:O2'	12:I:2273:A:N3	2.37	0.53
22:S:73:ASP:OD1	22:S:75:SER:OG	2.26	0.53
36:g:49:ASP:O	36:g:53:VAL:HG23	2.08	0.53
6:C:976:G:OP2	6:C:1358:U:O2'	2.25	0.53
12:I:1009:A:N3	12:I:1153:C:O2'	2.40	0.53
12:I:1682:G:OP2	12:I:1699:G:N2	2.39	0.53
54:y:27:ARG:NH1	54:y:42:THR:OG1	2.42	0.53
55:z:37:GLY:O	55:z:63:ARG:NH2	2.40	0.53
12:I:1047:G:HO2'	12:I:1110:G:H1	1.57	0.53
43:n:129:GLU:OE2	43:n:129:GLU:HA	2.09	0.53
6:C:275:G:P	54:y:16:LYS:HZ1	2.31	0.53
12:I:2116:G:O6	12:I:2171:A:N6	2.42	0.53
12:I:2335:A:H5'	26:W:13:ARG:HH22	1.74	0.53
30:a:34:ASP:OD2	38:i:37:LYS:NZ	2.40	0.53
18:O:72:LEU:HD23	18:O:75:MET:HE3	1.90	0.53
23:T:132:ARG:HD3	23:T:142:ILE:HD13	1.91	0.53
45:p:19:VAL:HA	45:p:65:ILE:HG22	1.90	0.53
54:y:40:ARG:NE	54:y:40:ARG:HA	2.23	0.53
2:2:55:GLN:NE2	6:C:193:C:O4'	2.42	0.53
9:F:99:ASP:OD2	9:F:99:ASP:C	2.52	0.53
13:J:66:A:OP2	13:J:108:A:N6	2.41	0.53
22:S:92:GLU:HG3	22:S:92:GLU:O	2.09	0.53
1:1:19:VAL:HG21	1:1:44:MET:HG2	1.90	0.53
12:I:1352:U:O2'	12:I:1353:A:O5'	2.27	0.53
12:I:2788:C:O2'	12:I:2809:A:N3	2.38	0.53
20:Q:62:LYS:O	20:Q:65:ASN:ND2	2.42	0.53
6:C:656:G:O2'	52:w:28:GLN:OE1	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:1141:U:OP2	21:R:65:THR:OG1	2.27	0.53
22:S:63:VAL:HG12	22:S:107:LEU:HD11	1.90	0.53
44:o:11:LEU:HD22	44:o:75:ILE:HD11	1.91	0.53
1:1:11:ILE:HD13	1:1:16:LEU:HD13	1.91	0.52
6:C:427:U:OP1	9:F:13:ARG:NH2	2.42	0.52
7:D:40:ILE:HD12	7:D:40:ILE:C	2.34	0.52
12:I:2640:G:OP1	21:R:96:ARG:NH1	2.43	0.52
45:p:55:VAL:HG22	45:p:56:ASP:N	2.23	0.52
20:Q:58:ASP:OD1	20:Q:58:ASP:N	2.36	0.52
38:i:52:ARG:HB3	38:i:52:ARG:NH1	2.24	0.52
46:q:99:GLN:C	46:q:100:ILE:HD13	2.34	0.52
6:C:115:G:H4'	6:C:116:A:O5'	2.08	0.52
12:I:1527:G:N1	12:I:1544:A:OP2	2.40	0.52
13:J:42:C:C6	17:N:66:LEU:HD21	2.45	0.52
6:C:563:A:HO2'	6:C:566:G:HO2'	1.58	0.52
6:C:846:G:O2'	6:C:847:G:P	2.66	0.52
11:H:61:LEU:HD13	11:H:62:MET:N	2.25	0.52
12:I:1417:C:HO2'	12:I:1587:G:HO2'	1.48	0.52
15:L:46:ARG:NH1	15:L:85:ALA:O	2.43	0.52
21:R:50:THR:O	21:R:50:THR:HG22	2.10	0.52
49:t:110:ARG:NH2	49:t:112:GLN:O	2.40	0.52
3:3:24:GLU:OE1	3:3:24:GLU:C	2.53	0.52
11:H:23:GLU:CD	11:H:23:GLU:H	2.18	0.52
12:I:249:C:O2	41:l:12:LYS:NZ	2.41	0.52
12:I:1378:A:O2'	12:I:1380:G:OP2	2.28	0.52
19:P:94:ILE:O	19:P:94:ILE:HG22	2.09	0.52
12:I:74:A:O2'	12:I:88:G:OP1	2.27	0.52
22:S:111:LYS:HZ3	22:S:111:LYS:HB2	1.75	0.52
12:I:617:G:OP1	16:M:102:ARG:NH1	2.42	0.52
12:I:1475:G:O2'	12:I:1514:G:O6	2.21	0.52
29:Z:37:GLU:HA	29:Z:37:GLU:OE2	2.09	0.52
6:C:1229:A:OP2	50:u:113:ARG:NH1	2.43	0.52
7:D:166:ALA:HB2	7:D:187:VAL:HG22	1.91	0.52
12:I:160:A:N3	12:I:2208:C:O2'	2.41	0.52
12:I:743:A:O2'	12:I:1659:G:OP1	2.25	0.52
12:I:1311:G:OP2	12:I:1311:G:N2	2.33	0.52
12:I:1755:A:OP1	27:X:103:ARG:NH2	2.38	0.52
45:p:55:VAL:HG13	45:p:56:ASP:H	1.74	0.52
47:r:67:ALA:HB2	47:r:96:THR:HG23	1.91	0.52
50:u:39:ILE:HD12	50:u:56:LEU:HD21	1.92	0.52
53:x:4:ILE:HG13	53:x:21:VAL:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:586:A:N1	12:I:809:G:O2'	2.34	0.52
12:I:2305:U:O2'	17:N:133:ARG:NH2	2.39	0.52
43:n:15:ASP:OD2	43:n:23:LEU:HD23	2.09	0.52
11:H:39:LEU:HD13	11:H:39:LEU:C	2.34	0.51
12:I:84:A:N1	12:I:98:G:O2'	2.33	0.51
15:L:99:GLU:OE2	15:L:99:GLU:N	2.32	0.51
12:I:1447:C:O2'	12:I:1544:A:N3	2.39	0.51
46:q:24:GLU:OE1	46:q:92:LEU:HD22	2.10	0.51
5:A:10:G:HO2'	5:A:11:C:P	2.34	0.51
6:C:1328:C:H5''	50:u:28:THR:HG21	1.92	0.51
7:D:118:GLU:OE2	7:D:118:GLU:HA	2.11	0.51
12:I:1954:G:O2'	12:I:1956:U:O4	2.16	0.51
51:v:64:CYS:SG	51:v:79:LEU:HD23	2.51	0.51
6:C:664:G:H22	6:C:741:G:H1	1.58	0.51
6:C:1238:A:H5'	6:C:1336:C:H41	1.76	0.51
54:y:15:ASP:OD2	54:y:55:ILE:N	2.44	0.51
12:I:463:G:N2	12:I:466:A:OP2	2.42	0.51
12:I:2854:G:O2'	12:I:2855:C:P	2.69	0.51
31:b:3:ARG:HG3	31:b:3:ARG:HH11	1.76	0.51
37:h:40:ASP:OD1	37:h:40:ASP:C	2.54	0.51
43:n:68:ASN:ND2	43:n:130:ASN:OD1	2.44	0.51
7:D:50:PHE:O	7:D:54:LEU:HD23	2.11	0.50
8:E:5:VAL:HG11	8:E:10:ILE:HD11	1.93	0.50
10:G:106:ILE:HD11	10:G:124:LEU:CD1	2.41	0.50
15:L:48:ILE:HG23	15:L:84:LEU:HD11	1.92	0.50
52:w:24:SER:OG	52:w:26:GLU:OE1	2.26	0.50
7:D:113:ARG:NH1	7:D:117:LEU:HD11	2.26	0.50
35:f:17:ASN:OD1	35:f:17:ASN:N	2.44	0.50
43:n:27:VAL:O	43:n:31:MET:N	2.43	0.50
6:C:993:G:O2'	6:C:994:A:N7	2.44	0.50
34:e:11:ARG:O	34:e:14:ARG:NH1	2.41	0.50
7:D:122:GLN:OE1	7:D:122:GLN:HA	2.12	0.50
12:I:468:G:N7	40:k:39:ARG:NH2	2.56	0.50
12:I:1604:C:O2'	12:I:1610:A:N1	2.44	0.50
30:a:96:ILE:HD12	30:a:96:ILE:C	2.36	0.50
7:D:113:ARG:O	7:D:117:LEU:HD12	2.11	0.50
12:I:1329:U:OP2	12:I:1330:C:N4	2.45	0.50
12:I:2445:2MG:OP1	16:M:69:ARG:NH1	2.35	0.50
12:I:818:G:N1	12:I:1188:U:OP2	2.37	0.50
15:L:18:ASP:N	15:L:18:ASP:OD1	2.43	0.50
12:I:636:G:N2	23:T:76:GLU:OE1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:v:93:ILE:HG21	51:v:96:LEU:HD22	1.94	0.50
6:C:574:A:HO2'	6:C:882:C:HO2'	1.57	0.50
12:I:1813:G:HO2'	12:I:1814:G:P	2.35	0.50
31:b:28:ASN:ND2	31:b:88:LYS:O	2.45	0.50
33:d:7:GLU:N	33:d:7:GLU:OE1	2.45	0.50
5:A:46:G:HO2'	5:A:47:U:C1'	2.24	0.49
12:I:182:A:O2'	12:I:183:C:OP1	2.28	0.49
12:I:2756:U:OP2	42:m:19:ARG:NH1	2.41	0.49
32:c:50:PRO:O	32:c:54:GLN:NE2	2.44	0.49
55:z:62:ALA:HB3	55:z:68:LEU:HD12	1.93	0.49
17:N:46:ASP:OD1	17:N:47:LYS:N	2.45	0.49
6:C:205:A:N1	6:C:206:C:N4	2.61	0.49
6:C:1016:A:HO2'	6:C:1217:C:HO2'	1.45	0.49
5:A:61:C:O2'	5:A:62:C:P	2.70	0.49
6:C:31:G:O2'	6:C:48:C:N4	2.45	0.49
9:F:35:GLU:OE1	9:F:35:GLU:N	2.41	0.49
12:I:1755:A:N6	12:I:2694:G:O2'	2.45	0.49
31:b:89:GLU:N	31:b:89:GLU:OE1	2.43	0.49
6:C:739:C:O2'	52:w:42:HIS:ND1	2.41	0.49
14:K:142:HIS:ND1	14:K:193:GLY:O	2.43	0.49
36:g:58:ASN:C	36:g:58:ASN:OD1	2.55	0.49
6:C:563:A:O2'	6:C:566:G:O3'	2.31	0.49
8:E:43:LEU:HD21	8:E:68:ILE:HD11	1.95	0.49
13:J:8:C:OP1	26:W:15:ARG:NH2	2.42	0.49
26:W:55:GLU:OE2	26:W:81:ARG:NH2	2.46	0.49
36:g:36:GLN:OE1	36:g:36:GLN:N	2.46	0.49
6:C:653:U:O4'	44:o:56:LYS:NZ	2.43	0.49
19:P:111:ALA:HB3	19:P:114:GLU:HB2	1.95	0.49
6:C:951:G:OP2	50:u:101:ARG:NH2	2.45	0.49
21:R:31:GLU:HA	21:R:31:GLU:OE2	2.13	0.49
12:I:1799:G:OP1	14:K:258:ARG:NH1	2.42	0.49
12:I:1980:G:O2'	12:I:1982:U:OP2	2.27	0.49
12:I:2104:C:H42	12:I:2184:A:H61	1.61	0.49
12:I:2430:A:N3	12:I:2430:A:H2'	2.28	0.49
6:C:769:G:H4'	6:C:1513:A:H4'	1.95	0.49
5:A:10:G:O2'	5:A:11:C:P	2.71	0.48
12:I:1266:G:OP1	38:i:16:ARG:NE	2.35	0.48
39:j:9:ILE:HG21	39:j:25:LYS:HB3	1.95	0.48
52:w:74:ASP:OD1	52:w:74:ASP:C	2.56	0.48
6:C:1491:G:O2'	6:C:1492:A:P	2.71	0.48
7:D:26:LYS:NZ	7:D:194:ASP:OD2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:n:25:LYS:HB3	43:n:101:MET:HE1	1.95	0.48
10:G:65:GLU:OE1	10:G:69:ARG:NE	2.46	0.48
12:I:18:U:O2'	12:I:554:U:OP1	2.27	0.48
16:M:121:VAL:O	16:M:190:ALA:N	2.47	0.48
16:M:198:GLU:OE1	16:M:198:GLU:N	2.46	0.48
17:N:38:MET:HE3	17:N:57:LEU:HD21	1.94	0.48
33:d:55:GLU:CD	33:d:55:GLU:H	2.22	0.48
8:E:112:ASP:OD1	8:E:112:ASP:C	2.57	0.48
9:F:145:ILE:HD13	9:F:178:MET:HB3	1.94	0.48
11:H:22:ILE:H	11:H:22:ILE:HD12	1.77	0.48
12:I:578:G:OP1	12:I:1255:U:O2'	2.21	0.48
12:I:784:G:H5'	12:I:785:G:OP1	2.12	0.48
43:n:15:ASP:OD1	43:n:17:LYS:N	2.46	0.48
54:y:52:GLU:O	54:y:81:LYS:NZ	2.46	0.48
12:I:1047:G:O2'	12:I:1110:G:N1	2.46	0.48
12:I:1363:C:O2'	12:I:1809:A:N3	2.40	0.48
12:I:1846:G:O2'	12:I:1847:A:P	2.71	0.48
12:I:1965:C:OP1	12:I:1966:A:O2'	2.29	0.48
31:b:54:GLU:N	31:b:54:GLU:OE1	2.47	0.48
12:I:182:A:O2'	12:I:183:C:P	2.71	0.48
18:O:72:LEU:HD23	18:O:75:MET:CE	2.43	0.48
42:m:15:LYS:NZ	42:m:15:LYS:HB3	2.29	0.48
43:n:47:LEU:HD12	43:n:48:GLU:N	2.28	0.48
6:C:1422:G:O3'	22:S:49:ARG:NH2	2.47	0.48
12:I:1224:U:OP2	29:Z:68:ARG:NH2	2.45	0.48
12:I:2225:A:H1'	12:I:2226:C:OP2	2.13	0.48
16:M:21:ARG:HG3	16:M:21:ARG:HH11	1.78	0.48
54:y:17:MET:HE3	54:y:20:SER:HB3	1.94	0.48
7:D:54:LEU:HD12	7:D:220:THR:OG1	2.14	0.48
12:I:1025:G:O2'	12:I:1026:G:P	2.71	0.48
12:I:2688:G:N1	12:I:2720:U:OP2	2.40	0.48
37:h:8:THR:OG1	37:h:58:GLU:OE2	2.26	0.48
52:w:14:GLU:C	52:w:14:GLU:OE2	2.57	0.48
6:C:1178:G:N2	6:C:1181:G:OP2	2.46	0.48
12:I:2127:G:O2'	12:I:2128:G:P	2.71	0.48
17:N:152:LEU:C	17:N:152:LEU:HD12	2.38	0.48
19:P:4:ILE:HD11	19:P:37:VAL:HG23	1.95	0.48
12:I:2854:G:O2'	12:I:2855:C:OP1	2.28	0.48
22:S:12:ASP:C	22:S:12:ASP:OD1	2.57	0.48
15:L:74:GLU:HA	15:L:74:GLU:OE2	2.13	0.47
29:Z:10:LYS:NZ	29:Z:23:GLU:OE2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:66:LEU:CD1	2:2:67:ILE:HG23	2.44	0.47
12:I:1654:A:O2'	15:L:118:PHE:O	2.31	0.47
20:Q:8:LYS:NZ	20:Q:8:LYS:HB3	2.29	0.47
6:C:1239:A:H62	6:C:1299:A:N6	2.12	0.47
12:I:2639:A:O3'	21:R:96:ARG:NH1	2.46	0.47
6:C:766:A:OP2	6:C:812:G:N2	2.48	0.47
2:2:70:ASN:OD1	2:2:70:ASN:N	2.48	0.47
6:C:1201:A:H1'	6:C:1202:U:OP2	2.13	0.47
17:N:112:ARG:HG2	17:N:112:ARG:HH11	1.79	0.47
26:W:14:ALA:O	26:W:18:LEU:HG	2.15	0.47
46:q:14:ASP:OD1	46:q:14:ASP:C	2.58	0.47
9:F:145:ILE:N	9:F:145:ILE:HD12	2.30	0.47
12:I:555:G:H4'	12:I:556:A:OP1	2.14	0.47
12:I:1420:A:N1	12:I:2211:A:N6	2.63	0.47
21:R:7:LYS:O	21:R:11:VAL:HG13	2.15	0.47
51:v:16:LEU:C	51:v:16:LEU:HD23	2.39	0.47
6:C:60:A:N1	6:C:107:G:O2'	2.42	0.47
6:C:96:U:O2'	6:C:97:G:P	2.72	0.47
12:I:629:G:N3	12:I:639:U:O2'	2.47	0.47
12:I:1068:G:N2	12:I:1095:A:O2'	2.48	0.47
12:I:2305:U:O2'	17:N:133:ARG:NH1	2.47	0.47
12:I:2348:U:C5'	39:j:42:VAL:HG13	2.44	0.47
26:W:112:GLU:OE2	26:W:112:GLU:HA	2.14	0.47
6:C:1109:C:OP2	8:E:176:HIS:ND1	2.45	0.47
6:C:1317:C:O2'	6:C:1318:A:OP1	2.33	0.47
7:D:13:GLY:O	7:D:15:HIS:N	2.37	0.47
12:I:1266:G:O2'	12:I:1267:U:OP2	2.33	0.47
24:U:27:SER:N	24:U:104:GLU:OE2	2.44	0.47
7:D:216:ALA:O	7:D:220:THR:OG1	2.31	0.46
39:j:43:VAL:HG22	39:j:43:VAL:O	2.16	0.46
2:2:12:ILE:C	2:2:12:ILE:HD12	2.40	0.46
3:3:23:CYS:SG	3:3:24:GLU:N	2.88	0.46
12:I:1288:G:OP2	12:I:1288:G:N2	2.40	0.46
12:I:2029:G:N1	12:I:2033:A:OP2	2.46	0.46
17:N:10:ASP:HB2	17:N:11:GLU:OE1	2.15	0.46
21:R:10:THR:O	21:R:10:THR:HG22	2.15	0.46
51:v:24:ARG:NE	51:v:24:ARG:HA	2.30	0.46
7:D:214:LEU:HD12	7:D:215:GLY:N	2.29	0.46
11:H:16:GLU:C	11:H:16:GLU:OE1	2.58	0.46
11:H:41:ASP:OD1	11:H:58:HIS:NE2	2.41	0.46
30:a:4:ILE:HD11	30:a:104:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:t:35:THR:N	49:t:54:ARG:O	2.48	0.46
9:F:160:GLU:OE2	9:F:160:GLU:HA	2.16	0.46
10:G:94:VAL:HG13	10:G:111:MET:HE3	1.97	0.46
12:I:1077:A:H61	12:I:1088:A:H2'	1.81	0.46
18:O:16:ASP:OD1	18:O:16:ASP:C	2.59	0.46
27:X:30:VAL:CG2	27:X:80:VAL:HG12	2.45	0.46
9:F:203:LEU:HD23	9:F:203:LEU:O	2.15	0.46
12:I:1079:C:O2'	12:I:1080:A:P	2.74	0.46
12:I:1847:A:O2'	12:I:1848:A:P	2.73	0.46
19:P:42:LYS:O	19:P:42:LYS:NZ	2.45	0.46
22:S:110:GLU:CD	22:S:110:GLU:H	2.23	0.46
24:U:33:LEU:HD11	24:U:128:THR:CG2	2.45	0.46
53:x:21:VAL:O	53:x:33:ILE:N	2.47	0.46
12:I:1814:G:OP1	14:K:40:SER:OG	2.31	0.46
17:N:26:MET:O	17:N:30:ARG:NH2	2.48	0.46
42:m:7:VAL:CG1	42:m:25:VAL:HG23	2.46	0.46
43:n:15:ASP:OD1	43:n:15:ASP:C	2.58	0.46
53:x:23:ASP:OD2	53:x:24:SER:N	2.48	0.46
8:E:79:LYS:N	8:E:82:GLU:OE1	2.49	0.46
12:I:2348:U:H5'	39:j:42:VAL:HG13	1.96	0.46
19:P:47:PHE:O	19:P:51:ARG:N	2.49	0.46
6:C:525:C:OP1	49:t:86:ARG:NH2	2.47	0.46
12:I:301:G:O2'	12:I:302:C:O5'	2.33	0.46
12:I:2680:U:O2'	12:I:2681:C:P	2.74	0.46
18:O:26:ILE:HD13	18:O:26:ILE:N	2.31	0.46
26:W:46:GLU:OE1	26:W:46:GLU:HA	2.15	0.46
45:p:31:ASN:O	45:p:32:GLN:HG2	2.15	0.46
7:D:63:ARG:NH1	7:D:63:ARG:HB2	2.32	0.46
8:E:92:ALA:O	8:E:96:GLY:N	2.48	0.46
12:I:1869:G:N2	12:I:1871:A:O2'	2.48	0.46
52:w:26:GLU:H	52:w:26:GLU:CD	2.23	0.46
12:I:52:A:H8	12:I:178:G:H21	1.63	0.45
12:I:1352:U:O2'	12:I:1353:A:P	2.74	0.45
10:G:106:ILE:HD11	10:G:124:LEU:HD12	1.97	0.45
14:K:117:GLN:N	14:K:128:ASN:OD1	2.44	0.45
6:C:401:C:OP2	9:F:70:ARG:NH1	2.48	0.45
7:D:127:ASP:N	7:D:127:ASP:OD1	2.49	0.45
10:G:109:GLY:O	10:G:110:ALA:HB3	2.17	0.45
17:N:36:LEU:HD13	17:N:57:LEU:HD22	1.98	0.45
22:S:73:ASP:CG	22:S:75:SER:HG	2.24	0.45
22:S:103:VAL:CG1	22:S:107:LEU:HD12	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:121:THR:HG21	8:E:187:SER:OG	2.16	0.45
12:I:177:G:OP2	12:I:177:G:N2	2.33	0.45
12:I:1750:G:O2'	12:I:2860:A:N1	2.36	0.45
29:Z:74:ILE:HD12	29:Z:74:ILE:N	2.32	0.45
43:n:90:GLU:OE2	43:n:91:VAL:N	2.49	0.45
53:x:42:ILE:O	53:x:42:ILE:HG22	2.16	0.45
10:G:24:THR:HA	10:G:29:ARG:HA	1.99	0.45
12:I:603:A:H5'	12:I:655:A:H61	1.81	0.45
12:I:2286:G:N2	39:j:12:VAL:HG22	2.31	0.45
12:I:2876:G:OP1	27:X:2:SER:N	2.49	0.45
51:v:80:SER:O	51:v:84:VAL:HG23	2.16	0.45
11:H:69:GLU:H	11:H:69:GLU:CD	2.23	0.45
16:M:136:GLN:NE2	16:M:140:ASP:OD1	2.50	0.45
1:I:48:THR:HG23	1:I:48:THR:O	2.17	0.45
6:C:565:U:OP2	6:C:566:G:O2'	2.32	0.45
6:C:1516:G:N2	6:C:1519:A:OP2	2.49	0.45
12:I:1797:G:O2'	14:K:257:THR:OG1	2.18	0.45
12:I:1816:C:N4	14:K:35:GLU:OE2	2.39	0.45
20:Q:26:SER:OG	20:Q:28:VAL:HG23	2.17	0.45
26:W:117:PHE:CD1	26:W:117:PHE:C	2.95	0.45
36:g:4:LYS:H	36:g:4:LYS:HD2	1.81	0.45
43:n:47:LEU:HD12	43:n:47:LEU:C	2.42	0.45
8:E:112:ASP:OD1	8:E:114:LYS:N	2.49	0.45
9:F:78:GLU:OE2	9:F:81:ARG:NH1	2.50	0.45
10:G:105:ILE:HD11	10:G:120:VAL:O	2.17	0.45
12:I:249:C:OP2	12:I:2394:C:O2'	2.25	0.45
12:I:545:U:O2'	12:I:546:U:O5'	2.33	0.45
19:P:95:GLY:O	19:P:99:ILE:HD12	2.17	0.45
45:p:28:ILE:HG23	45:p:63:LEU:HD11	1.98	0.45
6:C:280:C:N3	54:y:41:THR:HG21	2.32	0.45
37:h:4:THR:HG23	37:h:37:GLU:HG2	1.99	0.45
47:r:37:ARG:HG3	47:r:37:ARG:HH11	1.81	0.45
6:C:1280:A:OP1	46:q:9:ARG:NH1	2.50	0.45
12:I:223:A:N1	12:I:407:G:O2'	2.46	0.45
12:I:2306:C:N4	17:N:39:GLY:O	2.44	0.45
16:M:16:GLU:O	16:M:20:GLY:N	2.50	0.45
5:A:9:A:H5'	5:A:46:G:H21	1.82	0.44
6:C:1124:G:HO2'	6:C:1145:A:N6	2.13	0.44
7:D:178:ASN:C	7:D:178:ASN:OD1	2.60	0.44
12:I:624:C:O2'	12:I:657:U:OP1	2.33	0.44
17:N:46:ASP:OD1	17:N:46:ASP:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:76:GLU:C	23:T:77:ILE:HD13	2.41	0.44
12:I:2305:U:O4	17:N:39:GLY:N	2.50	0.44
14:K:168:ASP:OD1	14:K:168:ASP:C	2.60	0.44
29:Z:45:GLU:OE1	29:Z:45:GLU:N	2.48	0.44
53:x:23:ASP:OD1	53:x:25:ARG:NH1	2.51	0.44
2:2:57:ILE:HD12	2:2:57:ILE:C	2.42	0.44
9:F:161:LEU:C	9:F:161:LEU:HD12	2.41	0.44
12:I:668:A:H2'	12:I:670:A:H62	1.82	0.44
32:c:35:ILE:HD13	32:c:64:ALA:HA	2.00	0.44
45:p:35:LEU:HD23	45:p:35:LEU:O	2.17	0.44
6:C:130:A:O2'	6:C:131:A:O5'	2.31	0.44
10:G:151:GLU:OE1	10:G:151:GLU:N	2.50	0.44
15:L:24:VAL:HG12	15:L:178:VAL:HG21	1.99	0.44
15:L:181:ASP:OD2	15:L:181:ASP:C	2.60	0.44
16:M:155:GLU:OE1	16:M:155:GLU:N	2.42	0.44
18:O:137:ASP:OD1	18:O:137:ASP:C	2.61	0.44
31:b:30:ILE:HD12	31:b:32:LEU:HD21	2.00	0.44
6:C:279:A:OP1	6:C:280:C:O2'	2.31	0.44
6:C:978:A:HO2'	6:C:1322:C:H5	1.61	0.44
12:I:2299:U:OP2	17:N:71:ARG:NH2	2.51	0.44
18:O:173:GLU:OE2	18:O:173:GLU:C	2.60	0.44
46:q:45:ARG:NH2	46:q:47:GLU:OE1	2.51	0.44
50:u:50:GLU:OE2	50:u:50:GLU:HA	2.17	0.44
1:1:30:PRO:HA	1:1:48:THR:HG23	2.00	0.44
12:I:1141:U:H4'	12:I:1142:A:O4'	2.18	0.44
