



## Full wwPDB EM Validation Report ⓘ

Nov 1, 2025 – 07:09 am GMT

PDB ID : 9RTV / pdb\_00009rtv  
EMDB ID : EMD-54254  
Title : Structure of the 70S-EF-G(P610L)-GDP-Pi ribosome complex with tRNAs in hybrid state 2 (H2-EF-G(P610L)-GDP-Pi)  
Authors : Ghosh Dastidar, N.; Freyer, N.; Petrychenko, V.; Schwarzer, A.C.; Peng, B.Z.; Samatova, E.; Kothe, C.; Schmidt, M.; Peske, F.; Politi, A.; Urlaub, H.; Fischer, N.; Rodnina, M.V.; Wohlgemuth, I.  
Deposited on : 2025-07-03  
Resolution : 3.60 Å(reported)  
Based on initial model : 7PJW

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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)

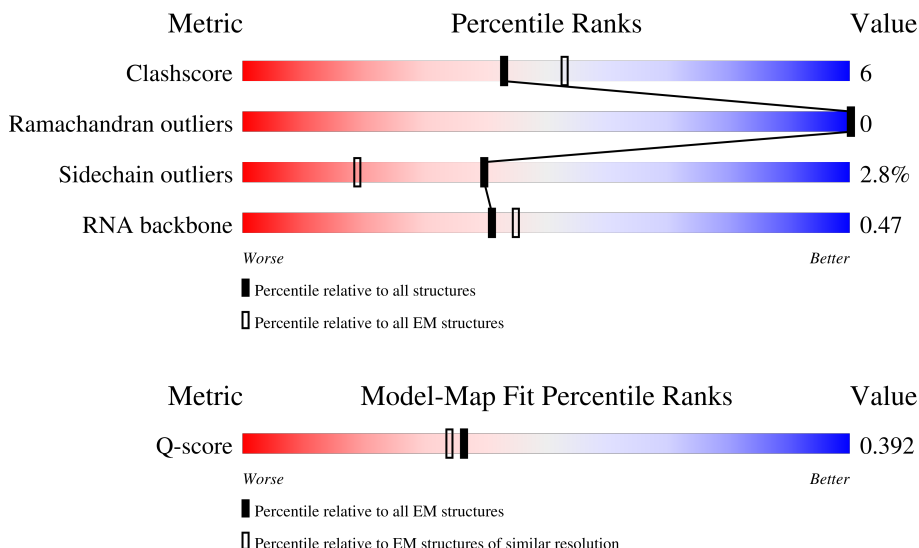
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*


The reported resolution of this entry is 3.60 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.














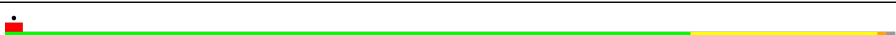


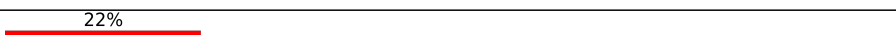
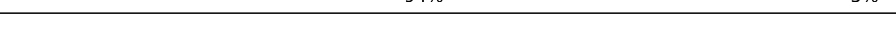

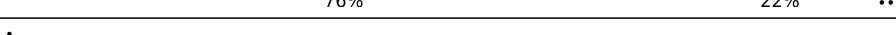







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	12797 ( 3.10 - 4.10 )

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  $\geq 3$ , 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	0	57	







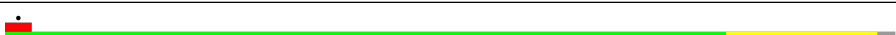
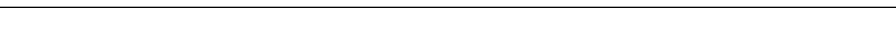
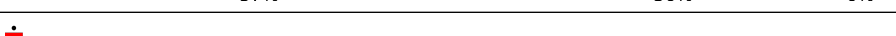
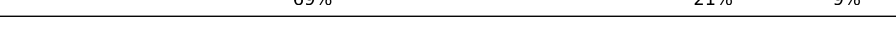
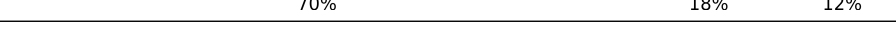
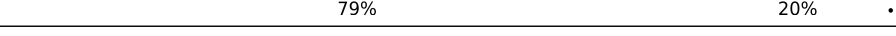













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Mol	Chain	Length	Quality of chain
2	1	55	
3	2	46	
4	3	65	
5	4	38	
6	5	165	
7	6	70	
8	A	2903	
9	B	120	
10	C	273	
11	D	209	
12	E	201	
13	F	179	
14	G	177	
15	H	149	
16	I	142	
17	J	142	
18	K	123	
19	L	144	
20	M	136	
21	N	127	
22	O	117	
23	P	115	
24	Q	118	
25	R	103	
26	S	110	

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Mol	Chain	Length	Quality of chain
27	T	100	
28	U	104	
29	V	94	
30	W	85	
31	X	78	
32	Y	63	
33	Z	59	
34	a	1542	
35	b	240	
36	c	233	
37	d	206	
38	e	167	
39	f	135	
40	g	179	
41	h	130	
42	i	130	
43	j	103	
44	k	129	
45	l	124	
46	m	118	
47	n	102	
48	o	89	
49	p	82	
50	q	84	
51	r	75	

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Mol	Chain	Length	Quality of chain
52	s	92	<div><div></div><div>67%21%11%</div></div>
53	t	87	<div><div></div><div>83%15%</div></div>
54	u	71	<div><div></div><div>76%15%8%</div></div>
55	v	77	<div><div></div><div>65%25%9%</div></div>
56	w	76	<div><div></div><div>15%47%43%9%</div></div>
57	x	704	<div><div></div><div>73%25%</div></div>
58	y	2	<div><div></div><div>100%</div></div>
59	z	33	<div><div></div><div>21%9%67%</div></div>

## 2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 153146 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 2 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 3 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 6 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	5	131	Total	C	N	O	0	0
			647	385	131	131		

- Molecule 7 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	2903	Total	C	N	O	P	0	0
			62338	27816	11471	20148	2903		

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 10 is a protein called 50S ribosomal protein L2.

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

- Molecule 11 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 12 is a protein called 50S ribosomal protein L4.

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

- Molecule 13 is a protein called 50S ribosomal protein L5.

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

- Molecule 14 is a protein called 50S ribosomal protein L6.

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

- Molecule 15 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 16 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	141	Total	C	N	O	S	0	0
			693	411	141	141			

- Molecule 17 is a protein called 50S ribosomal protein L13.

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

- Molecule 18 is a protein called 50S ribosomal protein L14.

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

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 20 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 21 is a protein called 50S ribosomal protein L17.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 22 is a protein called 50S ribosomal protein L18.

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

- Molecule 23 is a protein called 50S ribosomal protein L19.

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

- Molecule 24 is a protein called 50S ribosomal protein L20.

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

- Molecule 25 is a protein called 50S ribosomal protein L21.

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

- Molecule 26 is a protein called 50S ribosomal protein L22.

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

- Molecule 27 is a protein called 50S ribosomal protein L23.

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

- Molecule 28 is a protein called 50S ribosomal protein L24.

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

- Molecule 29 is a protein called 50S ribosomal protein L25.

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

- Molecule 30 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	75	Total	C	N	O	S		
			575	356	116	102	1	0	0

- Molecule 31 is a protein called 50S ribosomal protein L28.

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

- Molecule 32 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	63	Total	C	N	O	S		
			509	313	99	95	2	0	0

- Molecule 33 is a protein called 50S ribosomal protein L30.

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

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1540	Total	C	N	O	P		
			33050	14748	6057	10705	1540	0	0

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 36 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 37 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called 30S ribosomal protein S9.

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

- Molecule 43 is a protein called 30S ribosomal protein S10.

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

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 48 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			506	313	105	87	1		

- Molecule 55 is a RNA chain called P/E-site tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
55	v	76	Total	C	N	O	P	S	0	0
			1622	724	295	526	76	1		

- Molecule 56 is a RNA chain called A/P-site tRNA(Phe).

Mol	Chain	Residues	Atoms						AltConf	Trace
56	w	76	Total	C	N	O	P	S	0	0
			1631	731	291	531	76	2		

- Molecule 57 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	x	703	Total	C	N	O	S	0	0
			5445	3430	942	1048	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	609	LEU	PRO	conflict	UNP C4ZUJ5

- Molecule 58 is a protein called Dipeptide (FME-PHE).

Mol	Chain	Residues	Atoms					AltConf	Trace
58	y	2	Total	C	N	O	S	0	0
			21	15	2	3	1		

- Molecule 59 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	z	11	Total	C	N	O	P	0	0
			230	103	35	81	11		

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	0	1	Total	Mg	0
			1	1	
60	A	260	Total	Mg	0
			260	260	
60	B	7	Total	Mg	0
			7	7	

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Mol	Chain	Residues	Atoms		AltConf
60	C	3	Total 3	Mg 3	0
60	D	1	Total 1	Mg 1	0
60	N	1	Total 1	Mg 1	0
60	O	1	Total 1	Mg 1	0
60	P	1	Total 1	Mg 1	0
60	Q	2	Total 2	Mg 2	0
60	Z	1	Total 1	Mg 1	0
60	a	86	Total 86	Mg 86	0
60	m	1	Total 1	Mg 1	0
60	n	1	Total 1	Mg 1	0
60	v	1	Total 1	Mg 1	0
60	w	1	Total 1	Mg 1	0
60	x	1	Total 1	Mg 1	0

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

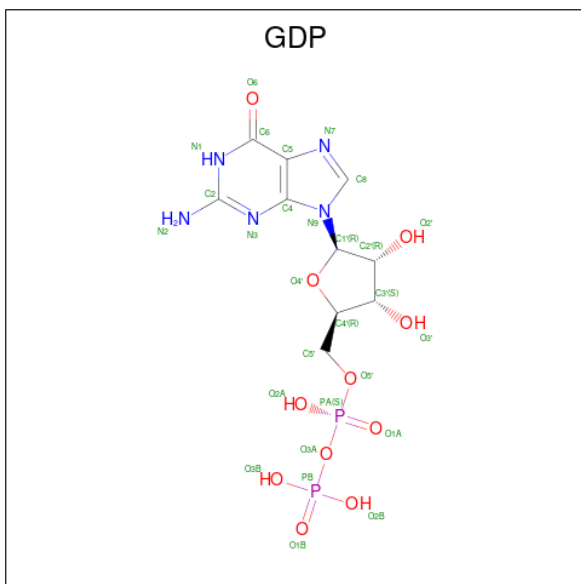
Mol	Chain	Residues	Atoms		AltConf
61	4	1	Total 1	Zn 1	0
61	6	1	Total 1	Zn 1	0

- Molecule 62 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
62	A	1	Total 1	Na 1	0
62	B	1	Total 1	Na 1	0

- [illegible]

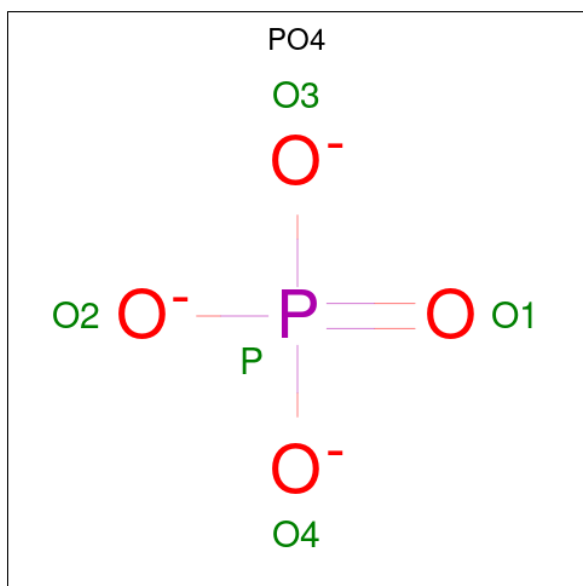
- Molecule 64 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$ ).





Mol	Chain	Residues	Atoms					AltConf
64	x	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 65 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).




Mol	Chain	Residues	Atoms			AltConf
65	x	1	Total	O	P	0
			5	4	1	

### 3 Residue-property plots [i](#)


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

- Molecule 1: 50S ribosomal protein L32

Chain 0:  77% 19% ..




- Molecule 2: Large ribosomal subunit protein bL33

Chain 1:  78% 13% 9%




- Molecule 3: Large ribosomal subunit protein bL34

Chain 2:  85% 15%




- Molecule 4: 50S ribosomal protein L35

Chain 3:  86% 12% .

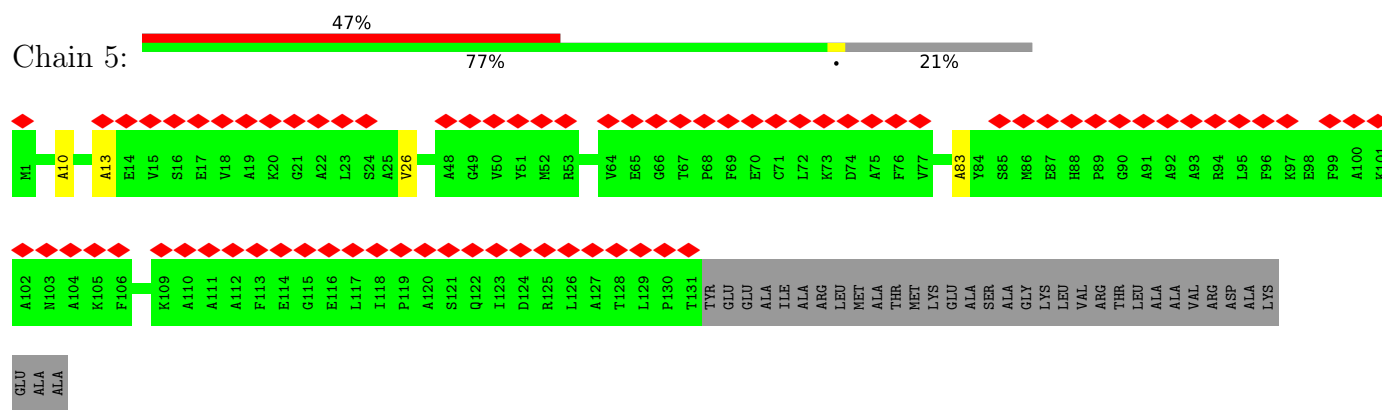


- Molecule 5: 50S ribosomal protein L36

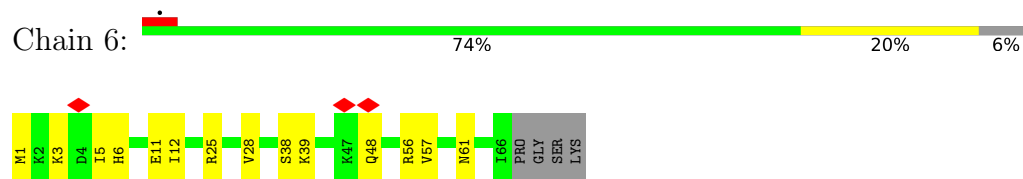
Chain 4:  89% 11%



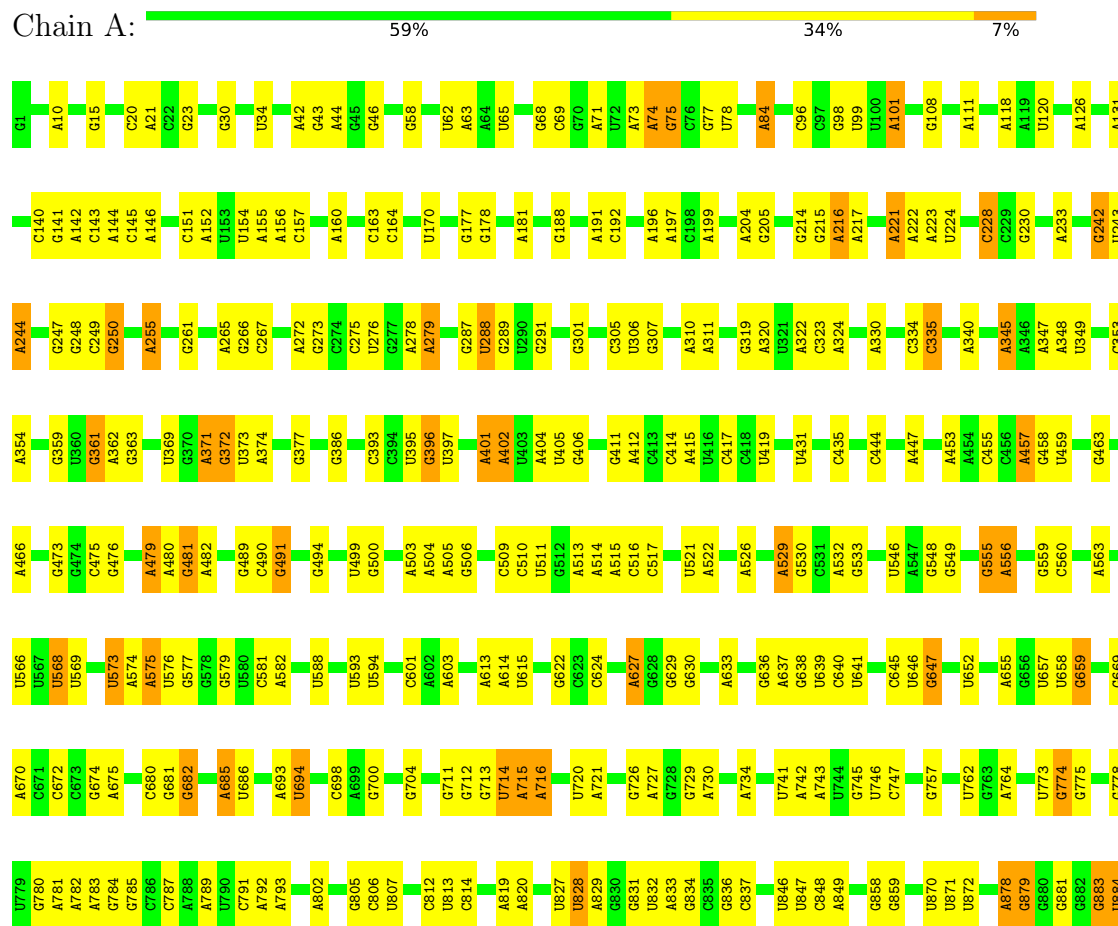
- Molecule 6: 50S ribosomal protein L10



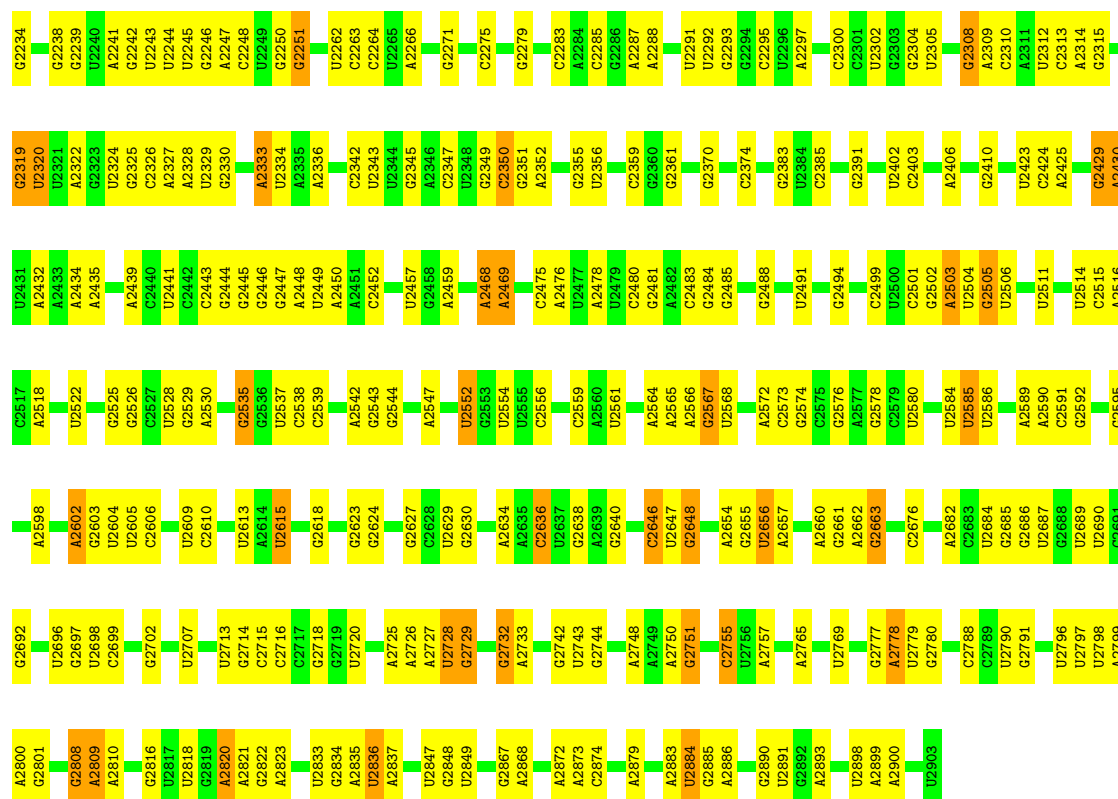
- Molecule 7: 50S ribosomal protein L31



- Molecule 8: 23S ribosomal RNA

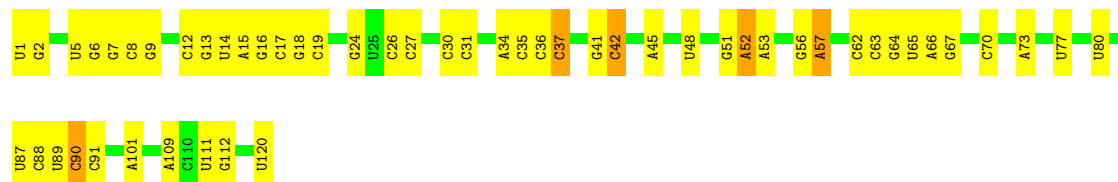


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U2155	C2091	C1996	C1909	G1682	U1578	G1471	G1380	A1264	G1139	A1070	G989	A886
G2157	U2092	C1997	U1783	U1683	A1579	A1783	U1579	A1265	C1140	C1071	A990	A887
A2158	G2093	C2006	A1912	G1684	A1580	U1474	A1383	G1266	U1141	C1072	C991	C888
G2159	U2099	G2012	A1913	U1688	U1584	G1475	C1386	C1270	A1142	A1073	C992	C889
C2160	A2101	A2013	U1917	U1693	C1585	U1476	A1387	G1271	G1153	C1075	C994	C890
G2162	G2102	A2014	A1918	U1699	U1586	A1477	A1392	A1272	G1154	C1076	C995	G891
A2163	C2103	A2015	A1919	A1698	G1587	A1478	A1393	U1273	A1155	A1077	A996	A892
C2164	C2104	A2016	C1920	G1699	G1588	G1482	U1394	G1278	G1168	U1078	C996	C893
C2165	U2105	U2017	U1796	G1699	U1589	G1482	A1395	G1279	A1169	A1080	U894	U895
U2166	G2108	G2018	G1797	A1700	U1590	C1488	A1403	C1278	C1170	U1081	A1000	A896
U2167	U2106	A2019	U1798	G1700	A1591	C1489	A1404	G1279	G1171	U1082	A1001	C897
G2168	G2107	A2020	G1799	U1709	C1592	C1490	U1405	A1284	U1174	U1083	C1005	C898
A2169	A2108	C2021	C1800	G1710	A1593	G1491	U1406	G1288	U1175	A1084	A1009	A899
G2170	U2109	U2022	A1801	A1711	U1594	A1494	U1409	G1300	U1176	A1085	U1012	C903
A2171	G2110	C2023	C1927	G1715	C1595	U1497	G1410	A1301	A1177	A1086	C1013	G907
U2172	U2111	G2029	A1802	U1716	A1596	U1497	G1411	G1301	G1178	A1087	A1014	A918
A2173	G2112	A2030	A1803	U1716	A1597	U1497	G1412	A1301	U1180	A1088	U1023	G926
C2174	U2113	G2031	G1807	G1724	A1598	G1501	A1413	G1309	G1179	A1089	G1024	A927
A2176	G2114	A2032	A1808	U1725	A1608	G1501	A1414	G1310	U1181	A1090	G1025	U931
U2180	C2115	G2033	A1809	C1726	G1609	A1504	U1415	G1311	G1187	G1091	G1026	U932
U2181	G2116	A2034	A1937	G1727	A1610	A1508	G1416	U1312	U1188	A1092	A1027	A933
U2182	U2118	G2035	U1939	C1728	C1611	A1509	C1417	C1315	G1189	A1093	A1028	U934
A2183	A2119	C2036	U1940	U1729	C1612	A1509	G1418	G1316	U1197	A1094	U1033	G946
G2184	G2120	A2037	C1817	G1730	G1613	G1510	G1419	G1317	U198	A1095	U1033	A947
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G2186	U2122	U2039	U1818	C1732	A1614	G1512	G1432	G1320	U1203	A1097	G1042	A941
U2187	G2123	G2040	G1823	G1733	A1618	G1514	A1433	G1331	G1212	A1098	G1043	C946
G2190	A2126	C2043	G1826	G1734	G1631	A1515	A1434	G1334	A1213	C1109	C1044	A947
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G2193	C2128	C2045	U1837	U1736	A1633	G1517	C1437	C1335	U1219	A1111	A1046	G953
U2198	C2129	G2046	A1829	G1738	A1634	G1524	U1438	G1339	G1220	A1112	G1047	U955
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G2201	U2131	G2056	G1835	A1745	C1638	G1532	G1442	G1341	G1226	C1114	C1053	C961
U2202	A2132	G2057	C1836	U1746	U1647	A1533	G1446	C1346	G1227	G1115	A1054	C965
U2203	A2133	A2060	U1837	U1747	U1648	A1535	C1447	A1353	U1234	G1116	G1056	G971
G2204	A2135	G2061	U1864	U1751	U1649	G1536	G1448	A1354	G1235	U1119	U1058	A972
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G2212	U2139	G2067	G1869	U1757	A1654	G1540	U1459	C1376	G1252	A1134	U1065	G976
C2215	G2140	U2068	U1869	A1757	U1662	G1544	G1459	A1377	A1254	U1135	U1066	A983
G2216	A2142	G2069	G1894	C1760	G1663	A1544	U1460	G1377	A1254	G1136	A1067	A984
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A2225	G2144	A2071	G1891	U1769	A1665	U1554	U1461					
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G2230	G2148	U2079	A1899	C1771	A1668	C1557	U1461					
U2231	U2149	A2080	A1900	A1772	A1669	C1558	U1461					
C2232	C2150	U2081	A1901	A1773	C1670	C1558	U1461					
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	C2153											



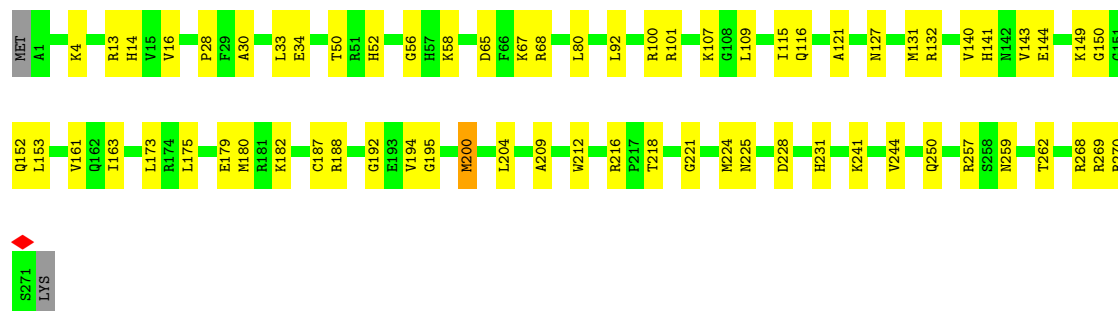
• Molecule 9: 5S ribosomal RNA

Chain B: 56% 40%

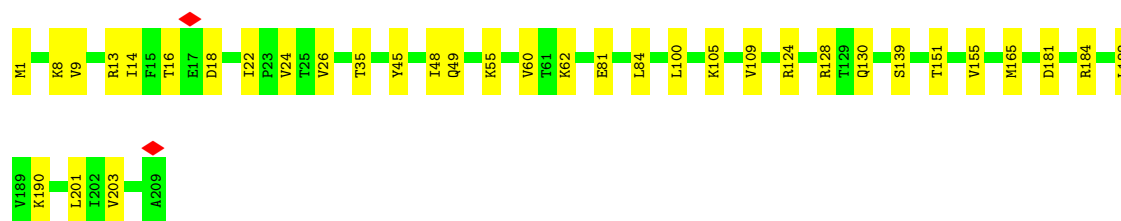
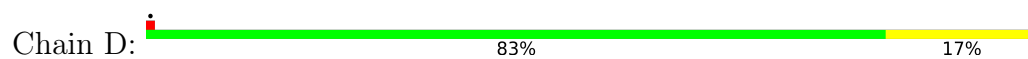


• Molecule 10: 50S ribosomal protein L2

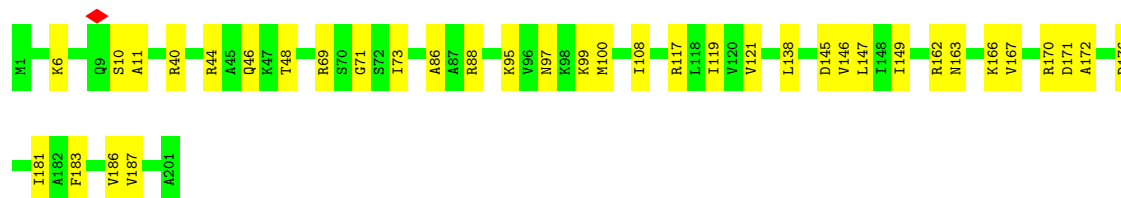
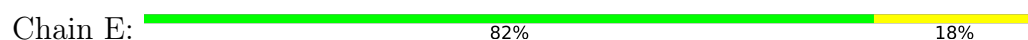
Chain C: 75% 24%



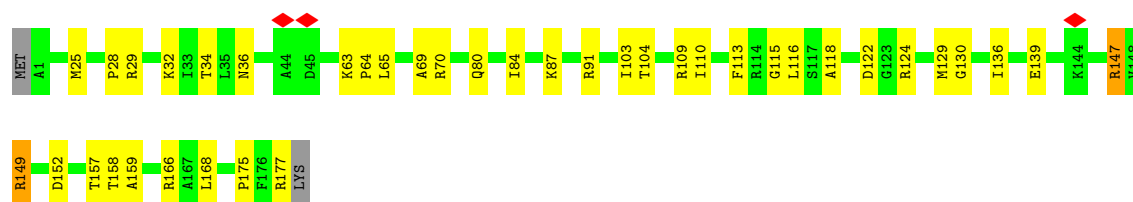
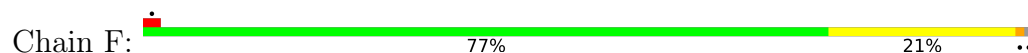
• Molecule 11: 50S ribosomal protein L3



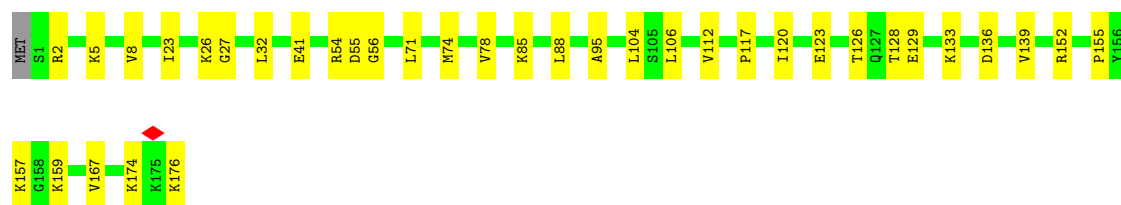
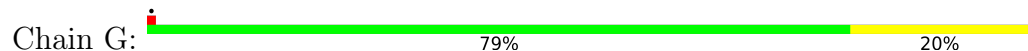
- Molecule 12: 50S ribosomal protein L4



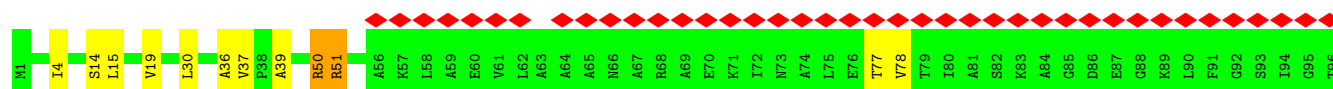
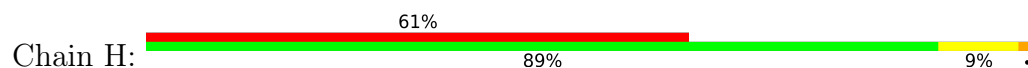
- Molecule 13: 50S ribosomal protein L5

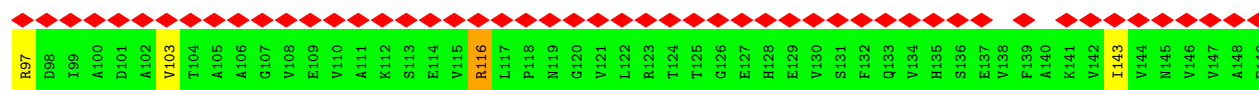


- Molecule 14: 50S ribosomal protein L6

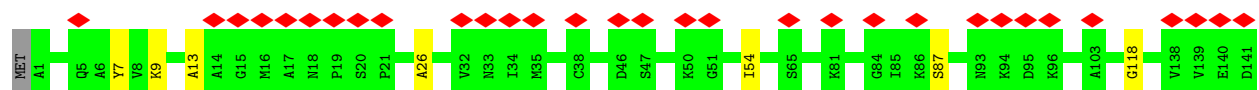


- Molecule 15: 50S ribosomal protein L9

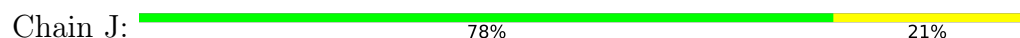




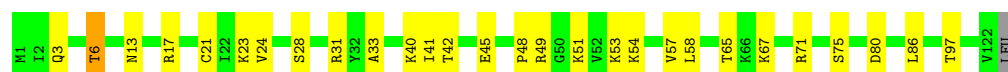
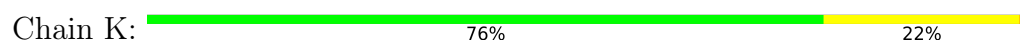
- Molecule 16: 50S ribosomal protein L11



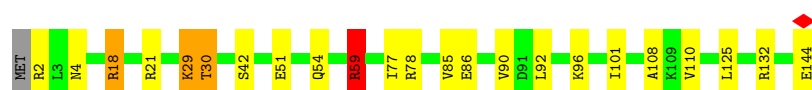
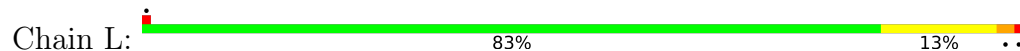
- Molecule 17: 50S ribosomal protein L13



- Molecule 18: 50S ribosomal protein L14



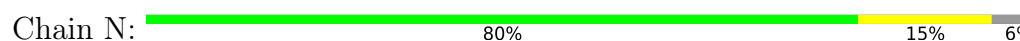
- Molecule 19: 50S ribosomal protein L15



- Molecule 20: 50S ribosomal protein L16



- Molecule 21: 50S ribosomal protein L17




- Molecule 22: 50S ribosomal protein L18

Chain O:  86% 13%




- Molecule 23: 50S ribosomal protein L19

Chain P:  78% 20%




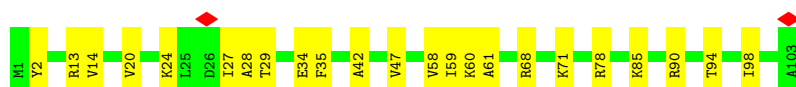
- Molecule 24: 50S ribosomal protein L20

Chain Q:  78% 20%



- Molecule 25: 50S ribosomal protein L21

Chain R:  78% 22%



- Molecule 26: 50S ribosomal protein L22

Chain S:  78% 22%




- Molecule 27: 50S ribosomal protein L23

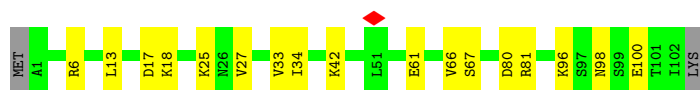
Chain T:  74% 17% 7%



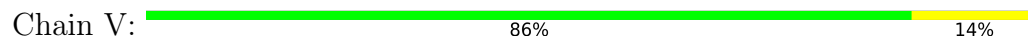
- Molecule 28: 50S ribosomal protein L24

Chain U:  82% 16%

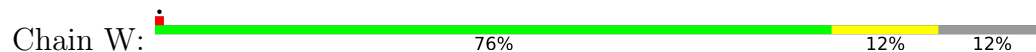




- Molecule 29: 50S ribosomal protein L25



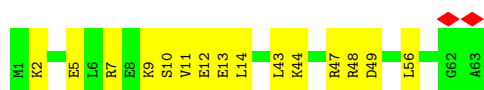
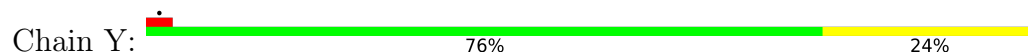
- Molecule 30: Large ribosomal subunit protein bL27



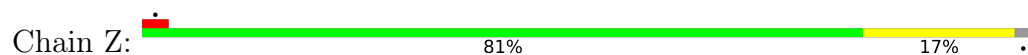
- Molecule 31: 50S ribosomal protein L28



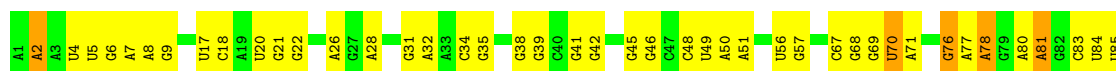
- Molecule 32: 50S ribosomal protein L29



- Molecule 33: 50S ribosomal protein L30



- Molecule 34: 16S ribosomal RNA



C1539	A1465	C1378	U1295	G1184	U1090	U1007	U921	C811	A563	A478	A393	C307	G202
U1540	G1473	G1379	C1296	G1190	U1091	U1008	G222	G812	C564	U479	G394	C308	G203
U	U1474	U1298	U1297	U1092	U1010	U1009	A923	U813	A572	U480	A397	G310	G204
A	C1475	C1382	A1196	A1093	C1011	C1012	G927	A816	A573	G713	C401	C316	A205
	A1476	C1383	G1300	G1094	A1012	G1013	G928	A815	A482	G714	U405	A321	C206
	U1477	G1386	U1301	U1095	G1014	G1015	C932	G818	C576	A817	U406	C207	U208
	U1478	C1302	C1200	C1096	U1015	G1016	G933	A819	G577	U716	U407	A322	U209
	C1305	G1305	G1207	G1099	A1016	U1017	G934	C935	C582	U718	U408	G324	C210
	U1308	U1308	C1208	A1101	U1018	U1019	A935	U822	G587	G720	U409	A327	G212
	G1309	G1309	C1209	G1108	G1020	C940	C940	A825	A586	G721	U410	C328	C215
	G1312	U1211	U1211	C1109	U1021	G945	G945	C826	G597	G722	A411	C329	G220
	U1313	U1212	A1213	A1022	A1022	A946	A946	G829	U598	U723	A412	C330	C221
	C1314	C1214	C1214	U1115	U1023	G947	G947	G832	G605	G724	A413	C331	C222
	U1315	G1217	C1217	G1124	G1024	C948	C948	G832	U605	G733	C419	C335	C223
	G1316	C1317	C1317	U1125	U1025	A949	A949	U835	G606	G734	U420	A336	A223
	C1320	C1320	C1320	U1126	C1026	A958	A958	C841	A607	G735	U421	G337	G226
	G1323	G1222	G1222	G1127	U1028	A959	A959	U842	C613	C736	U422	C339	G227
	U1326	G1226	A1227	G1131	C1031	U961	U961	G844	G615	G742	U426	U343	G230
	C1327	A1227	A1227	G1134	G1032	C965	C965	A845	C618	G743	U427	A344	U231
	G1331	A1238	A1238	C1137	A1035	C967	C967	G846	U619	G744	G428	C345	G232
	U1332	U1240	U1240	G1139	A1036	A968	A968	A846	G620	G745	U429	G346	C235
	A1333	G1241	G1241	U1144	U1040	G971	G971	G844	A621	G746	U436	G347	A236
	G1334	C1242	C1242	A1145	G1041	C972	C972	A845	G628	G747	U437	G351	A237
	U1335	C1243	C1243	C1146	A1042	A974	A974	G846	A629	G748	U438	C352	A238
	C1336	G1244	G1244	C1147	G1043	A975	A975	A846	U632	U751	U439	A353	U239
	U1344	C1249	C1249	U1148	A1046	A976	A976	G867	U634	G752	U440	C355	G240
	A1345	A1250	A1250	C1149	G1047	A977	A977	U870	C634	G753	G446	A356	U244
	G1347	A1251	A1251	A1150	U1059	A978	A978	A873	A635	G754	G447	G357	U245
	U1348	A1254	A1254	A1151	C1060	C979	C979	U874	U636	G755	A448	G358	A246
	C1352	G1260	G1260	A1157	G1061	U981	U981	U875	U637	G756	G449	G359	G247
	G1353	A1261	A1261	U1159	U1065	U982	U982	C879	A642	G757	U450	G360	G251
	U1354	C1267	C1267	G1160	U1071	C984	C984	C890	G650	G758	G455	A363	G259
	G1355	G1268	G1268	A1167	C1072	C985	C985	U899	U653	G759	A456	A366	A262
	A1357	A1269	A1269	U1168	U1073	U992	U992	C895	U662	G773	A459	U367	A263
	A1360	A1271	A1271	A1169	G1074	G993	G993	G885	U663	G776	A460	U368	C264
	G1361	C1272	C1272	U1170	U1075	A994	A994	C885	A663	A777	A461	G372	G265
	A1362	G1275	G1275	A1171	U1076	C995	C995	A901	G664	G778	G462	A373	G266
	U1363	A1275	A1275	G1175	U1077	A996	A996	G902	A665	U781	U464	A374	U268
	A1364	A1280	A1280	U1176	U1078	C999	C999	A909	A673	A792	A465	U375	C269
	C1369	A1287	A1287	G1177	U1079	A1000	A1000	A913	G674	U793	A468	G376	A270
	U1370	U1286	U1286	U1178	A1080	C1001	C1001	A914	A675	U794	U471	G377	G281
	G1371	A1287	A1287	A1179	A1081	G1002	G1002	A914	A553	A795	U472	G378	G289
	U1372	A1288	A1288	U1180	G1084	G1003	G1003	A918	G588	C795	U473	A388	U296
	A1375	G1294	G1294	U1183	U1085	A1004	A1004	A919	A559	G796	U474	U390	G391
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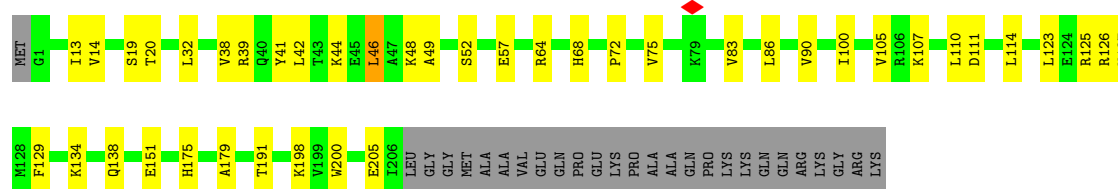
- Molecule 35: 30S ribosomal protein S2

Chain b: 




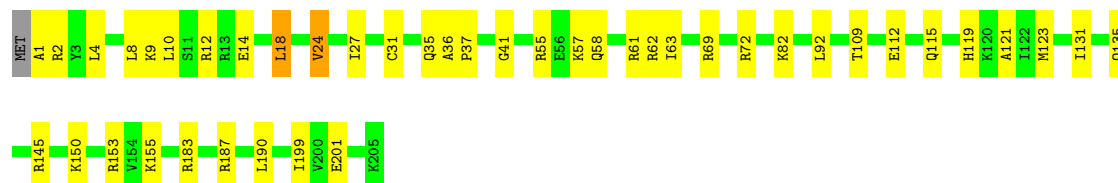
- Molecule 36: Small ribosomal subunit protein uS3

Chain c: 



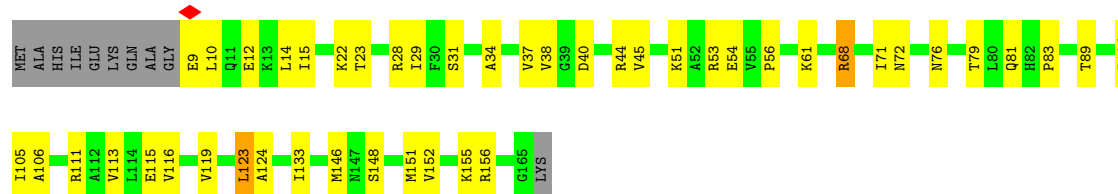
- Molecule 37: Small ribosomal subunit protein uS4

Chain d: 



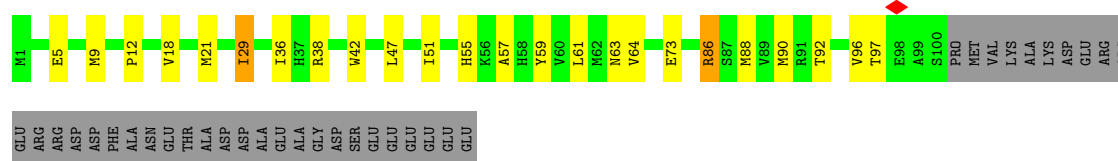
- Molecule 38: 30S ribosomal protein S5

Chain e: 

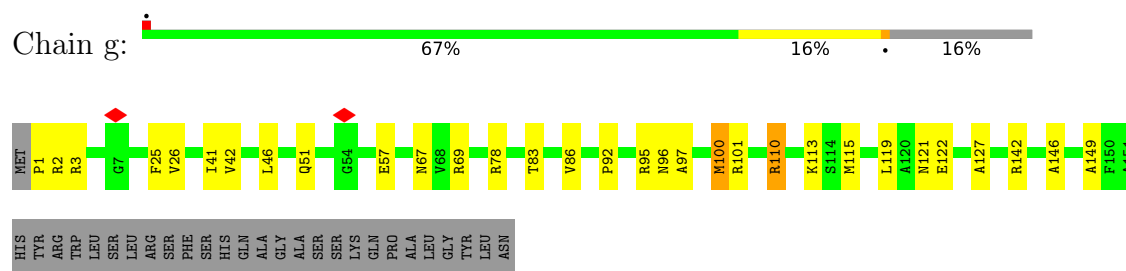


- Molecule 39: 30S ribosomal protein S6

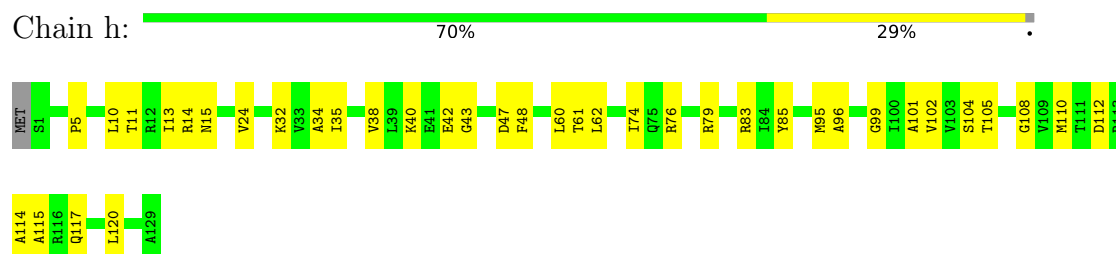
Chain f: 



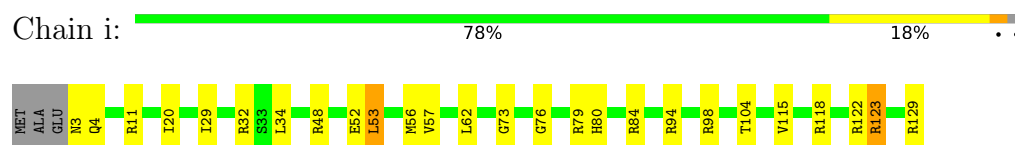
- Molecule 40: 30S ribosomal protein S7



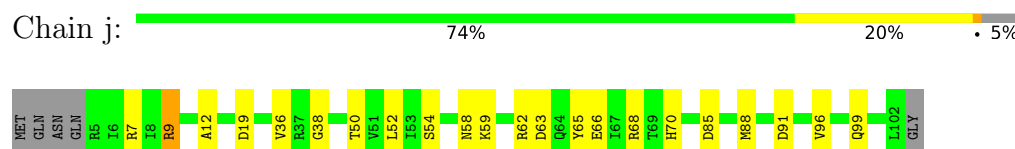
- Molecule 41: 30S ribosomal protein S8



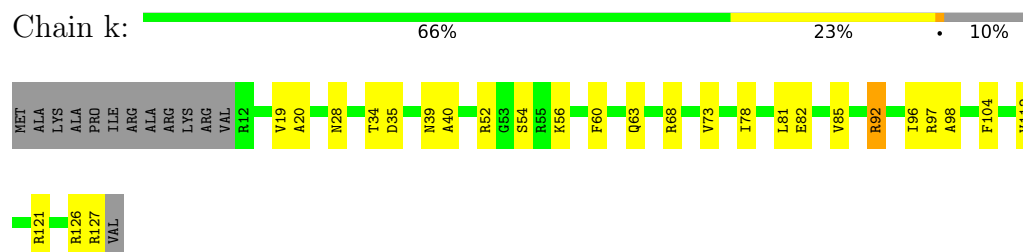
- Molecule 42: 30S ribosomal protein S9



- Molecule 43: 30S ribosomal protein S10

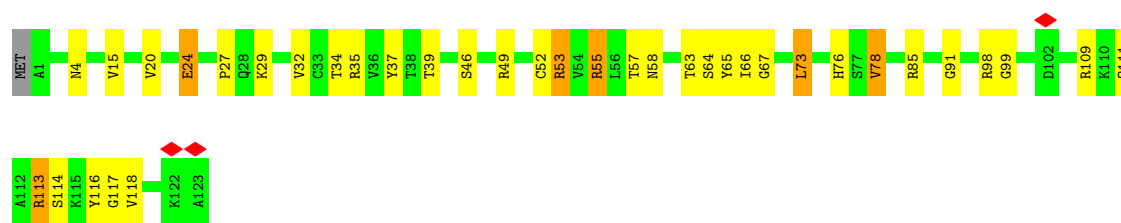


- Molecule 44: 30S ribosomal protein S11



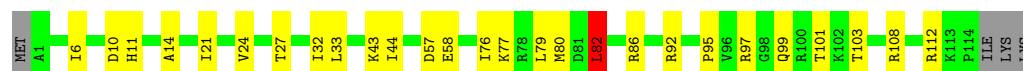
- Molecule 45: 30S ribosomal protein S12





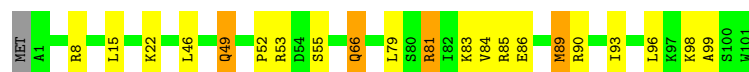
- Molecule 46: 30S ribosomal protein S13

Chain m: 74% 22% ..



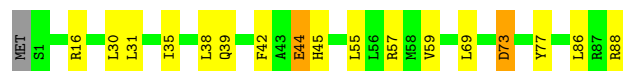
- Molecule 47: 30S ribosomal protein S14

Chain n: 78% 17% ..



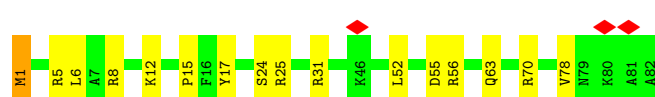
- Molecule 48: Small ribosomal subunit protein uS15

Chain o: 80% 17% ..



- Molecule 49: 30S ribosomal protein S16

Chain p: 80% 18% .



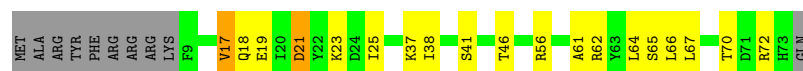
- Molecule 50: 30S ribosomal protein S17

Chain q: 77% 18% 5%



- Molecule 51: 30S ribosomal protein S18

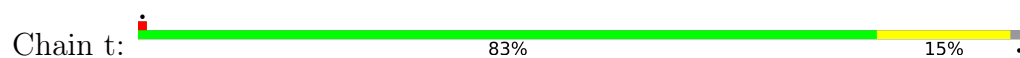
Chain r: 61% 23% 13%



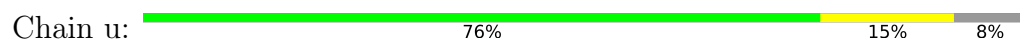
- Molecule 52: 30S ribosomal protein S19



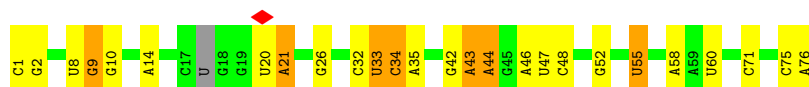
- Molecule 53: 30S ribosomal protein S20



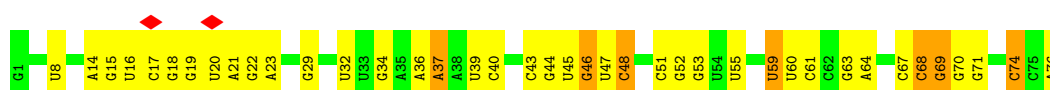
- Molecule 54: 30S ribosomal protein S21



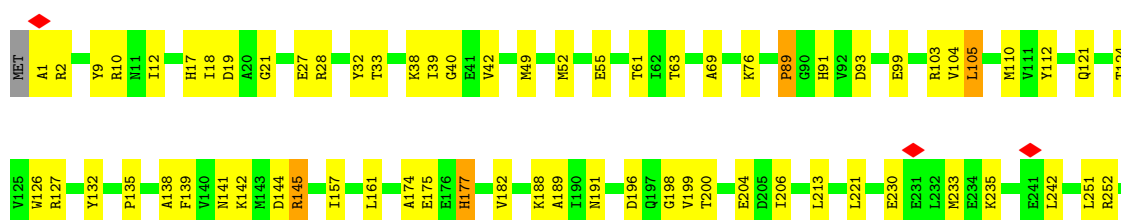
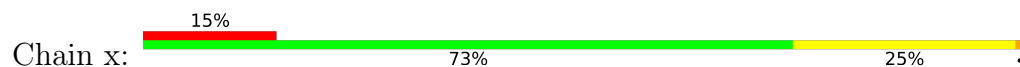
- Molecule 55: P/E-site tRNA(fMet)

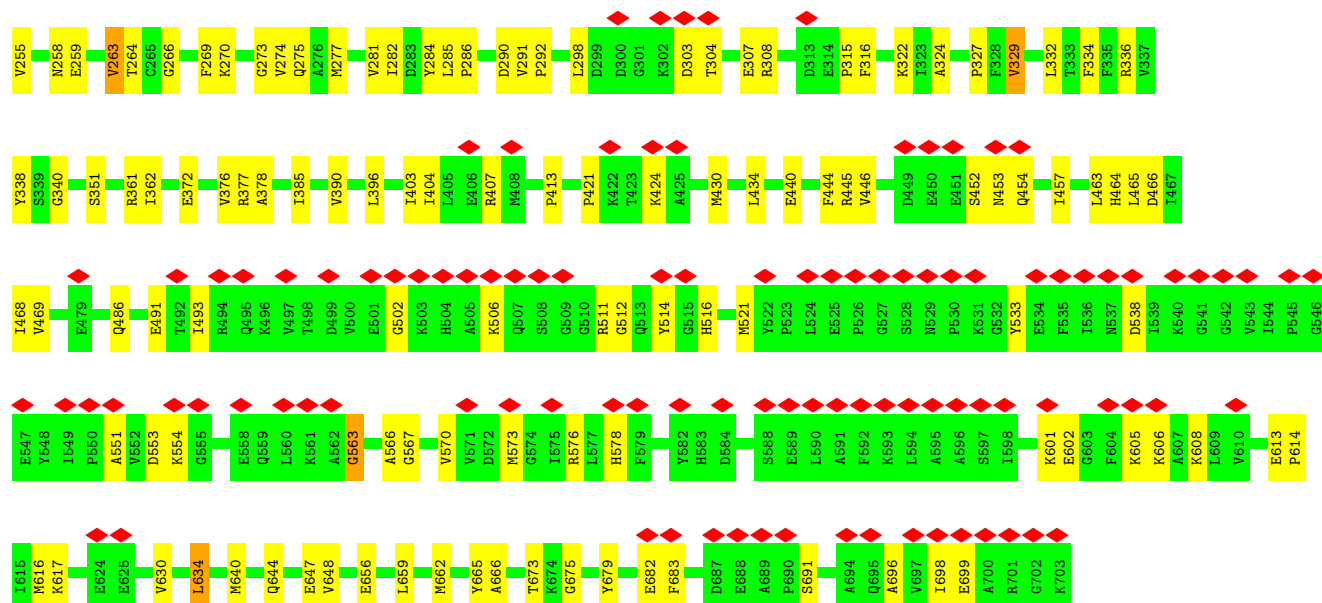


- Molecule 56: A/P-site tRNA(Phe)



- Molecule 57: Elongation factor G





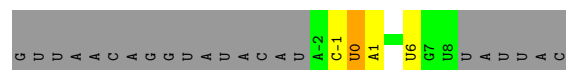
- Molecule 58: Dipeptide (FME-PHE)

Chain y: 100%

There are no outlier residues recorded for this chain.

- Molecule 59: mRNA

Chain z: 21% 9% 67%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20261	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	334.08, 334.08, 334.08	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, G7M, GDP, 2MA, 4SU, 5MU, 5MC, H2U, FME, MA6, PO4, OMU, UR3, ZN, PSU, 3TD, AM2, NA, OMC, MIA, 6MZ, 1MG, 4OC, OMG, 2MG

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	0	0.23	0/450	0.55	0/599
2	1	0.20	0/416	0.56	0/554
3	2	0.18	0/380	0.54	0/498
4	3	0.21	0/513	0.57	0/676
5	4	0.19	0/303	0.58	0/397
6	5	0.16	0/646	0.57	0/898
7	6	0.25	0/531	0.76	0/709
8	A	0.19	1/69266 (0.0%)	0.41	2/108055 (0.0%)
9	B	0.17	0/2873	0.40	0/4478
10	C	0.28	1/2121 (0.0%)	0.61	1/2852 (0.0%)
11	D	0.23	0/1586	0.58	0/2134
12	E	0.20	0/1571	0.50	0/2113
13	F	0.25	0/1434	0.67	0/1926
14	G	0.18	0/1343	0.50	0/1816
15	H	0.24	0/1122	0.70	1/1515 (0.1%)
16	I	0.17	0/692	0.58	0/960
17	J	0.20	0/1152	0.52	0/1551
18	K	0.27	0/947	0.62	0/1268
19	L	0.24	0/1054	0.63	2/1403 (0.1%)
20	M	0.26	0/1093	0.68	1/1460 (0.1%)
21	N	0.23	0/973	0.61	0/1301
22	O	0.21	0/902	0.59	0/1209
23	P	0.22	0/929	0.57	0/1242
24	Q	0.23	0/960	0.53	0/1278
25	R	0.22	0/829	0.60	0/1107
26	S	0.26	0/864	0.67	1/1156 (0.1%)
27	T	0.25	0/744	0.65	0/994
28	U	0.22	0/787	0.69	0/1051
29	V	0.21	0/766	0.61	0/1025
30	W	0.25	0/582	0.59	0/769
31	X	0.22	0/635	0.53	0/848

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Y	0.26	0/510	0.63	0/677
33	Z	0.23	0/453	0.67	0/605
34	a	0.19	1/36725 (0.0%)	0.40	1/57285 (0.0%)
35	b	0.25	0/1735	0.64	0/2338
36	c	0.21	0/1651	0.55	0/2225
37	d	0.25	0/1665	0.64	0/2227
38	e	0.24	0/1154	0.66	0/1554
39	f	0.29	0/835	0.75	4/1128 (0.4%)
40	g	0.26	0/1195	0.71	4/1602 (0.2%)
41	h	0.26	0/989	0.67	0/1326
42	i	0.24	0/1034	0.66	0/1375
43	j	0.23	0/796	0.65	0/1077
44	k	0.21	0/885	0.59	0/1195
45	l	0.28	0/969	0.77	2/1300 (0.2%)
46	m	0.24	0/892	0.67	1/1193 (0.1%)
47	n	0.26	0/811	0.67	0/1081
48	o	0.25	0/722	0.65	0/964
49	p	0.21	0/659	0.60	0/884
50	q	0.22	0/657	0.66	0/881
51	r	0.22	0/544	0.68	2/731 (0.3%)
52	s	0.25	0/675	0.67	0/908
53	t	0.23	0/671	0.53	0/888
54	u	0.26	0/512	0.66	0/683
55	v	0.22	0/1722	0.43	0/2678
56	w	0.27	1/1650 (0.1%)	0.50	0/2569
57	x	0.34	0/5546	0.74	1/7503 (0.0%)
58	y	0.11	0/11	0.35	0/13
59	z	0.19	0/255	0.37	0/394
All	All	0.21	4/164387 (0.0%)	0.48	23/245126 (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
10	C	0	1
13	F	0	1
15	H	0	2
26	S	0	1
27	T	0	2
30	W	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
37	d	0	1
39	f	0	1
42	i	0	2
45	l	0	2
51	r	0	1
57	x	0	1
All	All	0	16

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	30	ALA	C-N	5.57	1.40	1.34
34	a	527	G7M	O3'-P	5.32	1.61	1.56
8	A	2069	G7M	O3'-P	5.26	1.61	1.56
56	w	46	G7M	O3'-P	5.02	1.61	1.56

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	59	ARG	CG-CD-NE	-7.98	94.44	112.00
57	x	563	GLY	N-CA-C	7.45	127.54	112.34
19	L	86	GLU	CA-CB-CG	6.61	127.33	114.10
45	l	24	GLU	CA-CB-CG	6.09	126.28	114.10
26	S	52	GLU	N-CA-CB	6.07	119.05	110.12
51	r	17	VAL	CA-C-N	6.03	133.05	121.54
51	r	17	VAL	C-N-CA	6.03	133.05	121.54
39	f	73	GLU	N-CA-CB	5.99	119.03	110.16
15	H	50	ARG	CA-CB-CG	5.85	125.80	114.10
40	g	110	ARG	CA-CB-CG	5.83	125.77	114.10
45	l	55	ARG	CB-CG-CD	5.83	124.70	111.30
40	g	51	GLN	N-CA-CB	5.64	118.25	110.07
10	C	200	MET	CB-CG-SD	-5.47	96.28	112.70
8	A	894	U	P-O3'-C3'	5.42	128.33	120.20
40	g	51	GLN	CA-CB-CG	5.27	124.64	114.10
40	g	100	MET	CB-CG-SD	5.25	128.45	112.70
34	a	703	G	P-O3'-C3'	5.19	127.98	120.20
39	f	73	GLU	CA-CB-CG	5.16	124.43	114.10
20	M	47	GLU	N-CA-CB	5.16	117.79	110.16
8	A	1328	A	N9-C1'-C2'	5.15	119.73	112.00
39	f	92	THR	CA-C-N	5.11	131.30	121.54
39	f	92	THR	C-N-CA	5.11	131.30	121.54
46	m	82	LEU	CA-CB-CG	5.10	134.14	116.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	C	132	ARG	Sidechain
13	F	147	ARG	Sidechain
15	H	116	ARG	Sidechain
15	H	51	ARG	Sidechain
26	S	11	ARG	Sidechain
27	T	3	ARG	Sidechain
27	T	6	ARG	Sidechain
30	W	10	ARG	Sidechain
37	d	72	ARG	Sidechain
39	f	86	ARG	Sidechain
42	i	123	ARG	Sidechain
42	i	94	ARG	Sidechain
45	l	113	ARG	Sidechain
45	l	85	ARG	Sidechain
51	r	56	ARG	Sidechain
57	x	145	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	444	0	461	15	0
2	1	409	0	440	4	0
3	2	377	0	418	5	0
4	3	504	0	574	7	0
5	4	302	0	340	3	0
6	5	647	0	336	2	0
7	6	522	0	520	9	0
8	A	62338	0	31367	541	0
9	B	2570	0	1301	22	0
10	C	2082	0	2155	46	0
11	D	1565	0	1616	25	0
12	E	1552	0	1619	24	0
13	F	1410	0	1447	28	0
14	G	1323	0	1374	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	H	1111	0	1148	9	0
16	I	693	0	347	6	0
17	J	1129	0	1162	23	0
18	K	938	0	1012	20	0
19	L	1045	0	1117	16	0
20	M	1074	0	1157	23	0
21	N	960	0	1000	12	0
22	O	892	0	923	13	0
23	P	917	0	965	17	0
24	Q	947	0	1022	18	0
25	R	816	0	839	14	0
26	S	857	0	921	16	0
27	T	738	0	807	14	0
28	U	779	0	834	10	0
29	V	753	0	780	7	0
30	W	575	0	592	8	0
31	X	625	0	655	15	0
32	Y	509	0	543	10	0
33	Z	449	0	490	7	0
34	a	33050	0	16653	323	0
35	b	1704	0	1732	30	0
36	c	1624	0	1699	22	0
37	d	1643	0	1710	36	0
38	e	1141	0	1170	36	0
39	f	817	0	808	14	0
40	g	1181	0	1240	22	0
41	h	979	0	1034	25	0
42	i	1022	0	1070	17	0
43	j	786	0	828	19	0
44	k	869	0	878	20	0
45	l	955	0	1019	26	0
46	m	883	0	944	16	0
47	n	799	0	841	18	0
48	o	714	0	737	12	0
49	p	649	0	666	11	0
50	q	648	0	691	12	0
51	r	535	0	552	16	0
52	s	658	0	685	13	0
53	t	665	0	714	9	0
54	u	506	0	502	10	0
55	v	1622	0	831	12	0
56	w	1631	0	835	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	x	5445	0	5420	121	0
58	y	21	0	19	0	0
59	z	230	0	116	2	0
60	0	1	0	0	0	0
60	A	260	0	0	0	0
60	B	7	0	0	0	0
60	C	3	0	0	0	0
60	D	1	0	0	0	0
60	N	1	0	0	0	0
60	O	1	0	0	0	0
60	P	1	0	0	0	0
60	Q	2	0	0	0	0
60	Z	1	0	0	0	0
60	a	86	0	0	0	0
60	m	1	0	0	0	0
60	n	1	0	0	0	0
60	v	1	0	0	0	0
60	w	1	0	0	0	0
60	x	1	0	0	0	0
61	4	1	0	0	0	0
61	6	1	0	0	0	0
62	A	1	0	0	0	0
62	B	1	0	0	0	0
63	a	111	0	123	6	0
64	x	28	0	12	7	0
65	x	5	0	0	0	0
All	All	153146	0	103811	1557	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 6.