12:I:2581:G:OP2	12:I:2581:G:N2	2.48	0.44
18:O:25:THR:C	18:O:26:ILE:HD13	2.42	0.44
18:O:166:ASP:OD1	18:O:166:ASP:N	2.46	0.44
19:P:27:ARG:NH1	35:f:60:ASP:OD2	2.51	0.44
19:P:70:GLU:OE1	19:P:70:GLU:N	2.50	0.44
6:C:1086:U:H3	6:C:1099:G:H22	1.63	0.44
18:O:121:ILE:HD11	18:O:140:VAL:HG23	1.99	0.44
22:S:111:LYS:NZ	22:S:111:LYS:HB2	2.32	0.44
14:K:79:GLU:OE1	14:K:101:ARG:NH1	2.50	0.44
20:Q:10:GLU:OE2	20:Q:10:GLU:N	2.50	0.44
45:p:56:ASP:OD1	45:p:58:VAL:HG22	2.18	0.44
46:q:79:PRO:O	46:q:80:THR:C	2.61	0.44
10:G:94:VAL:HG13	10:G:111:MET:CE	2.48	0.44
12:I:205:G:O2'	12:I:206:U:OP2	2.31	0.44
12:I:1913:A:H1'	12:I:1914:C:P	2.58	0.44
15:L:110:THR:HG22	15:L:171:THR:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:V:2:ARG:NH1	25:V:5:LYS:O	2.50	0.44
45:p:21:ILE:HD13	45:p:63:LEU:HB3	2.00	0.44
6:C:346:G:OP1	27:X:39:ARG:NH1	2.46	0.43
16:M:144:GLU:OE1	16:M:144:GLU:HA	2.18	0.43
19:P:99:ILE:O	19:P:103:VAL:HG23	2.18	0.43
36:g:12:GLU:OE2	36:g:12:GLU:HA	2.18	0.43
2:2:32:ILE:HD13	2:2:54:MET:HG3	1.99	0.43
10:G:70:ASN:C	10:G:70:ASN:OD1	2.60	0.43
10:G:132:ASN:OD1	10:G:134:ILE:HG13	2.19	0.43
12:I:2523:G:O2'	12:I:2764:A:O2'	2.32	0.43
23:T:82:LEU:HD23	23:T:82:LEU:C	2.42	0.43
45:p:57:MET:N	45:p:57:MET:SD	2.91	0.43
6:C:935:A:O2'	6:C:1383:C:N3	2.48	0.43
7:D:197:ASP:OD1	7:D:197:ASP:N	2.51	0.43
19:P:6:LEU:N	19:P:35:LYS:O	2.46	0.43
24:U:47:GLU:OE1	24:U:50:ARG:NH1	2.51	0.43
46:q:97:ASP:OD1	46:q:97:ASP:C	2.62	0.43
2:2:39:ILE:HD12	2:2:39:ILE:H	1.83	0.43
6:C:115:G:H1'	6:C:116:A:OP2	2.19	0.43
9:F:27:ALA:O	9:F:28:ILE:O	2.36	0.43
9:F:78:GLU:OE1	9:F:78:GLU:HA	2.17	0.43
12:I:1012:U:O2	21:R:27:ARG:NH1	2.51	0.43
12:I:2181:U:O2'	12:I:2182:U:O4'	2.28	0.43
19:P:95:GLY:N	19:P:98:ASP:OD2	2.51	0.43
51:v:88:ALA:CB	51:v:96:LEU:HD23	2.47	0.43
12:I:1094:U:N3	12:I:1097:U:OP2	2.51	0.43
7:D:63:ARG:O	7:D:63:ARG:CG	2.66	0.43
12:I:1315:C:O2'	12:I:1392:A:N3	2.50	0.43
25:V:98:LEU:O	25:V:112:TYR:N	2.47	0.43
50:u:59:GLU:OE2	50:u:59:GLU:HA	2.18	0.43
6:C:1347:G:O6	45:p:12:ARG:NH2	2.51	0.43
12:I:182:A:HO2'	12:I:183:C:P	2.41	0.43
34:e:18:ALA:O	34:e:20:ARG:NH1	2.47	0.43
6:C:1233:G:OP1	45:p:119:ARG:NH1	2.51	0.43
8:E:181:ASP:OD2	8:E:181:ASP:C	2.62	0.43
12:I:138:U:HO2'	12:I:139:U:P	2.32	0.43
12:I:636:G:N1	23:T:76:GLU:OE1	2.46	0.43
12:I:2854:G:HO2'	12:I:2855:C:P	2.42	0.43
14:K:136:PRO:O	14:K:139:SER:OG	2.21	0.43
19:P:40:THR:HG23	19:P:43:ASN:H	1.82	0.43
19:P:41:LYS:H	19:P:41:LYS:CD	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:t:73:ASN:OD1	49:t:73:ASN:N	2.49	0.43
54:y:72:SER:O	54:y:72:SER:OG	2.31	0.43
11:H:9:MET:HE3	11:H:86:ARG:O	2.19	0.43
11:H:88:MET:HG2	55:z:65:LEU:HD21	2.00	0.43
12:I:479:A:H4'	12:I:480:A:OP1	2.19	0.43
17:N:112:ARG:HG2	17:N:112:ARG:NH1	2.34	0.43
28:Y:91:ASP:OD1	28:Y:91:ASP:C	2.61	0.43
7:D:154:MET:CE	7:D:158:PRO:HD3	2.49	0.43
12:I:1789:A:OP2	14:K:221:ARG:NH1	2.52	0.43
22:S:71:ARG:NH1	22:S:106:GLU:OE2	2.46	0.43
6:C:1397:C:OP2	10:G:29:ARG:NH2	2.48	0.42
12:I:2543:G:O2'	12:I:2544:G:P	2.77	0.42
18:O:39:ASP:OD1	18:O:39:ASP:N	2.51	0.42
43:n:111:ARG:NH1	43:n:123:GLU:OE1	2.48	0.42
47:r:56:ARG:HB2	47:r:56:ARG:NH1	2.34	0.42
8:E:3:GLN:N	8:E:3:GLN:OE1	2.52	0.42
8:E:131:ARG:HD2	8:E:168:TYR:OH	2.19	0.42
12:I:1326:U:O2'	12:I:2010:G:O2'	2.36	0.42
20:Q:12:ILE:C	20:Q:12:ILE:HD12	2.44	0.42
12:I:87:U:H5''	12:I:88:G:OP2	2.19	0.42
19:P:62:LEU:HD23	19:P:62:LEU:O	2.20	0.42
19:P:86:ASP:O	19:P:87:GLU:HB3	2.18	0.42
54:y:26:GLU:HA	54:y:26:GLU:OE1	2.18	0.42
7:D:21:ARG:HG3	7:D:21:ARG:HH11	1.84	0.42
7:D:27:MET:CE	7:D:187:VAL:HG12	2.47	0.42
10:G:69:ARG:O	10:G:70:ASN:OD1	2.36	0.42
12:I:52:A:H2	12:I:119:A:H62	1.66	0.42
12:I:247:G:O2'	12:I:386:G:N1	2.51	0.42
12:I:984:A:N3	12:I:984:A:H2'	2.34	0.42
16:M:21:ARG:HG3	16:M:21:ARG:NH1	2.34	0.42
30:a:1:MET:HE3	30:a:1:MET:HA	2.00	0.42
39:j:9:ILE:HD12	39:j:10:LYS:N	2.34	0.42
12:I:2600:A:OP2	14:K:236:GLU:OE1	2.38	0.42
15:L:183:GLU:H	15:L:183:GLU:CD	2.27	0.42
19:P:121:VAL:O	19:P:121:VAL:HG13	2.20	0.42
36:g:17:GLU:OE2	36:g:17:GLU:HA	2.20	0.42
46:q:8:ILE:HD13	46:q:8:ILE:N	2.35	0.42
46:q:29:ALA:O	46:q:33:GLY:N	2.43	0.42
1:1:50:ALA:HB1	1:1:57:HIS:HB3	2.02	0.42
17:N:51:ASP:N	17:N:51:ASP:OD1	2.52	0.42
39:j:9:ILE:HG21	39:j:25:LYS:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:7:A:O2'	5:A:49:C:O4'	2.37	0.42
6:C:923:A:N6	6:C:1392:G:O6	2.53	0.42
7:D:13:GLY:C	7:D:14:VAL:HG12	2.44	0.42
9:F:49:SER:OG	9:F:50:ASP:N	2.51	0.42
11:H:97:THR:C	11:H:98:GLU:CD	2.87	0.42
12:I:2401:U:O2	12:I:2401:U:O5'	2.38	0.42
29:Z:45:GLU:H	29:Z:45:GLU:CD	2.28	0.42
1:1:29:LYS:H	1:1:29:LYS:HD3	1.85	0.42
11:H:69:GLU:CD	11:H:69:GLU:N	2.77	0.42
12:I:2159:G:O2'	12:I:2160:C:O4'	2.21	0.42
45:p:54:LEU:O	45:p:55:VAL:C	2.63	0.42
54:y:68:SER:OG	54:y:69:LYS:N	2.53	0.42
5:A:56:C:O2'	17:N:75:ALA:N	2.47	0.42
7:D:117:LEU:HB3	7:D:141:LEU:HD11	2.01	0.42
7:D:131:LYS:HE2	7:D:131:LYS:CA	2.49	0.42
7:D:200:ILE:HD13	7:D:200:ILE:N	2.35	0.42
12:I:2060:A:O2'	12:I:2061:G:OP2	2.36	0.42
15:L:86:GLU:OE2	15:L:86:GLU:HA	2.18	0.42
19:P:101:ASP:OD1	19:P:101:ASP:N	2.52	0.42
22:S:104:THR:CG2	22:S:106:GLU:OE1	2.68	0.42
23:T:86:GLU:C	23:T:86:GLU:CD	2.87	0.42
25:V:106:ASP:OD1	25:V:106:ASP:N	2.53	0.42
26:W:47:VAL:O	26:W:47:VAL:HG13	2.19	0.42
31:b:91:GLN:C	31:b:91:GLN:OE1	2.62	0.42
46:q:10:LEU:CD2	46:q:98:VAL:HG23	2.50	0.42
49:t:109:ASP:OD1	49:t:109:ASP:N	2.53	0.42
53:x:53:ASP:OD2	53:x:53:ASP:C	2.62	0.42
6:C:528:C:N4	49:t:46:ASN:OD1	2.39	0.42
6:C:966:G:O2'	45:p:129:LYS:O	2.38	0.42
10:G:94:VAL:HG11	10:G:96:MET:HE2	2.01	0.42
12:I:76:C:O2'	36:g:55:THR:HG21	2.20	0.42
12:I:2751:G:OP1	12:I:2751:G:N2	2.46	0.42
36:g:8:GLU:OE1	36:g:8:GLU:C	2.63	0.42
6:C:946:A:O2'	6:C:1333:A:N3	2.49	0.41
32:c:98:SER:O	32:c:99:ASN:CG	2.62	0.41
39:j:6:ARG:NH1	39:j:24:THR:O	2.53	0.41
39:j:10:LYS:HB3	39:j:53:LYS:N	2.35	0.41
43:n:67:GLU:OE2	43:n:67:GLU:O	2.38	0.41
45:p:22:LYS:NZ	45:p:22:LYS:HB3	2.36	0.41
6:C:404:G:O6	9:F:2:ALA:N	2.54	0.41
8:E:5:VAL:HG11	8:E:10:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:646:U:H3'	12:I:647:G:C5'	2.50	0.41
12:I:1754:A:O2'	12:I:1755:A:P	2.78	0.41
12:I:1799:G:O2'	14:K:180:GLU:OE2	2.22	0.41
12:I:1813:G:O2'	12:I:1814:G:P	2.78	0.41
18:O:24:ILE:HG21	18:O:72:LEU:CD2	2.46	0.41
6:C:686:U:O2'	6:C:687:A:OP2	2.34	0.41
6:C:796:C:O3'	47:r:127:ARG:NH1	2.54	0.41
6:C:825:A:O2'	44:o:9:ASP:OD1	2.29	0.41
16:M:122:GLU:HG2	16:M:123:LYS:HD3	2.03	0.41
22:S:17:ARG:N	22:S:17:ARG:HD2	2.35	0.41
49:t:80:ILE:C	49:t:80:ILE:HD12	2.45	0.41
53:x:45:GLU:C	53:x:45:GLU:OE2	2.62	0.41
1:1:65:GLU:OE1	1:1:65:GLU:HA	2.21	0.41
19:P:4:ILE:HD11	19:P:37:VAL:CG2	2.50	0.41
19:P:41:LYS:H	19:P:41:LYS:HE2	1.84	0.41
32:c:83:VAL:HG11	32:c:94:ARG:HG2	2.02	0.41
12:I:1754:A:C2'	12:I:1755:A:O5'	2.69	0.41
23:T:55:MET:O	23:T:60:ARG:NH1	2.50	0.41
27:X:30:VAL:HG23	27:X:80:VAL:HG12	2.02	0.41
8:E:35:SER:HG	8:E:59:ARG:HH12	1.68	0.41
12:I:2660:A:HO2'	12:I:2661:G:P	2.38	0.41
18:O:101:ASN:OD1	18:O:116:GLN:NE2	2.46	0.41
19:P:99:ILE:HD12	19:P:99:ILE:H	1.85	0.41
19:P:132:PHE:N	19:P:140:ALA:O	2.49	0.41
24:U:47:GLU:CD	24:U:47:GLU:C	2.88	0.41
27:X:111:LYS:NZ	27:X:111:LYS:HB3	2.36	0.41
51:v:42:TRP:HB2	51:v:46:LEU:HD23	2.01	0.41
53:x:4:ILE:N	53:x:4:ILE:HD12	2.35	0.41
5:A:41:C:O2	5:A:41:C:O5'	2.39	0.41
6:C:328:C:O2	6:C:328:C:O2'	2.35	0.41
11:H:18:VAL:N	11:H:19:PRO:HD2	2.36	0.41
12:I:2756:U:H4'	12:I:2757:A:OP1	2.21	0.41
14:K:133:ARG:CZ	19:P:123:ARG:NH2	2.83	0.41
18:O:81:GLU:OE2	18:O:81:GLU:HA	2.21	0.41
51:v:28:LYS:O	51:v:32:SER:OG	2.31	0.41
1:1:13:LEU:HD21	51:v:47:LYS:HG2	2.03	0.41
12:I:2543:G:HO2'	12:I:2544:G:P	2.43	0.41
18:O:60:ASP:OD1	18:O:60:ASP:N	2.48	0.41
18:O:153:ARG:HG2	18:O:153:ARG:HH11	1.85	0.41
34:e:17:GLU:O	34:e:19:LYS:NZ	2.54	0.41
54:y:20:SER:OG	54:y:71:LYS:NZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:2:PRO:N	55:z:72:ASP:OD2	2.54	0.41
9:F:121:LYS:O	9:F:146:ARG:NH1	2.47	0.41
12:I:971:G:O2'	12:I:983:A:N3	2.48	0.41
12:I:1629:U:O4	12:I:1630:A:N6	2.54	0.41
22:S:122:VAL:O	22:S:122:VAL:HG23	2.21	0.41
51:v:90:ARG:HG3	51:v:92:GLU:OE2	2.21	0.41
7:D:82:ASP:OD2	7:D:82:ASP:N	2.53	0.40
7:D:151:ILE:O	7:D:151:ILE:HG23	2.21	0.40
12:I:504:A:C4'	12:I:505:A:OP2	2.69	0.40
12:I:2011:U:OP1	30:a:42:LYS:NZ	2.46	0.40
12:I:2623:G:OP1	12:I:2826:A:O2'	2.22	0.40
14:K:84:ASP:OD2	14:K:87:ARG:NE	2.50	0.40
21:R:131:ASN:OD1	21:R:131:ASN:N	2.53	0.40
30:a:74:ILE:HD12	30:a:105:VAL:HG22	2.03	0.40
43:n:48:GLU:O	43:n:48:GLU:OE1	2.38	0.40
44:o:118:GLN:HA	44:o:118:GLN:OE1	2.21	0.40
54:y:80:GLU:N	54:y:80:GLU:CD	2.79	0.40
5:A:63:G:H2'	5:A:64:A:O4'	2.21	0.40
6:C:523:A:H61	49:t:89:ASP:HB2	1.86	0.40
23:T:91:ASP:OD1	23:T:94:THR:OG1	2.30	0.40
1:1:13:LEU:HD21	51:v:47:LYS:CG	2.51	0.40
6:C:1081:A:OP2	10:G:52:LYS:NZ	2.52	0.40
7:D:13:GLY:O	7:D:14:VAL:CG1	2.66	0.40
12:I:87:U:H4'	12:I:88:G:OP2	2.21	0.40
12:I:243:U:OP2	41:l:8:ARG:NH1	2.55	0.40
12:I:910:A:N3	12:I:2264:C:O2'	2.45	0.40
12:I:2104:C:N4	12:I:2184:A:H61	2.19	0.40
17:N:112:ARG:C	17:N:113:ASP:OD2	2.63	0.40
32:c:83:VAL:HG12	32:c:84:GLY:N	2.37	0.40
6:C:667:G:O2'	52:w:49:ASP:OD1	2.34	0.40
7:D:44:GLU:OE2	7:D:44:GLU:HA	2.22	0.40
12:I:1044:C:O2'	12:I:1111:A:N1	2.50	0.40
12:I:2286:G:H5'	39:j:10:LYS:HD3	2.03	0.40
12:I:2357:G:N2	12:I:2360:G:OP2	2.44	0.40
12:I:2447:G:H1'	12:I:2448:A:OP2	2.20	0.40
15:L:12:THR:CG2	15:L:13:ARG:N	2.84	0.40
47:r:56:ARG:NH1	47:r:56:ARG:CB	2.85	0.40
54:y:8:LEU:HD12	54:y:8:LEU:O	2.21	0.40
2:2:39:ILE:HD11	2:2:83:ILE:HD11	2.04	0.40
6:C:816:A:OP1	6:C:1526:G:O2'	2.33	0.40
31:b:13:ALA:HB1	36:g:33:ALA:HB1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:78:SER:O	31:b:80:TRP:NE1	2.55	0.40
35:f:59:ILE:O	35:f:63:GLY:N	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
2	2	83/87 (95%)	79 (95%)	4 (5%)	0	100	100
3	3	68/71 (96%)	68 (100%)	0	0	100	100
7	D	216/241 (90%)	209 (97%)	6 (3%)	1 (0%)	24	40
8	E	204/233 (88%)	199 (98%)	5 (2%)	0	100	100
9	F	203/206 (98%)	196 (97%)	6 (3%)	1 (0%)	24	40
10	G	148/167 (89%)	142 (96%)	6 (4%)	0	100	100
11	H	98/135 (73%)	96 (98%)	2 (2%)	0	100	100
14	K	271/273 (99%)	260 (96%)	11 (4%)	0	100	100
15	L	207/209 (99%)	200 (97%)	7 (3%)	0	100	100
16	M	199/201 (99%)	198 (100%)	1 (0%)	0	100	100
17	N	175/179 (98%)	172 (98%)	3 (2%)	0	100	100
18	O	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
19	P	147/149 (99%)	139 (95%)	8 (5%)	0	100	100
20	Q	56/70 (80%)	55 (98%)	1 (2%)	0	100	100
21	R	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
22	S	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
23	T	142/144 (99%)	140 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	U	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
25	V	118/127 (93%)	118 (100%)	0	0	100	100
26	W	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
27	X	112/115 (97%)	112 (100%)	0	0	100	100
28	Y	115/118 (98%)	115 (100%)	0	0	100	100
29	Z	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
30	a	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
31	b	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
32	c	100/104 (96%)	99 (99%)	1 (1%)	0	100	100
33	d	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
34	e	73/85 (86%)	73 (100%)	0	0	100	100
35	f	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
36	g	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
37	h	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
38	i	54/57 (95%)	54 (100%)	0	0	100	100
39	j	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
40	k	44/46 (96%)	44 (100%)	0	0	100	100
41	l	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
42	m	36/38 (95%)	36 (100%)	0	0	100	100
43	n	149/179 (83%)	148 (99%)	1 (1%)	0	100	100
44	o	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
45	p	125/130 (96%)	120 (96%)	4 (3%)	1 (1%)	16	28
46	q	96/103 (93%)	89 (93%)	6 (6%)	1 (1%)	12	22
47	r	115/129 (89%)	113 (98%)	2 (2%)	0	100	100
48	s	3/5 (60%)	3 (100%)	0	0	100	100
49	t	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
50	u	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
51	v	92/101 (91%)	90 (98%)	2 (2%)	0	100	100
52	w	86/89 (97%)	86 (100%)	0	0	100	100
53	x	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
54	y	78/84 (93%)	76 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	z	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
All	All	5558/5918 (94%)	5429 (98%)	125 (2%)	4 (0%)	49	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	F	28	ILE
45	p	55	VAL
46	q	57	VAL
7	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%)	70 (100%)	0	100	100
2	2	65/66 (98%)	63 (97%)	2 (3%)	35	60
3	3	60/61 (98%)	60 (100%)	0	100	100
7	D	180/199 (90%)	177 (98%)	3 (2%)	53	75
8	E	170/190 (90%)	169 (99%)	1 (1%)	78	90
9	F	172/173 (99%)	171 (99%)	1 (1%)	78	90
10	G	113/126 (90%)	111 (98%)	2 (2%)	51	74
11	H	87/116 (75%)	87 (100%)	0	100	100
14	K	218/218 (100%)	218 (100%)	0	100	100
15	L	164/164 (100%)	163 (99%)	1 (1%)	78	90
16	M	165/165 (100%)	161 (98%)	4 (2%)	43	67
17	N	148/150 (99%)	145 (98%)	3 (2%)	48	72
18	O	137/138 (99%)	135 (98%)	2 (2%)	57	78
19	P	114/114 (100%)	112 (98%)	2 (2%)	51	74
20	Q	55/62 (89%)	54 (98%)	1 (2%)	51	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	R	116/116 (100%)	116 (100%)	0	100	100
22	S	103/104 (99%)	102 (99%)	1 (1%)	68	84
23	T	103/103 (100%)	103 (100%)	0	100	100
24	U	108/108 (100%)	108 (100%)	0	100	100
25	V	100/103 (97%)	99 (99%)	1 (1%)	68	84
26	W	86/87 (99%)	86 (100%)	0	100	100
27	X	99/100 (99%)	98 (99%)	1 (1%)	68	84
28	Y	89/90 (99%)	89 (100%)	0	100	100
29	Z	84/84 (100%)	83 (99%)	1 (1%)	63	81
30	a	93/93 (100%)	91 (98%)	2 (2%)	45	70
31	b	80/84 (95%)	79 (99%)	1 (1%)	61	80
32	c	83/85 (98%)	82 (99%)	1 (1%)	63	81
33	d	78/78 (100%)	78 (100%)	0	100	100
34	e	57/63 (90%)	57 (100%)	0	100	100
35	f	67/68 (98%)	67 (100%)	0	100	100
36	g	54/55 (98%)	54 (100%)	0	100	100
37	h	48/49 (98%)	47 (98%)	1 (2%)	47	71
38	i	47/48 (98%)	47 (100%)	0	100	100
39	j	45/49 (92%)	44 (98%)	1 (2%)	45	70
40	k	38/38 (100%)	38 (100%)	0	100	100
41	l	51/52 (98%)	51 (100%)	0	100	100
42	m	34/34 (100%)	34 (100%)	0	100	100
43	n	124/147 (84%)	123 (99%)	1 (1%)	73	87
44	o	104/105 (99%)	103 (99%)	1 (1%)	68	84
45	p	105/107 (98%)	104 (99%)	1 (1%)	68	84
46	q	86/90 (96%)	85 (99%)	1 (1%)	63	81
47	r	90/99 (91%)	89 (99%)	1 (1%)	65	83
48	s	4/4 (100%)	4 (100%)	0	100	100
49	t	103/104 (99%)	102 (99%)	1 (1%)	68	84
50	u	93/96 (97%)	92 (99%)	1 (1%)	65	83
51	v	79/84 (94%)	78 (99%)	1 (1%)	61	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	w	75/77 (97%)	75 (100%)	0	100	100
53	x	65/65 (100%)	64 (98%)	1 (2%)	57	78
54	y	74/78 (95%)	74 (100%)	0	100	100
55	z	48/65 (74%)	48 (100%)	0	100	100
All	All	4631/4833 (96%)	4590 (99%)	41 (1%)	68	86