All (1557) 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)
56:w:15:G:N2	56:w:59:U:H3	1.63	0.97
8:A:1071:G:H21	8:A:1089:A:N6	1.71	0.87
34:a:765:G:H1	34:a:812:G:HO2'	1.29	0.81
57:x:576:ARG:HH12	57:x:578:HIS:HB2	1.45	0.79
39:f:5:GLU:HB3	39:f:90:MET:HB2	1.65	0.79
8:A:1716:U:H3	8:A:1744:A:H62	1.31	0.78
8:A:1071:G:N2	8:A:1089:A:H61	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2140:G:H1	8:A:2151:U:H3	1.35	0.75
8:A:1071:G:N2	8:A:1089:A:N6	2.35	0.73
34:a:1530:G:N7	54:u:45:LYS:NZ	2.34	0.73
34:a:409:U:H5''	37:d:24:VAL:HG11	1.70	0.73
27:T:69:ARG:NH2	27:T:73:ARG:O	2.23	0.72
39:f:38:ARG:HH12	51:r:23:LYS:HE3	1.54	0.72
8:A:1270:C:H5''	8:A:1271:G:H5'	1.72	0.72
57:x:434:LEU:HB3	57:x:446:VAL:HG21	1.72	0.71
8:A:1102:C:H3'	8:A:1103:A:H8	1.56	0.71
35:b:100:LEU:HB2	35:b:174:GLU:HG2	1.73	0.70
34:a:1375:A:O2'	40:g:101:ARG:NH2	2.24	0.70
8:A:397:U:H5''	31:X:31:ASN:HB2	1.74	0.70
34:a:177:G:OP1	53:t:59:ARG:NH1	2.25	0.70
50:q:63:CYS:HG	50:q:73:THR:HG1	1.40	0.69
12:E:145:ASP:HB2	12:E:166:LYS:HE2	1.74	0.69
37:d:109:THR:HG23	37:d:112:GLU:H	1.58	0.69
47:n:49:GLN:HA	47:n:53:ARG:HH12	1.58	0.69
24:Q:48:ASP:HA	24:Q:51:GLN:HB2	1.74	0.68
34:a:501:C:OP1	45:l:113:ARG:NH2	2.27	0.68
5:4:1:MET:N	8:A:2526:G:N3	2.41	0.68
57:x:17:HIS:HA	57:x:121:GLN:HB2	1.75	0.68
38:e:54:GLU:HG3	38:e:56:PRO:HD2	1.75	0.67
46:m:95:PRO:HG2	46:m:101:THR:HG22	1.76	0.67
34:a:127:G:O2'	50:q:5:ARG:NH2	2.27	0.67
8:A:1779:U:OP2	8:A:1784:A:N6	2.27	0.67
25:R:2:TYR:H	25:R:42:ALA:HB3	1.60	0.66
34:a:344:A:OP1	57:x:38:LYS:NZ	2.27	0.66
8:A:1936:A:H2	8:A:1943:U:H3	1.42	0.66
4:3:32:LEU:HD12	4:3:40:LYS:HD3	1.78	0.66
10:C:200:MET:SD	10:C:200:MET:N	2.68	0.66
34:a:1522:U:OP1	44:k:127:ARG:NH1	2.28	0.66
1:0:21:LEU:HD11	26:S:41:LYS:HE3	1.78	0.65
8:A:475:C:O2	8:A:479:A:N6	2.29	0.65
34:a:742:G:OP1	48:o:57:ARG:NH2	2.29	0.65
8:A:250:G:OP2	19:L:59:ARG:NH2	2.30	0.65
8:A:99:U:O2	28:U:6:ARG:NH1	2.30	0.65
34:a:436:C:O2	37:d:153:ARG:NH2	2.30	0.65
34:a:1297:G:N2	40:g:113:LYS:O	2.29	0.65
38:e:15:ILE:HD11	38:e:37:VAL:HG22	1.77	0.65
38:e:156:ARG:NH2	41:h:42:GLU:O	2.29	0.65
40:g:67:ASN:HD21	40:g:127:ALA:HA	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:x:21:GLY:HA3	57:x:141:ASN:HD22	1.62	0.65
8:A:627:A:H5''	19:L:78:ARG:HH22	1.62	0.65
8:A:780:G:N1	10:C:228:ASP:OD2	2.25	0.65
34:a:1497:G:H1'	34:a:1518:MA6:H2	1.78	0.65
34:a:1500:A:H5''	34:a:1508:A:H5''	1.79	0.65
34:a:1491:G:N2	63:a:1663:AM2:OB6	2.30	0.65
34:a:722:G:H1	34:a:733:G:H1	1.42	0.64
34:a:516:PSU:OP2	57:x:511:ARG:NH2	2.31	0.64
8:A:793:A:OP2	8:A:2071:A:O2'	2.15	0.64
8:A:2676:C:OP1	18:K:31:ARG:NH2	2.30	0.64
20:M:73:ILE:HD11	20:M:93:VAL:HG22	1.78	0.64
46:m:10:ASP:O	46:m:11:HIS:ND1	2.30	0.64
8:A:279:A:H8	8:A:361:G:H21	1.44	0.64
10:C:107:LYS:HD2	10:C:195:GLY:HA2	1.78	0.64
8:A:2032:G:N2	11:D:151:THR:OG1	2.31	0.64
12:E:147:LEU:HB3	12:E:186:VAL:HG12	1.78	0.64
34:a:993:G:O2'	34:a:994:A:N7	2.31	0.64
34:a:1009:U:H3	34:a:1020:G:H1	1.46	0.64
57:x:27:GLU:HG2	57:x:49:MET:HE1	1.78	0.64
12:E:108:ILE:HD11	12:E:181:ILE:HB	1.80	0.63
42:i:115:VAL:HG11	43:j:62:ARG:HB2	1.80	0.63
57:x:49:MET:SD	57:x:49:MET:N	2.71	0.63
9:B:77:U:OP1	29:V:21:ARG:NH2	2.29	0.63
34:a:921:U:O2	38:e:23:THR:OG1	2.16	0.63
38:e:14:LEU:HD11	38:e:34:ALA:HB1	1.81	0.63
56:w:15:G:H22	56:w:59:U:H3	1.41	0.63
45:l:24:GLU:OE1	45:l:58:ASN:ND2	2.32	0.63
40:g:26:VAL:HG22	40:g:42:VAL:HG11	1.79	0.63
45:l:99:GLY:HA3	45:l:117:GLY:HA3	1.81	0.63
57:x:602:GLU:OE1	57:x:606:LYS:NZ	2.31	0.63
33:Z:15:ARG:HG3	33:Z:53:MET:HE1	1.81	0.62
8:A:75:G:H22	8:A:111:A:H2	1.47	0.62
8:A:994:C:OP1	24:Q:52:ARG:NH2	2.32	0.62
8:A:2131:U:H4'	8:A:2133:G:H4'	1.82	0.62
8:A:1799:G:OP1	10:C:257:ARG:NH1	2.32	0.62
8:A:2618:G:H21	11:D:155:VAL:HG21	1.63	0.62
43:j:36:VAL:HG22	43:j:38:GLY:H	1.64	0.62
8:A:1042:G:H1	8:A:1113:U:H3	1.47	0.62
27:T:91:GLN:NE2	27:T:92:ASN:O	2.33	0.62
37:d:10:LEU:HG	37:d:62:ARG:HE	1.65	0.62
38:e:9:GLU:HG2	38:e:10:LEU:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:x:329:VAL:HG21	57:x:385:ILE:HG23	1.81	0.62
10:C:143:VAL:HB	10:C:153:LEU:HB2	1.82	0.62
28:U:33:VAL:HG13	28:U:66:VAL:HG22	1.82	0.62
8:A:1668:A:N1	8:A:1676:A:N6	2.47	0.62
34:a:1004:A:H62	34:a:1024:G:H2'	1.63	0.62
57:x:390:VAL:HG21	57:x:396:LEU:HD11	1.81	0.62
42:i:56:MET:HG2	42:i:57:VAL:HG23	1.80	0.62
12:E:170:ARG:NH2	12:E:176:ASP:OD2	2.32	0.62
56:w:48:C:N4	56:w:59:U:C4	2.68	0.62
57:x:93:ASP:HB3	57:x:464:HIS:HB2	1.81	0.62
57:x:104:VAL:O	57:x:336:ARG:NH1	2.33	0.61
8:A:574:A:N6	8:A:2034:U:OP1	2.34	0.61
35:b:93:HIS:ND1	35:b:145:ASN:O	2.33	0.61
38:e:83:PRO:HD2	41:h:96:ALA:HB2	1.82	0.61
8:A:320:A:N3	12:E:163:ASN:ND2	2.47	0.61
52:s:24:SER:O	52:s:27:LYS:NZ	2.33	0.61
8:A:78:U:H3	8:A:108:G:H1	1.46	0.61
34:a:826:C:O2	41:h:15:ASN:ND2	2.33	0.61
34:a:1494:G:N7	63:a:1663:AM2:NC6	2.48	0.61
10:C:28:PRO:HG2	10:C:33:LEU:HD11	1.82	0.61
8:A:242:G:N2	8:A:255:A:OP2	2.30	0.61
8:A:2728:U:H2'	8:A:2729:G:H8	1.65	0.61
34:a:1524:C:OP1	44:k:121:ARG:NH2	2.33	0.61
34:a:1081:A:OP2	38:e:51:LYS:NZ	2.34	0.61
36:c:134:LYS:O	36:c:138:GLN:NE2	2.34	0.61
34:a:310:G:H5''	49:p:31:ARG:HB2	1.83	0.61
34:a:984:C:N3	34:a:1222:G:N2	2.48	0.61
37:d:201:GLU:OE1	38:e:111:ARG:NH1	2.34	0.61
8:A:566:U:OP1	19:L:29:LYS:NZ	2.34	0.61
8:A:1417:C:O2'	8:A:1587:G:O2'	2.19	0.61
10:C:109:LEU:HD21	10:C:115:ILE:HD11	1.83	0.61
8:A:301:G:O5'	28:U:81:ARG:NH2	2.33	0.60
34:a:851:G:O6	63:a:1614:AM2:NA2	2.34	0.60
38:e:37:VAL:HG11	38:e:113:VAL:HG22	1.83	0.60
1:0:12:ARG:NH2	8:A:517:C:OP1	2.34	0.60
8:A:279:A:H5''	8:A:361:G:H22	1.67	0.60
8:A:529:A:OP2	17:J:116:ARG:NH2	2.33	0.60
8:A:629:G:N3	8:A:639:U:O2'	2.33	0.60
34:a:1180:A:OP2	42:i:98:ARG:NH2	2.33	0.60
57:x:144:ASP:O	57:x:175:GLU:HB2	2.01	0.60
34:a:1149:C:H2'	34:a:1150:A:H8	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:x:1:ALA:HB1	57:x:377:ARG:HH22	1.65	0.60
57:x:616:MET:HG3	57:x:683:PHE:HA	1.84	0.60
34:a:776:G:N2	34:a:802:A:OP2	2.34	0.60
8:A:918:A:N3	9:B:80:U:O2'	2.33	0.60
8:A:2816:G:N3	8:A:2883:A:O2'	2.32	0.60
57:x:191:ASN:ND2	57:x:204:GLU:OE2	2.28	0.60
8:A:716:A:OP2	48:o:88:ARG:NH2	2.33	0.60
8:A:781:A:O2'	8:A:1788:C:O2	2.20	0.60
8:A:995:C:O2	17:J:3:THR:OG1	2.19	0.60
8:A:1087:G:N3	8:A:1102:C:N4	2.50	0.60
8:A:2692:G:H1'	8:A:2847:U:H1'	1.82	0.60
34:a:1295:U:O2'	34:a:1302:C:N4	2.34	0.60
8:A:1798:U:OP2	10:C:270:ARG:NH2	2.35	0.60
9:B:30:C:H1'	9:B:57:A:H61	1.66	0.60
11:D:1:MET:HE1	11:D:100:LEU:HD21	1.84	0.60
31:X:31:ASN:HD22	31:X:52:ALA:HB2	1.65	0.60
35:b:8:MET:HG3	35:b:9:LEU:H	1.66	0.60
40:g:41:ILE:HG21	40:g:115:MET:HE2	1.83	0.60
57:x:142:LYS:HG2	64:x:801:GDP:C6	2.37	0.60
3:2:26:ASN:HD21	8:A:682:G:H5''	1.67	0.60
14:G:85:LYS:NZ	14:G:129:GLU:OE1	2.35	0.60
45:l:113:ARG:HG3	45:l:118:VAL:HB	1.84	0.60
57:x:493:ILE:HD13	57:x:521:MET:HE3	1.83	0.60
8:A:307:G:O6	28:U:18:LYS:NZ	2.34	0.59
8:A:340:A:O2'	12:E:162:ARG:NH2	2.35	0.59
34:a:1086:U:H3	34:a:1099:G:H22	1.49	0.59
34:a:1179:A:OP2	42:i:98:ARG:NH1	2.35	0.59
17:J:92:MET:SD	17:J:95:ARG:NH2	2.75	0.59
34:a:481:G:O2'	34:a:483:C:N4	2.35	0.59
57:x:444:PHE:HE1	57:x:457:ILE:HG23	1.67	0.59
34:a:812:G:OP1	34:a:902:G:N2	2.36	0.59
57:x:316:PHE:HA	57:x:340:GLY:HA3	1.83	0.59
9:B:52:A:N7	22:O:33:ARG:NH1	2.51	0.59
34:a:1060:U:H2'	34:a:1061:G:H8	1.67	0.59
44:k:92:ARG:HH22	54:u:28:LEU:HD13	1.68	0.59
8:A:848:C:H2'	8:A:849:A:H8	1.68	0.59
8:A:2139:U:C4	8:A:2152:G:O6	2.55	0.59
8:A:2439:A:N6	8:A:2585:U:O2'	2.36	0.59
10:C:259:ASN:ND2	10:C:262:THR:OG1	2.36	0.59
34:a:516:PSU:H5'	57:x:511:ARG:HH22	1.68	0.59
8:A:577:G:O2'	8:A:1254:A:OP1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:s:30:LEU:HB3	52:s:48:ILE:HG22	1.85	0.58
8:A:324:A:OP2	8:A:1205:A:N6	2.36	0.58
34:a:238:A:OP1	50:q:39:ARG:NH2	2.36	0.58
34:a:427:U:OP1	37:d:12:ARG:NH2	2.35	0.58
34:a:673:A:H2'	34:a:674:G:C8	2.38	0.58
1:0:9:ARG:NH2	8:A:516:C:OP1	2.36	0.58
34:a:1241:G:H2'	34:a:1242:G:H8	1.68	0.58
2:1:5:ARG:NH1	8:A:2285:C:OP2	2.35	0.58
8:A:1392:A:H61	27:T:18:GLU:HG3	1.68	0.58
43:j:63:ASP:OD1	47:n:98:LYS:NZ	2.32	0.58
12:E:119:ILE:HB	12:E:187:VAL:HG22	1.85	0.58
27:T:1:MET:SD	27:T:3:ARG:NH2	2.77	0.58
44:k:63:GLN:HG3	44:k:98:ALA:HB2	1.84	0.58
1:0:53:VAL:HG23	1:0:54:ILE:HG23	1.85	0.58
8:A:447:A:OP1	24:Q:4:LYS:NZ	2.36	0.58
8:A:1754:A:N1	8:A:2716:C:O2'	2.34	0.58
8:A:2743:U:OP2	8:A:2755:C:N4	2.36	0.58
34:a:1209:C:O2'	34:a:1214:C:N4	2.37	0.58
45:l:67:GLY:O	45:l:98:ARG:NH1	2.36	0.58
8:A:463:G:N2	8:A:466:A:OP2	2.30	0.58
8:A:974:G:O2'	8:A:989:G:N2	2.37	0.58
34:a:2:A:N3	34:a:613:C:O2'	2.37	0.58
34:a:1000:A:N6	34:a:1041:G:O6	2.37	0.58
34:a:768:A:N3	34:a:1512:U:O2'	2.36	0.58
34:a:985:C:O2'	52:s:54:ARG:NH1	2.36	0.58
8:A:494:G:H4'	26:S:6:LYS:HB2	1.85	0.58
15:H:30:LEU:HB3	15:H:36:ALA:HB3	1.84	0.58
34:a:1115:U:H5'	43:j:68:ARG:HH22	1.69	0.58
37:d:115:GLN:O	37:d:119:HIS:ND1	2.34	0.58
8:A:143:C:H2'	8:A:144:A:H8	1.69	0.57
10:C:161:VAL:HG12	10:C:175:LEU:HA	1.86	0.57
15:H:78:VAL:HG21	15:H:103:VAL:HG22	1.85	0.57
34:a:552:U:H2'	34:a:553:A:H8	1.69	0.57
57:x:351:SER:HB2	57:x:403:ILE:HA	1.85	0.57
8:A:659:G:O2'	12:E:95:LYS:O	2.22	0.57
8:A:987:C:O2'	8:A:1000:A:N3	2.33	0.57
34:a:356:A:N3	34:a:368:U:O2'	2.35	0.57
57:x:21:GLY:HA3	57:x:141:ASN:ND2	2.19	0.57
8:A:1474:U:H3	8:A:1517:G:H1	1.51	0.57
37:d:183:ARG:HB3	37:d:183:ARG:HH11	1.69	0.57
8:A:1080:A:O2'	8:A:1082:U:O4	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1992:G:N2	8:A:1996:C:O2'	2.38	0.57
8:A:2780:G:O6	17:J:99:ARG:NH1	2.37	0.57
34:a:875:U:O2'	41:h:14:ARG:NH1	2.37	0.57
8:A:2127:G:N2	8:A:2128:G:O6	2.37	0.57
14:G:88:LEU:HD12	14:G:128:THR:HA	1.86	0.57
34:a:210:C:HO2'	34:a:211:G:H21	1.51	0.57
8:A:714:U:OP2	48:o:88:ARG:NH1	2.35	0.57
8:A:1816:C:N4	10:C:34:GLU:OE1	2.35	0.57
37:d:121:ALA:HA	37:d:145:ARG:HG3	1.87	0.57
41:h:110:MET:HE3	41:h:115:ALA:HA	1.87	0.57
35:b:56:LEU:HD23	35:b:59:ILE:HD11	1.87	0.57
57:x:666:ALA:HB2	57:x:679:TYR:HE1	1.68	0.57
8:A:1791:A:N6	8:A:1828:G:O2'	2.30	0.57
8:A:1829:A:N3	10:C:14:HIS:NE2	2.52	0.57
34:a:553:A:H5''	45:l:20:VAL:HG21	1.86	0.57
44:k:113:THR:O	51:r:72:ARG:NH1	2.28	0.57
8:A:1248:G:OP1	12:E:44:ARG:NH1	2.36	0.57
25:R:24:LYS:HA	25:R:94:THR:HG23	1.87	0.57
8:A:2661:G:H4'	57:x:18:ILE:HD13	1.86	0.56
11:D:48:ILE:HG23	11:D:84:LEU:HD21	1.87	0.56
31:X:5:GLN:NE2	31:X:75:GLU:OE2	2.37	0.56
31:X:17:ARG:HH11	31:X:23:ALA:HB2	1.69	0.56
8:A:2874:C:OP1	21:N:4:ARG:NH1	2.38	0.56
34:a:1175:G:H2'	34:a:1176:A:H8	1.69	0.56
38:e:152:VAL:HG22	38:e:155:LYS:HZ3	1.70	0.56
34:a:401:C:OP2	37:d:69:ARG:NH2	2.38	0.56
34:a:835:U:O4	63:a:1614:AM2:NA2	2.39	0.56
34:a:1492:A:N6	45:l:46:SER:OG	2.39	0.56
35:b:41:ASN:HD22	35:b:44:LYS:HB2	1.70	0.56
38:e:81:GLN:H	38:e:146:MET:HE3	1.70	0.56
42:i:3:ASN:OD1	42:i:4:GLN:N	2.38	0.56
57:x:142:LYS:HD2	57:x:145:ARG:HD3	1.88	0.56
8:A:2126:A:N3	8:A:2173:A:N6	2.53	0.56
10:C:244:VAL:HG12	10:C:250:GLN:HA	1.87	0.56
40:g:149:ALA:HA	44:k:60:PHE:HB3	1.88	0.56
8:A:693:A:O2'	8:A:1353:A:N3	2.32	0.56
8:A:2646:C:OP2	8:A:2732:G:O2'	2.24	0.56
34:a:1344:C:OP1	42:i:123:ARG:NH1	2.39	0.56
46:m:14:ALA:HA	46:m:44:ILE:HD11	1.87	0.56
7:6:28:VAL:HG12	13:F:139:GLU:HA	1.88	0.56
34:a:1074:G:OP1	38:e:68:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1386:C:H2'	8:A:1387:A:C8	2.41	0.56
8:A:1927:A:H2'	8:A:1928:A:C8	2.41	0.56
8:A:1995:U:OP1	11:D:128:ARG:NH2	2.30	0.56
8:A:2450:A:N6	8:A:2501:C:O2	2.39	0.56
57:x:132:TYR:OH	57:x:407:ARG:NH1	2.38	0.56
13:F:110:ILE:HB	13:F:113:PHE:HB2	1.88	0.56
23:P:87:ARG:NH2	23:P:109:ILE:O	2.39	0.56
26:S:4:ILE:HG12	26:S:106:VAL:HG22	1.88	0.56
55:v:8:4SU:O2'	55:v:21:A:N1	2.35	0.56
8:A:2898:U:O2'	17:J:136:GLN:NE2	2.37	0.56
34:a:1218:C:H2'	34:a:1219:A:C8	2.41	0.56
8:A:1597:A:H5'	8:A:1598:A:H5'	1.88	0.55
10:C:4:LYS:NZ	10:C:13:ARG:O	2.39	0.55
10:C:92:LEU:HD11	10:C:100:ARG:HB3	1.88	0.55
34:a:1001:C:H2'	34:a:1002:G:H8	1.70	0.55
38:e:12:GLU:HG2	38:e:38:VAL:HG12	1.88	0.55
48:o:73:ASP:N	48:o:73:ASP:OD1	2.36	0.55
8:A:396:G:OP2	31:X:9:LYS:NZ	2.39	0.55
8:A:2627:G:N2	8:A:2777:G:OP2	2.35	0.55
34:a:309:A:O2'	34:a:607:A:N1	2.38	0.55
37:d:8:LEU:HD13	37:d:31:CYS:HB3	1.87	0.55
38:e:44:ARG:NH1	38:e:72:ASN:OD1	2.39	0.55
57:x:99:GLU:HG2	57:x:407:ARG:HH12	1.69	0.55
24:Q:71:ASN:HB3	24:Q:109:VAL:HG11	1.89	0.55
34:a:539:A:OP2	45:l:111:GLN:NE2	2.35	0.55
49:p:6:LEU:HB3	49:p:17:TYR:HB3	1.87	0.55
4:3:44:ARG:NH1	8:A:2350:C:OP2	2.39	0.55
8:A:489:G:N2	8:A:1320:C:OP1	2.35	0.55
24:Q:66:ALA:O	24:Q:70:GLN:NE2	2.40	0.55
35:b:65:LYS:HE2	35:b:157:PRO:HA	1.88	0.55
8:A:2728:U:H2'	8:A:2729:G:C8	2.42	0.55
12:E:6:LYS:HG2	12:E:121:VAL:HG12	1.89	0.55
34:a:972:C:OP2	43:j:59:LYS:NZ	2.37	0.55
34:a:1218:C:H2'	34:a:1219:A:H8	1.72	0.55
11:D:9:VAL:HG11	23:P:3:ILE:HD13	1.89	0.55
23:P:90:ALA:HB3	23:P:110:LYS:HG3	1.89	0.55
34:a:210:C:O2'	34:a:211:G:N2	2.37	0.55
8:A:1664:A:N3	18:K:67:LYS:NZ	2.51	0.55
32:Y:9:LYS:HD2	32:Y:14:LEU:HB3	1.88	0.55
53:t:34:VAL:HG11	53:t:78:LEU:HD13	1.89	0.55
57:x:10:ARG:NH2	57:x:282:ILE:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:c:13:ILE:HG22	36:c:14:VAL:HG13	1.88	0.55
35:b:119:GLN:HA	35:b:123:GLY:HA3	1.88	0.55
8:A:84:A:H62	8:A:101:A:H2	1.55	0.54
8:A:250:G:H5'	19:L:59:ARG:NH2	2.22	0.54
8:A:334:C:O2'	28:U:81:ARG:NH2	2.41	0.54
8:A:807:U:O2'	8:A:2060:A:N1	2.37	0.54
8:A:1278:C:H2'	8:A:1279:G:H8	1.72	0.54
11:D:16:THR:OG1	11:D:18:ASP:OD1	2.24	0.54
36:c:46:LEU:HB3	36:c:49:ALA:HB3	1.89	0.54
8:A:1900:A:H1'	8:A:1970:A:H2'	1.89	0.54
19:L:51:GLU:OE1	19:L:54:GLN:NE2	2.41	0.54
19:L:108:ALA:HB3	19:L:125:LEU:HD22	1.88	0.54
24:Q:49:ARG:O	24:Q:53:LYS:NZ	2.40	0.54
34:a:401:C:O2'	34:a:621:A:N3	2.35	0.54
34:a:1211:U:H5'	34:a:1212:U:H5'	1.88	0.54
8:A:1187:G:OP1	25:R:85:LYS:NZ	2.39	0.54
8:A:1445:G:O6	8:A:1466:U:O2	2.25	0.54
10:C:56:GLY:HA2	10:C:212:TRP:HA	1.89	0.54
14:G:174:LYS:HE2	14:G:176:LYS:HG2	1.88	0.54
15:H:50:ARG:HH11	15:H:51:ARG:HB2	1.72	0.54
20:M:25:ASP:O	20:M:66:ARG:NH1	2.40	0.54
8:A:2469:A:N6	8:A:2481:G:O2'	2.39	0.54
9:B:14:U:OP2	9:B:70:C:O2'	2.25	0.54
22:O:111:ARG:NH2	22:O:117:PHE:OXT	2.40	0.54
8:A:1913:A:N1	56:w:37:MIA:O2'	2.39	0.54
10:C:116:GLN:O	10:C:127:ASN:ND2	2.37	0.54
20:M:17:ASN:O	20:M:38:ARG:NH1	2.39	0.54
34:a:1445:U:H3	34:a:1457:G:H1	1.56	0.54
42:i:118:ARG:HB2	42:i:122:ARG:HB3	1.89	0.54
43:j:65:TYR:HB3	47:n:96:LEU:HD11	1.89	0.54
8:A:781:A:OP1	10:C:216:ARG:NH2	2.38	0.54
8:A:1918:A:O2'	8:A:1920:C:N4	2.39	0.54
8:A:2295:C:OP2	22:O:9:ARG:NH2	2.40	0.54
9:B:90:C:H5''	20:M:18:ARG:HG2	1.90	0.54
34:a:674:G:H2'	34:a:675:A:H8	1.73	0.54
47:n:86:GLU:OE1	47:n:90:ARG:NH2	2.41	0.54
11:D:124:ARG:HG3	11:D:165:MET:HB3	1.89	0.54
21:N:77:ALA:O	21:N:81:ASN:HB2	2.08	0.54
34:a:1506:U:O2	44:k:127:ARG:NH1	2.41	0.54
36:c:19:SER:OG	36:c:39:ARG:NH2	2.40	0.54
37:d:187:ARG:O	37:d:187:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:o:44:GLU:OE1	48:o:45:HIS:ND1	2.40	0.54
57:x:696:ALA:HA	57:x:699:GLU:HG2	1.90	0.54
8:A:1339:G:H5''	27:T:19:LYS:HD3	1.90	0.54
8:A:1386:C:H2'	8:A:1387:A:H8	1.73	0.54
8:A:2898:U:O2'	17:J:134:ALA:O	2.24	0.54
34:a:393:A:OP2	49:p:12:LYS:NZ	2.31	0.54
10:C:144:GLU:HB2	10:C:187:CYS:HB3	1.90	0.54
34:a:473:U:H2'	34:a:474:G:H8	1.72	0.54
40:g:110:ARG:NH2	40:g:122:GLU:OE2	2.41	0.54
8:A:1076:C:N4	8:A:1078:U:O4	2.41	0.54
8:A:1432:G:H2'	8:A:1433:A:C8	2.43	0.54
9:B:48:U:OP2	22:O:30:ARG:NH2	2.41	0.54
10:C:131:MET:HE1	10:C:140:VAL:HG21	1.89	0.54
34:a:923:A:O2'	34:a:1399:C:OP2	2.24	0.54
8:A:1734:G:H2'	8:A:1735:A:H8	1.73	0.53
18:K:23:LYS:HB3	18:K:40:LYS:HB3	1.90	0.53
35:b:166:ASP:HB3	35:b:190:SER:HA	1.90	0.53
34:a:713:G:H2'	34:a:714:G:C8	2.43	0.53
57:x:103:ARG:NH1	57:x:338:TYR:OH	2.40	0.53
8:A:2220:U:H4'	15:H:97:ARG:HH12	1.73	0.53
4:3:44:ARG:NH2	8:A:2349:G:OP1	2.41	0.53
8:A:1131:G:N2	8:A:1132:U:O4	2.37	0.53
8:A:1138:G:H21	17:J:108:MET:HE2	1.74	0.53
8:A:2006:C:O2'	8:A:2823:A:N3	2.41	0.53
8:A:2245:U:H5''	8:A:2246:G:H5'	1.90	0.53
13:F:28:PRO:HB2	13:F:168:LEU:HD22	1.89	0.53
13:F:115:GLY:O	13:F:177:ARG:NH1	2.41	0.53
34:a:1064:G:H21	34:a:1190:G:H1'	1.74	0.53
8:A:2333:A:OP2	30:W:73:ARG:NH2	2.37	0.53
13:F:130:GLY:HA2	13:F:152:ASP:HA	1.91	0.53
17:J:31:GLU:HB3	17:J:142:ILE:HD12	1.91	0.53
35:b:113:LEU:HD13	35:b:143:LEU:HD22	1.89	0.53
37:d:92:LEU:HA	37:d:135:GLN:HE22	1.74	0.53
38:e:104:ILE:HD13	38:e:115:GLU:HG2	1.90	0.53
8:A:560:C:O2'	24:Q:47:ARG:NH2	2.41	0.53
10:C:65:ASP:HB2	10:C:101:ARG:HG2	1.90	0.53
34:a:358:U:O2'	57:x:327:PRO:O	2.27	0.53
8:A:1070:A:H61	16:I:26:ALA:HB3	1.73	0.53
8:A:2314:A:OP1	13:F:87:LYS:NZ	2.42	0.53
12:E:117:ARG:NH2	12:E:183:PHE:O	2.42	0.53
41:h:10:LEU:HD22	41:h:74:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:k:97:ARG:NH1	54:u:12:ASP:OD1	2.41	0.53
57:x:602:GLU:HA	57:x:605:LYS:HZ3	1.74	0.53
10:C:68:ARG:O	10:C:188:ARG:NH2	2.41	0.53
19:L:132:ARG:NH2	19:L:144:GLU:OE1	2.42	0.53
32:Y:9:LYS:HG3	32:Y:14:LEU:HD23	1.91	0.53
34:a:719:C:O2'	51:r:38:ILE:O	2.25	0.53
34:a:979:C:H41	34:a:1360:A:H62	1.57	0.53
8:A:1070:A:N7	8:A:1095:A:O2'	2.42	0.53
8:A:1081:U:H3	16:I:118:GLY:HA3	1.73	0.53
8:A:1682:G:OP2	8:A:1699:G:N2	2.42	0.53
8:A:1801:A:H5''	8:A:2203:U:H2'	1.91	0.53
30:W:55:LEU:HD12	30:W:76:ILE:HD12	1.91	0.53
34:a:694:A:H5''	44:k:54:SER:HB3	1.90	0.53
56:w:43:C:H2'	56:w:44:G:C8	2.44	0.53
11:D:45:TYR:OH	11:D:81:GLU:OE2	2.27	0.52
13:F:113:PHE:HZ	13:F:175:PRO:HG2	1.74	0.52
27:T:69:ARG:HH12	27:T:74:ILE:HD12	1.74	0.52
34:a:796:C:H4'	44:k:126:ARG:HH21	1.74	0.52
47:n:66:GLN:OE1	47:n:66:GLN:N	2.42	0.52
8:A:1138:G:N2	17:J:108:MET:HE2	2.24	0.52
8:A:2081:U:H2'	8:A:2082:A:H8	1.74	0.52
55:v:26:G:H1	55:v:44:A:H61	1.57	0.52
57:x:12:ILE:HD12	57:x:285:LEU:HD13	1.91	0.52
8:A:807:U:O2	12:E:69:ARG:NH2	2.43	0.52
8:A:990:A:N1	25:R:78:ARG:NH2	2.47	0.52
8:A:2142:A:N6	8:A:2150:C:O2'	2.43	0.52
9:B:8:C:O3'	22:O:25:ARG:NH2	2.42	0.52
8:A:1056:G:N3	8:A:1087:G:N1	2.58	0.52
8:A:1724:G:O6	8:A:1737:G:N2	2.40	0.52
41:h:35:ILE:HG13	41:h:102:VAL:HG11	1.92	0.52
8:A:1266:G:O2'	8:A:2012:G:O6	2.27	0.52
8:A:1429:G:H2'	8:A:1430:G:H8	1.74	0.52
8:A:2304:G:H22	8:A:2312:U:H3	1.57	0.52
37:d:14:GLU:OE2	37:d:62:ARG:NH1	2.42	0.52
40:g:78:ARG:HD3	40:g:83:THR:HG22	1.90	0.52
8:A:68:G:N2	8:A:74:A:OP2	2.43	0.52
8:A:568:U:H1'	8:A:2030:6MZ:H9C1	1.91	0.52
8:A:1153:C:OP1	24:Q:91:ARG:NH2	2.34	0.52
18:K:80:ASP:HB3	23:P:67:GLU:HB2	1.91	0.52
34:a:766:A:OP2	34:a:812:G:N2	2.42	0.52
8:A:1086:A:OP1	8:A:1087:G:N2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1187:G:N2	8:A:1188:U:O4	2.43	0.52
8:A:2595:G:N2	8:A:2598:A:OP2	2.35	0.52
10:C:4:LYS:HD2	10:C:16:VAL:HG22	1.91	0.52
12:E:10:SER:OG	12:E:11:ALA:N	2.41	0.52
14:G:27:GLY:HA3	14:G:78:VAL:HB	1.92	0.52
33:Z:15:ARG:O	33:Z:20:LYS:NZ	2.42	0.52
34:a:1287:A:H2	34:a:1353:G:H1'	1.75	0.52
57:x:18:ILE:HG12	57:x:91:HIS:HD2	1.75	0.52
57:x:221:LEU:HD11	57:x:251:LEU:HD11	1.91	0.52
57:x:308:ARG:NH2	57:x:315:PRO:O	2.42	0.52
8:A:371:A:N3	31:X:60:LYS:NZ	2.52	0.52
34:a:1125:U:H2'	34:a:1126:U:H2'	1.91	0.52
41:h:101:ALA:HB3	41:h:112:ASP:HB3	1.91	0.52
57:x:269:PHE:HB2	64:x:801:GDP:C5	2.45	0.52
1:O:3:GLN:NE2	8:A:2016:U:O2	2.42	0.52
20:M:109:PRO:HD2	20:M:112:LEU:HD13	1.92	0.52
36:c:32:LEU:HD11	47:n:93:ILE:HG12	1.91	0.52
45:l:52:CYS:HB3	45:l:66:ILE:HD11	1.90	0.52
8:A:601:C:O2'	12:E:99:LYS:NZ	2.40	0.52
8:A:837:C:N3	8:A:941:A:N6	2.57	0.52
8:A:2682:A:H61	8:A:2728:U:H1'	1.75	0.52
8:A:2899:A:H2'	8:A:2900:A:H8	1.75	0.52
18:K:3:GLN:O	18:K:6:THR:OG1	2.16	0.52
18:K:49:ARG:HH22	34:a:1423:G:H5''	1.74	0.52
34:a:562:U:H5''	34:a:563:A:C5	2.45	0.52
57:x:274:VAL:HA	57:x:277:MET:HG3	1.92	0.52
8:A:247:G:OP2	8:A:249:C:N4	2.43	0.51
8:A:1323:C:OP1	26:S:98:LYS:NZ	2.33	0.51
8:A:2079:U:O2'	31:X:22:ASN:ND2	2.43	0.51
41:h:13:ILE:HD11	41:h:60:LEU:HD22	1.93	0.51
50:q:63:CYS:SG	50:q:73:THR:OG1	2.57	0.51
52:s:63:ASP:OD1	52:s:63:ASP:N	2.39	0.51
8:A:2144:G:O2'	8:A:2147:A:N6	2.35	0.51
12:E:46:GLN:O	12:E:88:ARG:NH2	2.43	0.51
23:P:89:GLY:O	23:P:112:ARG:NH1	2.43	0.51
45:l:29:LYS:NZ	45:l:57:THR:OG1	2.41	0.51
8:A:883:G:N2	8:A:884:U:O2'	2.43	0.51
8:A:2183:A:H2'	8:A:2184:A:C8	2.46	0.51
8:A:2391:G:O2'	8:A:2429:G:N2	2.42	0.51
57:x:322:LYS:HB3	57:x:334:PHE:HB2	1.91	0.51
4:3:53:ASP:OD2	8:A:2359:C:O2'	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1666:G:H4'	18:K:6:THR:HG22	1.91	0.51
29:V:20:LEU:HD22	29:V:25:LYS:HB2	1.92	0.51
34:a:1522:U:H2'	34:a:1523:G:H8	1.76	0.51
8:A:2636:C:HO2'	11:D:45:TYR:HH	1.42	0.51
34:a:227:G:O2'	49:p:63:GLN:NE2	2.38	0.51
50:q:22:VAL:HG21	50:q:60:ILE:HD13	1.91	0.51
55:v:33:U:O2'	55:v:35:A:OP2	2.25	0.51
3:2:9:VAL:HG22	3:2:12:ARG:HH12	1.76	0.51
8:A:511:U:H4'	8:A:1235:G:H4'	1.92	0.51
8:A:2602:A:H8	56:w:74:C:H5''	1.75	0.51
29:V:77:VAL:HG22	29:V:89:ILE:HG12	1.93	0.51
32:Y:2:LYS:N	32:Y:5:GLU:OE1	2.39	0.51
57:x:538:ASP:OD2	57:x:576:ARG:NH1	2.44	0.51
8:A:500:G:N1	8:A:503:A:OP2	2.39	0.51
8:A:675:A:N3	8:A:2443:C:O2'	2.37	0.51
8:A:2170:A:H2'	8:A:2171:A:H4'	1.93	0.51
34:a:197:A:N1	34:a:220:G:O2'	2.41	0.51
34:a:618:C:H5'	34:a:619:U:H5''	1.92	0.51
55:v:9:G:O2'	55:v:10:G:N7	2.39	0.51
8:A:2229:U:H2'	8:A:2230:G:H8	1.75	0.51
8:A:197:A:H62	8:A:2430:A:H2'	1.76	0.51
8:A:1796:U:H2'	8:A:1797:G:H8	1.76	0.51
8:A:1834:U:H5''	8:A:1835:2MG:H5'	1.93	0.51
26:S:86:MET:HB2	26:S:96:ILE:HG12	1.92	0.51
34:a:927:G:O2'	34:a:1503:A:N7	2.37	0.51
45:l:98:ARG:HB2	45:l:116:TYR:HA	1.93	0.51
8:A:20:C:H2'	8:A:21:A:H8	1.76	0.51
8:A:2561:U:O3'	18:K:40:LYS:NZ	2.43	0.51
20:M:10:ARG:HG3	20:M:11:LYS:HG3	1.92	0.51
34:a:455:G:H2'	34:a:456:A:H8	1.75	0.51
36:c:83:VAL:HG13	36:c:100:ILE:HB	1.91	0.51
8:A:569:U:O2'	8:A:983:A:N1	2.36	0.50
8:A:1141:U:OP2	17:J:68:LYS:NZ	2.44	0.50
20:M:20:LEU:HD22	29:V:81:PRO:HG2	1.93	0.50
34:a:517:G:N2	34:a:530:G:OP1	2.43	0.50
34:a:1152:A:OP1	43:j:70:HIS:ND1	2.44	0.50
29:V:62:THR:OG1	29:V:69:GLU:OE1	2.22	0.50
34:a:107:G:N7	53:t:9:ARG:NH1	2.60	0.50
51:r:25:ILE:HD11	51:r:66:LEU:HD13	1.93	0.50
57:x:303:ASP:OD1	57:x:304:THR:N	2.40	0.50
8:A:1437:C:O2'	8:A:1516:G:O2'	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1478:G:H1	8:A:1513:U:H3	1.58	0.50
34:a:202:G:H1	34:a:215:C:H41	1.58	0.50
8:A:84:A:N1	8:A:98:G:O2'	2.42	0.50
9:B:37:C:O2	22:O:100:HIS:NE2	2.37	0.50
14:G:136:ASP:HB3	14:G:139:VAL:HG12	1.94	0.50
15:H:77:THR:HA	15:H:143:ILE:HG23	1.94	0.50
17:J:125:TYR:OH	17:J:132:HIS:NE2	2.39	0.50
34:a:366:A:H1'	34:a:394:G:H22	1.76	0.50
34:a:1280:A:OP1	43:j:9:ARG:NH2	2.45	0.50
34:a:1391:U:H2'	34:a:1392:G:C8	2.46	0.50
36:c:107:LYS:HB3	36:c:110:LEU:HD13	1.94	0.50
52:s:62:THR:H	52:s:65:MET:HE2	1.75	0.50
35:b:150:ILE:HG22	35:b:153:MET:HE2	1.93	0.50
8:A:2788:C:O2'	8:A:2809:A:N3	2.36	0.50
20:M:110:GLU:OE2	20:M:114:ARG:NE	2.44	0.50
34:a:56:U:H2'	34:a:57:G:H8	1.77	0.50
34:a:335:C:O2'	34:a:1433:A:N3	2.36	0.50
34:a:437:U:O4'	37:d:153:ARG:NH1	2.42	0.50
34:a:1096:C:O2	34:a:1170:A:O2'	2.28	0.50
35:b:100:LEU:HD11	35:b:160:LEU:HD21	1.92	0.50
3:2:34:ARG:NE	3:2:42:LEU:O	2.43	0.50
8:A:514:A:N3	8:A:581:C:O2'	2.34	0.50
8:A:1509:A:H2'	8:A:1510:G:C8	2.47	0.50
8:A:1837:C:O2'	8:A:1927:A:N3	2.37	0.50
34:a:34:C:H2'	34:a:35:G:H8	1.75	0.50
54:u:3:ILE:HG23	54:u:4:LYS:H	1.76	0.50
57:x:110:MET:HE1	57:x:126:TRP:HE3	1.77	0.50
8:A:1036:G:H1	8:A:1119:U:H3	1.60	0.50
8:A:1171:G:H1	8:A:1177:G:H22	1.59	0.50
8:A:1278:C:H2'	8:A:1279:G:C8	2.47	0.50
8:A:2743:U:O2'	14:G:152:ARG:NH2	2.44	0.50
10:C:141:HIS:ND1	10:C:192:GLY:O	2.45	0.50
13:F:69:ALA:O	13:F:80:GLN:NE2	2.45	0.50
45:l:49:ARG:HB3	45:l:65:TYR:HE1	1.76	0.50
13:F:116:LEU:HD22	13:F:129:MET:HE2	1.93	0.50
24:Q:44:TYR:HD1	24:Q:47:ARG:HD3	1.77	0.50
34:a:1268:G:N3	34:a:1326:U:O2'	2.38	0.50
47:n:52:PRO:O	47:n:55:SER:OG	2.27	0.50
49:p:52:LEU:HD23	49:p:78:VAL:HG21	1.93	0.50
8:A:870:U:O2	8:A:907:G:O6	2.30	0.49
32:Y:10:SER:OG	32:Y:12:GLU:OE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:187:G:N2	34:a:190:A:OP2	2.44	0.49
37:d:14:GLU:HB2	37:d:18:LEU:HD21	1.93	0.49
45:l:76:HIS:HB2	57:x:424:LYS:HD3	1.94	0.49
8:A:1532:A:N6	8:A:1540:G:O6	2.45	0.49
8:A:2204:G:H4'	10:C:149:LYS:HD3	1.93	0.49
20:M:42:THR:HA	20:M:93:VAL:HA	1.93	0.49
25:R:14:VAL:HG11	25:R:20:VAL:HG22	1.93	0.49
34:a:816:A:OP1	34:a:1526:G:O2'	2.31	0.49
34:a:1071:C:H2'	34:a:1072:G:H8	1.76	0.49
8:A:224:U:O4	8:A:419:U:O2'	2.29	0.49
8:A:700:G:O2'	8:A:1632:A:N3	2.38	0.49
8:A:1980:G:O2'	8:A:1982:U:OP2	2.28	0.49
8:A:2636:C:O2'	11:D:45:TYR:OH	2.16	0.49