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	6	SER
2	2	66	LEU
7	D	56	GLU
7	D	121	SER
7	D	199	VAL
8	E	35	SER
9	F	53	VAL
10	G	111	MET
10	G	120	VAL
15	L	110	THR
16	M	3	LEU
16	M	75	SER
16	M	165	HIS
16	M	198	GLU
17	N	37	ASN
17	N	51	ASP
17	N	74	VAL
18	O	48	ASN
18	O	114	ASP
19	P	14	SER
19	P	143	ILE
20	Q	20	ASN
22	S	75	SER
25	V	65	LEU
27	X	7	GLN
29	Z	20	VAL
30	a	30	SER
30	a	68	ASP
31	b	89	GLU
32	c	29	LEU
37	h	4	THR
39	j	14	SER

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Mol	Chain	Res	Type
43	n	72	THR
44	o	67	GLN
45	p	126	GLN
46	q	5	ARG
47	r	30	THR
49	t	87	VAL
50	u	20	THR
51	v	47	LYS
53	x	50	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
3	3	56	HIS
7	D	39	HIS
8	E	41	GLN
9	F	136	GLN
10	G	43	ASN
10	G	61	GLN
11	H	52	ASN
14	K	53	HIS
14	K	90	ASN
14	K	163	GLN
14	K	243	HIS
15	L	126	ASN
16	M	9	GLN
16	M	92	HIS
17	N	63	GLN
19	P	28	ASN
21	R	132	HIS
21	R	138	GLN
25	V	9	GLN
28	Y	59	GLN
30	a	9	HIS
31	b	59	ASN
32	c	27	ASN
35	f	36	HIS
36	g	27	ASN
36	g	31	GLN
36	g	41	HIS
39	j	46	HIS
43	n	148	ASN

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Mol	Chain	Res	Type
44	o	67	GLN
45	p	50	GLN
47	r	24	HIS
47	r	64	GLN
51	v	35	ASN
53	x	59	HIS
55	z	54	GLN
55	z	74	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	I	2896/2904 (99%)	352 (12%)	30 (1%)
13	J	117/120 (97%)	11 (9%)	0
4	4	5/15 (33%)	0	0
5	A	75/76 (98%)	17 (22%)	3 (4%)
6	C	1539/1540 (99%)	175 (11%)	9 (0%)
All	All	4632/4655 (99%)	555 (11%)	42 (0%)

All (555) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	3	C
5	A	5	G
5	A	11	C
5	A	17	A
5	A	18	G
5	A	20	U
5	A	21	A
5	A	22	G
5	A	43	C
5	A	47	U
5	A	54	U
5	A	58	A
5	A	61	C
5	A	62	C
5	A	63	G
5	A	68	C
5	A	76	A
6	C	4	U
6	C	9	G

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Mol	Chain	Res	Type
6	C	32	A
6	C	39	G
6	C	47	C
6	C	48	C
6	C	51	A
6	C	70	U
6	C	74	A
6	C	83	C
6	C	85	U
6	C	87	C
6	C	95	C
6	C	97	G
6	C	108	G
6	C	116	A
6	C	120	A
6	C	121	U
6	C	130	A
6	C	131	A
6	C	144	G
6	C	182	A
6	C	207	C
6	C	208	U
6	C	209	U
6	C	210	C
6	C	211	G
6	C	213	G
6	C	245	U
6	C	247	G
6	C	251	G
6	C	266	G
6	C	267	C
6	C	279	A
6	C	280	C
6	C	289	G
6	C	328	C
6	C	329	A
6	C	332	G
6	C	352	C
6	C	354	G
6	C	367	U
6	C	372	C
6	C	406	G

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Mol	Chain	Res	Type
6	C	412	A
6	C	413	G
6	C	421	U
6	C	422	C
6	C	424	G
6	C	429	U
6	C	439	U
6	C	459	A
6	C	467	U
6	C	468	A
6	C	478	A
6	C	479	U
6	C	485	U
6	C	497	G
6	C	511	C
6	C	518	C
6	C	527	G
6	C	532	A
6	C	533	A
6	C	547	A
6	C	564	C
6	C	572	A
6	C	573	A
6	C	576	C
6	C	577	G
6	C	650	G
6	C	653	U
6	C	665	A
6	C	687	A
6	C	721	G
6	C	723	U
6	C	731	G
6	C	747	A
6	C	755	G
6	C	793	U
6	C	794	A
6	C	815	A
6	C	817	C
6	C	828	U
6	C	829	G
6	C	841	C
6	C	842	U

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Mol	Chain	Res	Type
6	C	843	U
6	C	844	G
6	C	845	A
6	C	846	G
6	C	847	G
6	C	885	G
6	C	914	A
6	C	926	G
6	C	934	C
6	C	935	A
6	C	960	U
6	C	969	A
6	C	975	A
6	C	976	G
6	C	977	A
6	C	983	A
6	C	993	G
6	C	1004	A
6	C	1008	U
6	C	1030	U
6	C	1032	G
6	C	1033	G
6	C	1034	G
6	C	1043	G
6	C	1048	G
6	C	1054	C
6	C	1065	U
6	C	1085	U
6	C	1094	G
6	C	1095	U
6	C	1101	A
6	C	1133	G
6	C	1134	G
6	C	1136	C
6	C	1137	C
6	C	1139	G
6	C	1140	C
6	C	1141	C
6	C	1142	G
6	C	1145	A
6	C	1146	A
6	C	1159	U

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Mol	Chain	Res	Type
6	C	1167	A
6	C	1196	A
6	C	1197	A
6	C	1202	U
6	C	1212	U
6	C	1213	A
6	C	1227	A
6	C	1238	A
6	C	1240	U
6	C	1241	G
6	C	1275	A
6	C	1280	A
6	C	1286	U
6	C	1287	A
6	C	1293	C
6	C	1299	A
6	C	1300	G
6	C	1302	C
6	C	1305	G
6	C	1317	C
6	C	1318	A
6	C	1320	C
6	C	1337	G
6	C	1346	A
6	C	1353	G
6	C	1362	A
6	C	1364	U
6	C	1378	C
6	C	1398	A
6	C	1419	G
6	C	1446	A
6	C	1452	C
6	C	1492	A
6	C	1493	A
6	C	1494	G
6	C	1497	G
6	C	1503	A
6	C	1506	U
6	C	1517	G
6	C	1529	G
6	C	1530	G
6	C	1533	C

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Mol	Chain	Res	Type
6	C	1534	A
6	C	1537	U
6	C	1538	C
6	C	1539	C
6	C	1540	U
12	I	10	A
12	I	26	G
12	I	34	U
12	I	42	A
12	I	45	G
12	I	46	G
12	I	51	G
12	I	63	A
12	I	71	A
12	I	72	U
12	I	74	A
12	I	75	G
12	I	88	G
12	I	101	A
12	I	102	U
12	I	110	G
12	I	118	A
12	I	120	U
12	I	137	U
12	I	139	U
12	I	163	C
12	I	174	U
12	I	183	C
12	I	196	A
12	I	199	A
12	I	209	C
12	I	216	A
12	I	220	G
12	I	221	A
12	I	222	A
12	I	228	C
12	I	236	C
12	I	238	C
12	I	240	C
12	I	248	G
12	I	266	G
12	I	272	A

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Mol	Chain	Res	Type
12	I	276	U
12	I	302	C
12	I	307	G
12	I	309	A
12	I	311	A
12	I	329	G
12	I	330	A
12	I	345	A
12	I	353	C
12	I	361	G
12	I	362	A
12	I	371	A
12	I	372	G
12	I	376	G
12	I	379	G
12	I	386	G
12	I	391	A
12	I	396	G
12	I	404	A
12	I	405	U
12	I	411	G
12	I	437	U
12	I	443	A
12	I	456	C
12	I	457	A
12	I	475	C
12	I	481	G
12	I	491	G
12	I	504	A
12	I	505	A
12	I	509	C
12	I	532	A
12	I	533	G
12	I	546	U
12	I	548	G
12	I	549	G
12	I	556	A
12	I	562	U
12	I	563	A
12	I	573	U
12	I	575	A
12	I	587	C

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Mol	Chain	Res	Type
12	I	603	A
12	I	607	U
12	I	614	A
12	I	616	A
12	I	627	A
12	I	637	A
12	I	647	G
12	I	654	A
12	I	655	A
12	I	686	U
12	I	730	A
12	I	747	5MU
12	I	765	C
12	I	775	G
12	I	776	G
12	I	782	A
12	I	784	G
12	I	785	G
12	I	805	G
12	I	812	C
12	I	819	A
12	I	827	U
12	I	828	U
12	I	845	A
12	I	846	U
12	I	847	U
12	I	858	G
12	I	859	G
12	I	896	A
12	I	897	C
12	I	910	A
12	I	914	G
12	I	915	C
12	I	931	U
12	I	941	A
12	I	946	C
12	I	961	C
12	I	974	G
12	I	983	A
12	I	996	A
12	I	1012	U
12	I	1013	C