18:K:58:LEU:HD11	18:K:86:LEU:HD12	1.94	0.49
34:a:324:G:N2	34:a:327:A:OP2	2.41	0.49
34:a:405:U:O4	37:d:1:ALA:N	2.44	0.49
34:a:1298:U:O2	34:a:1299:A:N6	2.45	0.49
45:l:32:VAL:HG22	45:l:55:ARG:HB3	1.94	0.49
47:n:83:LYS:HA	47:n:86:GLU:HG3	1.93	0.49
8:A:151:C:H2'	8:A:152:A:H8	1.77	0.49
8:A:2328:A:H2'	8:A:2329:U:C6	2.47	0.49
8:A:2662:A:H2'	8:A:2663:G:O4'	2.13	0.49
11:D:130:GLN:OE1	11:D:139:SER:OG	2.31	0.49
19:L:85:VAL:HG11	19:L:90:VAL:HG22	1.93	0.49
23:P:33:GLU:HG3	23:P:36:LYS:HB2	1.93	0.49
8:A:2515:C:H2'	8:A:2516:A:H8	1.76	0.49
12:E:171:ASP:OD1	12:E:172:ALA:N	2.45	0.49
13:F:118:ALA:O	13:F:166:ARG:NH2	2.40	0.49
8:A:2565:A:N6	18:K:28:SER:OG	2.46	0.49
10:C:231:HIS:HA	10:C:241:LYS:HE3	1.94	0.49
13:F:29:ARG:H	13:F:158:THR:HG1	1.60	0.49
34:a:718:A:H4'	54:u:34:ARG:HH22	1.77	0.49
34:a:1401:G:O6	34:a:1504:G:N2	2.46	0.49
34:a:1412:C:H2'	34:a:1413:A:C8	2.47	0.49
36:c:125:ARG:HG3	36:c:127:VAL:HG23	1.95	0.49
8:A:1826:G:O2'	8:A:1971:U:OP2	2.31	0.49
10:C:204:LEU:HB3	10:C:209:ALA:HB3	1.94	0.49
11:D:109:VAL:HG22	11:D:203:VAL:HG22	1.94	0.49
15:H:50:ARG:NH1	15:H:51:ARG:HB2	2.27	0.49
18:K:17:ARG:HB2	18:K:45:GLU:HG2	1.94	0.49
18:K:21:CYS:HA	18:K:41:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:K:53:LYS:HD3	18:K:54:LYS:H	1.77	0.49
23:P:28:LYS:HB3	23:P:39:LEU:HD21	1.95	0.49
34:a:2:A:H4'	37:d:82:LYS:HE2	1.95	0.49
34:a:455:G:H2'	34:a:456:A:C8	2.48	0.49
34:a:920:U:O2'	34:a:1081:A:O2'	2.29	0.49
50:q:59:GLU:OE1	50:q:76:ARG:NE	2.45	0.49
57:x:18:ILE:HG12	57:x:91:HIS:CD2	2.48	0.49
57:x:104:VAL:HG23	57:x:105:LEU:HD13	1.94	0.49
8:A:576:U:H2'	8:A:577:G:C8	2.48	0.49
8:A:713:G:H5''	48:o:88:ARG:HD3	1.95	0.49
8:A:1364:G:OP2	31:X:49:ARG:NH1	2.43	0.49
8:A:1667:G:N2	8:A:1992:G:OP2	2.33	0.49
8:A:2312:U:H5'	13:F:84:ILE:HD11	1.94	0.49
18:K:13:ASN:ND2	18:K:97:THR:OG1	2.39	0.49
27:T:9:LYS:O	27:T:12:ARG:NH2	2.45	0.49
34:a:21:G:H2'	34:a:22:G:C8	2.48	0.49
34:a:210:C:HO2'	34:a:211:G:N2	2.11	0.49
15:H:50:ARG:HH12	15:H:51:ARG:HH11	1.61	0.49
31:X:2:ARG:HD2	31:X:29:LEU:HD12	1.95	0.49
8:A:1093:G:N2	8:A:1097:U:OP2	2.46	0.49
8:A:2246:G:H2'	8:A:2247:A:H8	1.78	0.49
32:Y:7:ARG:HG3	32:Y:56:LEU:HD11	1.95	0.49
34:a:358:U:H2'	34:a:359:G:H8	1.78	0.49
34:a:502:A:OP1	45:l:114:SER:N	2.32	0.49
4:3:7:ARG:NH2	8:A:244:A:OP2	2.46	0.48
8:A:1060:U:O2'	8:A:1062:G:OP2	2.31	0.48
8:A:1415:U:H3	8:A:1587:G:H1	1.61	0.48
8:A:1941:C:N4	8:A:1965:C:O4'	2.45	0.48
8:A:2898:U:H2'	8:A:2899:A:H8	1.77	0.48
26:S:59:GLU:HB3	26:S:66:ILE:HD11	1.94	0.48
34:a:429:U:H3'	37:d:8:LEU:HD12	1.95	0.48
34:a:1238:A:H5'	34:a:1336:C:H41	1.77	0.48
39:f:18:VAL:HA	39:f:21:MET:HE3	1.94	0.48
52:s:55:GLN:OE1	52:s:55:GLN:N	2.46	0.48
5:4:3:VAL:HG21	8:A:2539:C:H5'	1.95	0.48
8:A:820:A:H4'	8:A:836:G:H22	1.78	0.48
8:A:1054:A:H2'	8:A:1055:G:C8	2.48	0.48
8:A:2175:C:H2'	8:A:2176:A:H8	1.77	0.48
18:K:51:LYS:NZ	34:a:339:C:OP1	2.33	0.48
23:P:40:GLN:NE2	23:P:41:ALA:O	2.46	0.48
32:Y:9:LYS:HD3	32:Y:13:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:28:A:O2'	34:a:296:U:OP1	2.23	0.48
34:a:674:G:H21	44:k:117:HIS:HB2	1.78	0.48
34:a:1356:G:H2'	34:a:1357:A:C8	2.48	0.48
8:A:526:A:O2'	8:A:2043:C:O2	2.31	0.48
8:A:1068:G:O6	8:A:1070:A:N6	2.46	0.48
8:A:1638:C:O2	8:A:2698:U:O2'	2.32	0.48
8:A:2638:G:H1'	8:A:2778:A:H61	1.78	0.48
21:N:103:ARG:HG3	21:N:110:MET:HE2	1.95	0.48
34:a:235:C:H2'	34:a:236:A:C8	2.48	0.48
37:d:9:LYS:HZ2	37:d:37:PRO:HB3	1.77	0.48
39:f:29:ILE:HD12	39:f:64:VAL:HG21	1.94	0.48
8:A:1361:G:O2'	8:A:2215:C:O2'	2.30	0.48
34:a:909:A:N3	34:a:1413:A:O2'	2.44	0.48
45:l:52:CYS:SG	45:l:64:SER:OG	2.72	0.48
5:4:24:ARG:NH2	8:A:2742:G:OP2	2.45	0.48
8:A:926:G:H2'	8:A:927:A:C8	2.48	0.48
8:A:1753:G:H5''	23:P:92:ARG:HD3	1.95	0.48
11:D:14:ILE:HD12	11:D:24:VAL:HG11	1.95	0.48
28:U:98:ASN:ND2	28:U:100:GLU:OE2	2.46	0.48
34:a:264:C:O2'	50:q:65:PRO:O	2.26	0.48
34:a:946:A:OP1	46:m:112:ARG:NH1	2.47	0.48
36:c:72:PRO:HA	36:c:75:VAL:HG12	1.96	0.48
37:d:18:LEU:HD13	37:d:63:ILE:HG13	1.94	0.48
8:A:2522:U:O2'	8:A:2647:U:OP1	2.23	0.48
34:a:477:C:H2'	34:a:478:A:C8	2.48	0.48
34:a:751:U:OP1	48:o:16:ARG:NH2	2.47	0.48
34:a:932:C:OP1	40:g:3:ARG:HB2	2.14	0.48
34:a:1239:A:N6	34:a:1299:A:C2	2.80	0.48
8:A:2202:U:O2'	8:A:2204:G:OP1	2.23	0.48
20:M:41:LEU:HD13	20:M:96:ILE:HG13	1.96	0.48
24:Q:77:LYS:HE3	24:Q:116:LEU:HD13	1.96	0.48
34:a:542:G:OP1	37:d:9:LYS:NZ	2.26	0.48
57:x:61:THR:O	57:x:89:PRO:HB3	2.14	0.48
3:2:19:ARG:HG3	8:A:126:A:H5'	1.95	0.48
8:A:742:A:H2'	8:A:743:A:C8	2.48	0.48
20:M:17:ASN:OD1	20:M:97:GLN:NE2	2.47	0.48
34:a:269:C:H2'	34:a:270:A:C8	2.48	0.48
36:c:134:LYS:HE3	36:c:138:GLN:HE22	1.79	0.48
43:j:52:LEU:HB2	47:n:81:ARG:NE	2.28	0.48
52:s:52:ASN:HB3	52:s:74:ALA:HB1	1.95	0.48
56:w:69:G:H2'	56:w:70:G:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:30:G:O2'	8:A:1214:A:N3	2.40	0.48
8:A:453:A:N3	8:A:457:A:O2'	2.46	0.48
11:D:14:ILE:HD11	11:D:188:LEU:HD13	1.95	0.48
34:a:335:C:H2'	34:a:336:A:H8	1.78	0.48
34:a:746:A:H2'	34:a:747:A:C8	2.48	0.48
8:A:1072:C:OP1	8:A:1088:A:O2'	2.24	0.48
8:A:1800:C:O2'	10:C:152:GLN:OE1	2.32	0.48
8:A:1807:G:N2	8:A:1810:A:OP2	2.45	0.48
8:A:2215:C:H2'	8:A:2216:G:C8	2.48	0.48
8:A:2450:A:N6	8:A:2501:C:C2	2.81	0.48
20:M:69:PRO:HA	20:M:94:ALA:HB2	1.96	0.48
35:b:99:MET:HA	35:b:106:VAL:HG21	1.95	0.48
42:i:80:HIS:CE1	42:i:84:ARG:HE	2.32	0.48
8:A:444:C:OP1	12:E:40:ARG:NH2	2.46	0.47
8:A:1069:A:O2'	8:A:1095:A:O2'	2.31	0.47
8:A:2251:OMG:HM23	8:A:2251:OMG:H1'	1.73	0.47
10:C:52:HIS:CE1	10:C:218:THR:HA	2.48	0.47
34:a:946:A:H2'	34:a:947:G:C8	2.49	0.47
57:x:157:ILE:HG23	57:x:161:LEU:HD12	1.96	0.47
1:O:15:ARG:HH22	8:A:1265:A:H3'	1.79	0.47
8:A:976:G:O2'	8:A:1155:A:O2'	2.29	0.47
8:A:1378:A:O2'	8:A:1380:G:OP2	2.32	0.47
8:A:1590:A:H2'	8:A:1591:A:H8	1.79	0.47
28:U:25:LYS:HB2	28:U:34:ILE:HG23	1.96	0.47
34:a:49:U:H3	34:a:362:G:H1'	1.79	0.47
34:a:269:C:H2'	34:a:270:A:H8	1.79	0.47
34:a:587:G:OP1	41:h:83:ARG:NH2	2.46	0.47
37:d:150:LYS:HA	37:d:155:LYS:HE3	1.95	0.47
57:x:291:VAL:HG22	57:x:292:PRO:HD2	1.96	0.47
8:A:774:G:N2	8:A:787:C:O2'	2.47	0.47
8:A:833:A:H2'	8:A:834:G:C8	2.49	0.47
8:A:1038:G:H2'	8:A:1039:A:C8	2.49	0.47
8:A:2120:G:H2'	8:A:2121:G:H8	1.78	0.47
57:x:138:ALA:HB3	57:x:263:VAL:HG13	1.95	0.47
57:x:463:LEU:O	57:x:464:HIS:C	2.56	0.47
8:A:1818:U:O2'	10:C:152:GLN:O	2.24	0.47
8:A:2013:A:O2'	26:S:94:ASP:OD2	2.25	0.47
8:A:2355:G:H5'	30:W:21:ARG:HH12	1.79	0.47
11:D:22:ILE:HG23	11:D:190:LYS:HG3	1.96	0.47
34:a:67:C:H2'	34:a:68:G:C8	2.49	0.47
36:c:41:TYR:HD1	36:c:44:LYS:HE3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:46:GLY:HA3	1:0:54:ILE:HG12	1.97	0.47
8:A:191:A:H2'	8:A:192:C:H6	1.80	0.47
8:A:848:C:H2'	8:A:849:A:C8	2.49	0.47
8:A:1042:G:N2	8:A:1113:U:O2	2.40	0.47
8:A:1614:A:N6	26:S:92:ARG:O	2.44	0.47
8:A:2308:G:H2'	8:A:2310:C:H5	1.80	0.47
8:A:2713:U:H3'	8:A:2714:G:H5''	1.97	0.47
34:a:126:G:OP1	34:a:605:U:O2'	2.27	0.47
35:b:56:LEU:HA	35:b:59:ILE:HG12	1.96	0.47
2:1:32:LYS:HD3	2:1:50:GLU:HB3	1.95	0.47
8:A:221:A:H1'	8:A:233:A:H1'	1.95	0.47
8:A:641:U:O4	8:A:647:G:O6	2.32	0.47
35:b:68:PHE:HB3	35:b:79:VAL:HG13	1.96	0.47
8:A:1203:U:H1'	19:L:4:ASN:HB3	1.96	0.47
8:A:1474:U:O4	8:A:1517:G:O6	2.33	0.47
8:A:2106:U:H2'	8:A:2107:G:H8	1.80	0.47
8:A:2134:A:N6	8:A:2156:G:O2'	2.47	0.47
8:A:2233:U:H2'	8:A:2234:G:C8	2.49	0.47
8:A:2314:A:H2'	8:A:2315:G:C8	2.50	0.47
8:A:2327:A:H2'	8:A:2328:A:C8	2.50	0.47
8:A:2543:G:H2'	8:A:2544:G:C8	2.50	0.47
10:C:179:GLU:HB2	10:C:270:ARG:HB3	1.97	0.47
20:M:40:ARG:HB3	20:M:93:VAL:HG21	1.96	0.47
31:X:6:VAL:HG13	31:X:7:THR:HG23	1.96	0.47
34:a:50:A:O2'	34:a:360:G:N2	2.47	0.47
34:a:832:G:H1	34:a:854:U:H3	1.61	0.47
34:a:1090:U:HO2'	34:a:1171:A:HO2'	1.61	0.47
34:a:1512:U:H2'	34:a:1513:A:C8	2.50	0.47
50:q:77:VAL:HG11	50:q:80:LYS:HE3	1.96	0.47
56:w:63:G:H2'	56:w:64:A:C8	2.50	0.47
57:x:32:TYR:HE2	57:x:274:VAL:HB	1.79	0.47
57:x:506:LYS:HD3	57:x:514:TYR:HA	1.96	0.47
8:A:641:U:O2'	8:A:2350:C:OP1	2.33	0.47
8:A:1009:A:N3	8:A:1153:C:O2'	2.40	0.47
22:O:49:VAL:HG21	22:O:81:ARG:HB3	1.96	0.47
34:a:202:G:H22	34:a:215:C:H5	1.63	0.47
34:a:714:G:H2'	34:a:715:A:C8	2.50	0.47
57:x:614:PRO:HG2	57:x:659:LEU:HB3	1.96	0.47
8:A:1796:U:H2'	8:A:1797:G:C8	2.50	0.47
8:A:2657:A:O3'	14:G:159:LYS:NZ	2.48	0.47
34:a:129:A:H2	34:a:232:G:H22	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:l:32:VAL:HG12	45:l:78:VAL:HG13	1.97	0.47
8:A:636:G:O2'	8:A:638:G:O2'	2.32	0.47
8:A:907:G:N2	20:M:70:ASP:OD2	2.48	0.47
8:A:1791:A:O2'	10:C:204:LEU:O	2.19	0.47
8:A:1802:A:H2'	8:A:1803:A:C8	2.50	0.47
13:F:109:ARG:HD2	13:F:136:ILE:HA	1.97	0.47
14:G:104:LEU:HD13	14:G:106:LEU:HD11	1.97	0.47
34:a:363:A:C6	45:l:27:PRO:HD2	2.50	0.47
34:a:405:U:OP2	37:d:2:ARG:NH1	2.48	0.47
34:a:1249:C:N4	34:a:1288:A:OP2	2.47	0.47
1:0:3:GLN:HA	8:A:2615:U:C2	2.50	0.46
8:A:2136:G:H2'	8:A:2137:U:C6	2.50	0.46
8:A:2514:U:H2'	8:A:2515:C:C6	2.50	0.46
34:a:373:A:O2'	34:a:451:A:N7	2.47	0.46
34:a:948:C:H2'	34:a:949:A:H8	1.80	0.46
57:x:33:THR:HG21	57:x:69:ALA:HB1	1.97	0.46
57:x:491:GLU:HB2	57:x:570:VAL:HG13	1.97	0.46
8:A:143:C:H2'	8:A:144:A:C8	2.50	0.46
8:A:579:G:O2'	8:A:2019:A:OP1	2.33	0.46
8:A:2128:G:C2	8:A:2174:C:H5'	2.50	0.46
8:A:2215:C:H2'	8:A:2216:G:H8	1.80	0.46
34:a:81:A:N6	34:a:89:U:O2'	2.49	0.46
34:a:1414:U:H2'	34:a:1415:G:H8	1.80	0.46
38:e:106:ALA:HB2	38:e:124:ALA:HB3	1.97	0.46
40:g:25:PHE:HD1	40:g:100:MET:HG3	1.79	0.46
8:A:476:G:N1	8:A:479:A:OP2	2.46	0.46
8:A:1080:A:N6	8:A:1088:A:O4'	2.47	0.46
8:A:2243:U:H2'	8:A:2244:U:C6	2.51	0.46
8:A:2443:C:H2'	8:A:2444:G:H8	1.80	0.46
10:C:107:LYS:HE3	10:C:107:LYS:HB3	1.69	0.46
34:a:8:A:N6	37:d:201:GLU:O	2.48	0.46
34:a:1355:G:H2'	34:a:1356:G:H8	1.80	0.46
35:b:14:HIS:HB3	35:b:208:ALA:HB2	1.98	0.46
46:m:95:PRO:HD3	46:m:108:ARG:HB3	1.98	0.46
8:A:1587:G:H2'	8:A:1588:G:H8	1.81	0.46
8:A:2584:U:H3'	8:A:2585:U:H5''	1.97	0.46
9:B:1:U:H2'	9:B:2:G:H8	1.80	0.46
34:a:436:C:O2'	37:d:153:ARG:NH1	2.49	0.46
34:a:1003:G:H5'	34:a:1024:G:H1	1.80	0.46
40:g:92:PRO:HA	40:g:95:ARG:HD2	1.96	0.46
43:j:66:GLU:HB3	47:n:99:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:k:35:ASP:OD1	44:k:39:ASN:N	2.48	0.46
45:l:34:THR:N	45:l:53:ARG:O	2.48	0.46
51:r:18:GLN:NE2	51:r:19:GLU:OE1	2.49	0.46
8:A:310:A:HO2'	8:A:311:A:P	2.39	0.46
32:Y:43:LEU:O	32:Y:47:ARG:HB2	2.15	0.46
34:a:1077:G:N2	34:a:1080:A:OP2	2.41	0.46
36:c:179:ALA:HA	36:c:205:GLU:HA	1.97	0.46
41:h:38:VAL:O	41:h:42:GLU:HB3	2.15	0.46
57:x:452:SER:OG	57:x:453:ASN:N	2.47	0.46
8:A:2291:U:H2'	8:A:2292:U:C6	2.51	0.46
31:X:1:SER:O	31:X:49:ARG:NH2	2.49	0.46
34:a:1012:A:N6	34:a:1018:G:O6	2.48	0.46
34:a:1535:C:H5'	34:a:1536:C:H5''	1.97	0.46
35:b:163:ILE:HD11	35:b:213:LEU:HD11	1.98	0.46
57:x:465:LEU:HD23	57:x:465:LEU:HA	1.77	0.46
8:A:573:U:O4	8:A:2029:G:O2'	2.32	0.46
8:A:1392:A:N6	27:T:18:GLU:HG3	2.31	0.46
9:B:12:C:O2'	30:W:70:PRO:O	2.33	0.46
27:T:69:ARG:HH22	27:T:74:ILE:HA	1.79	0.46
34:a:235:C:H2'	34:a:236:A:H8	1.79	0.46
34:a:337:G:H2'	34:a:338:A:C8	2.51	0.46
34:a:933:G:O6	40:g:2:ARG:NH2	2.48	0.46
34:a:1270:G:H2'	34:a:1271:A:H8	1.80	0.46
8:A:188:G:O2'	8:A:1365:A:N6	2.49	0.46
8:A:953:G:OP2	20:M:18:ARG:NH2	2.44	0.46
8:A:1409:U:H2'	8:A:1410:G:H8	1.81	0.46
8:A:1437:C:H2'	8:A:1438:U:H6	1.80	0.46
8:A:1590:A:H2'	8:A:1591:A:C8	2.51	0.46
8:A:2093:G:N7	8:A:2225:A:H2'	2.31	0.46
8:A:2809:A:OP2	8:A:2890:G:N1	2.42	0.46
13:F:157:THR:HG22	13:F:159:ALA:H	1.81	0.46
14:G:55:ASP:OD1	14:G:56:GLY:N	2.48	0.46
34:a:205:A:H3'	34:a:206:C:H6	1.81	0.46
34:a:598:U:H4'	41:h:85:TYR:CG	2.50	0.46
39:f:51:ILE:HD11	51:r:65:SER:HB2	1.98	0.46
56:w:69:G:H2'	56:w:70:G:C8	2.51	0.46
20:M:53:MET:HB3	20:M:120:ALA:HB2	1.98	0.46
29:V:32:GLY:O	29:V:93:ARG:NH1	2.48	0.46
34:a:634:C:H2'	34:a:635:A:H8	1.81	0.46
34:a:718:A:C2	51:r:37:LYS:HG2	2.51	0.46
34:a:1464:U:H2'	34:a:1465:A:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:e:71:ILE:HG13	38:e:72:ASN:H	1.81	0.46
38:e:156:ARG:HH22	41:h:42:GLU:CD	2.24	0.46
8:A:228:C:N3	8:A:417:C:O2'	2.44	0.46
8:A:491:G:O6	26:S:49:LYS:NZ	2.44	0.46
8:A:720:U:H2'	8:A:721:A:C8	2.51	0.46
8:A:1734:G:H2'	8:A:1735:A:C8	2.51	0.46
8:A:1987:A:H2'	8:A:1988:G:H8	1.81	0.46
8:A:2231:U:OP1	31:X:26:ARG:NH2	2.49	0.46
8:A:2246:G:H2'	8:A:2247:A:C8	2.51	0.46
12:E:97:ASN:HB2	12:E:100:MET:HG3	1.98	0.46
25:R:61:ALA:HB2	25:R:98:ILE:HD13	1.98	0.46
53:t:34:VAL:HG21	53:t:53:MET:HG2	1.97	0.46
55:v:32:C:N4	55:v:33:U:O4	2.49	0.46
8:A:624:C:O2'	8:A:657:U:OP1	2.33	0.45
8:A:1683:U:H2'	8:A:1684:G:H8	1.81	0.45
8:A:2319:G:O2'	8:A:2320:U:O5'	2.31	0.45
8:A:2640:G:OP1	17:J:95:ARG:NH1	2.49	0.45
9:B:27:C:OP1	22:O:34:HIS:NE2	2.46	0.45
10:C:121:ALA:HB1	10:C:127:ASN:HB3	1.98	0.45
18:K:65:THR:HG22	18:K:67:LYS:H	1.81	0.45
34:a:34:C:H2'	34:a:35:G:C8	2.50	0.45
41:h:40:LYS:HD2	41:h:48:PHE:HD1	1.80	0.45
45:l:46:SER:OG	45:l:46:SER:O	2.33	0.45
8:A:813:U:H2'	8:A:814:C:C6	2.52	0.45
8:A:1097:U:HO2'	16:I:7:TYR:H	1.61	0.45
8:A:2086:U:H2'	8:A:2087:G:C8	2.52	0.45
8:A:2552:OMU:H5	8:A:2556:C:N4	2.31	0.45
8:A:2567:G:H2'	8:A:2568:U:C6	2.51	0.45
10:C:221:GLY:HA2	10:C:224:MET:HG3	1.99	0.45
13:F:32:LYS:HD3	13:F:91:ARG:NH2	2.31	0.45
57:x:235:LYS:HD2	57:x:242:LEU:HD23	1.98	0.45
8:A:581:C:H2'	8:A:582:A:H8	1.81	0.45
8:A:2172:U:O2'	8:A:2174:C:OP2	2.33	0.45
9:B:15:A:H3'	9:B:16:G:H8	1.81	0.45
21:N:29:VAL:HG11	21:N:75:ILE:HG23	1.99	0.45
34:a:473:U:H2'	34:a:474:G:C8	2.51	0.45
34:a:1226:C:OP2	46:m:101:THR:OG1	2.32	0.45
34:a:1530:G:H2'	34:a:1531:A:C8	2.51	0.45
37:d:58:GLN:HB3	37:d:62:ARG:NH1	2.31	0.45
40:g:142:ARG:O	40:g:146:ALA:CB	2.65	0.45
8:A:521:U:H2'	8:A:522:A:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2262:U:H2'	8:A:2263:C:H6	1.82	0.45
9:B:31:C:H5'	13:F:25:MET:HE1	1.98	0.45
11:D:26:VAL:HG21	23:P:4:ILE:HG22	1.99	0.45
14:G:123:GLU:OE2	14:G:133:LYS:NZ	2.49	0.45
19:L:29:LYS:HE2	19:L:30:THR:HG23	1.97	0.45
20:M:31:PHE:HD1	20:M:132:THR:HG22	1.81	0.45
34:a:545:C:OP2	37:d:61:ARG:NH2	2.48	0.45
34:a:628:G:H2'	34:a:629:A:C8	2.51	0.45
34:a:995:C:N3	34:a:1046:A:O2'	2.46	0.45
45:l:63:THR:OG1	45:l:91:GLY:O	2.34	0.45
8:A:77:G:O2'	32:Y:7:ARG:NH2	2.26	0.45
8:A:291:G:O6	8:A:349:U:O2	2.35	0.45
34:a:390:U:H2'	34:a:391:G:C8	2.52	0.45
35:b:59:ILE:O	35:b:62:ARG:HG2	2.17	0.45
44:k:28:ASN:HB2	44:k:56:LYS:HE3	1.97	0.45
54:u:15:LEU:HD23	54:u:16:ARG:HH11	1.81	0.45
57:x:269:PHE:HB2	64:x:801:GDP:C6	2.52	0.45
3:2:7:PRO:HG3	8:A:1612:C:H5'	1.99	0.45
8:A:288:U:H2'	8:A:289:G:H8	1.82	0.45
8:A:1683:U:H2'	8:A:1684:G:C8	2.52	0.45
8:A:1794:A:H2'	8:A:1795:C:C6	2.51	0.45
8:A:2356:U:H4'	30:W:16:ARG:HG3	1.98	0.45
8:A:2483:C:H1'	20:M:51:ARG:HH12	1.82	0.45
33:Z:4:ILE:HG23	33:Z:39:ASP:HB2	1.98	0.45
34:a:757:U:OP1	34:a:822:U:O2'	2.34	0.45
34:a:1009:U:O2	34:a:1020:G:N2	2.41	0.45
48:o:69:LEU:HG	48:o:77:TYR:HB2	1.98	0.45
49:p:5:ARG:HH12	49:p:24:SER:HA	1.82	0.45
57:x:576:ARG:NH1	57:x:578:HIS:HB2	2.23	0.45
2:1:43:ARG:NH2	8:A:2370:G:O2'	2.50	0.45
8:A:1341:G:OP2	8:A:1394:U:O2'	2.29	0.45
8:A:1791:A:H61	8:A:1828:G:HO2'	1.60	0.45
8:A:1929:G:OP2	8:A:1929:G:N2	2.44	0.45
8:A:2241:A:H2'	8:A:2242:G:C8	2.51	0.45
34:a:703:G:H4'	34:a:704:A:O5'	2.17	0.45
34:a:928:G:O2'	34:a:1533:C:OP1	2.35	0.45
34:a:1382:C:O2'	40:g:78:ARG:NH2	2.47	0.45
34:a:1513:A:H2'	34:a:1514:G:C8	2.51	0.45
40:g:69:ARG:NH2	40:g:96:ASN:OD1	2.50	0.45
42:i:115:VAL:HG13	43:j:62:ARG:HH11	1.80	0.45
51:r:21:ASP:OD1	51:r:21:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:x:198:GLY:O	57:x:275:GLN:NE2	2.49	0.45
57:x:361:ARG:HB2	57:x:385:ILE:HB	1.99	0.45
8:A:521:U:H2'	8:A:522:A:C8	2.51	0.45
8:A:1716:U:O4	8:A:1744:A:N7	2.49	0.45
8:A:1794:A:H2'	8:A:1795:C:H6	1.82	0.45
8:A:1799:G:OP2	10:C:269:ARG:NH2	2.50	0.45
8:A:1913:A:C6	34:a:1494:G:H5'	2.52	0.45
8:A:2055:C:N4	8:A:2499:C:O2'	2.50	0.45
8:A:2590:A:H2'	8:A:2591:C:H6	1.81	0.45
8:A:2698:U:H2'	8:A:2699:C:C6	2.51	0.45
14:G:41:GLU:HG2	14:G:54:ARG:HB2	1.97	0.45
33:Z:2:LYS:NZ	33:Z:39:ASP:OD2	2.39	0.45
34:a:147:G:H2'	34:a:148:G:C8	2.51	0.45
34:a:1042:A:H3'	34:a:1043:G:C8	2.52	0.45
34:a:1251:A:N3	34:a:1369:C:O2'	2.44	0.45
43:j:91:ASP:OD1	43:j:91:ASP:N	2.49	0.45
44:k:19:VAL:HG13	44:k:82:GLU:HG3	1.99	0.45
46:m:92:ARG:HA	46:m:92:ARG:HD2	1.88	0.45
57:x:52:MET:HB2	57:x:55:GLU:HG3	1.97	0.45
2:l:5:ARG:NH2	2:l:23:THR:O	2.41	0.45
8:A:69:C:O2	8:A:73:A:O2'	2.34	0.45
8:A:2329:U:H2'	8:A:2330:G:C8	2.52	0.45
8:A:2816:G:H5''	21:N:99:LYS:HE3	1.98	0.45
8:A:2836:U:H2'	8:A:2837:A:C8	2.52	0.45
28:U:80:ASP:OD1	28:U:96:LYS:N	2.50	0.45
34:a:56:U:H2'	34:a:57:G:C8	2.52	0.45
34:a:464:U:H2'	34:a:465:A:H2'	1.99	0.45
34:a:636:U:H2'	34:a:637:C:C6	2.52	0.45
34:a:811:C:O2'	34:a:901:A:N1	2.48	0.45
34:a:867:G:O2'	34:a:873:A:N1	2.39	0.45
34:a:1095:U:OP1	34:a:1108:G:N2	2.46	0.45
34:a:1125:U:O3'	43:j:7:ARG:NH2	2.50	0.45
35:b:18:GLN:HG3	35:b:20:ARG:H	1.82	0.45
57:x:19:ASP:HB3	64:x:801:GDP:H5'	1.99	0.45
8:A:1265:A:H61	8:A:2013:A:H3'	1.81	0.45
9:B:42:C:C6	13:F:65:LEU:HB2	2.52	0.45
13:F:147:ARG:HE	13:F:149:ARG:HG3	1.82	0.45
14:G:5:LYS:HE3	14:G:5:LYS:HB2	1.86	0.45
14:G:23:ILE:HD13	14:G:71:LEU:HD11	1.99	0.45
23:P:104:GLY:HA3	34:a:1431:A:H5''	1.99	0.45
27:T:6:ARG:O	27:T:10:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:537:G:OP1	45:l:109:ARG:NH2	2.46	0.45
51:r:41:SER:OG	51:r:46:THR:O	2.29	0.45
8:A:319:G:H1	8:A:323:C:H41	1.64	0.44
8:A:581:C:H2'	8:A:582:A:C8	2.52	0.44
8:A:1000:A:H2'	8:A:1001:A:C8	2.52	0.44
8:A:1215:G:H1	8:A:1234:U:H3	1.65	0.44
8:A:1953:A:O2'	8:A:2559:C:O2	2.33	0.44
16:I:13:ALA:HB1	16:I:54:ILE:N	2.32	0.44
21:N:106:ASP:N	21:N:106:ASP:OD1	2.50	0.44
34:a:259:G:OP2	53:t:77:ASN:ND2	2.51	0.44
34:a:628:G:H2'	34:a:629:A:H8	1.82	0.44
34:a:1005:A:H5'	34:a:1036:A:H2	1.83	0.44
35:b:103:TRP:CD1	35:b:107:ARG:HE	2.35	0.44
41:h:5:PRO:HB2	41:h:32:LYS:HE3	1.97	0.44
55:v:1:C:H2'	55:v:2:G:C8	2.52	0.44
56:w:51:C:H2'	56:w:52:G:H8	1.82	0.44
57:x:42:VAL:HG11	64:x:801:GDP:O2A	2.16	0.44
8:A:214:G:H1'	8:A:217:A:H5'	2.00	0.44
8:A:414:C:H1'	8:A:1864:U:H1'	2.00	0.44
26:S:73:LYS:HB2	26:S:106:VAL:HB	2.00	0.44
34:a:427:U:O2'	34:a:541:G:OP1	2.30	0.44
34:a:792:A:O2'	34:a:794:A:N7	2.44	0.44
34:a:1060:U:OP1	47:n:85:ARG:NH2	2.50	0.44
34:a:1078:U:C2	38:e:89:THR:HG21	2.52	0.44
34:a:1297:G:N2	34:a:1298:U:O4	2.42	0.44
34:a:1429:A:H2'	34:a:1430:A:C8	2.53	0.44
38:e:76:ASN:HB2	38:e:81:GLN:NE2	2.31	0.44
46:m:77:LYS:HA	46:m:77:LYS:HD3	1.76	0.44
7:6:12:ILE:HD12	7:6:12:ILE:HA	1.83	0.44
8:A:971:G:O2'	8:A:983:A:N3	2.44	0.44
8:A:1509:A:H2'	8:A:1510:G:H8	1.82	0.44
8:A:2291:U:O2'	8:A:2374:C:O2	2.36	0.44
23:P:90:ALA:HB2	23:P:112:ARG:HA	1.99	0.44
25:R:42:ALA:HA	25:R:47:VAL:HG12	2.00	0.44
34:a:449:G:H2'	34:a:450:G:C8	2.53	0.44
41:h:95:MET:HB3	41:h:99:GLY:H	1.83	0.44
57:x:617:LYS:HB3	57:x:682:GLU:HB2	1.99	0.44
8:A:639:U:H2'	8:A:640:C:C6	2.51	0.44
8:A:704:G:O2'	8:A:727:A:N6	2.51	0.44
8:A:1335:C:OP1	27:T:69:ARG:HB3	2.17	0.44
26:S:72:THR:OG1	26:S:106:VAL:O	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:230:G:O2'	49:p:25:ARG:NH2	2.50	0.44
34:a:377:G:H2'	34:a:378:G:H8	1.83	0.44
34:a:1217:C:OP1	47:n:8:ARG:NE	2.47	0.44
41:h:24:VAL:HG13	41:h:62:LEU:HD11	1.99	0.44
44:k:20:ALA:HB2	44:k:81:LEU:HD22	1.99	0.44
57:x:466:ASP:HA	57:x:469:VAL:HG22	1.99	0.44
8:A:579:G:H4'	8:A:2018:G:H5''	1.99	0.44
10:C:163:ILE:HA	10:C:173:LEU:HD23	1.99	0.44
34:a:26:A:H61	34:a:558:G:H1'	1.82	0.44
34:a:680:C:H2'	34:a:681:A:H8	1.83	0.44
34:a:1004:A:H2'	34:a:1005:A:C4	2.52	0.44
34:a:1513:A:H2'	34:a:1514:G:H8	1.83	0.44
38:e:22:LYS:HD3	38:e:29:ILE:HD11	1.98	0.44
42:i:48:ARG:HB3	42:i:52:GLU:OE2	2.18	0.44
57:x:196:ASP:OD2	57:x:200:THR:OG1	2.33	0.44
57:x:506:LYS:HB3	57:x:514:TYR:HA	2.00	0.44
59:z:0:U:H2'	59:z:1:A:C8	2.51	0.44
6:5:10:ALA:HA	6:5:13:ALA:HB3	1.98	0.44
7:6:6:HIS:CE1	13:F:63:LYS:H	2.36	0.44
8:A:414:C:H2'	8:A:415:A:C8	2.53	0.44
8:A:658:U:O2'	12:E:97:ASN:OD1	2.35	0.44
8:A:992:C:OP1	24:Q:46:TYR:OH	2.29	0.44
34:a:157:U:O2	34:a:164:G:O6	2.34	0.44
34:a:375:U:H5''	49:p:70:ARG:HG3	2.00	0.44
34:a:1126:U:O2'	34:a:1127:G:H5'	2.18	0.44
8:A:1316:U:H2'	8:A:1317:G:H8	1.82	0.44
34:a:69:G:H2'	34:a:70:U:C6	2.52	0.44
34:a:966:2MG:HM23	34:a:967:5MC:H1'	1.99	0.44
35:b:165:ALA:HB3	35:b:190:SER:HB3	2.00	0.44
36:c:38:VAL:HG23	36:c:90:VAL:HG22	1.99	0.44
38:e:111:ARG:O	38:e:115:GLU:HG3	2.17	0.44
42:i:76:GLY:HA2	42:i:79:ARG:NH1	2.33	0.44
46:m:99:GLN:N	46:m:99:GLN:OE1	2.51	0.44
57:x:19:ASP:HA	64:x:801:GDP:O3A	2.18	0.44
57:x:141:ASN:HA	57:x:266:GLY:O	2.17	0.44
8:A:197:A:H2	8:A:2434:A:H62	1.64	0.44
8:A:559:G:N2	24:Q:48:ASP:OD1	2.51	0.44
8:A:1710:G:H2'	8:A:1711:A:C8	2.53	0.44
8:A:2446:G:N2	8:A:2449:U:O2	2.49	0.44
34:a:674:G:H2'	34:a:675:A:C8	2.53	0.44
34:a:718:A:O2'	54:u:34:ARG:NH2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:j:52:LEU:HD23	43:j:62:ARG:HG2	1.98	0.44
44:k:85:VAL:HG11	44:k:92:ARG:HG3	2.00	0.44
57:x:454:GLN:NE2	57:x:486:GLN:HG3	2.32	0.44
8:A:694:U:OP1	10:C:58:LYS:NZ	2.34	0.44
8:A:932:U:O2'	8:A:934:U:O4	2.32	0.44
8:A:1923:U:H2'	8:A:1924:C:C6	2.53	0.44
8:A:2037:A:H2'	8:A:2038:G:C8	2.53	0.44
8:A:2167:U:N3	8:A:2170:A:OP2	2.47	0.44
8:A:2505:G:N2	8:A:2610:C:O2	2.50	0.44
8:A:2778:A:O2'	8:A:2780:G:O2'	2.35	0.44
13:F:115:GLY:HA3	13:F:177:ARG:HB3	2.00	0.44
15:H:116:ARG:HD3	15:H:116:ARG:HA	1.81	0.44
34:a:373:A:H1'	34:a:481:G:C8	2.53	0.44
37:d:187:ARG:HA	37:d:187:ARG:HD2	1.92	0.44
38:e:31:SER:HA	38:e:53:ARG:HD2	2.00	0.44
8:A:1752:C:H2'	8:A:1753:G:C8	2.53	0.43
34:a:4:U:H2'	34:a:5:U:H3'	2.00	0.43
34:a:45:G:OP1	34:a:307:C:O2'	2.34	0.43
34:a:222:C:H2'	34:a:223:A:H8	1.83	0.43
34:a:1417:G:O2'	34:a:1483:A:N6	2.51	0.43
35:b:152:ASP:OD1	35:b:152:ASP:N	2.42	0.43
46:m:79:LEU:HA	46:m:82:LEU:HD22	1.99	0.43
55:v:58:A:O2'	55:v:60:U:OP2	2.33	0.43
57:x:124:THR:HA	57:x:127:ARG:HE	1.83	0.43
8:A:481:G:H1'	8:A:506:G:H21	1.82	0.43
8:A:639:U:H2'	8:A:640:C:H6	1.83	0.43
8:A:1891:G:N2	55:v:71:C:O3'	2.51	0.43
8:A:2543:G:H2'	8:A:2544:G:H8	1.83	0.43
8:A:2589:A:N1	8:A:2606:C:N4	2.66	0.43
9:B:48:U:H4'	22:O:100:HIS:CD2	2.53	0.43
34:a:41:G:H2'	34:a:42:G:H8	1.83	0.43
34:a:825:A:H2	41:h:11:THR:HG21	1.82	0.43
34:a:1243:C:H2'	34:a:1244:G:C8	2.52	0.43
34:a:1308:U:H2'	34:a:1309:G:C8	2.53	0.43
36:c:111:ASP:HB3	36:c:114:LEU:HB2	1.99	0.43
39:f:9:MET:SD	39:f:86:ARG:HB3	2.58	0.43
42:i:11:ARG:HD3	42:i:76:GLY:HA3	1.99	0.43
8:A:145:C:H2'	8:A:146:A:C8	2.53	0.43
8:A:310:A:O2'	8:A:311:A:O5'	2.30	0.43
8:A:345:A:N3	8:A:347:A:N6	2.66	0.43
8:A:2039:U:H2'	8:A:2040:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:1:U:H2'	9:B:2:G:C8	2.53	0.43
23:P:105:LYS:HA	23:P:108:ARG:HG3	2.00	0.43
24:Q:77:LYS:HA	24:Q:77:LYS:HD2	1.75	0.43
34:a:20:U:O2'	34:a:573:A:N6	2.51	0.43
4:3:50:SER:OG	4:3:51:LYS:N	2.51	0.43
8:A:397:U:H3'	31:X:53:LYS:HZ3	1.82	0.43
8:A:956:G:H2'	8:A:957:C:H2'	2.00	0.43
8:A:2537:U:H2'	8:A:2538:C:C6	2.54	0.43
10:C:180:MET:HB3	10:C:268:ARG:H	1.83	0.43
13:F:103:ILE:HG23	13:F:104:THR:HG23	2.01	0.43
13:F:116:LEU:HD12	13:F:175:PRO:HD2	2.00	0.43
24:Q:23:TYR:HB2	24:Q:28:SER:HB3	2.00	0.43
33:Z:36:GLU:O	33:Z:37:ARG:NH1	2.52	0.43
34:a:459:A:H2'	34:a:460:A:C8	2.53	0.43
34:a:1022:A:H2'	34:a:1023:U:H5''	1.99	0.43
34:a:1079:G:H5'	38:e:133:ILE:HD13	2.01	0.43
34:a:1402:4OC:H6	34:a:1402:4OC:O5'	2.17	0.43
38:e:156:ARG:HH21	41:h:43:GLY:C	2.26	0.43
46:m:76:ILE:O	46:m:80:MET:HG3	2.18	0.43
52:s:53:GLY:O	52:s:54:ARG:HD3	2.19	0.43
57:x:570:VAL:HG11	57:x:573:MET:HE2	1.99	0.43
57:x:640:MET:HB3	57:x:656:GLU:HB2	2.00	0.43
1:0:15:ARG:NH2	8:A:1266:G:OP2	2.51	0.43
7:6:11:GLU:HA	7:6:25:ARG:HA	2.01	0.43
8:A:177:G:H3'	8:A:178:G:H8	1.83	0.43
8:A:401:A:H2'	8:A:402:A:C8	2.54	0.43
8:A:1437:C:H2'	8:A:1438:U:C6	2.54	0.43
8:A:1751:U:H2'	8:A:1752:C:C6	2.54	0.43
11:D:35:THR:N	11:D:49:GLN:O	2.50	0.43
14:G:117:PRO:HD2	14:G:120:ILE:HD12	2.00	0.43
34:a:642:A:N3	41:h:104:SER:OG	2.43	0.43
41:h:105:THR:OG1	41:h:108:GLY:O	2.32	0.43
53:t:2:ASN:HB3	53:t:3:ILE:H	1.64	0.43
54:u:39:LYS:O	54:u:42:THR:OG1	2.26	0.43
56:w:34:G:O6	59:z:6:U:O2	2.36	0.43
8:A:335:C:O2	28:U:67:SER:OG	2.27	0.43
8:A:828:U:H2'	8:A:829:A:C8	2.53	0.43
8:A:1061:U:C2	8:A:1068:G:H1'	2.53	0.43
8:A:1197:G:H2'	8:A:1198:U:H6	1.84	0.43
8:A:1682:G:H2'	8:A:1683:U:C6	2.53	0.43
8:A:2751:G:OP2	14:G:2:ARG:NH1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:109:LEU:HD23	10:C:109:LEU:HA	1.80	0.43