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Mol	Chain	Res	Type
12	I	1022	G
12	I	1025	G
12	I	1026	G
12	I	1033	U
12	I	1046	A
12	I	1047	G
12	I	1070	A
12	I	1071	G
12	I	1080	A
12	I	1088	A
12	I	1111	A
12	I	1112	G
12	I	1116	G
12	I	1132	U
12	I	1133	A
12	I	1135	C
12	I	1142	A
12	I	1150	C
12	I	1151	A
12	I	1173	U
12	I	1174	U
12	I	1175	A
12	I	1180	U
12	I	1206	G
12	I	1238	G
12	I	1250	G
12	I	1253	A
12	I	1256	G
12	I	1266	G
12	I	1271	G
12	I	1272	A
12	I	1300	G
12	I	1301	A
12	I	1314	C
12	I	1340	U
12	I	1352	U
12	I	1353	A
12	I	1365	A
12	I	1368	G
12	I	1379	U
12	I	1383	A
12	I	1386	C

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Mol	Chain	Res	Type
12	I	1416	G
12	I	1419	A
12	I	1428	C
12	I	1452	G
12	I	1461	C
12	I	1482	G
12	I	1493	C
12	I	1494	A
12	I	1506	U
12	I	1508	A
12	I	1510	G
12	I	1515	A
12	I	1534	U
12	I	1535	A
12	I	1536	C
12	I	1569	A
12	I	1578	U
12	I	1583	A
12	I	1608	A
12	I	1610	A
12	I	1618	6MZ
12	I	1646	C
12	I	1647	U
12	I	1648	U
12	I	1649	G
12	I	1674	G
12	I	1684	G
12	I	1692	U
12	I	1696	G
12	I	1699	G
12	I	1715	G
12	I	1729	U
12	I	1730	C
12	I	1738	G
12	I	1755	A
12	I	1758	U
12	I	1763	G
12	I	1764	C
12	I	1773	A
12	I	1791	A
12	I	1800	C
12	I	1801	A

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Mol	Chain	Res	Type
12	I	1808	A
12	I	1814	G
12	I	1816	C
12	I	1829	A
12	I	1847	A
12	I	1848	A
12	I	1869	G
12	I	1870	C
12	I	1872	A
12	I	1906	G
12	I	1909	C
12	I	1913	A
12	I	1914	C
12	I	1915	3TD
12	I	1929	G
12	I	1930	G
12	I	1936	A
12	I	1938	A
12	I	1955	U
12	I	1967	C
12	I	1970	A
12	I	1971	U
12	I	1972	G
12	I	1982	U
12	I	1991	U
12	I	1992	G
12	I	1993	U
12	I	1997	C
12	I	2022	U
12	I	2023	C
12	I	2030	6MZ
12	I	2031	A
12	I	2033	A
12	I	2043	C
12	I	2055	C
12	I	2056	G
12	I	2060	A
12	I	2061	G
12	I	2062	A
12	I	2069	G7M
12	I	2093	G
12	I	2111	U

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Mol	Chain	Res	Type
12	I	2112	G
12	I	2113	U
12	I	2115	G
12	I	2116	G
12	I	2117	A
12	I	2118	U
12	I	2119	A
12	I	2126	A
12	I	2128	G
12	I	2131	U
12	I	2132	U
12	I	2133	G
12	I	2134	A
12	I	2159	G
12	I	2160	C
12	I	2161	C
12	I	2163	A
12	I	2164	C
12	I	2165	C
12	I	2167	U
12	I	2169	A
12	I	2170	A
12	I	2171	A
12	I	2172	U
12	I	2177	C
12	I	2178	C
12	I	2181	U
12	I	2198	A
12	I	2204	G
12	I	2211	A
12	I	2225	A
12	I	2226	C
12	I	2238	G
12	I	2239	G
12	I	2283	C
12	I	2287	A
12	I	2297	A
12	I	2305	U
12	I	2322	A
12	I	2325	G
12	I	2333	A
12	I	2344	U

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Mol	Chain	Res	Type
12	I	2345	G
12	I	2347	C
12	I	2350	C
12	I	2361	G
12	I	2371	G
12	I	2383	G
12	I	2385	C
12	I	2403	C
12	I	2423	U
12	I	2425	A
12	I	2426	A
12	I	2428	G
12	I	2429	G
12	I	2430	A
12	I	2441	U
12	I	2448	A
12	I	2475	C
12	I	2476	A
12	I	2491	U
12	I	2498	OMC
12	I	2502	G
12	I	2504	PSU
12	I	2505	G
12	I	2518	A
12	I	2544	G
12	I	2547	A
12	I	2554	U
12	I	2566	A
12	I	2567	G
12	I	2572	A
12	I	2602	A
12	I	2605	PSU
12	I	2609	U
12	I	2613	U
12	I	2615	U
12	I	2661	G
12	I	2681	C
12	I	2682	A
12	I	2689	U
12	I	2690	U
12	I	2714	G
12	I	2718	G

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Mol	Chain	Res	Type
12	I	2726	A
12	I	2729	G
12	I	2744	G
12	I	2748	A
12	I	2765	A
12	I	2766	A
12	I	2778	A
12	I	2780	G
12	I	2781	A
12	I	2791	G
12	I	2793	C
12	I	2797	U
12	I	2800	A
12	I	2820	A
12	I	2855	C
12	I	2867	G
12	I	2880	C
12	I	2883	A
12	I	2884	U
12	I	2885	G
12	I	2887	A
13	J	15	A
13	J	25	U
13	J	32	U
13	J	35	C
13	J	56	G
13	J	88	C
13	J	89	U
13	J	90	C
13	J	99	A
13	J	109	A
13	J	119	A

All (42) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	10	G
5	A	21	A
5	A	61	C
6	C	96	U
6	C	115	G
6	C	206	C

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Mol	Chain	Res	Type
6	C	212	G
6	C	846	G
6	C	1145	A
6	C	1201	A
6	C	1317	C
6	C	1491	G
12	I	25	U
12	I	87	U
12	I	138	U
12	I	182	A
12	I	271	G
12	I	404	A
12	I	504	A
12	I	547	A
12	I	548	G
12	I	555	G
12	I	784	G
12	I	1025	G
12	I	1079	C
12	I	1352	U
12	I	1754	A
12	I	1813	G
12	I	1846	G
12	I	1847	A
12	I	1913	A
12	I	2127	G
12	I	2158	A
12	I	2159	G
12	I	2225	A
12	I	2425	A
12	I	2447	G
12	I	2506	U
12	I	2543	G
12	I	2660	A
12	I	2680	U
12	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$
12	PSU	I	2457	12	18,21,22	0.93	0	21,30,33	2.01	4 (19%)
12	3TD	I	1915	12	19,22,23	1.09	2 (10%)	23,32,35	1.88	2 (8%)
12	PSU	I	746	12,56	18,21,22	0.97	1 (5%)	21,30,33	1.89	4 (19%)
12	2MG	I	2445	12	23,26,27	0.77	0	33,38,41	2.19	11 (33%)
12	PSU	I	2604	12	18,21,22	0.92	1 (5%)	21,30,33	1.98	4 (19%)
12	6MZ	I	1618	12	22,25,26	1.09	1 (4%)	29,36,39	2.19	9 (31%)
12	1MG	I	745	12	23,26,27	0.91	2 (8%)	33,39,42	1.77	6 (18%)
12	OMU	I	2552	12	19,22,23	0.95	2 (10%)	25,31,34	1.95	6 (24%)
12	OMC	I	2498	12,56	19,22,23	0.89	1 (5%)	25,31,34	0.96	1 (4%)
12	PSU	I	955	12	18,21,22	0.93	0	21,30,33	1.98	4 (19%)
12	2MG	I	1835	12	23,26,27	0.76	0	33,38,41	2.17	10 (30%)
12	H2U	I	2449	12	18,21,22	0.43	0	19,30,33	0.68	0
12	PSU	I	1911	12	18,21,22	0.90	0	21,30,33	1.98	4 (19%)
12	PSU	I	2580	12,56	18,21,22	0.97	0	21,30,33	2.00	5 (23%)
12	G7M	I	2069	12	23,26,27	0.54	0	34,39,42	0.91	2 (5%)
12	5MC	I	1962	12	19,22,23	1.22	2 (10%)	26,32,35	1.10	3 (11%)
12	OMG	I	2251	12,5	23,26,27	0.73	0	32,38,41	1.96	10 (31%)
12	5MU	I	1939	12	19,22,23	1.04	2 (10%)	27,32,35	2.10	6 (22%)
12	PSU	I	2504	12,56	18,21,22	0.90	0	21,30,33	1.99	4 (19%)
12	5MU	I	747	12	19,22,23	1.02	2 (10%)	27,32,35	2.13	6 (22%)
24	4D4	U	81	24	9,11,12	2.13	2 (22%)	7,13,15	1.96	3 (42%)
12	6MZ	I	2030	12	22,25,26	1.11	1 (4%)	29,36,39	2.24	9 (31%)
12	PSU	I	2605	12	18,21,22	0.92	1 (5%)	21,30,33	1.96	4 (19%)
12	PSU	I	1917	12	18,21,22	0.90	0	21,30,33	2.00	4 (19%)
12	2MA	I	2503	12,56	22,25,26	1.36	3 (13%)	32,37,40	2.06	8 (25%)

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
12	PSU	I	2457	12	-	0/7/25/26	0/2/2/2
12	3TD	I	1915	12	-	2/7/25/26	0/2/2/2
12	PSU	I	746	12,56	-	1/7/25/26	0/2/2/2
12	2MG	I	2445	12	-	1/9/27/28	0/3/3/3
12	PSU	I	2604	12	-	0/7/25/26	0/2/2/2
12	6MZ	I	1618	12	-	2/9/27/28	0/3/3/3
12	1MG	I	745	12	-	0/7/25/26	0/3/3/3
12	OMU	I	2552	12	-	0/9/27/28	0/2/2/2
12	OMC	I	2498	12,56	-	1/9/27/28	0/2/2/2
12	PSU	I	955	12	-	0/7/25/26	0/2/2/2
12	2MG	I	1835	12	-	0/9/27/28	0/3/3/3
12	H2U	I	2449	12	-	0/7/38/39	0/2/2/2
12	PSU	I	1911	12	-	0/7/25/26	0/2/2/2
12	PSU	I	2580	12,56	-	0/7/25/26	0/2/2/2
12	G7M	I	2069	12	-	0/7/25/26	0/3/3/3
12	5MC	I	1962	12	-	0/7/25/26	0/2/2/2
12	OMG	I	2251	12,5	-	0/9/27/28	0/3/3/3
12	5MU	I	1939	12	-	0/7/25/26	0/2/2/2
12	PSU	I	2504	12,56	-	2/7/25/26	0/2/2/2
12	5MU	I	747	12	-	0/7/25/26	0/2/2/2
24	4D4	U	81	24	-	1/11/12/14	-
12	6MZ	I	2030	12	-	2/9/27/28	0/3/3/3
12	PSU	I	2605	12	-	2/7/25/26	0/2/2/2
12	PSU	I	1917	12	-	0/7/25/26	0/2/2/2
12	2MA	I	2503	12,56	-	2/7/25/26	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	U	81	4D4	CZ-NE	5.32	1.43	1.33
12	I	1962	5MC	C5-C4	-3.93	1.41	1.44
12	I	2503	2MA	C6-N1	3.88	1.40	1.35
12	I	2030	6MZ	C6-N6	3.85	1.38	1.34
12	I	1618	6MZ	C6-N6	3.82	1.38	1.34
12	I	2503	2MA	C5-N7	-2.96	1.33	1.39
24	U	81	4D4	CZ-NH1	2.82	1.44	1.34
12	I	2503	2MA	C5-C6	2.71	1.48	1.41
12	I	2498	OMC	C2-N1	-2.60	1.34	1.40
12	I	1915	3TD	C4-N3	-2.54	1.35	1.40
12	I	747	5MU	C2-N1	-2.46	1.34	1.38
12	I	1962	5MC	C2-N1	-2.44	1.35	1.40
12	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)
12	I	2552	OMU	C2-N1	-2.42	1.34	1.38
12	I	1939	5MU	C2-N1	-2.35	1.34	1.38
12	I	745	1MG	C6-N1	-2.32	1.35	1.40
12	I	1939	5MU	C4-N3	-2.16	1.34	1.38
12	I	746	PSU	O4'-C1'	-2.06	1.41	1.43
12	I	747	5MU	C4-N3	-2.06	1.35	1.38
12	I	2552	OMU	C4-N3	-2.05	1.35	1.38
12	I	745	1MG	C2-N2	2.04	1.37	1.34
12	I	2604	PSU	C4-N3	-2.03	1.35	1.38
12	I	2605	PSU	C4-N3	-2.00	1.35	1.38

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	I	2445	2MG	C2-N3-C4	7.30	121.13	112.00
12	I	1835	2MG	C2-N3-C4	7.29	121.11	112.00
12	I	1915	3TD	N1-C2-N3	6.61	120.94	116.13
12	I	2503	2MA	C5-C4-N3	-6.11	120.74	127.18
12	I	2457	PSU	N1-C2-N3	5.64	121.12	115.17
12	I	2504	PSU	N1-C2-N3	5.63	121.10	115.17
12	I	1917	PSU	N1-C2-N3	5.59	121.07	115.17
12	I	2580	PSU	N1-C2-N3	5.57	121.04	115.17
12	I	2030	6MZ	C5-C4-N3	-5.54	119.09	126.72
12	I	955	PSU	N1-C2-N3	5.54	121.01	115.17
12	I	745	1MG	C5-C4-N3	-5.53	119.58	128.39
12	I	2251	OMG	C5-C4-N3	-5.52	119.61	128.39
12	I	2605	PSU	N1-C2-N3	5.52	120.99	115.17
12	I	2604	PSU	N1-C2-N3	5.51	120.98	115.17
12	I	1618	6MZ	C5-C4-N3	-5.50	119.14	126.72
12	I	1911	PSU	N1-C2-N3	5.50	120.97	115.17
12	I	1835	2MG	C5-C4-N3	-5.47	119.68	128.39
12	I	747	5MU	C4-N3-C2	-5.45	120.20	127.34
12	I	746	PSU	N1-C2-N3	5.44	120.91	115.17
12	I	1939	5MU	C4-N3-C2	-5.38	120.29	127.34
12	I	2445	2MG	C5-C4-N3	-5.36	119.86	128.39
12	I	2552	OMU	C4-N3-C2	-5.22	120.13	126.61
12	I	2251	OMG	C2-N3-C4	5.16	121.19	112.30
12	I	747	5MU	N3-C2-N1	4.89	121.25	114.89
12	I	2503	2MA	N3-C4-N9	4.86	133.15	126.99
12	I	2552	OMU	N3-C2-N1	4.75	121.08	114.89
12	I	1939	5MU	N3-C2-N1	4.74	121.07	114.89
12	I	1939	5MU	C5-C4-N3	4.66	119.38	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	I	2503	2MA	N6-C6-N1	4.66	123.31	117.03
12	I	747	5MU	C5-C4-N3	4.58	119.31	115.32
12	I	2457	PSU	C4-N3-C2	-4.55	120.11	126.37
12	I	1917	PSU	C4-N3-C2	-4.55	120.11	126.37
12	I	1618	6MZ	N3-C4-N9	4.55	134.90	127.17
12	I	2604	PSU	C4-N3-C2	-4.51	120.15	126.37
12	I	2504	PSU	C4-N3-C2	-4.50	120.17	126.37
12	I	2605	PSU	C4-N3-C2	-4.50	120.17	126.37
12	I	955	PSU	C4-N3-C2	-4.49	120.18	126.37
12	I	1911	PSU	C4-N3-C2	-4.49	120.19	126.37
12	I	2580	PSU	C4-N3-C2	-4.47	120.21	126.37
12	I	746	PSU	C4-N3-C2	-4.46	120.22	126.37
12	I	2030	6MZ	N3-C4-N9	4.45	134.74	127.17
12	I	1915	3TD	C4-N3-C2	-4.28	120.08	124.61
12	I	2251	OMG	N9-C4-N3	4.18	134.31	125.95
12	I	745	1MG	C2-N3-C4	4.18	121.37	111.98
12	I	745	1MG	N9-C4-N3	4.15	134.25	125.95
12	I	1835	2MG	N9-C4-N3	4.14	134.23	125.95
12	I	2030	6MZ	N1-C2-N3	-4.05	122.45	128.58
12	I	1618	6MZ	N1-C2-N3	-4.02	122.50	128.58
12	I	1939	5MU	O4-C4-C5	-4.01	120.32	124.92
24	U	81	4D4	NE-CZ-NH2	4.01	127.56	120.67
12	I	2030	6MZ	C5-N7-C8	4.00	109.74	103.45
12	I	747	5MU	O4-C4-C5	-3.99	120.35	124.92
12	I	2445	2MG	N9-C4-N3	3.98	133.92	125.95
12	I	1618	6MZ	C5-N7-C8	3.86	109.52	103.45
12	I	2030	6MZ	C9-N6-C6	-3.65	119.47	122.85
12	I	2030	6MZ	C2-N3-C4	3.63	120.70	111.83
12	I	2503	2MA	C5-N7-C8	3.60	109.11	103.45
12	I	1618	6MZ	C2-N3-C4	3.60	120.62	111.83
12	I	2445	2MG	C2-N1-C6	-3.58	120.22	124.55
12	I	1835	2MG	C2-N1-C6	-3.57	120.23	124.55
12	I	747	5MU	C5-C6-N1	-3.39	119.63	123.31
12	I	1939	5MU	C5-C6-N1	-3.39	119.64	123.31
12	I	2552	OMU	C5-C4-N3	3.33	119.47	114.80
12	I	2504	PSU	O2-C2-N1	-3.25	119.44	122.79
12	I	1618	6MZ	C9-N6-C6	-3.25	119.84	122.85
12	I	1962	5MC	C5-C6-N1	-3.20	119.84	123.31
12	I	2030	6MZ	C4-C5-N7	-3.20	106.93	110.58
12	I	1917	PSU	O2-C2-N1	-3.18	119.51	122.79
12	I	955	PSU	O2-C2-N1	-3.15	119.54	122.79
12	I	2580	PSU	O2-C2-N1	-3.14	119.55	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	I	1911	PSU	O2-C2-N1	-3.12	119.57	122.79
12	I	2457	PSU	O2-C2-N1	-3.12	119.57	122.79
12	I	2069	G7M	C8-N7-C5	-3.12	103.88	107.78
12	I	2503	2MA	C5-C6-N1	-3.10	114.08	118.90
12	I	2552	OMU	CM2-O2'-C2'	-3.09	106.55	114.47
12	I	2604	PSU	O2-C2-N1	-3.06	119.63	122.79
12	I	746	PSU	O2-C2-N1	-3.04	119.66	122.79
12	I	2605	PSU	O2-C2-N1	-3.04	119.66	122.79
12	I	1618	6MZ	C4-C5-N7	-3.03	107.11	110.58
12	I	2030	6MZ	N9-C8-N7	-2.99	109.69	113.94
12	I	2503	2MA	N9-C8-N7	-2.98	109.71	113.94
12	I	1618	6MZ	N9-C8-N7	-2.85	109.89	113.94
12	I	2552	OMU	O4-C4-C5	-2.85	120.25	125.16
12	I	2251	OMG	C8-N7-C5	2.83	109.31	104.26
12	I	745	1MG	C8-N7-C5	2.83	109.31	104.26
12	I	747	5MU	O2-C2-N1	-2.81	119.14	122.80
12	I	2445	2MG	C8-N7-C5	2.79	109.23	104.26
12	I	2445	2MG	N1-C2-N2	2.78	119.40	116.56
12	I	1835	2MG	C8-N7-C5	2.76	109.18	104.26
12	I	2251	OMG	C2-N1-C6	-2.72	120.18	125.11
12	I	2552	OMU	O2-C2-N1	-2.62	119.39	122.80
12	I	2498	OMC	CM2-O2'-C2'	-2.45	108.18	114.47
12	I	2503	2MA	C4-C5-N7	-2.44	107.79	110.58
12	I	2030	6MZ	C6-C5-N7	2.39	135.03	132.43
12	I	1835	2MG	N1-C2-N2	2.34	118.95	116.56
12	I	2504	PSU	C6-N1-C2	-2.34	120.52	122.69
12	I	2580	PSU	C6-N1-C2	-2.32	120.54	122.69
12	I	2457	PSU	C6-N1-C2	-2.31	120.55	122.69
12	I	1917	PSU	C6-N1-C2	-2.30	120.55	122.69
12	I	1962	5MC	C5-C4-N3	-2.29	119.41	121.75
24	U	81	4D4	NH1-CZ-NE	-2.26	114.13	119.27
12	I	955	PSU	C6-N1-C2	-2.25	120.60	122.69
12	I	2605	PSU	C6-N1-C2	-2.24	120.62	122.69
12	I	1911	PSU	C6-N1-C2	-2.23	120.62	122.69
12	I	2604	PSU	C6-N1-C2	-2.22	120.63	122.69
12	I	1962	5MC	O2-C2-N3	-2.22	118.83	122.33
12	I	1835	2MG	O6-C6-C5	-2.18	120.78	126.53
12	I	1618	6MZ	C6-C5-N7	2.17	134.80	132.43
12	I	2445	2MG	C6-C5-N7	2.17	134.24	130.29
12	I	2445	2MG	O6-C6-C5	-2.17	120.80	126.53
12	I	1939	5MU	O2-C2-N1	-2.17	119.97	122.80
12	I	746	PSU	C6-N1-C2	-2.17	120.68	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	I	745	1MG	C4-C5-N7	-2.16	107.24	110.67
24	U	81	4D4	O-C-CA	-2.14	119.25	124.77
12	I	2580	PSU	O4'-C1'-C2'	2.14	108.11	105.15
12	I	2251	OMG	O6-C6-C5	-2.13	120.90	126.53
12	I	2445	2MG	C4-C5-N7	-2.13	107.29	110.67
12	I	2251	OMG	C4-C5-N7	-2.13	107.29	110.67
12	I	745	1MG	C6-C5-N7	2.13	134.09	129.36
12	I	2251	OMG	C6-C5-N7	2.09	134.10	130.29
12	I	2251	OMG	CM2-O2'-C2'	-2.09	109.12	114.47
12	I	2069	G7M	CN7-N7-C8	2.08	127.95	124.79
12	I	1835	2MG	C4-C5-N7	-2.08	107.38	110.67
12	I	2503	2MA	C2-N1-C6	2.06	121.27	118.10
12	I	1835	2MG	C6-C5-N7	2.04	134.00	130.29
12	I	1835	2MG	C5-C6-N1	2.03	118.42	113.25
12	I	2445	2MG	C5-C6-N1	2.03	118.42	113.25
12	I	2251	OMG	C5-C6-N1	2.02	118.40	113.25
12	I	2445	2MG	N9-C8-N7	-2.02	109.66	113.40

There are no chirality outliers.

All (16) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	I	2445	2MG	1	0
12	I	2030	6MZ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 212 ligands modelled in this entry, 211 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
57	RD8	I	3114	56	35,35,35	1.32	4 (11%)	45,48,48	1.77	10 (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
57	RD8	I	3114	56	-	0/19/31/31	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	I	3114	RD8	C30-N21	3.72	1.40	1.36
57	I	3114	RD8	O29-C23	-3.18	1.41	1.46
57	I	3114	RD8	C24-C23	3.16	1.55	1.51
57	I	3114	RD8	C13-N17	-2.54	1.31	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	I	3114	RD8	C13-N17-N16	-5.58	103.00	109.01
57	I	3114	RD8	C23-O29-C30	4.55	113.74	110.10
57	I	3114	RD8	C22-N21-C30	-4.02	108.20	111.17
57	I	3114	RD8	C23-C22-N21	3.01	104.69	101.85
57	I	3114	RD8	C22-C23-C24	2.79	116.54	113.38
57	I	3114	RD8	O29-C30-N21	-2.74	107.61	109.92
57	I	3114	RD8	O29-C23-C22	-2.70	101.88	104.50
57	I	3114	RD8	O31-C30-N21	2.52	131.13	128.80
57	I	3114	RD8	C23-C24-N25	2.14	116.25	111.98
57	I	3114	RD8	C24-N25-C26	2.00	125.55	122.64

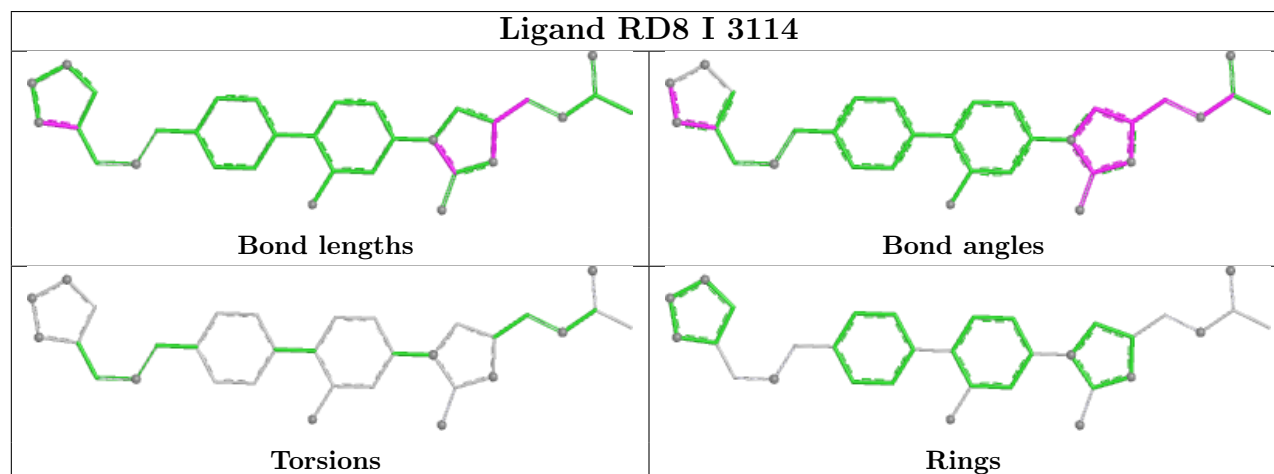
There are no chirality outliers.

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.

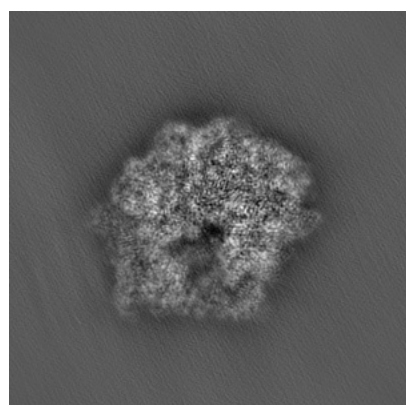
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24802. These allow visual inspection of the internal detail of the map and identification of artifacts.

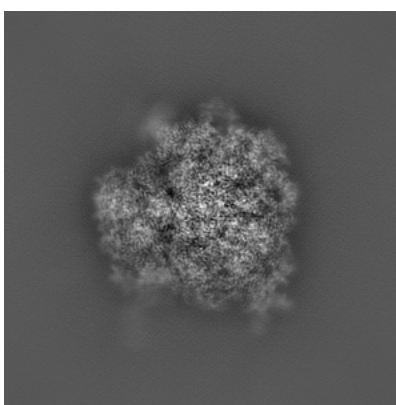
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

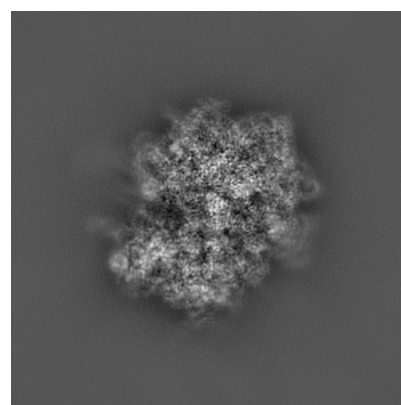
6.1.1 Primary map



X



Y

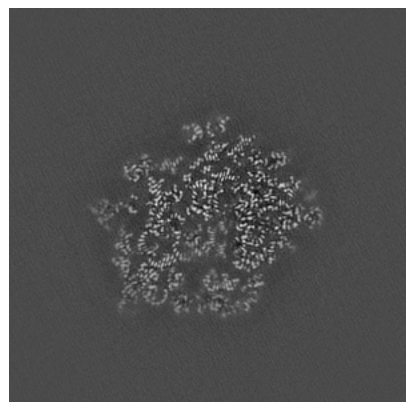


Z

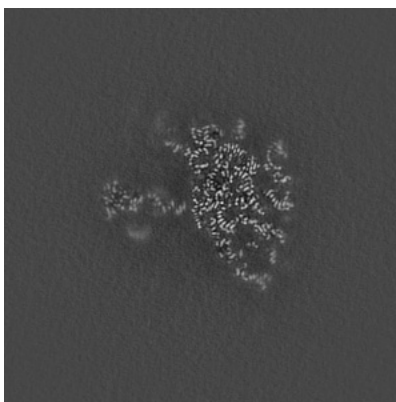
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

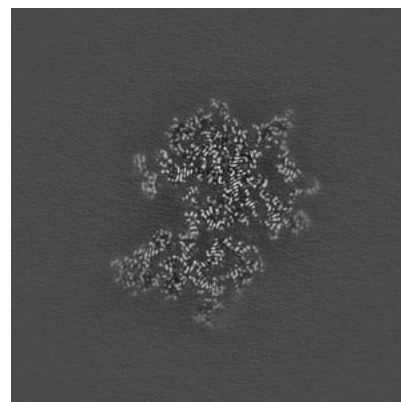
6.2.1 Primary map



X Index: 256



Y Index: 256

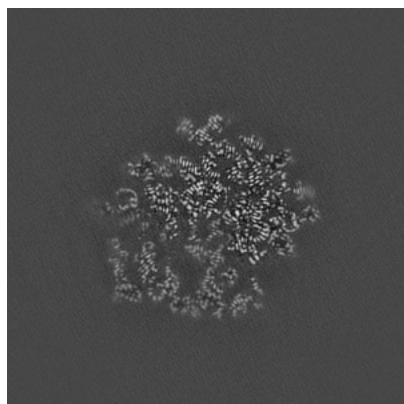


Z Index: 256

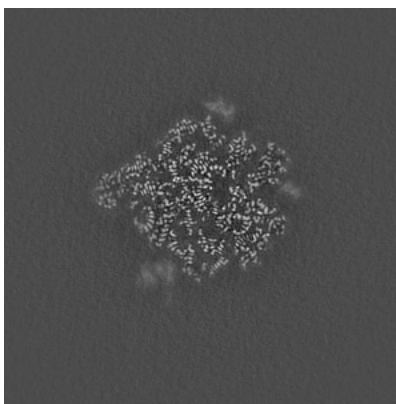
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

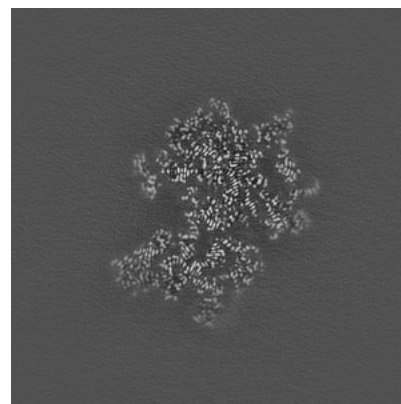
6.3.1 Primary map



X Index: 264



Y Index: 293

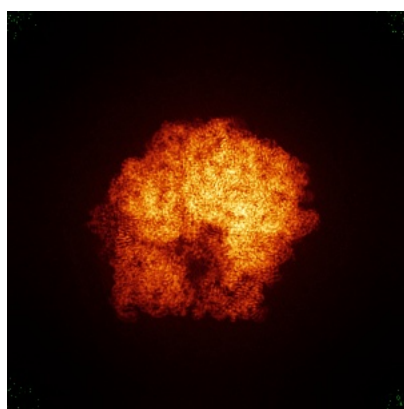


Z Index: 255

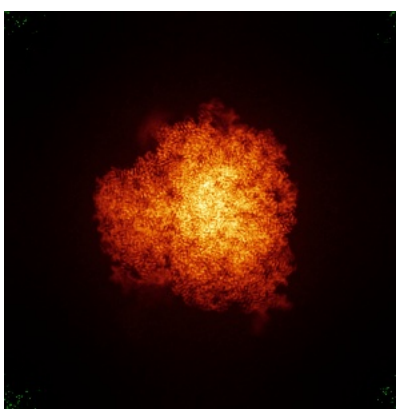
The images above show the largest variance slices of the map in three orthogonal directions.