25:R:71:LYS:HA	25:R:90:ARG:HG2	1.99	0.43
34:a:1144:G:N2	34:a:1146:A:H62	2.16	0.43
34:a:1179:A:H2'	34:a:1180:A:C8	2.53	0.43
38:e:23:THR:HG22	38:e:28:ARG:HG2	2.00	0.43
46:m:21:ILE:HB	46:m:24:VAL:HB	2.00	0.43
8:A:685:A:N1	8:A:787:C:H1'	2.34	0.43
8:A:1063:G:O2'	16:I:87:SER:O	2.37	0.43
8:A:1288:G:OP2	8:A:1288:G:N2	2.50	0.43
8:A:1688:U:O2'	8:A:1700:A:N7	2.47	0.43
8:A:2313:C:H2'	8:A:2314:A:H8	1.84	0.43
8:A:2696:U:H2'	8:A:2697:G:H8	1.84	0.43
10:C:200:MET:HE2	10:C:200:MET:HB2	1.96	0.43
10:C:209:ALA:HA	10:C:212:TRP:CE2	2.53	0.43
13:F:70:ARG:C	13:F:80:GLN:HE22	2.27	0.43
17:J:56:VAL:HB	17:J:124:VAL:HG12	1.99	0.43
21:N:24:MET:HE1	21:N:40:LYS:HB3	2.01	0.43
23:P:32:VAL:HG22	23:P:37:LYS:HD2	2.01	0.43
34:a:712:A:H2'	34:a:713:G:C8	2.54	0.43
34:a:718:A:H2	51:r:37:LYS:HG2	1.83	0.43
34:a:946:A:O2'	34:a:1333:A:N3	2.47	0.43
34:a:1169:A:OP2	34:a:1169:A:H8	2.02	0.43
45:l:29:LYS:HD2	45:l:29:LYS:HA	1.84	0.43
47:n:83:LYS:HA	47:n:83:LYS:HD3	1.86	0.43
57:x:252:ARG:NH2	57:x:290:ASP:OD2	2.51	0.43
8:A:414:C:H2'	8:A:415:A:H8	1.84	0.43
8:A:832:U:H2'	8:A:833:A:C8	2.53	0.43
8:A:1013:C:H2'	8:A:1014:A:H8	1.84	0.43
8:A:1403:A:O2'	8:A:1471:G:O2'	2.34	0.43
8:A:2312:U:OP1	13:F:70:ARG:N	2.41	0.43
10:C:67:LYS:HD3	10:C:150:GLY:HA2	2.01	0.43
40:g:96:ASN:HB3	40:g:100:MET:HE1	2.01	0.43
42:i:20:ILE:HG22	42:i:62:LEU:HG	2.00	0.43
42:i:129:ARG:NH1	55:v:32:C:OP2	2.52	0.43
44:k:115:ILE:HD12	44:k:116:PRO:HD2	2.00	0.43
57:x:281:VAL:HG13	57:x:285:LEU:HD12	2.00	0.43
1:0:49:ARG:NH1	8:A:2884:U:O4'	2.52	0.43
8:A:373:U:H2'	8:A:374:A:H8	1.84	0.43
8:A:773:U:O2	8:A:778:G:O2'	2.34	0.43
8:A:1447:C:H2'	8:A:1448:G:H8	1.84	0.43
8:A:2250:G:OP1	8:A:2275:C:O2'	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:49:ASP:HB2	17:J:114:LEU:HD11	2.00	0.43
34:a:864:A:O2'	34:a:1078:U:O4	2.28	0.43
34:a:1352:C:H2'	34:a:1353:G:C8	2.54	0.43
40:g:25:PHE:HE2	40:g:119:LEU:HD21	1.83	0.43
57:x:135:PRO:HG2	57:x:286:PRO:HG2	2.00	0.43
8:A:1453:A:N6	21:N:74:GLU:OE2	2.52	0.43
8:A:2111:U:H1'	8:A:2118:U:H1'	2.01	0.43
8:A:2638:G:H1'	8:A:2778:A:N6	2.34	0.43
12:E:48:THR:HG23	12:E:86:ALA:HB3	2.01	0.43
18:K:24:VAL:HG13	18:K:33:ALA:HB2	1.99	0.43
19:L:18:ARG:NH1	19:L:21:ARG:HG3	2.34	0.43
34:a:662:U:H2'	34:a:663:A:C8	2.53	0.43
42:i:29:ILE:N	42:i:32:ARG:O	2.52	0.43
55:v:43:A:H2'	55:v:44:A:O4'	2.19	0.43
57:x:174:ALA:HB3	57:x:177:HIS:CE1	2.53	0.43
8:A:2030:6MZ:N3	8:A:2499:C:H5''	2.34	0.42
8:A:2333:A:OP1	30:W:73:ARG:NH1	2.42	0.42
8:A:2820:A:OP1	21:N:2:ARG:NH2	2.51	0.42
34:a:203:G:N2	34:a:204:G:O6	2.49	0.42
34:a:680:C:H2'	34:a:681:A:C8	2.54	0.42
34:a:1308:U:H2'	34:a:1309:G:H8	1.84	0.42
34:a:1326:U:H2'	34:a:1327:C:H6	1.84	0.42
38:e:45:VAL:HG23	38:e:116:VAL:HG23	2.00	0.42
8:A:1309:G:O2'	8:A:1611:C:O2'	2.31	0.42
34:a:854:U:OP1	63:a:1605:AM2:OB6	2.38	0.42
51:r:61:ALA:HB1	51:r:67:LEU:HD23	1.99	0.42
53:t:23:ARG:HD3	53:t:26:MET:HE3	2.01	0.42
53:t:44:ALA:O	53:t:48:LYS:HG2	2.19	0.42
57:x:502:GLY:O	57:x:516:HIS:ND1	2.51	0.42
8:A:926:G:H2'	8:A:927:A:H8	1.83	0.42
8:A:1061:U:O2'	16:I:9:LYS:O	2.35	0.42
8:A:1447:C:O2'	8:A:1544:A:N3	2.38	0.42
8:A:2070:A:H2'	8:A:2071:A:C8	2.54	0.42
8:A:2134:A:N7	8:A:2157:G:O2'	2.53	0.42
17:J:60:ASP:OD1	17:J:60:ASP:N	2.52	0.42
34:a:744:C:H2'	34:a:745:G:H8	1.84	0.42
49:p:55:ASP:OD1	49:p:56:ARG:N	2.52	0.42
51:r:17:VAL:O	51:r:18:GLN:HG3	2.19	0.42
1:O:15:ARG:HA	8:A:2046:G:H5'	2.01	0.42
7:6:56:ARG:NH2	52:s:66:VAL:HG13	2.34	0.42
8:A:322:A:OP2	12:E:163:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:910:A:N3	8:A:2264:C:O2'	2.41	0.42
8:A:1265:A:N1	8:A:2013:A:H5''	2.35	0.42
8:A:1803:A:H2	8:A:1823:G:H1'	1.84	0.42
8:A:1962:5MC:O2'	8:A:1964:G:OP2	2.37	0.42
25:R:14:VAL:HG21	25:R:20:VAL:HG21	2.01	0.42
29:V:6:ALA:HB1	29:V:40:ILE:HB	2.00	0.42
34:a:77:A:H2'	34:a:78:A:C8	2.54	0.42
34:a:127:G:HO2'	50:q:5:ARG:NH2	2.13	0.42
34:a:208:U:H2'	34:a:209:U:H3'	2.01	0.42
34:a:524:G:H2'	34:a:525:C:C6	2.54	0.42
34:a:880:C:OP1	45:l:4:ASN:ND2	2.52	0.42
34:a:1309:G:N7	46:m:97:ARG:NH2	2.66	0.42
48:o:38:LEU:HD23	48:o:42:PHE:HE2	1.85	0.42
57:x:139:PHE:HA	57:x:264:THR:O	2.19	0.42
1:0:15:ARG:NH1	8:A:1266:G:OP1	2.52	0.42
7:6:1:MET:HE2	7:6:1:MET:HB2	1.90	0.42
19:L:77:ILE:HB	19:L:110:VAL:HA	2.01	0.42
26:S:3:THR:OG1	26:S:62:ASP:OD2	2.36	0.42
34:a:76:G:H1	34:a:93:U:H3	1.66	0.42
34:a:492:C:H2'	34:a:493:A:C8	2.54	0.42
34:a:719:C:H1'	51:r:37:LYS:HB3	2.01	0.42
34:a:815:A:O2'	34:a:1526:G:N2	2.36	0.42
35:b:69:VAL:HB	35:b:162:VAL:HA	2.01	0.42
44:k:81:LEU:HG	44:k:104:PHE:HB3	2.02	0.42
45:l:35:ARG:HG2	45:l:37:TYR:CD1	2.55	0.42
47:n:79:LEU:HB2	47:n:84:VAL:HG23	2.00	0.42
49:p:8:ARG:CZ	49:p:15:PRO:HB3	2.50	0.42
57:x:196:ASP:OD1	57:x:196:ASP:N	2.48	0.42
8:A:2302:U:O2'	13:F:122:ASP:O	2.27	0.42
8:A:2685:G:H2'	8:A:2686:G:H8	1.85	0.42
13:F:152:ASP:OD1	13:F:152:ASP:N	2.49	0.42
20:M:28:PHE:HB3	20:M:64:TRP:CE2	2.54	0.42
34:a:236:A:H2'	34:a:237:G:C8	2.54	0.42
34:a:634:C:H2'	34:a:635:A:C8	2.54	0.42
36:c:126:ARG:NH2	36:c:191:THR:HG21	2.34	0.42
37:d:123:MET:HE1	37:d:145:ARG:HG2	2.01	0.42
40:g:110:ARG:HH12	40:g:121:ASN:ND2	2.18	0.42
48:o:42:PHE:CD2	48:o:55:LEU:HD22	2.54	0.42
50:q:77:VAL:HG12	50:q:80:LYS:HG2	2.01	0.42
57:x:602:GLU:HA	57:x:605:LYS:NZ	2.35	0.42
8:A:1501:G:OP1	10:C:100:ARG:NH2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1527:G:N1	8:A:1544:A:OP2	2.44	0.42
8:A:1769:U:O2'	8:A:1958:C:OP1	2.36	0.42
8:A:2247:A:H2'	8:A:2248:C:H6	1.85	0.42
11:D:55:LYS:HD2	11:D:60:VAL:HG22	2.01	0.42
27:T:6:ARG:NH2	27:T:37:ASP:OD2	2.42	0.42
27:T:65:GLY:N	27:T:79:ASP:OD1	2.53	0.42
34:a:744:C:H2'	34:a:745:G:C8	2.54	0.42
34:a:1425:U:H3	34:a:1475:G:H1	1.66	0.42
36:c:57:GLU:HB2	36:c:64:ARG:HB3	2.01	0.42
57:x:112:TYR:O	57:x:141:ASN:N	2.49	0.42
7:6:3:LYS:HE2	7:6:3:LYS:HB2	1.89	0.42
8:A:715:A:C8	48:o:59:VAL:HG11	2.55	0.42
8:A:1168:G:H2'	8:A:1169:A:C8	2.55	0.42
8:A:1594:U:H2'	8:A:1595:C:C6	2.55	0.42
8:A:1709:U:H2'	8:A:1710:G:C8	2.54	0.42
8:A:1925:C:H42	8:A:1929:G:H22	1.68	0.42
8:A:2139:U:O4	8:A:2153:C:N3	2.53	0.42
8:A:2660:A:H1'	57:x:675:GLY:HA3	2.01	0.42
9:B:48:U:H4'	22:O:100:HIS:HD2	1.84	0.42
25:R:68:ARG:O	25:R:90:ARG:NH2	2.53	0.42
34:a:501:C:H2'	34:a:502:A:C8	2.53	0.42
34:a:501:C:H2'	34:a:502:A:H8	1.85	0.42
34:a:757:U:O2'	34:a:879:C:O2	2.34	0.42
34:a:1013:G:H21	34:a:1016:A:H8	1.67	0.42
34:a:1109:C:OP1	36:c:175:HIS:ND1	2.51	0.42
34:a:1243:C:H2'	34:a:1244:G:H8	1.85	0.42
36:c:48:LYS:HE2	36:c:48:LYS:HB2	1.90	0.42
41:h:40:LYS:HE3	41:h:47:ASP:HA	2.02	0.42
41:h:76:ARG:HE	41:h:79:ARG:HA	1.84	0.42
41:h:114:ALA:HA	41:h:117:GLN:HE21	1.84	0.42
43:j:12:ALA:HB2	43:j:96:VAL:HG12	2.01	0.42
56:w:70:G:H2'	56:w:71:G:H8	1.84	0.42
57:x:563:GLY:HA2	57:x:567:GLY:HA2	2.02	0.42
8:A:78:U:H5'	32:Y:7:ARG:NH2	2.35	0.42
8:A:672:C:OP2	19:L:42:SER:OG	2.24	0.42
8:A:878:A:H3'	8:A:879:G:C8	2.55	0.42
8:A:1170:C:H3'	8:A:1171:G:H8	1.85	0.42
8:A:1441:G:H2'	8:A:1442:U:C6	2.54	0.42
8:A:1631:G:N1	8:A:1634:A:OP2	2.46	0.42
8:A:2822:G:H2'	8:A:2823:A:H5''	2.02	0.42
8:A:2898:U:H2'	8:A:2899:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:52:HIS:HA	10:C:216:ARG:HB2	2.02	0.42
10:C:141:HIS:CD2	10:C:194:VAL:HG22	2.55	0.42
11:D:8:LYS:HB2	11:D:201:LEU:HD11	2.01	0.42
18:K:48:PRO:HA	34:a:1422:G:OP1	2.20	0.42
21:N:1:MET:HE3	21:N:1:MET:HB2	1.90	0.42
23:P:38:ARG:HG2	23:P:39:LEU:H	1.85	0.42
34:a:419:C:OP1	34:a:513:C:O2'	2.38	0.42
34:a:958:A:H62	52:s:78:THR:H	1.68	0.42
34:a:1074:G:H4'	35:b:101:THR:HB	2.02	0.42
34:a:1075:U:OP1	35:b:177:ASN:ND2	2.53	0.42
34:a:1208:C:HO2'	57:x:512:GLY:HA2	1.85	0.42
46:m:32:ILE:HD12	46:m:58:GLU:HB3	2.01	0.42
57:x:2:ARG:NH1	57:x:377:ARG:HB3	2.34	0.42
7:6:38:SER:OG	7:6:39:LYS:NZ	2.51	0.42
8:A:305:C:H2'	8:A:306:U:C6	2.54	0.42
8:A:322:A:H5'	8:A:340:A:H1'	2.01	0.42
8:A:680:C:H2'	8:A:681:G:C8	2.54	0.42
8:A:726:G:O5'	8:A:1432:G:O2'	2.36	0.42
8:A:1315:C:O2'	8:A:1392:A:N3	2.44	0.42
8:A:2618:G:O2'	11:D:155:VAL:O	2.37	0.42
19:L:2:ARG:HA	19:L:2:ARG:HD3	1.83	0.42
34:a:769:G:H4'	34:a:1513:A:H4'	2.01	0.42
34:a:1355:G:H2'	34:a:1356:G:C8	2.55	0.42
35:b:112:ARG:HH12	35:b:116:LEU:HD13	1.84	0.42
40:g:25:PHE:HZ	40:g:119:LEU:HD11	1.84	0.42
42:i:53:LEU:HA	42:i:53:LEU:HD13	1.85	0.42
43:j:54:SER:O	47:n:81:ARG:NH2	2.52	0.42
46:m:79:LEU:HD22	46:m:86:ARG:HB2	2.01	0.42
8:A:181:A:H1'	8:A:435:C:H5'	2.02	0.41
8:A:1044:C:H4'	8:A:1047:G:H4'	2.02	0.41
8:A:1431:A:H2'	8:A:1432:G:C8	2.55	0.41
8:A:1662:U:O2'	8:A:2687:U:OP1	2.36	0.41
8:A:2014:A:H5'	26:S:94:ASP:OD2	2.20	0.41
8:A:2123:G:N2	8:A:2172:U:O4'	2.53	0.41
8:A:2342:C:H2'	8:A:2343:U:O4'	2.20	0.41
8:A:2525:G:HO2'	8:A:2742:G:HO2'	1.67	0.41
9:B:111:U:H2'	9:B:112:G:H8	1.85	0.41
26:S:29:VAL:HB	26:S:55:ILE:HD11	2.02	0.41
34:a:113:G:H2'	34:a:114:U:C6	2.55	0.41
34:a:316:C:O5'	34:a:351:G:O2'	2.37	0.41
34:a:321:A:H2'	34:a:322:C:H6	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:587:G:N1	34:a:754:C:OP2	2.41	0.41
37:d:36:ALA:HB3	37:d:41:GLY:HA2	2.02	0.41
37:d:55:ARG:HH21	37:d:62:ARG:HH12	1.67	0.41
43:j:85:ASP:HA	43:j:88:MET:HE2	2.02	0.41
57:x:298:LEU:HD13	57:x:403:ILE:HG13	2.02	0.41
8:A:871:U:H2'	8:A:872:U:C6	2.54	0.41
8:A:1219:U:H2'	8:A:1220:G:C8	2.55	0.41
8:A:1771:C:H2'	8:A:1772:A:H8	1.84	0.41
8:A:2485:G:OP1	20:M:45:GLN:NE2	2.47	0.41
13:F:63:LYS:HA	13:F:64:PRO:HD3	1.93	0.41
17:J:95:ARG:HE	17:J:96:ARG:HB2	1.85	0.41
20:M:77:PRO:O	20:M:80:VAL:HG12	2.21	0.41
22:O:29:HIS:HB3	22:O:36:TYR:HB2	2.02	0.41
34:a:135:C:O2	49:p:1:MET:N	2.53	0.41
34:a:407:U:H2'	34:a:408:A:C8	2.55	0.41
6:5:26:VAL:HA	6:5:83:ALA:H	1.86	0.41
8:A:192:C:O2	8:A:802:A:O2'	2.35	0.41
8:A:1668:A:N3	8:A:1670:C:N4	2.68	0.41
34:a:343:U:O2'	34:a:346:G:O6	2.32	0.41
34:a:344:A:H5''	34:a:345:C:H5	1.85	0.41
34:a:918:A:H2'	34:a:919:A:C8	2.55	0.41
34:a:1314:C:H2'	34:a:1315:U:C6	2.55	0.41
43:j:59:LYS:HE2	43:j:62:ARG:NH2	2.35	0.41
45:l:73:LEU:HD13	45:l:73:LEU:HA	1.83	0.41
50:q:80:LYS:HE2	50:q:80:LYS:HB3	1.87	0.41
57:x:135:PRO:HB3	57:x:255:VAL:HG12	2.02	0.41
57:x:322:LYS:NZ	57:x:324:ALA:HB2	2.35	0.41
57:x:361:ARG:NE	57:x:372:GLU:OE2	2.37	0.41
1:0:14:MET:HB3	8:A:2045:C:H4'	2.02	0.41
4:3:41:ARG:NH1	8:A:2351:G:O6	2.53	0.41
8:A:154:U:H2'	8:A:155:A:C8	2.55	0.41
8:A:2021:C:H5''	24:Q:24:TYR:HE2	1.86	0.41
9:B:7:G:H21	22:O:38:GLN:HE22	1.68	0.41
14:G:32:LEU:HD13	14:G:74:MET:SD	2.60	0.41
25:R:34:GLU:OE2	25:R:60:LYS:NZ	2.35	0.41
34:a:426:U:OP1	37:d:35:GLN:NE2	2.53	0.41
34:a:1397:C:OP2	38:e:28:ARG:NH2	2.42	0.41
34:a:1436:U:H2'	34:a:1437:A:C8	2.55	0.41
35:b:58:LYS:O	35:b:61:SER:OG	2.36	0.41
37:d:8:LEU:O	37:d:12:ARG:HG2	2.21	0.41
38:e:148:SER:OG	38:e:151:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:f:38:ARG:HB2	39:f:63:ASN:HB2	2.02	0.41
44:k:96:ILE:HG22	54:u:11:PHE:HZ	1.85	0.41
56:w:68:C:H2'	56:w:69:G:C8	2.55	0.41
57:x:142:LYS:HG2	64:x:801:GDP:C5	2.55	0.41
57:x:285:LEU:HD23	57:x:285:LEU:HA	1.80	0.41
8:A:1176:U:H2'	8:A:1177:G:C8	2.55	0.41
8:A:1353:A:H2'	8:A:1354:A:C8	2.56	0.41
8:A:1754:A:O3'	23:P:102:ARG:NH2	2.53	0.41
8:A:1960:A:HO2'	34:a:1484:C:HO2'	1.42	0.41
20:M:50:ARG:HA	20:M:53:MET:HG2	2.01	0.41
30:W:33:ILE:HD11	30:W:78:ILE:HD11	2.02	0.41
33:Z:4:ILE:HG13	33:Z:6:ILE:HD11	2.01	0.41
34:a:17:U:H2'	34:a:18:C:C6	2.55	0.41
34:a:719:C:N3	51:r:62:ARG:NH1	2.46	0.41
34:a:1271:A:H2'	34:a:1272:G:C8	2.55	0.41
35:b:187:ASP:OD1	35:b:188:THR:N	2.38	0.41
39:f:9:MET:HE1	51:r:64:LEU:HD22	2.02	0.41
44:k:34:THR:HG22	44:k:40:ALA:HA	2.01	0.41
48:o:35:ILE:O	48:o:39:GLN:HG2	2.20	0.41
57:x:199:VAL:HG23	57:x:200:THR:HG23	2.02	0.41
57:x:281:VAL:HG22	57:x:285:LEU:HD12	2.03	0.41
57:x:647:GLU:HG2	57:x:648:VAL:H	1.86	0.41
1:O:29:VAL:O	8:A:2885:G:N1	2.42	0.41
8:A:154:U:H2'	8:A:155:A:H8	1.85	0.41
8:A:347:A:H2'	8:A:348:A:C8	2.55	0.41
8:A:2099:U:H3	8:A:2190:G:H1	1.68	0.41
8:A:2656:U:O5'	8:A:2656:U:H6	2.04	0.41
22:O:55:GLU:OE1	22:O:81:ARG:NH2	2.53	0.41
34:a:176:C:H2'	34:a:177:G:N3	2.34	0.41
37:d:190:LEU:HD23	37:d:190:LEU:HA	1.91	0.41
38:e:53:ARG:HD2	38:e:53:ARG:HA	1.87	0.41
39:f:12:PRO:HG3	39:f:55:HIS:O	2.21	0.41
40:g:97:ALA:HB1	40:g:101:ARG:NH1	2.36	0.41
54:u:12:ASP:O	54:u:16:ARG:HG2	2.21	0.41
57:x:39:ILE:HG13	57:x:40:GLY:H	1.85	0.41
57:x:76:LYS:HE2	57:x:76:LYS:HB3	1.89	0.41
57:x:230:GLU:HA	57:x:233:MET:HG2	2.02	0.41
57:x:270:LYS:HA	57:x:270:LYS:HD3	1.78	0.41
8:A:499:U:H5''	28:U:42:LYS:HD2	2.02	0.41
8:A:555:G:O2'	8:A:556:A:O5'	2.37	0.41
8:A:630:G:N2	8:A:633:A:OP2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1595:C:H2'	8:A:1596:A:H8	1.85	0.41
8:A:2848:G:H1'	8:A:2868:A:H61	1.85	0.41
9:B:5:U:H2'	9:B:6:G:H8	1.85	0.41
26:S:71:VAL:HG13	26:S:105:VAL:HG23	2.03	0.41
34:a:195:A:H1'	34:a:222:C:O2'	2.20	0.41
34:a:407:U:H2'	34:a:408:A:H8	1.85	0.41
34:a:531:U:N3	57:x:511:ARG:HA	2.36	0.41
34:a:1157:A:N7	34:a:1180:A:N6	2.68	0.41
34:a:1404:C:H2'	34:a:1405:G:C8	2.55	0.41
35:b:53:LEU:HA	35:b:56:LEU:HD12	2.02	0.41
57:x:182:VAL:HA	57:x:189:ALA:HA	2.03	0.41
57:x:266:GLY:HA3	57:x:273:GLY:HA3	2.02	0.41
8:A:155:A:H2'	8:A:156:A:H8	1.86	0.41
8:A:1198:U:H2'	8:A:1199:U:C6	2.56	0.41
8:A:1801:A:N6	8:A:2201:G:O2'	2.43	0.41
8:A:2505:G:N2	8:A:2610:C:C2	2.86	0.41
8:A:2661:G:N3	8:A:2661:G:H2'	2.35	0.41
8:A:2874:C:H5''	21:N:4:ARG:NH1	2.36	0.41
12:E:138:LEU:HD13	12:E:167:VAL:HG21	2.02	0.41
34:a:481:G:H8	34:a:482:A:H62	1.69	0.41
34:a:958:A:C2	52:s:54:ARG:HG2	2.56	0.41
34:a:1042:A:H3'	34:a:1043:G:H8	1.86	0.41
34:a:1372:U:OP1	42:i:73:GLY:N	2.49	0.41
37:d:57:LYS:HG3	37:d:199:ILE:HG23	2.03	0.41
38:e:76:ASN:HB2	38:e:81:GLN:CD	2.46	0.41
41:h:34:ALA:O	41:h:38:VAL:HG23	2.21	0.41
56:w:48:C:C4	56:w:59:U:C4	3.09	0.41
57:x:533:TYR:HE2	57:x:553:ASP:HB2	1.85	0.41
8:A:833:A:H2'	8:A:834:G:H8	1.85	0.41
8:A:1219:U:H2'	8:A:1220:G:H8	1.86	0.41
8:A:1614:A:C2	26:S:93:ALA:HB2	2.56	0.41
8:A:1899:A:H4'	8:A:1901:A:H5''	2.03	0.41
8:A:2564:A:OP1	8:A:2648:G:O2'	2.31	0.41
8:A:2810:A:H4'	11:D:62:LYS:HD2	2.03	0.41
13:F:122:ASP:OD1	13:F:124:ARG:N	2.53	0.41
15:H:4:ILE:HG23	15:H:39:ALA:HB2	2.02	0.41
17:J:1:MET:HE1	25:R:13:ARG:HH21	1.86	0.41
17:J:140:LEU:HG	17:J:142:ILE:HG12	2.03	0.41
18:K:42:THR:HG22	18:K:57:VAL:HG22	2.03	0.41
25:R:35:PHE:HB2	25:R:59:ILE:HB	2.03	0.41
34:a:76:G:O6	34:a:93:U:O4	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1312:G:H5'	52:s:4:LEU:HD11	2.02	0.41
35:b:114:LYS:O	35:b:118:THR:HG23	2.21	0.41
39:f:38:ARG:HH11	39:f:61:LEU:HD21	1.86	0.41
39:f:38:ARG:HH21	39:f:96:VAL:HG13	1.86	0.41
39:f:42:TRP:HB2	39:f:59:TYR:HB2	2.03	0.41
39:f:88:MET:HB2	51:r:64:LEU:HD21	2.02	0.41
47:n:22:LYS:HE3	47:n:22:LYS:HB2	1.88	0.41
53:t:56:ILE:HD13	53:t:59:ARG:HH21	1.86	0.41
55:v:33:U:O2'	55:v:34:C:O5'	2.39	0.41
57:x:2:ARG:NH2	57:x:378:ALA:O	2.43	0.41
57:x:413:PRO:HG3	57:x:445:ARG:HE	1.86	0.41
57:x:421:PRO:HD3	57:x:430:MET:SD	2.61	0.41
57:x:506:LYS:NZ	57:x:511:ARG:HE	2.19	0.41
57:x:551:ALA:HB1	57:x:554:LYS:HE2	2.02	0.41
57:x:566:ALA:HB2	57:x:698:ILE:HD13	2.02	0.41
1:0:2:VAL:HG23	8:A:2015:A:C6	2.56	0.41
7:6:57:VAL:HA	7:6:61:ASN:HB2	2.02	0.41
8:A:1155:A:H5''	24:Q:54:ARG:HD3	2.02	0.41
8:A:2064:C:O2'	8:A:2251:OMG:N2	2.52	0.41
8:A:2514:U:H4'	17:J:81:ILE:HG12	2.02	0.41
34:a:1238:A:H2'	34:a:1239:A:H5'	2.03	0.41
39:f:47:LEU:HD21	39:f:57:ALA:HB3	2.03	0.41
47:n:89:MET:HE1	47:n:98:LYS:HD2	2.03	0.41
50:q:9:GLY:HA3	50:q:24:ILE:HD13	2.03	0.41
57:x:403:ILE:HB	57:x:404:ILE:HD12	2.03	0.41
57:x:601:LYS:HE2	57:x:605:LYS:HD3	2.03	0.41
8:A:674:G:H5''	12:E:71:GLY:N	2.36	0.40
8:A:1071:G:N2	8:A:1089:A:C6	2.87	0.40
8:A:1435:G:H2'	8:A:1436:G:C8	2.56	0.40
8:A:2108:A:O2'	8:A:2109:U:O4'	2.35	0.40
8:A:2328:A:H2'	8:A:2329:U:H6	1.86	0.40
8:A:2780:G:N1	17:J:102:GLU:OE1	2.46	0.40
8:A:2808:G:O2'	8:A:2809:A:H8	2.04	0.40
12:E:146:VAL:HG12	12:E:167:VAL:HG22	2.03	0.40
14:G:88:LEU:HD11	14:G:95:ALA:HB2	2.02	0.40
31:X:21:LEU:HD23	55:v:75:C:N4	2.36	0.40
34:a:945:G:N2	34:a:1334:G:O2'	2.54	0.40
38:e:40:ASP:N	38:e:40:ASP:OD1	2.50	0.40
43:j:54:SER:HB3	43:j:58:ASN:HB2	2.02	0.40
57:x:61:THR:HG22	57:x:63:THR:O	2.21	0.40
57:x:613:GLU:OE2	57:x:691:SER:OG	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:x:630:VAL:O	57:x:634:LEU:HD22	2.22	0.40
8:A:216:A:N7	8:A:431:U:O2	2.55	0.40
8:A:372:G:N2	8:A:401:A:OP2	2.49	0.40
8:A:741:U:H2'	8:A:742:A:C8	2.56	0.40
8:A:813:U:H2'	8:A:814:C:H6	1.86	0.40
8:A:2572:A:OP1	8:A:2574:G:O2'	2.36	0.40
18:K:71:ARG:HB2	18:K:75:SER:HB2	2.02	0.40
19:L:92:LEU:HD12	19:L:92:LEU:HA	1.96	0.40
19:L:96:LYS:HG3	19:L:101:ILE:HD11	2.04	0.40
21:N:57:THR:HG23	21:N:62:ASN:ND2	2.36	0.40
31:X:9:LYS:HE3	31:X:53:LYS:HG2	2.04	0.40
34:a:715:A:H2'	34:a:716:A:C8	2.56	0.40
36:c:198:LYS:HE2	36:c:200:TRP:CH2	2.56	0.40
38:e:79:THR:HA	38:e:119:VAL:HG13	2.02	0.40
56:w:22:G:H2'	56:w:23:A:H8	1.86	0.40
8:A:20:C:H2'	8:A:21:A:C8	2.54	0.40
8:A:145:C:H2'	8:A:146:A:H8	1.87	0.40
8:A:353:C:H2'	8:A:354:A:H8	1.86	0.40
8:A:593:U:H2'	8:A:594:U:C6	2.57	0.40
8:A:698:C:O2'	8:A:734:A:N6	2.31	0.40
8:A:946:C:H2'	8:A:947:A:H8	1.86	0.40
8:A:1727:C:H2'	8:A:1728:C:C6	2.57	0.40
8:A:2391:G:H2'	8:A:2424:C:H41	1.86	0.40
8:A:2511:U:H1'	11:D:130:GLN:HE21	1.86	0.40
8:A:2530:A:N6	14:G:155:PRO:HG3	2.36	0.40
20:M:16:ARG:HA	20:M:16:ARG:HD3	1.97	0.40
34:a:38:G:H22	34:a:397:A:H5'	1.86	0.40
34:a:736:C:H2'	34:a:737:C:H6	1.86	0.40
34:a:1009:U:H2'	34:a:1010:U:H6	1.86	0.40
34:a:1408:A:N1	63:a:1663:AM2:OA6	2.47	0.40
35:b:101:THR:HG23	35:b:174:GLU:HG3	2.03	0.40
36:c:52:SER:N	36:c:68:HIS:O	2.52	0.40
40:g:1:PRO:HB2	40:g:2:ARG:H	1.67	0.40
40:g:46:LEU:HD12	40:g:57:GLU:HB2	2.04	0.40
8:A:514:A:H2'	8:A:515:A:H8	1.86	0.40
8:A:575:A:OP2	8:A:2055:C:N4	2.54	0.40
8:A:948:C:H2'	8:A:949:G:H8	1.86	0.40
8:A:1252:G:N2	24:Q:32:ARG:HB3	2.35	0.40
8:A:1316:U:H2'	8:A:1317:G:C8	2.55	0.40
8:A:1405:U:H2'	8:A:1406:U:C6	2.56	0.40
8:A:1710:G:H2'	8:A:1711:A:H8	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2110:G:N1	8:A:2120:G:N7	2.70	0.40
8:A:2468:A:O2'	8:A:2469:A:O5'	2.30	0.40
8:A:2661:G:H3'	8:A:2662:A:C8	2.57	0.40
9:B:63:C:H2'	9:B:64:G:C8	2.56	0.40
17:J:40:HIS:NE2	17:J:52:ASP:OD2	2.45	0.40
17:J:130:HIS:HD2	17:J:132:HIS:HB2	1.85	0.40
24:Q:61:ILE:HG23	24:Q:75:TYR:CZ	2.57	0.40
25:R:27:ILE:HG22	25:R:28:ALA:H	1.86	0.40
34:a:1148:U:H2'	34:a:1149:C:O4'	2.21	0.40
36:c:46:LEU:HD11	36:c:86:LEU:HD11	2.04	0.40
36:c:123:LEU:HD11	36:c:129:PHE:HB3	2.04	0.40
38:e:61:LYS:HB3	38:e:61:LYS:HE2	1.88	0.40
46:m:11:HIS:HA	46:m:43:LYS:HD3	2.04	0.40
52:s:45:GLY:H	52:s:61:VAL:HG23	1.86	0.40
57:x:28:ARG:NH1	57:x:39:ILE:HB	2.37	0.40
57:x:252:ARG:HG3	57:x:284:TYR:HA	2.02	0.40
8:A:65:U:H5'	27:T:75:GLY:HA2	2.02	0.40
8:A:1209:U:O2'	8:A:1237:A:N1	2.49	0.40
8:A:1746:A:H2'	8:A:1747:U:C6	2.57	0.40
8:A:2070:A:H2'	8:A:2071:A:H8	1.86	0.40
8:A:2135:A:H3'	8:A:2136:G:C8	2.56	0.40
8:A:2292:U:H2'	8:A:2293:G:H8	1.87	0.40
8:A:2528:U:O2	8:A:2535:G:O6	2.40	0.40
11:D:13:ARG:HH21	23:P:55:HIS:HA	1.86	0.40
11:D:181:ASP:OD2	11:D:184:ARG:HB3	2.21	0.40
17:J:37:ARG:HA	17:J:118:MET:SD	2.61	0.40
30:W:74:LYS:HB3	30:W:74:LYS:HE2	1.88	0.40
32:Y:44:LYS:O	32:Y:48:ARG:HG2	2.21	0.40
33:Z:4:ILE:HG22	33:Z:58:GLU:HG3	2.04	0.40
34:a:1059:C:O3'	47:n:85:ARG:NH1	2.55	0.40
34:a:1241:G:H2'	34:a:1242:G:C8	2.51	0.40
38:e:105:ILE:HB	38:e:123:LEU:HA	2.03	0.40
57:x:662:MET:HB2	57:x:665:TYR:HB2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
2	1	48/55 (87%)	48 (100%)	0	0	100	100
3	2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
4	3	62/65 (95%)	56 (90%)	6 (10%)	0	100	100
5	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
6	5	129/165 (78%)	113 (88%)	16 (12%)	0	100	100
7	6	64/70 (91%)	57 (89%)	7 (11%)	0	100	100
10	C	269/273 (98%)	256 (95%)	13 (5%)	0	100	100
11	D	207/209 (99%)	193 (93%)	14 (7%)	0	100	100
12	E	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
13	F	175/179 (98%)	157 (90%)	18 (10%)	0	100	100
14	G	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
15	H	147/149 (99%)	130 (88%)	17 (12%)	0	100	100
16	I	139/142 (98%)	118 (85%)	21 (15%)	0	100	100
17	J	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
18	K	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
19	L	141/144 (98%)	133 (94%)	8 (6%)	0	100	100
20	M	134/136 (98%)	125 (93%)	9 (7%)	0	100	100
21	N	118/127 (93%)	110 (93%)	8 (7%)	0	100	100
22	O	114/117 (97%)	106 (93%)	8 (7%)	0	100	100
23	P	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
24	Q	115/118 (98%)	112 (97%)	3 (3%)	0	100	100
25	R	101/103 (98%)	91 (90%)	10 (10%)	0	100	100
26	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
27	T	91/100 (91%)	90 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	U	100/104 (96%)	91 (91%)	9 (9%)	0	100	100
29	V	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
30	W	73/85 (86%)	70 (96%)	3 (4%)	0	100	100
31	X	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
32	Y	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
33	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
35	b	216/240 (90%)	204 (94%)	12 (6%)	0	100	100
36	c	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
37	d	203/206 (98%)	193 (95%)	10 (5%)	0	100	100
38	e	155/167 (93%)	151 (97%)	4 (3%)	0	100	100
39	f	98/135 (73%)	88 (90%)	10 (10%)	0	100	100
40	g	149/179 (83%)	138 (93%)	11 (7%)	0	100	100
41	h	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
42	i	125/130 (96%)	117 (94%)	8 (6%)	0	100	100
43	j	96/103 (93%)	86 (90%)	10 (10%)	0	100	100
44	k	114/129 (88%)	107 (94%)	7 (6%)	0	100	100
45	l	121/124 (98%)	108 (89%)	13 (11%)	0	100	100
46	m	112/118 (95%)	104 (93%)	8 (7%)	0	100	100
47	n	99/102 (97%)	94 (95%)	5 (5%)	0	100	100
48	o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
49	p	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
50	q	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
51	r	63/75 (84%)	59 (94%)	4 (6%)	0	100	100
52	s	80/92 (87%)	75 (94%)	5 (6%)	0	100	100
53	t	83/87 (95%)	80 (96%)	3 (4%)	0	100	100
54	u	63/71 (89%)	61 (97%)	2 (3%)	0	100	100
57	x	701/704 (100%)	657 (94%)	44 (6%)	0	100	100
All	All	6551/6924 (95%)	6146 (94%)	405 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	0	47/48 (98%)	46 (98%)	1 (2%)	48	71
2	1	45/49 (92%)	43 (96%)	2 (4%)	24	53
3	2	38/38 (100%)	38 (100%)	0	100	100
4	3	51/52 (98%)	51 (100%)	0	100	100
5	4	34/34 (100%)	33 (97%)	1 (3%)	37	63
7	6	59/62 (95%)	57 (97%)	2 (3%)	32	60
10	C	216/218 (99%)	212 (98%)	4 (2%)	52	73
11	D	164/164 (100%)	163 (99%)	1 (1%)	84	92
12	E	165/165 (100%)	163 (99%)	2 (1%)	67	82
13	F	148/150 (99%)	145 (98%)	3 (2%)	50	72
14	G	137/138 (99%)	131 (96%)	6 (4%)	24	53
15	H	114/114 (100%)	110 (96%)	4 (4%)	31	60
17	J	116/116 (100%)	112 (97%)	4 (3%)	32	60
18	K	103/104 (99%)	102 (99%)	1 (1%)	73	85
19	L	102/103 (99%)	98 (96%)	4 (4%)	27	57
20	M	109/109 (100%)	106 (97%)	3 (3%)	38	64
21	N	100/103 (97%)	97 (97%)	3 (3%)	36	63
22	O	86/87 (99%)	85 (99%)	1 (1%)	67	82
23	P	99/100 (99%)	98 (99%)	1 (1%)	73	85
24	Q	89/90 (99%)	86 (97%)	3 (3%)	32	60
25	R	84/84 (100%)	82 (98%)	2 (2%)	44	67
26	S	93/93 (100%)	92 (99%)	1 (1%)	70	83
27	T	80/84 (95%)	78 (98%)	2 (2%)	42	66
28	U	83/85 (98%)	79 (95%)	4 (5%)	21	51
29	V	78/78 (100%)	77 (99%)	1 (1%)	65	81
30	W	57/63 (90%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	X	67/68 (98%)	66 (98%)	1 (2%)	60	78
32	Y	55/55 (100%)	53 (96%)	2 (4%)	30	59
33	Z	48/49 (98%)	48 (100%)	0	100	100
35	b	180/198 (91%)	176 (98%)	4 (2%)	47	69
36	c	170/190 (90%)	165 (97%)	5 (3%)	37	63
37	d	172/173 (99%)	167 (97%)	5 (3%)	37	63
38	e	114/126 (90%)	112 (98%)	2 (2%)	54	74
39	f	87/116 (75%)	84 (97%)	3 (3%)	32	60
40	g	124/147 (84%)	123 (99%)	1 (1%)	79	88
41	h	104/105 (99%)	102 (98%)	2 (2%)	52	73
42	i	105/107 (98%)	102 (97%)	3 (3%)	37	63
43	j	86/90 (96%)	82 (95%)	4 (5%)	22	51
44	k	89/99 (90%)	83 (93%)	6 (7%)	13	41
45	l	103/104 (99%)	98 (95%)	5 (5%)	21	50
46	m	92/96 (96%)	86 (94%)	6 (6%)	14	42
47	n	79/84 (94%)	73 (92%)	6 (8%)	11	37
48	o	76/77 (99%)	71 (93%)	5 (7%)	14	42
49	p	65/65 (100%)	64 (98%)	1 (2%)	60	78
50	q	74/78 (95%)	72 (97%)	2 (3%)	40	65
51	r	56/65 (86%)	54 (96%)	2 (4%)	30	59
52	s	72/79 (91%)	68 (94%)	4 (6%)	17	47
53	t	65/66 (98%)	65 (100%)	0	100	100
54	u	46/61 (75%)	46 (100%)	0	100	100
57	x	577/578 (100%)	556 (96%)	21 (4%)	30	59
58	y	1/1 (100%)	1 (100%)	0	100	100
All	All	5204/5408 (96%)	5058 (97%)	146 (3%)	40	64