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

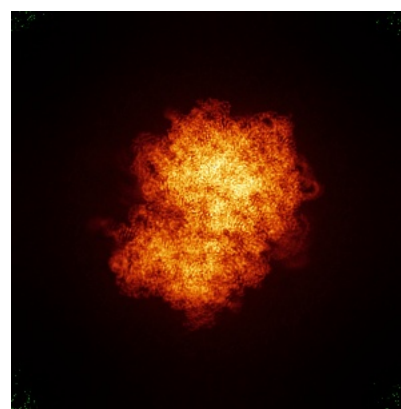
6.4.1 Primary map



X



Y

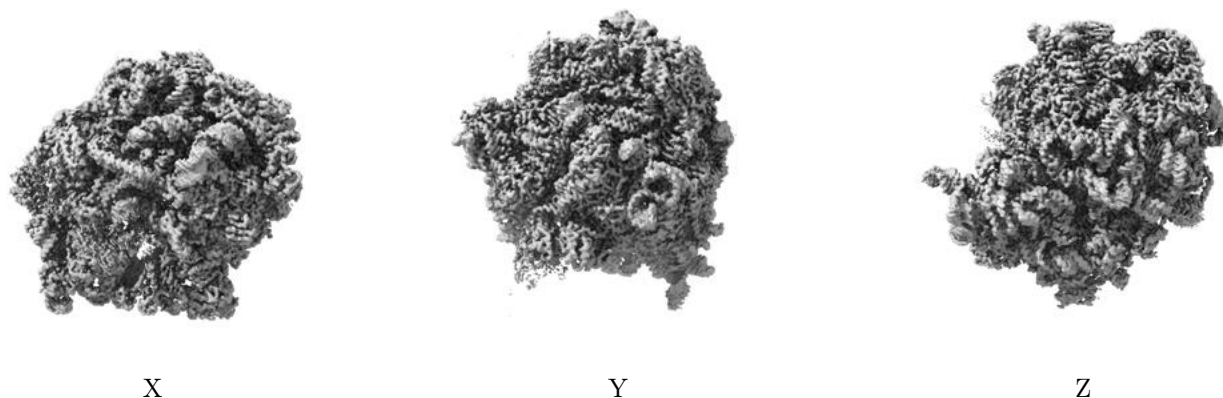


Z

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.

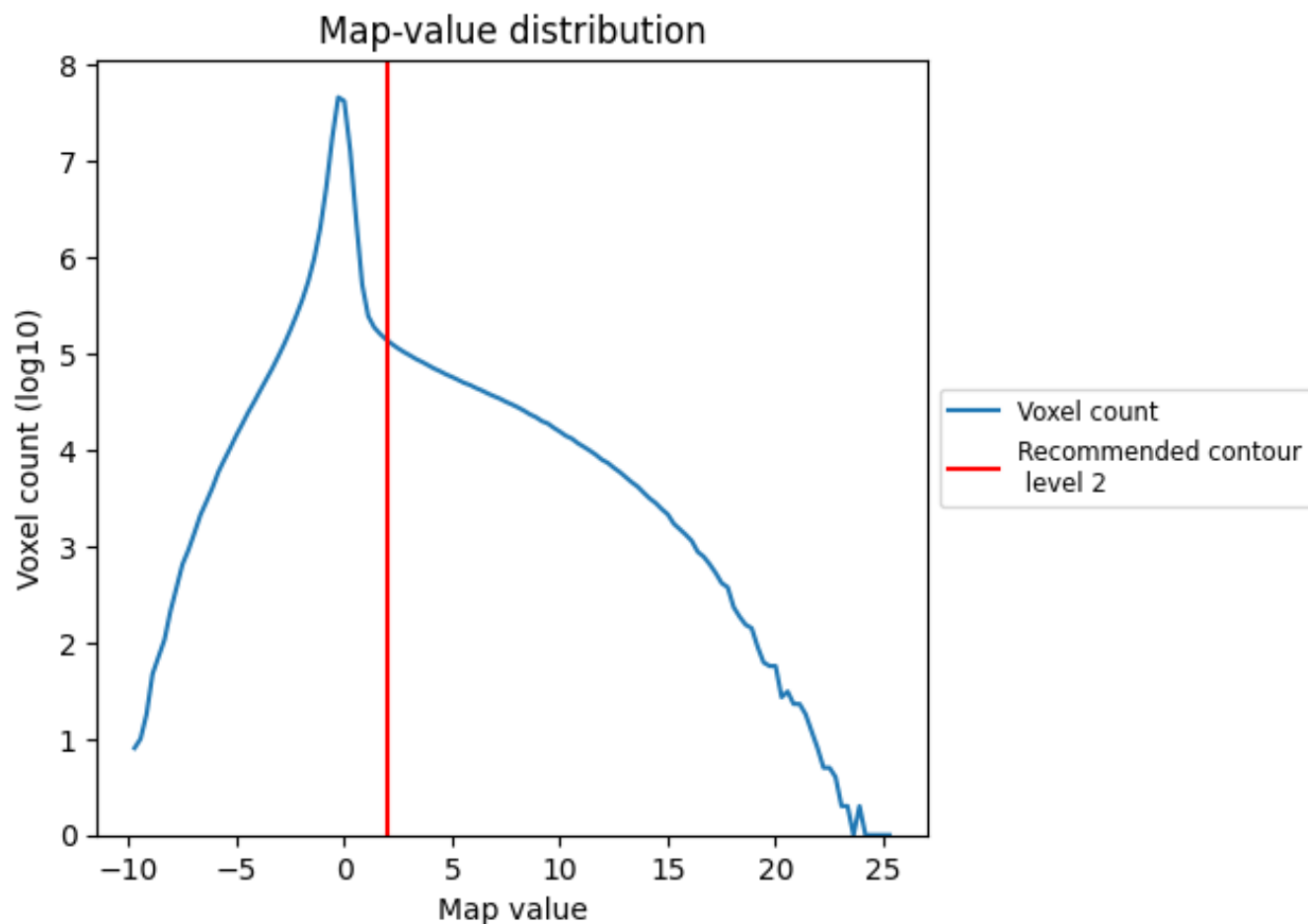
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

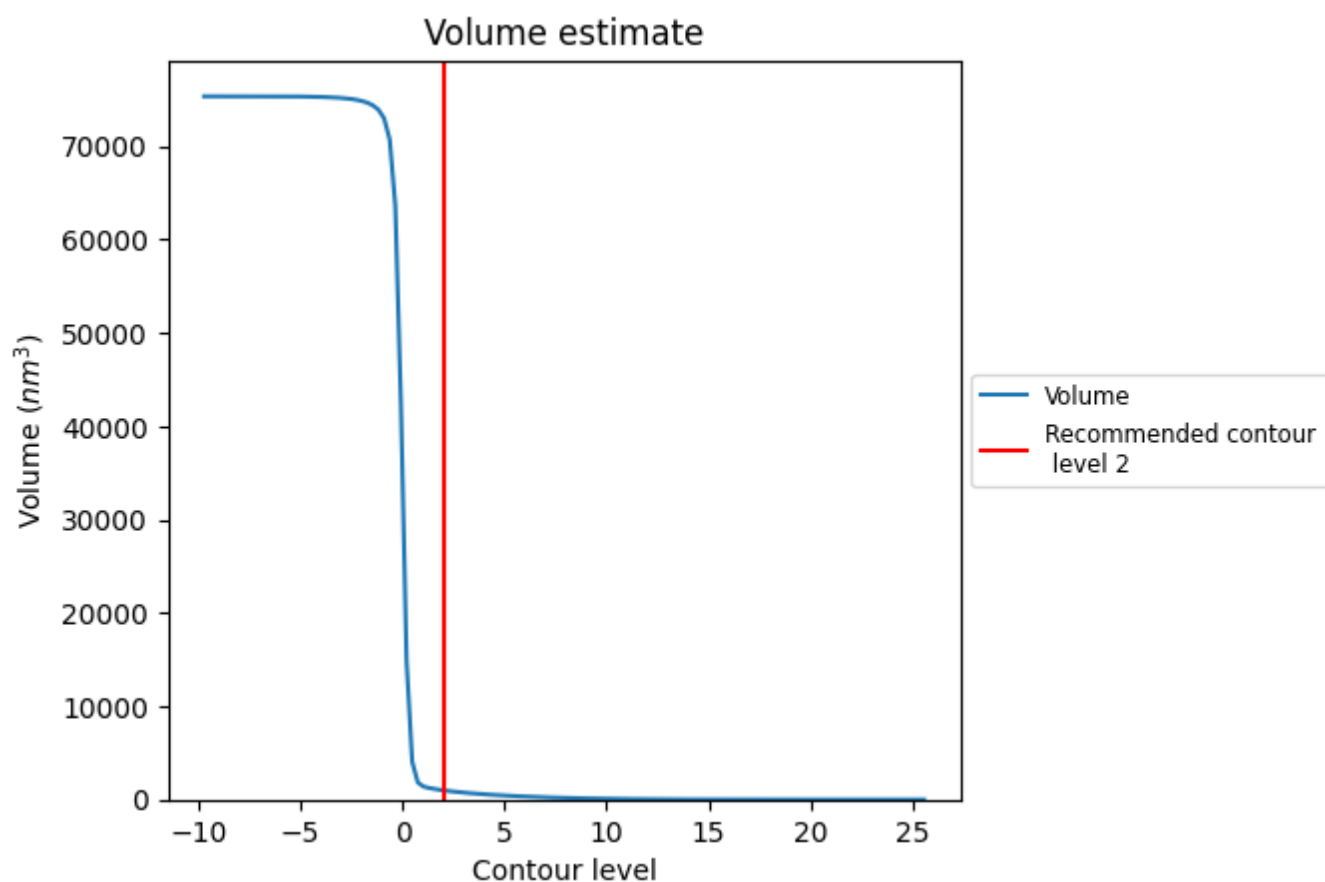
This section contains the results of statistical analysis of the map.

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.

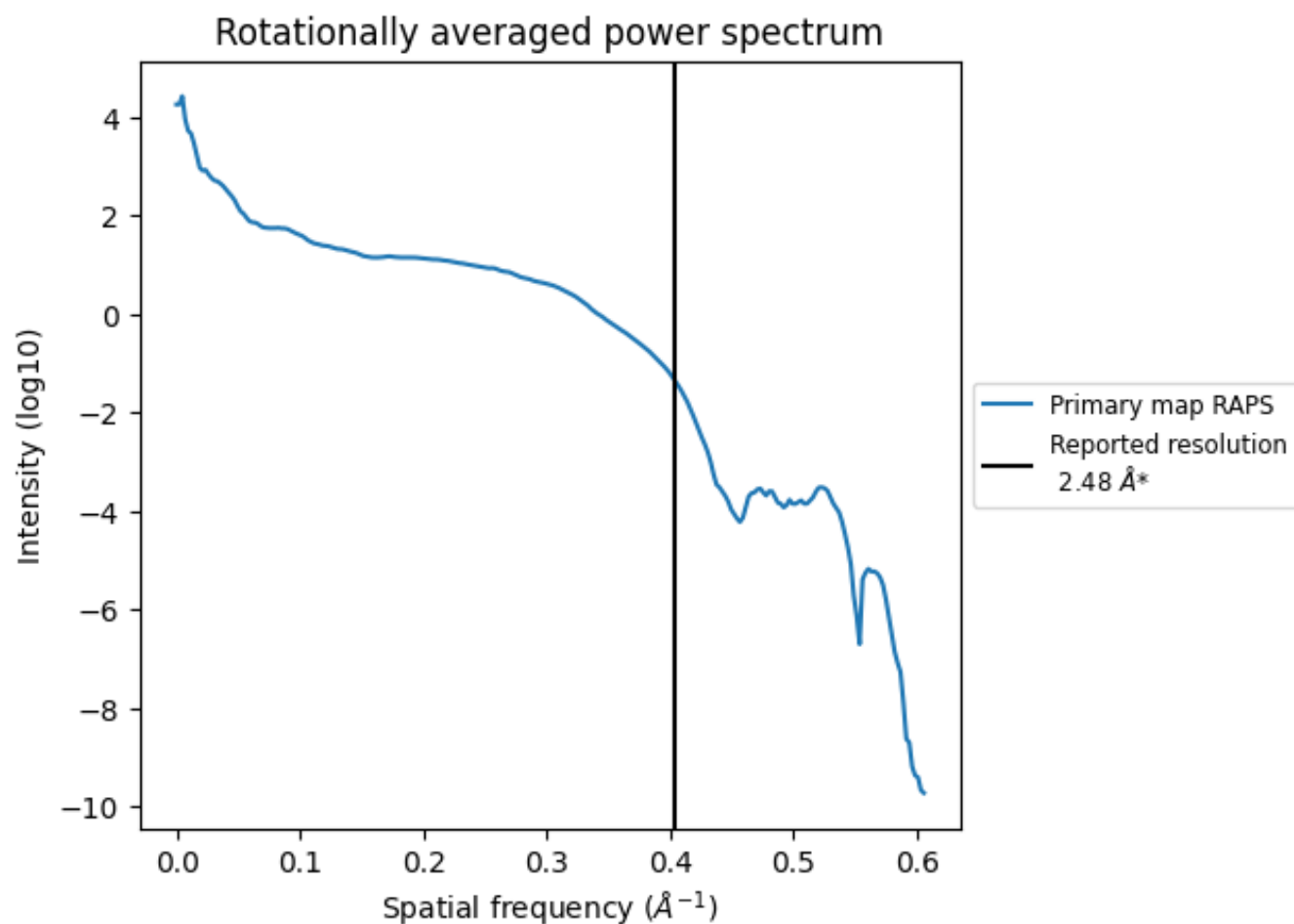
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 988 nm³; this corresponds to an approximate mass of 893 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 ⓘ