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	29	VAL
2	1	4	ILE
2	1	27	ARG

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Mol	Chain	Res	Type
5	4	22	VAL
7	6	5	ILE
7	6	48	GLN
10	C	50	THR
10	C	80	LEU
10	C	182	LYS
10	C	225	ASN
11	D	105	LYS
12	E	73	ILE
12	E	149	ILE
13	F	34	THR
13	F	36	ASN
13	F	149	ARG
14	G	8	VAL
14	G	26	LYS
14	G	112	VAL
14	G	126	THR
14	G	157	LYS
14	G	167	VAL
15	H	14	SER
15	H	15	LEU
15	H	19	VAL
15	H	37	VAL
17	J	5	THR
17	J	37	ARG
17	J	88	THR
17	J	139	VAL
18	K	6	THR
19	L	18	ARG
19	L	29	LYS
19	L	30	THR
19	L	59	ARG
20	M	24	THR
20	M	112	LEU
20	M	136	MET
21	N	35	LYS
21	N	76	VAL
21	N	83	LEU
22	O	98	GLN
23	P	3	ILE
24	Q	7	VAL
24	Q	51	GLN

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Mol	Chain	Res	Type
24	Q	103	VAL
25	R	29	THR
25	R	58	VAL
26	S	97	LEU
27	T	39	THR
27	T	57	VAL
28	U	13	LEU
28	U	17	ASP
28	U	27	VAL
28	U	61	GLU
29	V	1	MET
31	X	3	VAL
32	Y	11	VAL
32	Y	49	ASP
35	b	67	LEU
35	b	135	MET
35	b	213	LEU
35	b	219	THR
36	c	20	THR
36	c	42	LEU
36	c	46	LEU
36	c	105	VAL
36	c	151	GLU
37	d	4	LEU
37	d	18	LEU
37	d	24	VAL
37	d	27	ILE
37	d	131	ILE
38	e	68	ARG
38	e	123	LEU
39	f	29	ILE
39	f	36	ILE
39	f	97	THR
40	g	86	VAL
41	h	61	THR
41	h	120	LEU
42	i	34	LEU
42	i	53	LEU
42	i	104	THR
43	j	9	ARG
43	j	19	ASP
43	j	50	THR

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Mol	Chain	Res	Type
43	j	99	GLN
44	k	52	ARG
44	k	68	ARG
44	k	73	VAL
44	k	78	ILE
44	k	92	ARG
44	k	112	VAL
45	l	15	VAL
45	l	39	THR
45	l	53	ARG
45	l	73	LEU
45	l	78	VAL
46	m	6	ILE
46	m	27	THR
46	m	33	LEU
46	m	57	ASP
46	m	82	LEU
46	m	103	THR
47	n	15	LEU
47	n	46	LEU
47	n	49	GLN
47	n	66	GLN
47	n	81	ARG
47	n	89	MET
48	o	30	LEU
48	o	31	LEU
48	o	44	GLU
48	o	73	ASP
48	o	86	LEU
49	p	1	MET
50	q	11	VAL
50	q	21	VAL
51	r	21	ASP
51	r	70	THR
52	s	43	MET
52	s	47	THR
52	s	57	VAL
52	s	66	VAL
57	x	9	TYR
57	x	89	PRO
57	x	105	LEU
57	x	177	HIS

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Mol	Chain	Res	Type
57	x	188	LYS
57	x	206	ILE
57	x	213	LEU
57	x	258	ASN
57	x	259	GLU
57	x	263	VAL
57	x	307	GLU
57	x	329	VAL
57	x	332	LEU
57	x	362	ILE
57	x	376	VAL
57	x	440	GLU
57	x	468	ILE
57	x	608	LYS
57	x	634	LEU
57	x	644	GLN
57	x	673	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	27	ASN
10	C	133	ASN
10	C	259	ASN
11	D	36	GLN
11	D	136	ASN
13	F	80	GLN
14	G	29	ASN
17	J	138	GLN
20	M	3	GLN
20	M	88	ASN
21	N	73	ASN
22	O	98	GLN
23	P	14	GLN
23	P	55	HIS
24	Q	51	GLN
25	R	18	GLN
26	S	9	HIS
27	T	28	ASN
27	T	48	GLN
27	T	91	GLN
28	U	26	ASN

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Mol	Chain	Res	Type
28	U	39	ASN
28	U	53	GLN
28	U	73	ASN
29	V	87	GLN
30	W	46	ASN
31	X	22	ASN
31	X	31	ASN
32	Y	58	ASN
35	b	18	GLN
35	b	41	ASN
35	b	102	ASN
35	b	121	GLN
37	d	39	GLN
37	d	40	HIS
37	d	53	GLN
37	d	70	GLN
37	d	88	ASN
40	g	67	ASN
40	g	121	ASN
40	g	147	ASN
41	h	15	ASN
41	h	17	GLN
43	j	99	GLN
44	k	80	ASN
57	x	169	GLN
57	x	177	HIS
57	x	197	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	a	1539/1542 (99%)	334 (21%)	0
55	v	74/77 (96%)	15 (20%)	0
56	w	75/76 (98%)	24 (32%)	0
59	z	10/33 (30%)	2 (20%)	0
8	A	2902/2903 (99%)	640 (22%)	39 (1%)
9	B	119/120 (99%)	29 (24%)	3 (2%)
All	All	4719/4751 (99%)	1044 (22%)	42 (0%)

All (1044) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	10	A
8	A	15	G
8	A	23	G
8	A	34	U
8	A	42	A
8	A	43	G
8	A	44	A
8	A	46	G
8	A	58	G
8	A	62	U
8	A	63	A
8	A	71	A
8	A	74	A
8	A	75	G
8	A	84	A
8	A	96	C
8	A	101	A
8	A	118	A
8	A	120	U
8	A	131	A
8	A	140	C
8	A	141	G
8	A	142	A
8	A	157	C
8	A	160	A
8	A	163	C
8	A	164	C
8	A	170	U
8	A	196	A
8	A	199	A
8	A	204	A
8	A	205	G
8	A	215	G
8	A	216	A
8	A	221	A
8	A	222	A
8	A	223	A
8	A	228	C
8	A	230	G
8	A	242	G
8	A	243	U
8	A	244	A
8	A	248	G

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Mol	Chain	Res	Type
8	A	250	G
8	A	255	A
8	A	261	G
8	A	265	A
8	A	266	G
8	A	267	C
8	A	272	A
8	A	273	G
8	A	275	C
8	A	276	U
8	A	278	A
8	A	279	A
8	A	287	G
8	A	288	U
8	A	330	A
8	A	335	C
8	A	345	A
8	A	359	G
8	A	361	G
8	A	362	A
8	A	363	G
8	A	369	U
8	A	371	A
8	A	372	G
8	A	377	G
8	A	386	G
8	A	393	C
8	A	395	U
8	A	396	G
8	A	401	A
8	A	402	A
8	A	404	A
8	A	405	U
8	A	406	G
8	A	411	G
8	A	412	A
8	A	455	C
8	A	457	A
8	A	458	G
8	A	459	U
8	A	473	G
8	A	480	A

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Mol	Chain	Res	Type
8	A	481	G
8	A	482	A
8	A	490	C
8	A	491	G
8	A	504	A
8	A	505	A
8	A	509	C
8	A	510	C
8	A	513	A
8	A	529	A
8	A	530	G
8	A	532	A
8	A	533	G
8	A	546	U
8	A	548	G
8	A	549	G
8	A	556	A
8	A	563	A
8	A	568	U
8	A	573	U
8	A	575	A
8	A	588	U
8	A	603	A
8	A	613	A
8	A	614	A
8	A	615	U
8	A	622	G
8	A	627	A
8	A	637	A
8	A	645	C
8	A	646	U
8	A	647	G
8	A	655	A
8	A	659	G
8	A	669	G
8	A	670	A
8	A	682	G
8	A	685	A
8	A	686	U
8	A	694	U
8	A	711	G
8	A	712	G

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Mol	Chain	Res	Type
8	A	714	U
8	A	716	A
8	A	729	G
8	A	730	A
8	A	747	5MC
8	A	757	G
8	A	762	U
8	A	764	A
8	A	775	G
8	A	782	A
8	A	783	A
8	A	784	G
8	A	785	G
8	A	789	A
8	A	791	C
8	A	792	A
8	A	805	G
8	A	806	C
8	A	812	C
8	A	819	A
8	A	827	U
8	A	828	U
8	A	831	G
8	A	846	U
8	A	847	U
8	A	858	G
8	A	859	G
8	A	878	A
8	A	879	G
8	A	881	G
8	A	883	G
8	A	884	U
8	A	885	C
8	A	887	A
8	A	889	C
8	A	890	C
8	A	891	G
8	A	892	A
8	A	893	C
8	A	894	U
8	A	895	U
8	A	896	A