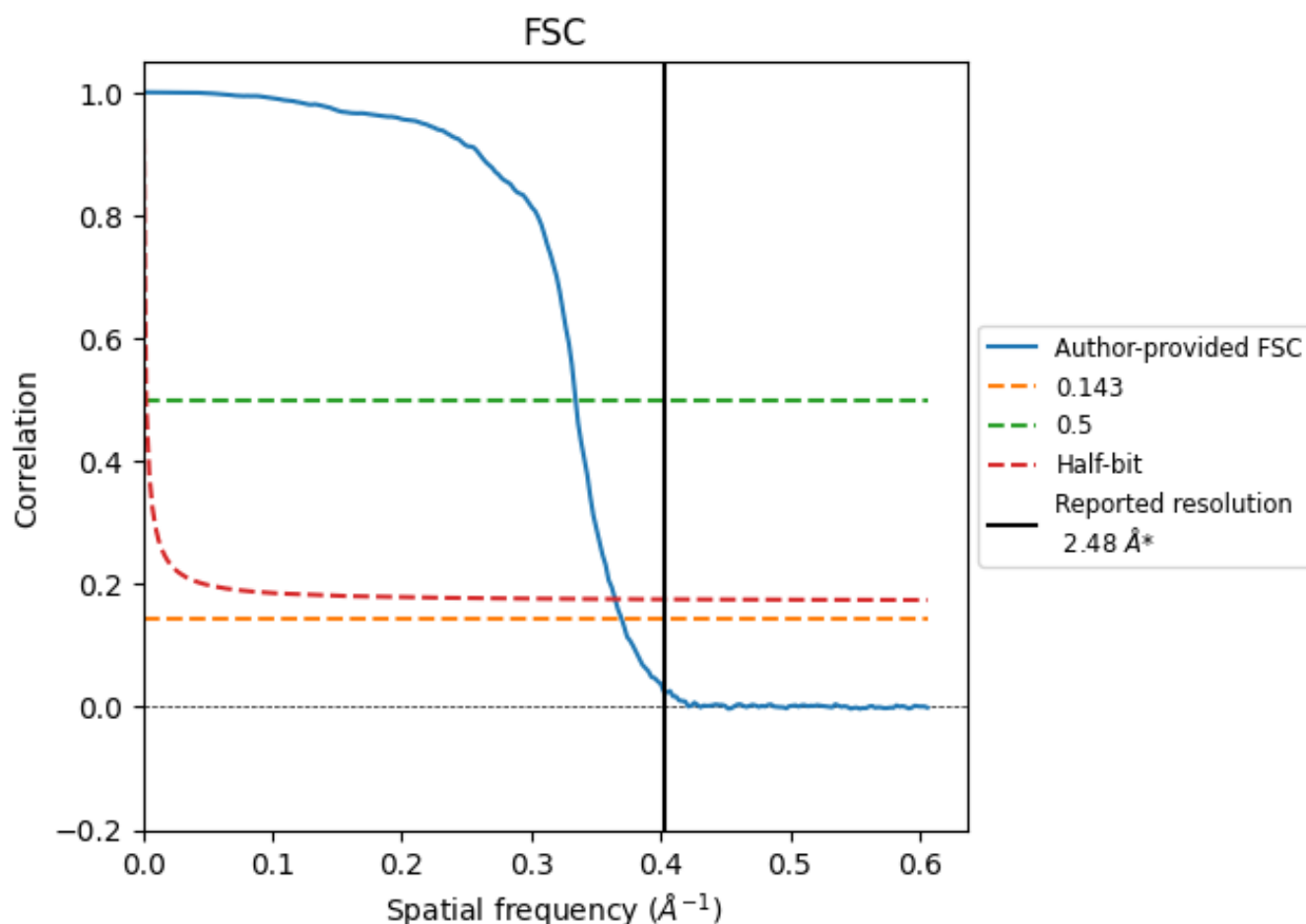


*Reported resolution corresponds to spatial frequency of 0.403 Å⁻¹

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 0.403 Å⁻¹

8.2 Resolution estimates [i](#)

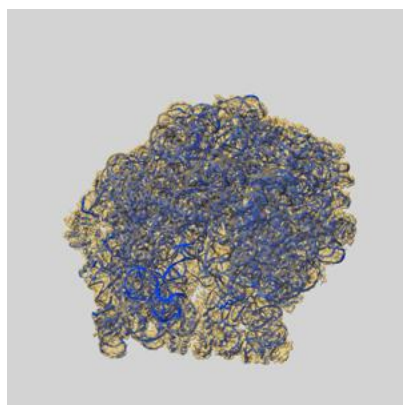
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.48	-	-
Author-provided FSC curve	2.70	2.99	2.74
Unmasked-calculated*	-	-	-

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

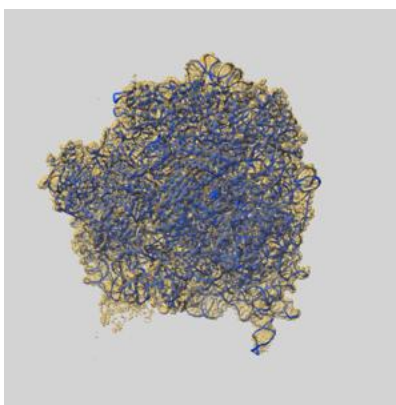
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24802 and PDB model 7S1I. Per-residue inclusion information can be found in section [3](#) on page [16](#).

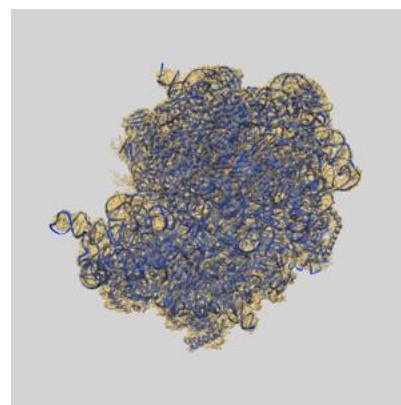
9.1 Map-model overlay [i](#)



X



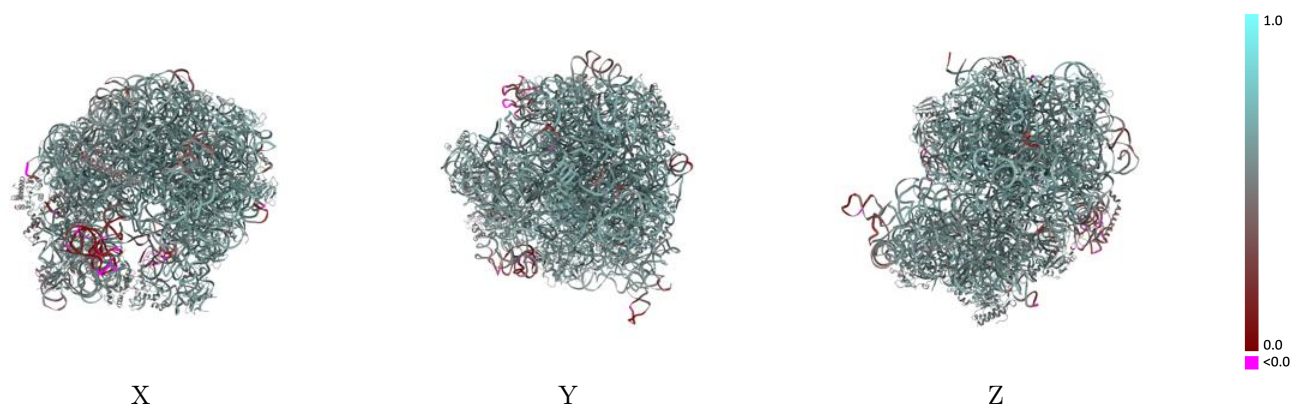
Y



Z

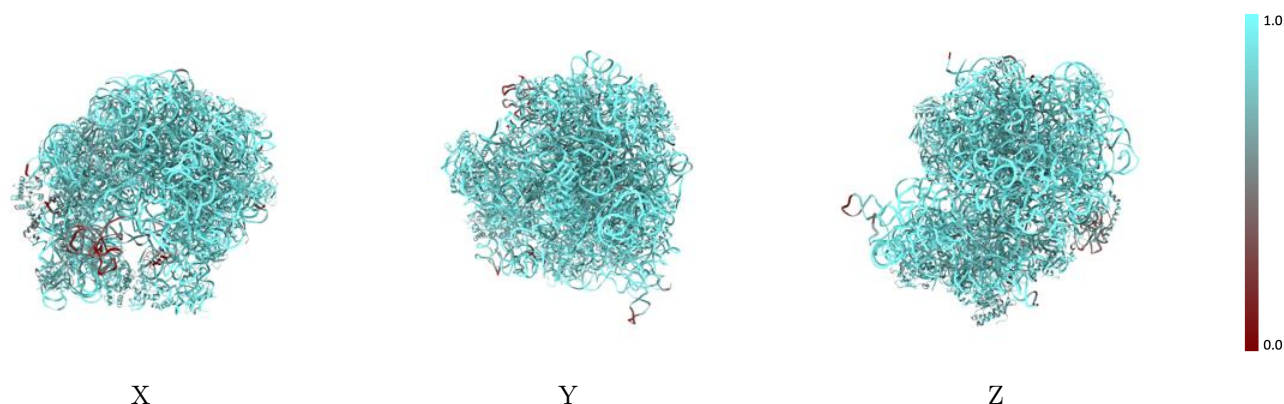
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



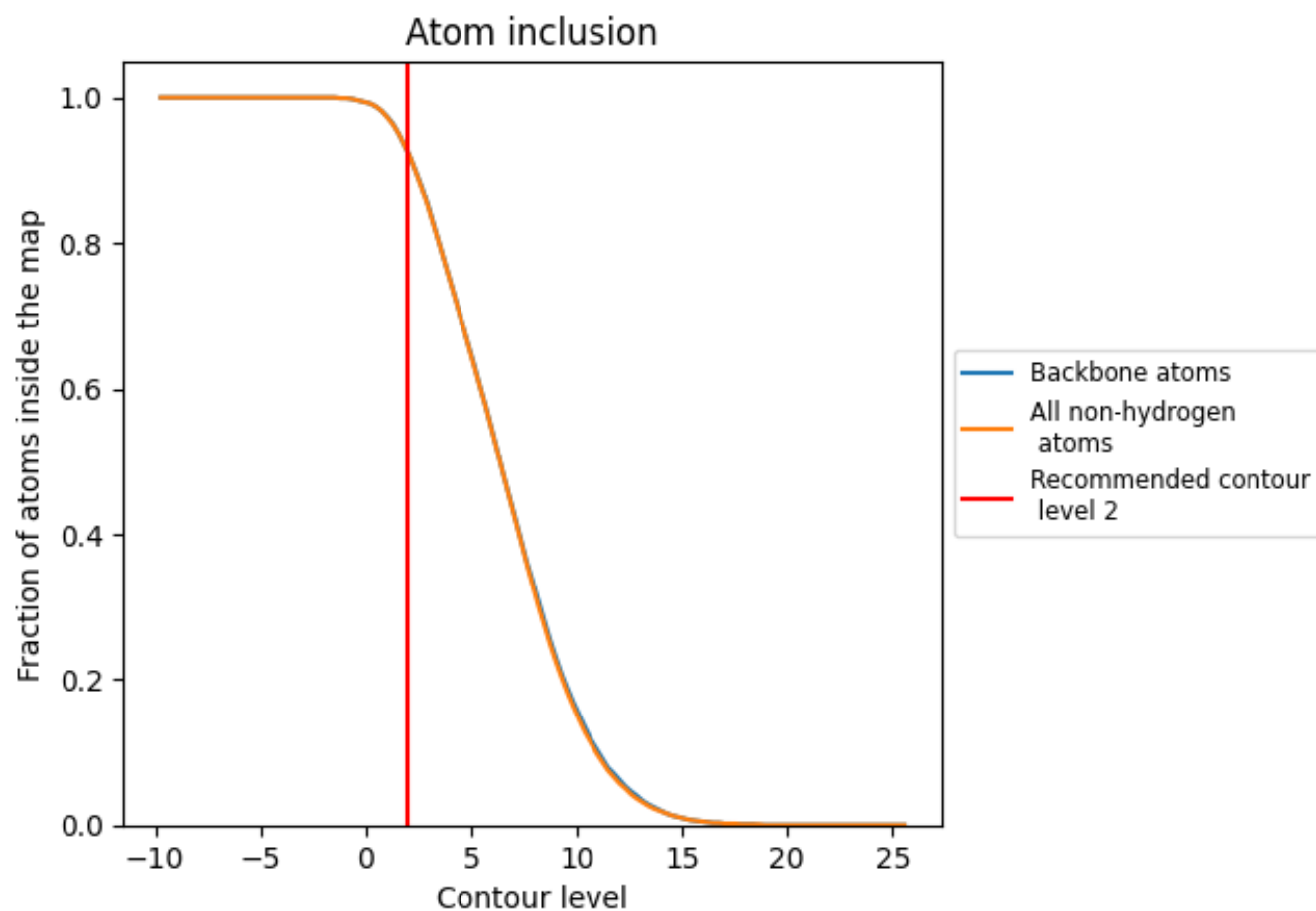
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 92% of all backbone atoms, 92% 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	 0.9250	 0.5750
1	 0.8440	 0.5300
2	 0.8450	 0.5410
3	 0.6540	 0.4820
4	 0.9040	 0.5620
A	 0.9200	 0.5500
C	 0.9610	 0.5770
D	 0.6860	 0.4960
E	 0.8270	 0.5550
F	 0.8040	 0.5340
G	 0.8860	 0.5790
H	 0.8930	 0.5400
I	 0.9560	 0.5830
J	 0.9800	 0.5910
K	 0.9420	 0.6190
L	 0.9300	 0.6150
M	 0.8820	 0.5800
N	 0.8480	 0.5330
O	 0.8470	 0.5420
P	 0.6840	 0.4550
Q	 0.8410	 0.5310
R	 0.9210	 0.6120
S	 0.9100	 0.6100
T	 0.9210	 0.6030
U	 0.9110	 0.6050
V	 0.9500	 0.6220
W	 0.8810	 0.5640
X	 0.9130	 0.6100
Y	 0.9580	 0.6290
Z	 0.9120	 0.6040
a	 0.8980	 0.6120
b	 0.8630	 0.5700
c	 0.8590	 0.5690
d	 0.8860	 0.5940
e	 0.9160	 0.6220



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Chain	Atom inclusion	Q-score
f	 0.9080	 0.6110
g	 0.8550	 0.5460
h	 0.8830	 0.5930
i	 0.9180	 0.6140
j	 0.1000	 0.0700
k	 0.9440	 0.6370
l	 0.9390	 0.6340
m	 0.8770	 0.6020
n	 0.7970	 0.5140
o	 0.8910	 0.5930
p	 0.7900	 0.5080
q	 0.6970	 0.5120
r	 0.8820	 0.5590
s	 0.7050	 0.6360
t	 0.8910	 0.5820
u	 0.8790	 0.5520
v	 0.8280	 0.5370
w	 0.9140	 0.5720
x	 0.8630	 0.5610
y	 0.8260	 0.5520
z	 0.9270	 0.5810