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Mol	Chain	Res	Type
8	A	897	C
8	A	899	A
8	A	903	C
8	A	907	G
8	A	910	A
8	A	931	U
8	A	933	A
8	A	941	A
8	A	946	C
8	A	961	C
8	A	965	C
8	A	973	A
8	A	974	G
8	A	975	A
8	A	983	A
8	A	984	A
8	A	990	A
8	A	995	C
8	A	996	A
8	A	1005	C
8	A	1012	U
8	A	1013	C
8	A	1024	G
8	A	1025	G
8	A	1026	G
8	A	1027	A
8	A	1028	A
8	A	1033	U
8	A	1040	A
8	A	1041	G
8	A	1042	G
8	A	1046	A
8	A	1047	G
8	A	1048	A
8	A	1053	C
8	A	1056	G
8	A	1057	A
8	A	1058	U
8	A	1059	G
8	A	1060	U
8	A	1061	U
8	A	1062	G

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Mol	Chain	Res	Type
8	A	1063	G
8	A	1064	C
8	A	1066	U
8	A	1067	A
8	A	1068	G
8	A	1069	A
8	A	1070	A
8	A	1071	G
8	A	1072	C
8	A	1073	A
8	A	1074	G
8	A	1077	A
8	A	1078	U
8	A	1079	C
8	A	1080	A
8	A	1083	U
8	A	1084	A
8	A	1085	A
8	A	1086	A
8	A	1087	G
8	A	1088	A
8	A	1089	A
8	A	1090	A
8	A	1091	G
8	A	1092	C
8	A	1094	U
8	A	1095	A
8	A	1096	A
8	A	1098	A
8	A	1100	C
8	A	1101	U
8	A	1102	C
8	A	1103	A
8	A	1105	U
8	A	1106	G
8	A	1109	C
8	A	1110	G
8	A	1111	A
8	A	1112	G
8	A	1115	G
8	A	1116	G
8	A	1121	C

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Mol	Chain	Res	Type
8	A	1130	U
8	A	1131	G
8	A	1132	U
8	A	1134	A
8	A	1135	C
8	A	1136	G
8	A	1139	G
8	A	1142	A
8	A	1169	A
8	A	1170	C
8	A	1171	G
8	A	1174	U
8	A	1175	A
8	A	1176	U
8	A	1179	G
8	A	1180	U
8	A	1188	U
8	A	1212	G
8	A	1225	G
8	A	1227	G
8	A	1234	U
8	A	1235	G
8	A	1247	A
8	A	1253	A
8	A	1255	U
8	A	1256	G
8	A	1264	A
8	A	1271	G
8	A	1272	A
8	A	1273	U
8	A	1284	A
8	A	1300	G
8	A	1301	A
8	A	1311	G
8	A	1312	U
8	A	1334	G
8	A	1340	U
8	A	1341	G
8	A	1345	C
8	A	1365	A
8	A	1368	G
8	A	1376	C

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Mol	Chain	Res	Type
8	A	1377	G
8	A	1379	U
8	A	1383	A
8	A	1386	C
8	A	1395	A
8	A	1409	U
8	A	1413	A
8	A	1415	U
8	A	1416	G
8	A	1419	A
8	A	1420	A
8	A	1421	G
8	A	1428	C
8	A	1432	G
8	A	1433	A
8	A	1434	A
8	A	1445	G
8	A	1452	G
8	A	1453	A
8	A	1458	U
8	A	1460	U
8	A	1461	C
8	A	1474	U
8	A	1476	U
8	A	1478	G
8	A	1482	G
8	A	1488	C
8	A	1490	A
8	A	1491	G
8	A	1494	A
8	A	1497	U
8	A	1504	A
8	A	1508	A
8	A	1515	A
8	A	1524	G
8	A	1532	A
8	A	1535	A
8	A	1536	C
8	A	1537	G
8	A	1538	G
8	A	1549	A
8	A	1554	U

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Mol	Chain	Res	Type
8	A	1555	G
8	A	1557	C
8	A	1558	C
8	A	1566	A
8	A	1569	A
8	A	1578	U
8	A	1580	A
8	A	1584	U
8	A	1585	C
8	A	1591	A
8	A	1592	C
8	A	1608	A
8	A	1610	A
8	A	1634	A
8	A	1635	A
8	A	1647	U
8	A	1648	U
8	A	1649	G
8	A	1651	G
8	A	1654	A
8	A	1674	G
8	A	1693	U
8	A	1698	A
8	A	1715	G
8	A	1716	U
8	A	1726	C
8	A	1727	C
8	A	1730	C
8	A	1731	G
8	A	1732	C
8	A	1738	G
8	A	1757	A
8	A	1760	C
8	A	1764	C
8	A	1773	A
8	A	1782	U
8	A	1784	A
8	A	1791	A
8	A	1800	C
8	A	1801	A
8	A	1802	A
8	A	1808	A

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Mol	Chain	Res	Type
8	A	1809	A
8	A	1811	G
8	A	1816	C
8	A	1829	A
8	A	1835	2MG
8	A	1866	A
8	A	1869	G
8	A	1884	G
8	A	1895	C
8	A	1900	A
8	A	1901	A
8	A	1906	G
8	A	1908	C
8	A	1910	G
8	A	1912	A
8	A	1913	A
8	A	1917	PSU
8	A	1922	G
8	A	1924	C
8	A	1925	C
8	A	1926	U
8	A	1927	A
8	A	1930	G
8	A	1936	A
8	A	1937	A
8	A	1938	A
8	A	1939	5MU
8	A	1955	U
8	A	1960	A
8	A	1964	G
8	A	1965	C
8	A	1967	C
8	A	1970	A
8	A	1971	U
8	A	1972	G
8	A	1982	U
8	A	1991	U
8	A	1992	G
8	A	1997	C
8	A	2020	A
8	A	2021	C
8	A	2022	U

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Mol	Chain	Res	Type
8	A	2023	C
8	A	2030	6MZ
8	A	2031	A
8	A	2032	G
8	A	2033	A
8	A	2036	C
8	A	2043	C
8	A	2046	G
8	A	2055	C
8	A	2056	G
8	A	2060	A
8	A	2061	G
8	A	2062	A
8	A	2067	G
8	A	2069	G7M
8	A	2077	A
8	A	2091	C
8	A	2093	G
8	A	2101	A
8	A	2102	G
8	A	2103	C
8	A	2104	C
8	A	2105	U
8	A	2107	G
8	A	2110	G
8	A	2111	U
8	A	2112	G
8	A	2114	A
8	A	2116	G
8	A	2118	U
8	A	2119	A
8	A	2120	G
8	A	2126	A
8	A	2127	G
8	A	2128	G
8	A	2129	C
8	A	2131	U
8	A	2132	U
8	A	2133	G
8	A	2134	A
8	A	2135	A
8	A	2136	G

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Mol	Chain	Res	Type
8	A	2137	U
8	A	2138	G
8	A	2139	U
8	A	2143	C
8	A	2145	C
8	A	2146	C
8	A	2147	A
8	A	2148	G
8	A	2149	U
8	A	2150	C
8	A	2151	U
8	A	2153	C
8	A	2154	A
8	A	2155	U
8	A	2158	A
8	A	2159	G
8	A	2161	C
8	A	2162	G
8	A	2164	C
8	A	2165	C
8	A	2169	A
8	A	2170	A
8	A	2171	A
8	A	2172	U
8	A	2173	A
8	A	2174	C
8	A	2176	A
8	A	2180	U
8	A	2181	U
8	A	2183	A
8	A	2184	A
8	A	2185	U
8	A	2186	G
8	A	2190	G
8	A	2193	G
8	A	2198	A
8	A	2204	G
8	A	2211	A
8	A	2212	A
8	A	2225	A
8	A	2226	C
8	A	2238	G

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Mol	Chain	Res	Type
8	A	2239	G
8	A	2266	A
8	A	2271	G
8	A	2279	G
8	A	2283	C
8	A	2287	A
8	A	2288	A
8	A	2297	A
8	A	2300	C
8	A	2305	U
8	A	2309	A
8	A	2320	U
8	A	2322	A
8	A	2325	G
8	A	2326	C
8	A	2333	A
8	A	2334	U
8	A	2336	A
8	A	2345	G
8	A	2347	C
8	A	2350	C
8	A	2352	A
8	A	2361	G
8	A	2383	G
8	A	2385	C
8	A	2402	U
8	A	2403	C
8	A	2406	A
8	A	2410	G
8	A	2423	U
8	A	2425	A
8	A	2429	G
8	A	2430	A
8	A	2432	A
8	A	2435	A
8	A	2441	U
8	A	2447	G
8	A	2448	A
8	A	2452	C
8	A	2459	A
8	A	2469	A
8	A	2475	C

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Mol	Chain	Res	Type
8	A	2476	A
8	A	2478	A
8	A	2480	C
8	A	2484	G
8	A	2488	G
8	A	2491	U
8	A	2494	G
8	A	2502	G
8	A	2503	2MA
8	A	2505	G
8	A	2506	U
8	A	2518	A
8	A	2529	G
8	A	2535	G
8	A	2542	A
8	A	2547	A
8	A	2552	OMU
8	A	2554	U
8	A	2566	A
8	A	2567	G
8	A	2573	C
8	A	2576	G
8	A	2578	G
8	A	2585	U
8	A	2586	U
8	A	2592	G
8	A	2602	A
8	A	2603	G
8	A	2609	U
8	A	2613	U
8	A	2615	U
8	A	2623	G
8	A	2624	G
8	A	2629	U
8	A	2630	G
8	A	2634	A
8	A	2636	C
8	A	2646	C
8	A	2648	G
8	A	2654	A
8	A	2655	G
8	A	2656	U

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Mol	Chain	Res	Type
8	A	2663	G
8	A	2684	U
8	A	2689	U
8	A	2690	U
8	A	2702	G
8	A	2707	U
8	A	2715	C
8	A	2718	G
8	A	2720	U
8	A	2725	A
8	A	2726	A
8	A	2727	A
8	A	2729	G
8	A	2732	G
8	A	2733	A
8	A	2744	G
8	A	2748	A
8	A	2750	A
8	A	2751	G
8	A	2755	C
8	A	2757	A
8	A	2765	A
8	A	2769	U
8	A	2778	A
8	A	2779	U
8	A	2790	U
8	A	2791	G
8	A	2796	U
8	A	2797	U
8	A	2798	U
8	A	2799	A
8	A	2800	A
8	A	2801	G
8	A	2808	G
8	A	2809	A
8	A	2818	U
8	A	2820	A
8	A	2821	A
8	A	2833	U
8	A	2834	G
8	A	2835	A
8	A	2836	U

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Mol	Chain	Res	Type
8	A	2849	U
8	A	2867	G
8	A	2872	A
8	A	2873	A
8	A	2879	A
8	A	2884	U
8	A	2886	A
8	A	2891	U
8	A	2893	A
9	B	9	G
9	B	13	G
9	B	17	C
9	B	18	G
9	B	19	C
9	B	24	G
9	B	26	C
9	B	34	A
9	B	35	C
9	B	37	C
9	B	41	G
9	B	42	C
9	B	45	A
9	B	51	G
9	B	53	A
9	B	56	G
9	B	57	A
9	B	62	C
9	B	65	U
9	B	67	G
9	B	73	A
9	B	87	U
9	B	88	C
9	B	89	U
9	B	90	C
9	B	91	C
9	B	101	A
9	B	109	A
9	B	120	U
34	a	2	A
34	a	6	G
34	a	7	A
34	a	9	G

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Mol	Chain	Res	Type
34	a	31	G
34	a	32	A
34	a	39	G
34	a	46	G
34	a	48	C
34	a	51	A
34	a	70	U
34	a	71	A
34	a	76	G
34	a	78	A
34	a	80	A
34	a	81	A
34	a	83	C
34	a	84	U
34	a	85	U
34	a	86	G
34	a	87	C
34	a	89	U
34	a	90	C
34	a	94	G
34	a	96	U
34	a	98	A
34	a	121	U
34	a	141	G
34	a	144	G
34	a	158	G
34	a	163	C
34	a	164	G
34	a	166	U
34	a	173	U
34	a	182	A
34	a	183	C
34	a	184	G
34	a	189	A
34	a	197	A
34	a	198	G
34	a	205	A
34	a	206	C
34	a	208	U
34	a	209	U
34	a	210	C
34	a	211	G

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Mol	Chain	Res	Type
34	a	212	G
34	a	226	G
34	a	240	G
34	a	244	U
34	a	245	U
34	a	247	G
34	a	251	G
34	a	262	A
34	a	266	G
34	a	267	C
34	a	270	A
34	a	281	G
34	a	289	G
34	a	306	A
34	a	316	C
34	a	321	A
34	a	327	A
34	a	328	C
34	a	329	A
34	a	330	C
34	a	344	A
34	a	347	G
34	a	351	G
34	a	352	C
34	a	353	A
34	a	354	G
34	a	356	A
34	a	360	G
34	a	367	U
34	a	372	C
34	a	375	U
34	a	388	G
34	a	397	A
34	a	406	G
34	a	411	A
34	a	412	A
34	a	413	G
34	a	421	U
34	a	423	G
34	a	428	G
34	a	429	U
34	a	439	U

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Mol	Chain	Res	Type
34	a	440	C
34	a	446	G
34	a	448	A
34	a	461	A
34	a	462	G
34	a	465	A
34	a	468	A
34	a	471	U
34	a	472	U
34	a	473	U
34	a	474	G
34	a	479	U
34	a	482	A
34	a	484	G
34	a	495	A
34	a	496	A
34	a	505	G
34	a	509	A
34	a	510	A
34	a	511	C
34	a	516	PSU
34	a	517	G
34	a	518	C
34	a	521	G
34	a	524	G
34	a	531	U
34	a	532	A
34	a	535	A
34	a	547	A
34	a	559	A
34	a	562	U
34	a	563	A
34	a	564	C
34	a	572	A
34	a	573	A
34	a	576	C
34	a	577	G
34	a	582	C
34	a	596	A
34	a	607	A
34	a	614	C
34	a	615	G

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Mol	Chain	Res	Type
34	a	629	A
34	a	632	U
34	a	642	A
34	a	650	G
34	a	653	U
34	a	665	A
34	a	703	G
34	a	704	A
34	a	721	G
34	a	723	U
34	a	724	G
34	a	734	G
34	a	747	A
34	a	748	G
34	a	753	A
34	a	755	G
34	a	773	G
34	a	777	A
34	a	781	A
34	a	792	A
34	a	793	U
34	a	794	A
34	a	814	A
34	a	815	A
34	a	816	A
34	a	817	C
34	a	819	A
34	a	829	G
34	a	841	C
34	a	842	U
34	a	843	U
34	a	844	G
34	a	845	A
34	a	846	G
34	a	849	G
34	a	851	G
34	a	870	U
34	a	875	U
34	a	885	G
34	a	902	G
34	a	913	A
34	a	914	A

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Mol	Chain	Res	Type
34	a	922	G
34	a	934	C
34	a	935	A
34	a	940	C
34	a	960	U
34	a	961	U
34	a	966	2MG
34	a	968	A
34	a	969	A
34	a	971	G
34	a	973	G
34	a	975	A
34	a	976	G
34	a	977	A
34	a	981	U
34	a	982	U
34	a	984	C
34	a	992	U
34	a	993	G
34	a	994	A
34	a	996	A
34	a	999	C
34	a	1003	G
34	a	1004	A
34	a	1005	A
34	a	1006	G
34	a	1007	U
34	a	1011	C
34	a	1014	A
34	a	1016	A
34	a	1017	U
34	a	1021	A
34	a	1022	A
34	a	1023	U
34	a	1025	U
34	a	1027	C
34	a	1028	C
34	a	1029	U
34	a	1030	U
34	a	1031	C
34	a	1032	G
34	a	1035	A

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Mol	Chain	Res	Type
34	a	1040	U
34	a	1043	G
34	a	1047	G
34	a	1065	U
34	a	1084	G
34	a	1085	U
34	a	1092	A
34	a	1094	G
34	a	1095	U
34	a	1101	A
34	a	1109	C
34	a	1124	G
34	a	1125	U
34	a	1126	U
34	a	1127	G
34	a	1131	G
34	a	1134	G
34	a	1137	C
34	a	1138	G
34	a	1139	G
34	a	1144	G
34	a	1145	A
34	a	1159	U
34	a	1160	G
34	a	1167	A
34	a	1168	U
34	a	1169	A
34	a	1171	A
34	a	1177	G
34	a	1179	A
34	a	1183	U
34	a	1184	G
34	a	1196	A
34	a	1197	A
34	a	1200	C
34	a	1212	U
34	a	1213	A
34	a	1214	C
34	a	1226	C
34	a	1227	A
34	a	1238	A
34	a	1239	A

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Mol	Chain	Res	Type
34	a	1240	U
34	a	1241	G
34	a	1251	A
34	a	1254	A
34	a	1260	G
34	a	1261	A
34	a	1267	C
34	a	1270	G
34	a	1275	A
34	a	1280	A
34	a	1286	U
34	a	1287	A
34	a	1294	G
34	a	1297	G
34	a	1300	G
34	a	1301	U
34	a	1302	C
34	a	1305	G
34	a	1317	C
34	a	1320	C
34	a	1323	G
34	a	1331	G
34	a	1332	A
34	a	1346	A
34	a	1347	G
34	a	1348	U
34	a	1360	A
34	a	1361	G
34	a	1363	A
34	a	1364	U
34	a	1370	G
34	a	1378	C
34	a	1379	G
34	a	1383	C
34	a	1386	G
34	a	1397	C
34	a	1398	A
34	a	1413	A
34	a	1423	G
34	a	1424	U
34	a	1433	A
34	a	1441	A

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Mol	Chain	Res	Type
34	a	1442	G
34	a	1443	C
34	a	1444	U
34	a	1446	A
34	a	1450	U
34	a	1451	U
34	a	1452	C
34	a	1453	G
34	a	1473	G
34	a	1474	U
34	a	1475	G
34	a	1476	A
34	a	1477	U
34	a	1479	C
34	a	1482	G
34	a	1483	A
34	a	1485	U
34	a	1486	G
34	a	1487	G
34	a	1488	G
34	a	1492	A
34	a	1494	G
34	a	1499	A
34	a	1503	A
34	a	1506	U
34	a	1517	G
34	a	1519	MA6
34	a	1529	G
34	a	1530	G
34	a	1534	A
34	a	1535	C
34	a	1536	C
34	a	1537	U
34	a	1538	C
34	a	1539	C
34	a	1540	U
55	v	9	G
55	v	14	A
55	v	20	H2U
55	v	21	A
55	v	33	U
55	v	34	C

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Mol	Chain	Res	Type
55	v	42	G
55	v	43	A
55	v	44	A
55	v	46	A
55	v	47	U
55	v	48	C
55	v	52	G
55	v	55	PSU
55	v	76	A
56	w	8	4SU
56	w	14	A
56	w	16	U
56	w	17	C
56	w	18	G
56	w	19	G
56	w	20	U
56	w	21	A
56	w	29	G
56	w	36	A
56	w	40	C
56	w	45	U
56	w	46	G7M
56	w	47	U
56	w	48	C
56	w	53	G
56	w	59	U
56	w	60	U
56	w	61	C
56	w	67	C
56	w	68	C
56	w	69	G
56	w	74	C
56	w	76	A
59	z	-1	C
59	z	0	U

All (42) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	242	G
8	A	361	G
8	A	458	G

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Mol	Chain	Res	Type
8	A	479	A
8	A	481	G
8	A	555	G
8	A	652	U
8	A	715	A
8	A	774	G
8	A	784	G
8	A	883	G
8	A	894	U
8	A	1023	U
8	A	1024	G
8	A	1082	U
8	A	1090	A
8	A	1093	G
8	A	1300	G
8	A	1331	G
8	A	1432	G
8	A	1451	C
8	A	1475	G
8	A	1490	A
8	A	1715	G
8	A	1730	C
8	A	1907	G
8	A	1926	U
8	A	2067	G
8	A	2192	U
8	A	2287	A
8	A	2308	G
8	A	2319	G
8	A	2324	U
8	A	2468	A
8	A	2505	G
8	A	2655	G
8	A	2728	U
8	A	2796	U
8	A	2808	G
9	B	36	C
9	B	52	A
9	B	66	A

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

46 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$
8	PSU	A	2504	8	18,21,22	1.11	1 (5%)	22,30,33	1.80	4 (18%)
8	1MG	A	745	8	18,26,27	0.90	1 (5%)	19,39,42	0.50	0
8	G7M	A	2069	8	20,26,27	0.52	0	17,39,42	0.61	0
34	2MG	a	1516	34	18,26,27	0.94	1 (5%)	16,38,41	0.68	0
34	4OC	a	1402	34	20,23,24	0.35	0	26,32,35	0.61	0
8	2MA	A	2503	8,60	19,25,26	1.01	2 (10%)	21,37,40	3.07	5 (23%)
56	MIA	w	37	56	24,31,32	0.63	0	26,44,47	1.10	4 (15%)
8	6MZ	A	1618	8	18,25,26	0.74	0	16,36,39	0.80	1 (6%)
34	G7M	a	527	34	20,26,27	0.52	0	17,39,42	0.49	0
8	2MG	A	2445	8	18,26,27	1.01	1 (5%)	16,38,41	0.60	0
8	OMU	A	2552	8	19,22,23	0.36	0	26,31,34	0.58	0
56	5MU	w	54	56	19,22,23	0.29	0	28,32,35	0.35	0
55	PSU	v	55	55	18,21,22	1.08	1 (5%)	22,30,33	1.63	5 (22%)
34	2MG	a	1207	34	18,26,27	0.93	1 (5%)	16,38,41	0.67	0
34	UR3	a	1498	34	19,22,23	0.35	0	26,32,35	0.66	0
8	PSU	A	746	8,60	18,21,22	1.12	1 (5%)	22,30,33	1.72	4 (18%)
8	3TD	A	1915	8	18,22,23	0.38	0	22,32,35	0.62	0
8	2MG	A	1835	8	18,26,27	0.95	1 (5%)	16,38,41	0.64	0
34	2MG	a	966	34	18,26,27	0.94	2 (11%)	16,38,41	0.77	0
8	PSU	A	1911	8	18,21,22	1.07	1 (5%)	22,30,33	1.70	4 (18%)
8	OMG	A	2251	8,60,56	18,26,27	0.94	1 (5%)	19,38,41	0.61	0
56	4SU	w	8	56	18,21,22	0.30	0	26,30,33	0.41	0
34	5MC	a	1407	34	18,22,23	0.35	0	26,32,35	0.50	0
34	PSU	a	516	34,60	18,21,22	0.88	1 (5%)	22,30,33	1.72	4 (18%)
8	5MU	A	1939	8,60	19,22,23	0.29	0	28,32,35	0.54	0
8	PSU	A	955	8	18,21,22	1.06	1 (5%)	22,30,33	1.71	4 (18%)
56	G7M	w	46	56	20,26,27	0.50	0	17,39,42	0.47	0
8	OMC	A	2498	8,60	19,22,23	0.34	0	26,31,34	0.43	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
55	5MU	v	54	55	19,22,23	0.28	0	28,32,35	0.45	0
56	PSU	w	55	56	18,21,22	1.16	1 (5%)	22,30,33	1.65	4 (18%)
8	5MC	A	1962	8	18,22,23	0.29	0	26,32,35	0.48	0
8	PSU	A	1917	8	18,21,22	1.00	1 (5%)	22,30,33	1.77	4 (18%)
55	H2U	v	20	55	18,21,22	0.45	0	21,30,33	0.55	0
56	PSU	w	32	56	18,21,22	1.06	1 (5%)	22,30,33	1.60	4 (18%)
8	PSU	A	2605	8	18,21,22	1.13	1 (5%)	22,30,33	1.72	4 (18%)
56	PSU	w	39	56	18,21,22	1.12	1 (5%)	22,30,33	1.68	5 (22%)
34	5MC	a	967	34	18,22,23	0.29	0	26,32,35	0.45	0
8	PSU	A	2580	8	18,21,22	1.11	2 (11%)	22,30,33	1.83	5 (22%)
55	4SU	v	8	55	18,21,22	0.35	0	26,30,33	0.34	0
34	MA6	a	1518	34	18,26,27	0.78	0	19,38,41	0.84	1 (5%)
8	6MZ	A	2030	8	18,25,26	0.78	0	16,36,39	0.97	1 (6%)
8	PSU	A	2457	8	18,21,22	1.02	1 (5%)	22,30,33	1.83	5 (22%)
8	PSU	A	2604	8	18,21,22	1.03	1 (5%)	22,30,33	1.70	4 (18%)
58	FME	y	101	58	8,9,10	0.95	0	7,9,11	0.94	0
34	MA6	a	1519	34	18,26,27	0.78	0	19,38,41	0.84	1 (5%)
8	5MC	A	747	8	18,22,23	0.32	0	26,32,35	0.46	0

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
8	PSU	A	2504	8	-	0/7/25/26	0/2/2/2
8	1MG	A	745	8	-	0/3/25/26	0/3/3/3
8	G7M	A	2069	8	-	1/3/25/26	0/3/3/3
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2
8	2MA	A	2503	8,60	-	1/3/25/26	0/3/3/3
56	MIA	w	37	56	-	2/11/33/34	0/3/3/3
8	6MZ	A	1618	8	-	0/5/27/28	0/3/3/3
34	G7M	a	527	34	-	2/3/25/26	0/3/3/3
8	2MG	A	2445	8	-	0/5/27/28	0/3/3/3
8	OMU	A	2552	8	-	2/9/27/28	0/2/2/2
56	5MU	w	54	56	-	0/7/25/26	0/2/2/2
55	PSU	v	55	55	-	1/7/25/26	0/2/2/2
34	2MG	a	1207	34	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
8	PSU	A	746	8,60	-	4/7/25/26	0/2/2/2
8	3TD	A	1915	8	-	2/7/25/26	0/2/2/2
8	2MG	A	1835	8	-	2/5/27/28	0/3/3/3
34	2MG	a	966	34	-	2/5/27/28	0/3/3/3
8	PSU	A	1911	8	-	0/7/25/26	0/2/2/2
8	OMG	A	2251	8,60,56	-	1/5/27/28	0/3/3/3
56	4SU	w	8	56	-	0/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
34	PSU	a	516	34,60	-	0/7/25/26	0/2/2/2
8	5MU	A	1939	8,60	-	2/7/25/26	0/2/2/2
8	PSU	A	955	8	-	0/7/25/26	0/2/2/2
56	G7M	w	46	56	-	1/3/25/26	0/3/3/3
8	OMC	A	2498	8,60	-	0/9/27/28	0/2/2/2
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
56	PSU	w	55	56	-	0/7/25/26	0/2/2/2
8	5MC	A	1962	8	-	0/7/25/26	0/2/2/2
8	PSU	A	1917	8	-	4/7/25/26	0/2/2/2
55	H2U	v	20	55	-	6/7/38/39	0/2/2/2
56	PSU	w	32	56	-	3/7/25/26	0/2/2/2
8	PSU	A	2605	8	-	0/7/25/26	0/2/2/2
56	PSU	w	39	56	-	2/7/25/26	0/2/2/2
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
8	PSU	A	2580	8	-	0/7/25/26	0/2/2/2
55	4SU	v	8	55	-	0/7/25/26	0/2/2/2
34	MA6	a	1518	34	-	0/7/29/30	0/3/3/3
8	6MZ	A	2030	8	-	2/5/27/28	0/3/3/3
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
8	PSU	A	2604	8	-	0/7/25/26	0/2/2/2
58	FME	y	101	58	-	5/7/9/11	-
34	MA6	a	1519	34	-	1/7/29/30	0/3/3/3
8	5MC	A	747	8	-	1/7/25/26	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	55	PSU	C6-C5	3.99	1.40	1.35
8	A	2605	PSU	C6-C5	3.82	1.39	1.35
55	v	55	PSU	C6-C5	3.73	1.39	1.35
56	w	39	PSU	C6-C5	3.68	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2504	PSU	C6-C5	3.58	1.39	1.35
8	A	746	PSU	C6-C5	3.56	1.39	1.35
56	w	32	PSU	C6-C5	3.53	1.39	1.35
8	A	1911	PSU	C6-C5	3.47	1.39	1.35
8	A	955	PSU	C6-C5	3.44	1.39	1.35
8	A	2604	PSU	C6-C5	3.43	1.39	1.35
8	A	1917	PSU	C6-C5	3.27	1.39	1.35
8	A	2580	PSU	C6-C5	3.22	1.39	1.35
8	A	2457	PSU	C6-C5	2.94	1.38	1.35
34	a	516	PSU	C6-C5	2.89	1.38	1.35
34	a	966	2MG	C5-C6	-2.50	1.42	1.47
8	A	1835	2MG	C5-C6	-2.49	1.42	1.47
8	A	2445	2MG	C5-C6	-2.41	1.42	1.47
8	A	2580	PSU	O4'-C1'	-2.39	1.40	1.43
8	A	745	1MG	C5-C4	-2.32	1.37	1.43
34	a	1516	2MG	C5-C6	-2.30	1.42	1.47
8	A	2251	OMG	C5-C6	-2.26	1.42	1.47
8	A	2503	2MA	C6-N6	-2.14	1.26	1.34
34	a	1207	2MG	C5-C6	-2.13	1.43	1.47
8	A	2503	2MA	C6-N1	2.12	1.37	1.33
34	a	966	2MG	C8-N7	-2.11	1.31	1.35

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2503	2MA	C5-C6-N1	-12.35	112.90	121.01
8	A	2504	PSU	N1-C2-N3	4.83	120.60	115.13
8	A	2457	PSU	C4-N3-C2	-4.68	119.59	126.34
8	A	2457	PSU	N1-C2-N3	4.53	120.27	115.13
8	A	746	PSU	C4-N3-C2	-4.52	119.82	126.34
8	A	1911	PSU	C4-N3-C2	-4.45	119.93	126.34
8	A	2604	PSU	C4-N3-C2	-4.45	119.93	126.34
8	A	1917	PSU	C4-N3-C2	-4.45	119.93	126.34
8	A	2605	PSU	C4-N3-C2	-4.42	119.97	126.34
8	A	2580	PSU	N1-C2-N3	4.41	120.13	115.13
8	A	2504	PSU	C4-N3-C2	-4.41	119.98	126.34
8	A	2605	PSU	N1-C2-N3	4.37	120.08	115.13
8	A	746	PSU	N1-C2-N3	4.37	120.08	115.13
8	A	955	PSU	N1-C2-N3	4.36	120.07	115.13
8	A	2604	PSU	N1-C2-N3	4.35	120.06	115.13
56	w	55	PSU	C4-N3-C2	-4.35	120.07	126.34
8	A	1911	PSU	N1-C2-N3	4.30	120.00	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1917	PSU	N1-C2-N3	4.29	120.00	115.13
8	A	2580	PSU	C4-N3-C2	-4.28	120.17	126.34
56	w	55	PSU	N1-C2-N3	4.24	119.93	115.13
8	A	955	PSU	C4-N3-C2	-4.21	120.27	126.34
55	v	55	PSU	N1-C2-N3	4.19	119.88	115.13
56	w	39	PSU	N1-C2-N3	4.12	119.80	115.13
56	w	32	PSU	N1-C2-N3	4.04	119.70	115.13
34	a	516	PSU	N1-C2-N3	3.97	119.63	115.13
56	w	39	PSU	C4-N3-C2	-3.97	120.62	126.34
55	v	55	PSU	C4-N3-C2	-3.93	120.67	126.34
56	w	32	PSU	C4-N3-C2	-3.92	120.69	126.34
8	A	2503	2MA	C2-N3-C4	-3.91	112.34	115.52
34	a	516	PSU	C4-N3-C2	-3.90	120.72	126.34
8	A	2503	2MA	C2-N1-C6	3.80	124.00	118.08
8	A	2580	PSU	O2-C2-N1	-3.17	119.30	122.79
8	A	1917	PSU	O2-C2-N1	-3.02	119.46	122.79
8	A	955	PSU	O2-C2-N1	-2.99	119.50	122.79
8	A	1917	PSU	C6-N1-C2	-2.90	119.72	122.68
34	a	516	PSU	C6-N1-C2	-2.85	119.77	122.68
34	a	516	PSU	O2-C2-N1	-2.76	119.75	122.79
56	w	37	MIA	C2-N3-C4	-2.73	111.56	115.32
8	A	955	PSU	C6-N1-C2	-2.65	119.98	122.68
8	A	2504	PSU	C6-N1-C2	-2.64	119.98	122.68
8	A	2457	PSU	O2-C2-N1	-2.64	119.89	122.79
8	A	2605	PSU	O2-C2-N1	-2.63	119.89	122.79
56	w	37	MIA	C5-C6-N1	-2.62	118.63	120.81
8	A	2580	PSU	O4'-C1'-C2'	2.61	108.83	105.14
8	A	2580	PSU	C6-N1-C2	-2.59	120.03	122.68
8	A	1911	PSU	O2-C2-N1	-2.59	119.94	122.79
56	w	39	PSU	O4-C4-N3	-2.59	115.16	120.12
34	a	1519	MA6	C9-N6-C6	2.55	127.24	119.51
8	A	746	PSU	O2-C2-N1	-2.54	120.00	122.79
55	v	55	PSU	C6-N1-C2	-2.50	120.12	122.68
56	w	32	PSU	O2-C2-N1	-2.46	120.08	122.79
8	A	2605	PSU	C6-N1-C2	-2.43	120.20	122.68
55	v	55	PSU	O2-C2-N1	-2.42	120.12	122.79
56	w	32	PSU	C6-N1-C2	-2.39	120.24	122.68
34	a	1518	MA6	C9-N6-C6	2.36	126.66	119.51
8	A	2604	PSU	O2-C2-N1	-2.36	120.20	122.79
8	A	2504	PSU	O2-C2-N1	-2.34	120.21	122.79
8	A	2457	PSU	O4'-C1'-C2'	2.34	108.45	105.14
8	A	2503	2MA	N6-C6-N1	2.33	123.41	117.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	39	PSU	C6-N1-C2	-2.32	120.32	122.68
56	w	39	PSU	O4'-C1'-C2'	2.28	108.37	105.14
56	w	55	PSU	O2-C2-N1	-2.27	120.30	122.79
56	w	55	PSU	C6-N1-C2	-2.24	120.40	122.68
8	A	1911	PSU	C6-N1-C2	-2.22	120.41	122.68
8	A	2503	2MA	C5-C6-N6	2.20	123.69	120.35
8	A	746	PSU	C6-N1-C2	-2.15	120.49	122.68
8	A	2457	PSU	C6-N1-C2	-2.12	120.52	122.68
55	v	55	PSU	O4'-C1'-C2'	2.11	108.11	105.14
8	A	2604	PSU	C6-N1-C2	-2.07	120.56	122.68
8	A	1618	6MZ	C2-N1-C6	2.04	118.34	116.59
8	A	2030	6MZ	C2-N1-C6	2.04	118.34	116.59
56	w	37	MIA	C12-C13-C14	2.01	131.06	127.14
56	w	37	MIA	C12-N6-C6	-2.01	119.57	122.55

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	a	1498	UR3	O4'-C1'-N1-C2
55	v	20	H2U	O4'-C4'-C5'-O5'
55	v	20	H2U	O4'-C1'-N1-C6
8	A	746	PSU	C2'-C1'-C5-C4
8	A	746	PSU	C2'-C1'-C5-C6
8	A	1915	3TD	O4'-C1'-C5-C4
8	A	1915	3TD	O4'-C1'-C5-C6
8	A	2030	6MZ	O4'-C4'-C5'-O5'
8	A	2030	6MZ	C3'-C4'-C5'-O5'
8	A	2251	OMG	C1'-C2'-O2'-CM2
8	A	2552	OMU	O4'-C1'-N1-C2
56	w	32	PSU	O4'-C1'-C5-C4
56	w	32	PSU	O4'-C1'-C5-C6
56	w	37	MIA	C12-C13-C14-C15
56	w	37	MIA	C12-C13-C14-C16
56	w	39	PSU	O4'-C1'-C5-C4
56	w	39	PSU	O4'-C1'-C5-C6
58	y	101	FME	O1-CN-N-CA
58	y	101	FME	O-C-CA-CB
8	A	2552	OMU	O4'-C1'-N1-C6
55	v	20	H2U	C3'-C4'-C5'-O5'
8	A	1917	PSU	C3'-C4'-C5'-O5'
8	A	1917	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
8	A	1939	5MU	O4'-C4'-C5'-O5'
58	y	101	FME	CA-CB-CG-SD
8	A	1835	2MG	O4'-C4'-C5'-O5'
8	A	1835	2MG	C3'-C4'-C5'-O5'
55	v	20	H2U	C2'-C1'-N1-C6
34	a	527	G7M	C3'-C4'-C5'-O5'
58	y	101	FME	N-CA-CB-CG
55	v	20	H2U	C2'-C1'-N1-C2
34	a	1498	UR3	O4'-C1'-N1-C6
34	a	966	2MG	C3'-C4'-C5'-O5'
8	A	1939	5MU	C3'-C4'-C5'-O5'
34	a	966	2MG	O4'-C4'-C5'-O5'
56	w	46	G7M	C4'-C5'-O5'-P
34	a	527	G7M	O4'-C4'-C5'-O5'
8	A	2503	2MA	O4'-C4'-C5'-O5'
55	v	55	PSU	C4'-C5'-O5'-P
8	A	2069	G7M	O4'-C4'-C5'-O5'
55	v	20	H2U	O4'-C1'-N1-C2
58	y	101	FME	C-CA-CB-CG
34	a	1519	MA6	C4'-C5'-O5'-P
8	A	746	PSU	O4'-C1'-C5-C4
8	A	1917	PSU	O4'-C1'-C5-C4
56	w	32	PSU	O4'-C4'-C5'-O5'
34	a	1402	4OC	C3'-C4'-C5'-O5'
8	A	746	PSU	O4'-C1'-C5-C6
8	A	1917	PSU	O4'-C1'-C5-C6
8	A	747	5MC	C4'-C5'-O5'-P
34	a	1402	4OC	O4'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	a	1402	4OC	1	0
56	w	37	MIA	1	0
8	A	2552	OMU	1	0
8	A	1835	2MG	1	0
34	a	966	2MG	1	0
8	A	2251	OMG	2	0
34	a	516	PSU	2	0
8	A	1962	5MC	1	0
34	a	967	5MC	1	0

*Continued on next page...*

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	v	8	4SU	1	0
34	a	1518	MA6	1	0
8	A	2030	6MZ	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 378 ligands modelled in this entry, 373 are monoatomic - leaving 5 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	$\# Z  > 2$
63	AM2	a	1614	-	40,40,40	0.56	0	53,60,60	1.26	5 (9%)
65	PO4	x	802	60	4,4,4	0.79	0	6,6,6	0.40	0
63	AM2	a	1605	-	40,40,40	0.52	0	53,60,60	1.11	3 (5%)
64	GDP	x	801	60	24,30,30	0.98	2 (8%)	30,47,47	0.69	1 (3%)
63	AM2	a	1663	-	40,40,40	0.61	0	53,60,60	1.12	3 (5%)

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
63	AM2	a	1605	-	-	4/12/84/84	0/4/4/4
64	GDP	x	801	60	-	0/12/32/32	0/3/3/3
63	AM2	a	1614	-	-	5/12/84/84	0/4/4/4
63	AM2	a	1663	-	-	1/12/84/84	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	x	801	GDP	C5-C6	-2.71	1.41	1.47
64	x	801	GDP	C8-N7	-2.01	1.31	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	a	1605	AM2	OA4-CA1-CA2	5.04	121.48	110.25
63	a	1614	AM2	CB1-OB1-CB5	4.23	121.99	113.69
63	a	1614	AM2	CB3-CB4-CB5	3.70	118.38	110.67
63	a	1663	AM2	CC6-CC5-CC4	3.67	118.71	111.18
63	a	1663	AM2	OA4-CA1-CA2	3.36	117.73	110.25
63	a	1663	AM2	OA1-CA1-CA2	3.34	113.82	108.23
63	a	1614	AM2	OA1-CC1-CC6	-3.12	101.74	109.18
63	a	1614	AM2	OA1-CA1-CA2	2.99	113.24	108.23
63	a	1605	AM2	CA1-OA4-CA5	2.46	117.02	113.06
63	a	1614	AM2	OA5-CA8-CA7	2.13	114.73	110.58
63	a	1605	AM2	OA4-CA5-CA4	2.04	111.98	108.88
64	x	801	GDP	O6-C6-C5	2.03	128.34	124.37

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
63	a	1614	AM2	CB4-CB5-CB6-OB6
63	a	1614	AM2	OB1-CB5-CB6-OB6
63	a	1614	AM2	OA4-CA1-OA1-CC1
63	a	1614	AM2	OB1-CB1-OA8-CA8
63	a	1614	AM2	CC2-CC1-OA1-CA1
63	a	1605	AM2	OB1-CB5-CB6-OB6
63	a	1605	AM2	CB2-CB1-OA8-CA8
63	a	1605	AM2	OB1-CB1-OA8-CA8
63	a	1663	AM2	OA4-CA1-OA1-CC1
63	a	1605	AM2	CC2-CC1-OA1-CA1

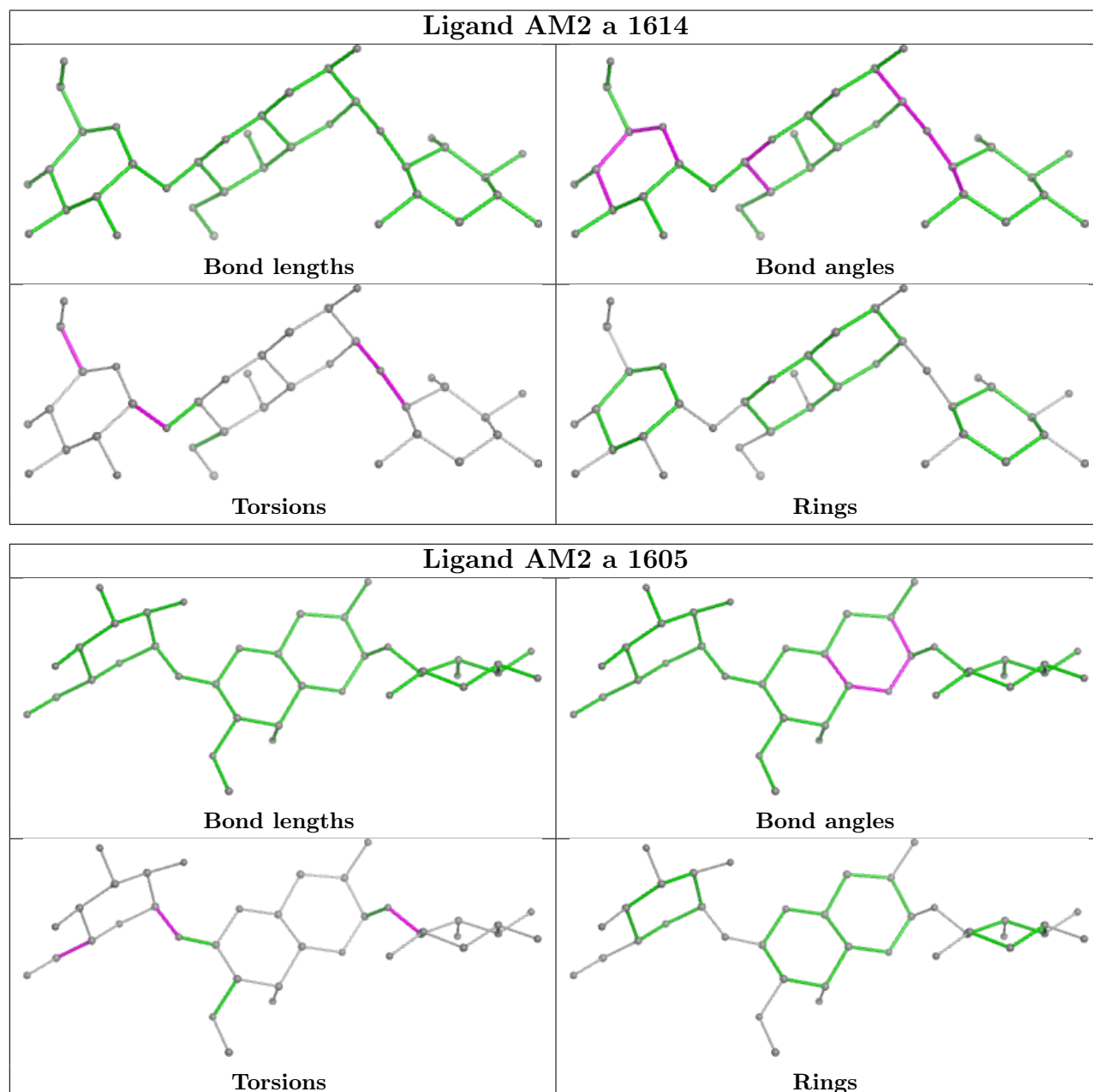
There are no ring outliers.

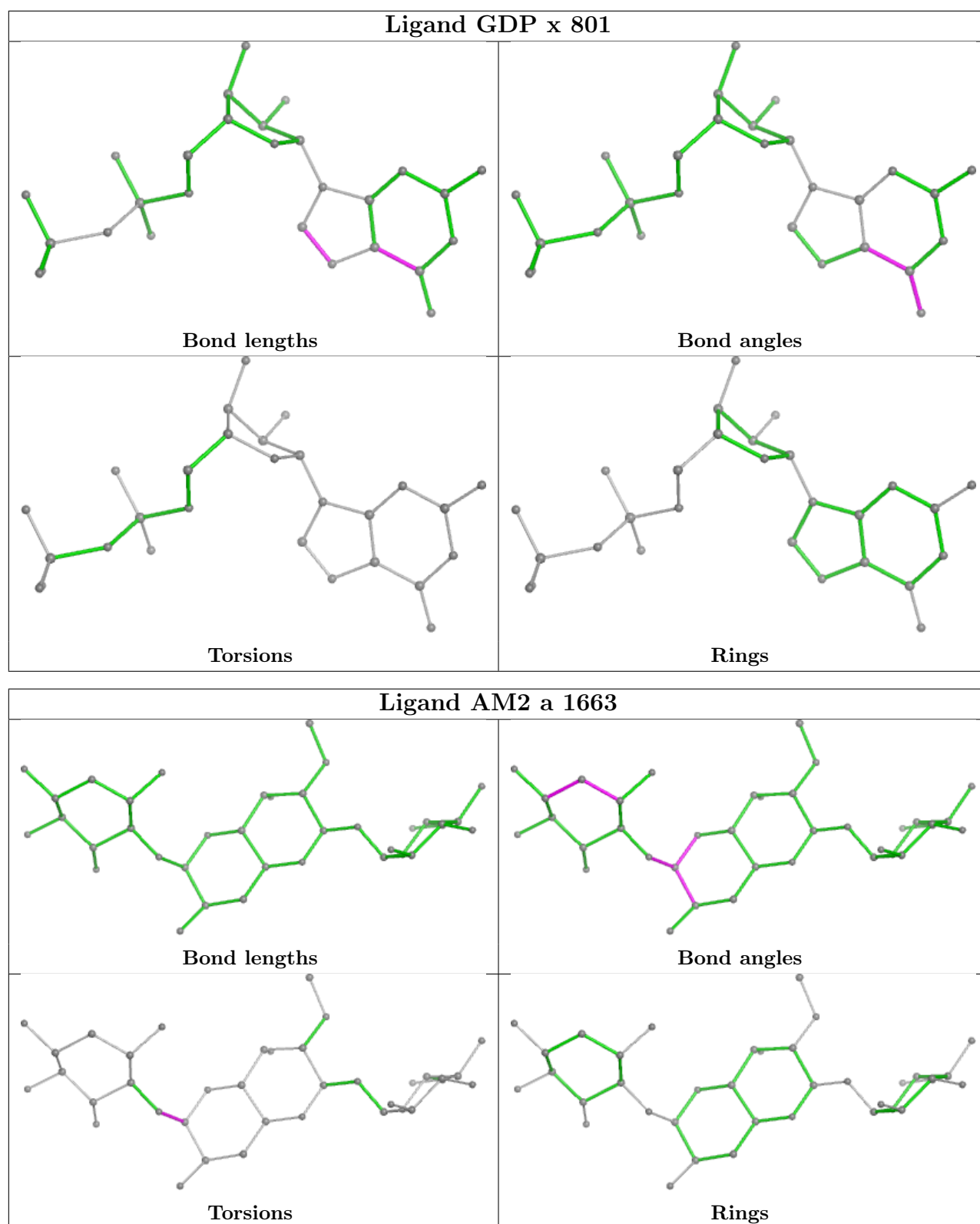
4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	a	1614	AM2	2	0
63	a	1605	AM2	1	0
64	x	801	GDP	7	0
63	a	1663	AM2	3	0



The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

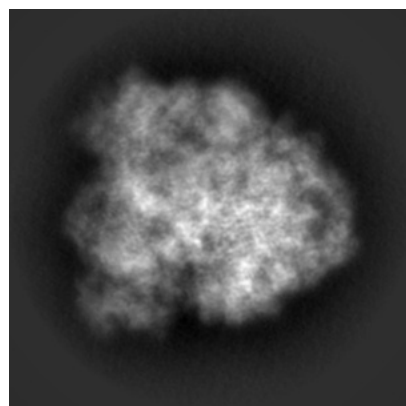
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54254. These allow visual inspection of the internal detail of the map and identification of artifacts.

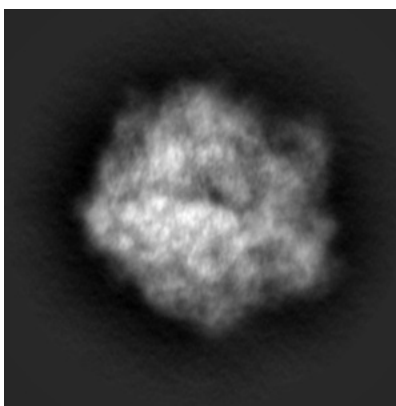
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

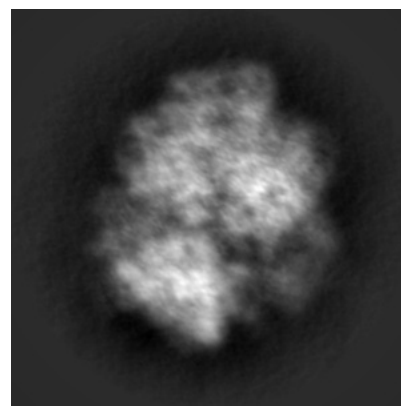
#### 6.1.1 Primary map



X

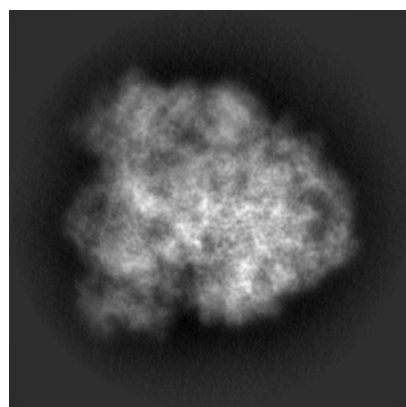


Y

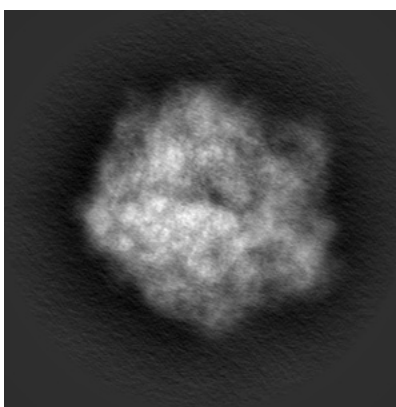


Z

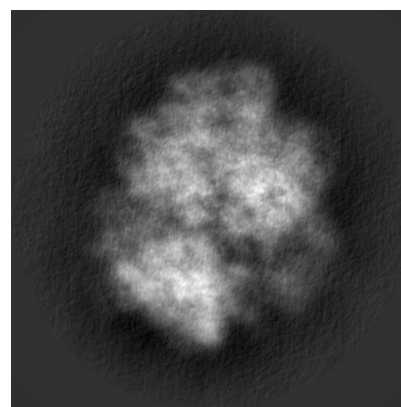
#### 6.1.2 Raw map



X



Y

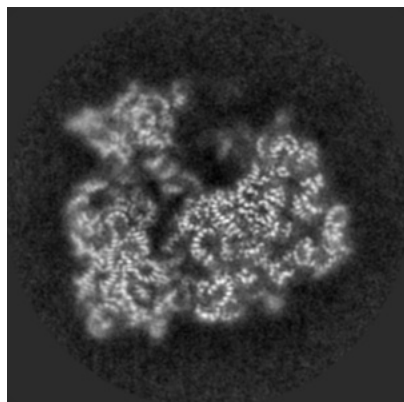


Z

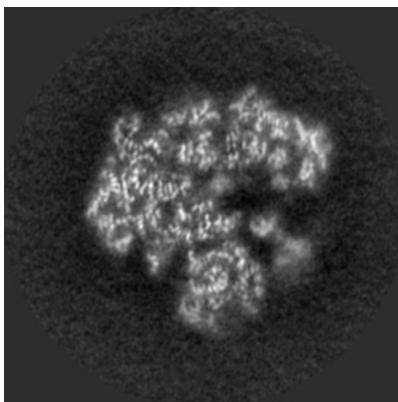
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

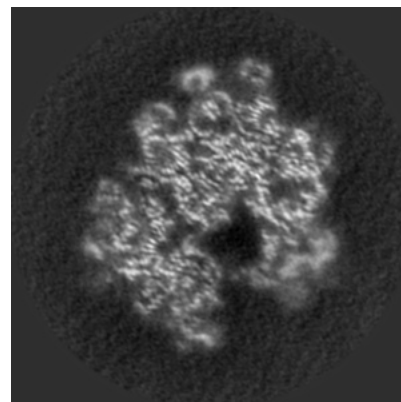
### 6.2.1 Primary map



X Index: 144

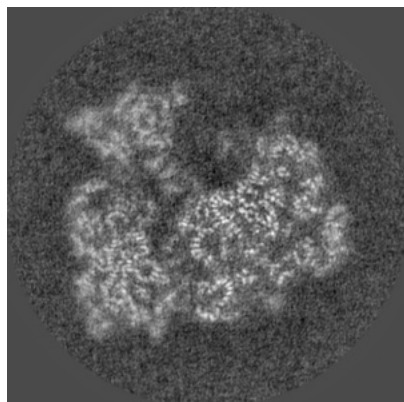


Y Index: 144

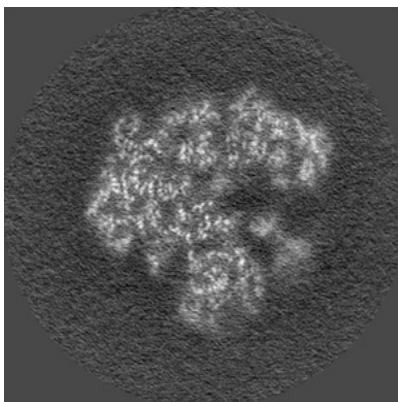


Z Index: 144

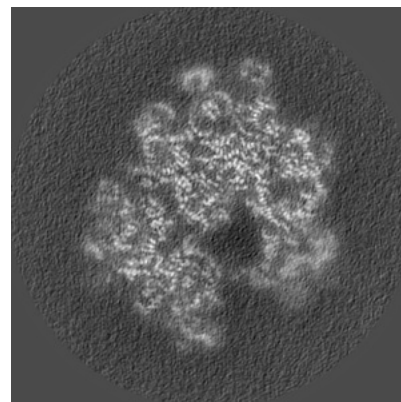
### 6.2.2 Raw map



X Index: 144



Y Index: 144

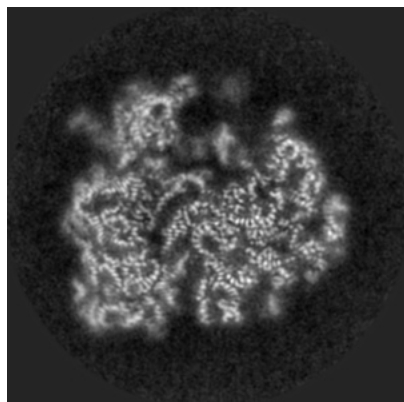


Z Index: 144

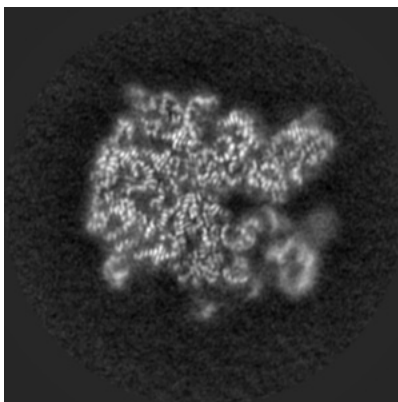
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

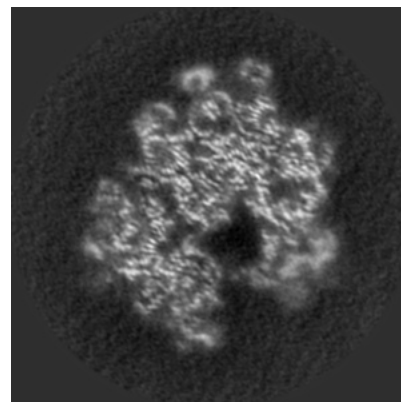
### 6.3.1 Primary map



X Index: 138

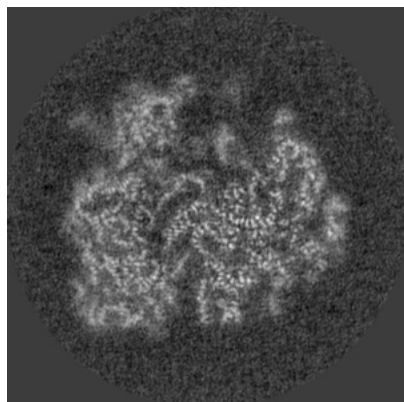


Y Index: 161

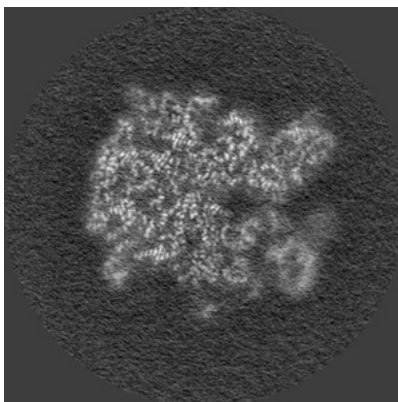


Z Index: 144

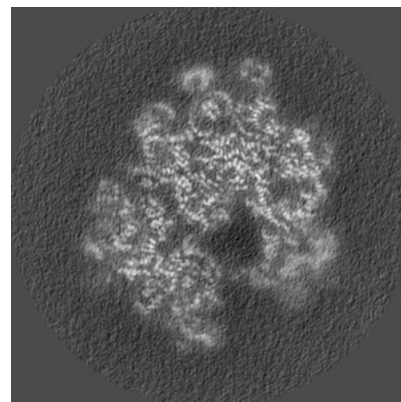
### 6.3.2 Raw map



X Index: 138



Y Index: 161



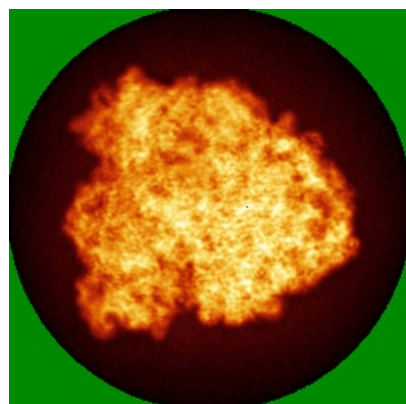
Z Index: 144

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

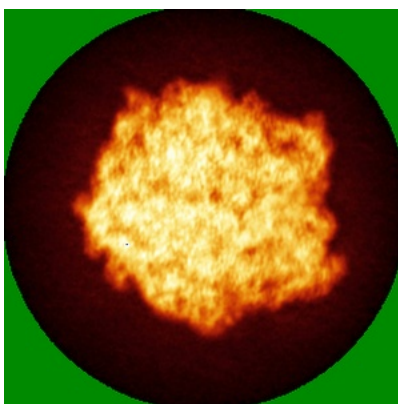


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

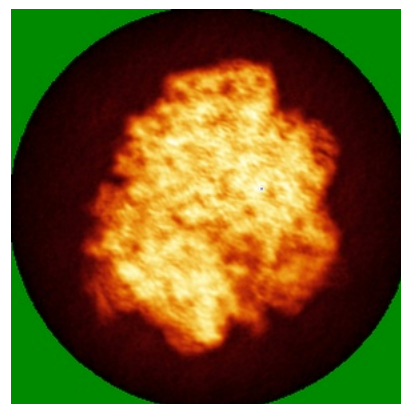
### 6.4.1 Primary map



X

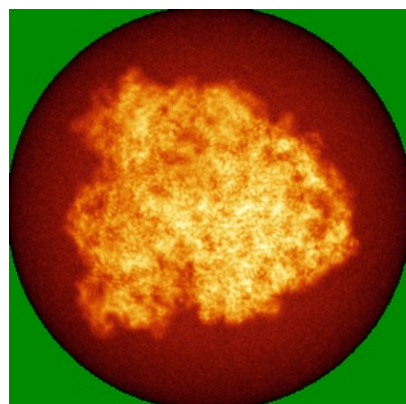


Y

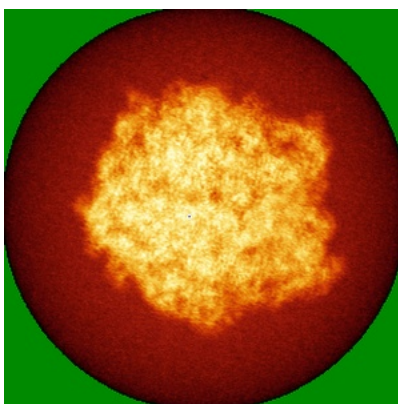


Z

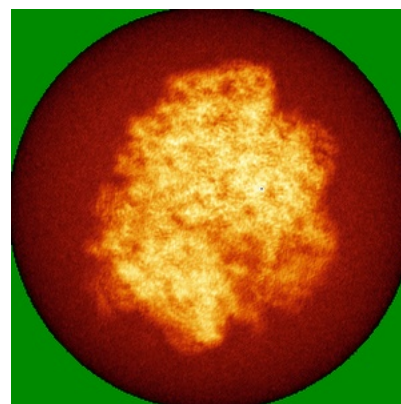
### 6.4.2 Raw map



X



Y



Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



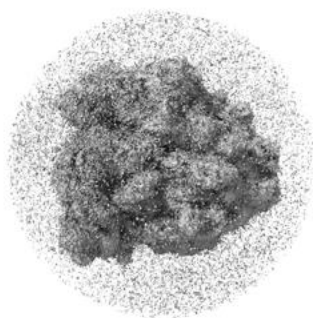
Y



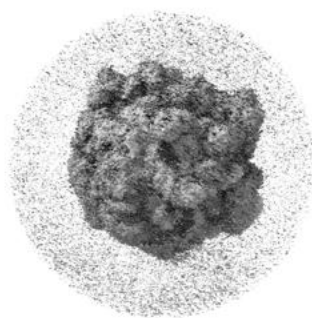
Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

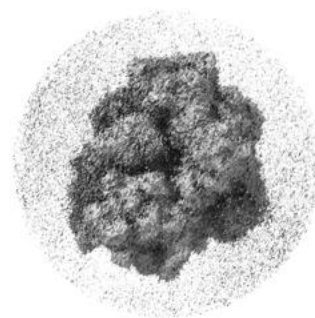
### 6.5.2 Raw map



X



Y



Z

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



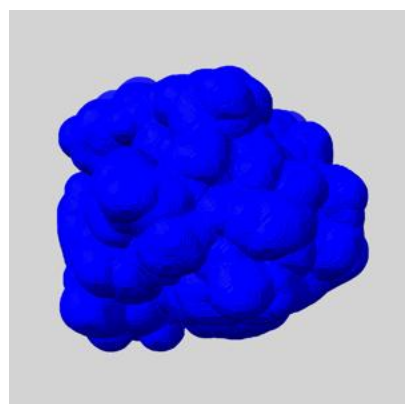
## 6.6 Mask visualisation [i](#)

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

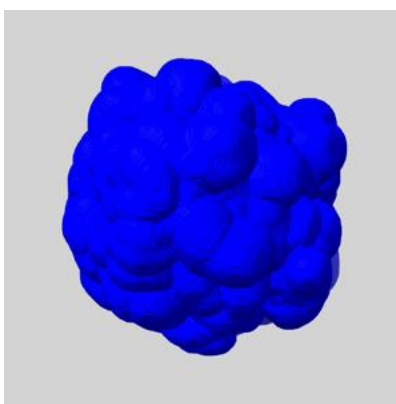
A mask typically either:

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

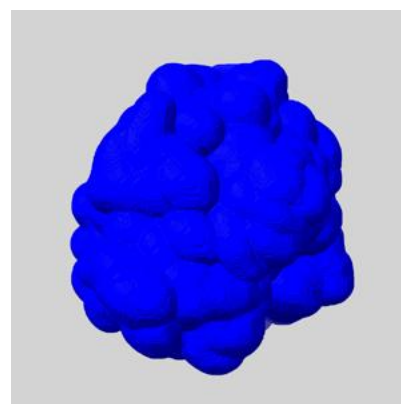
### 6.6.1 emd\_54254\_msk\_1.map [i](#)



X



Y

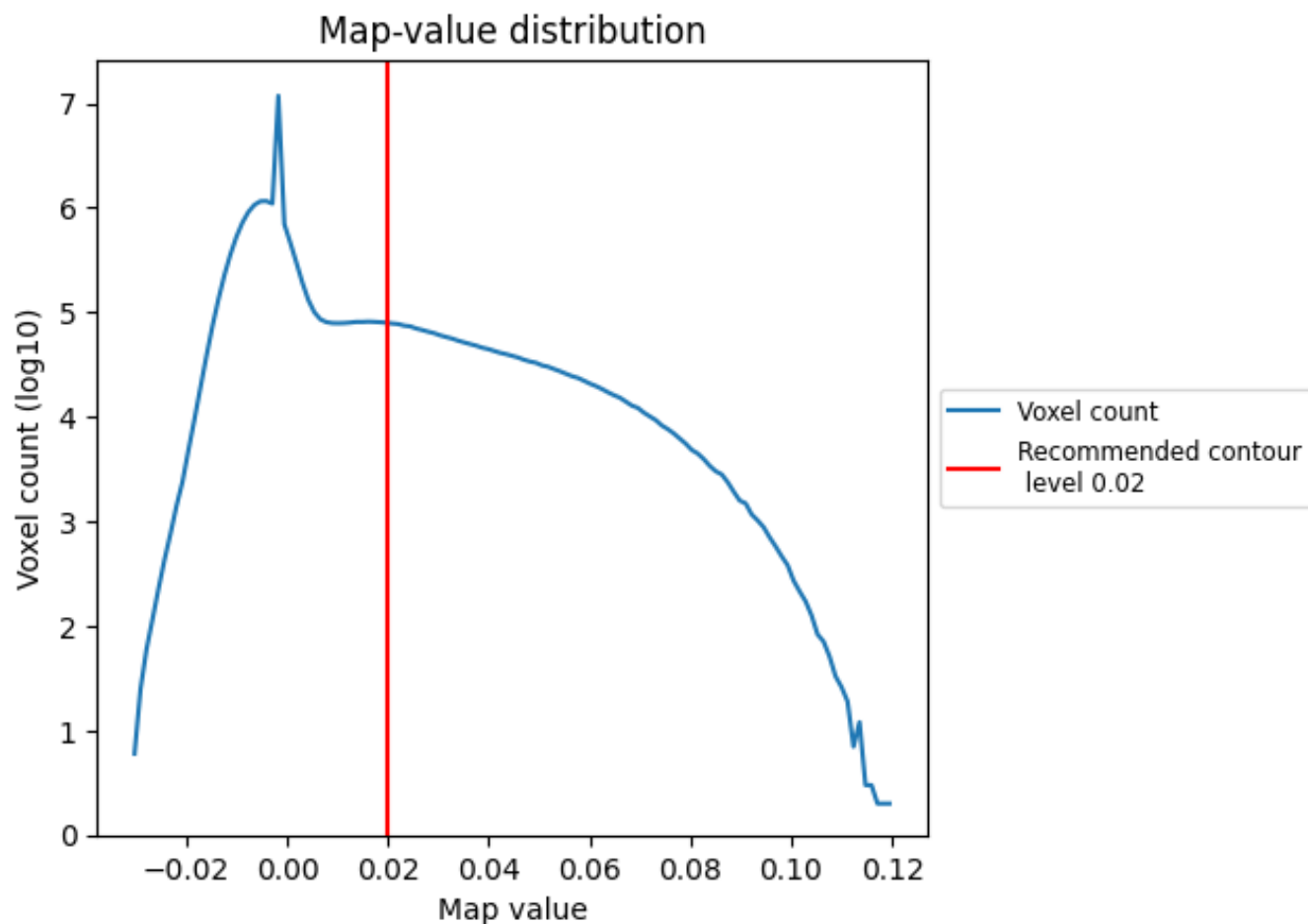


Z

## 7 Map analysis [i](#)

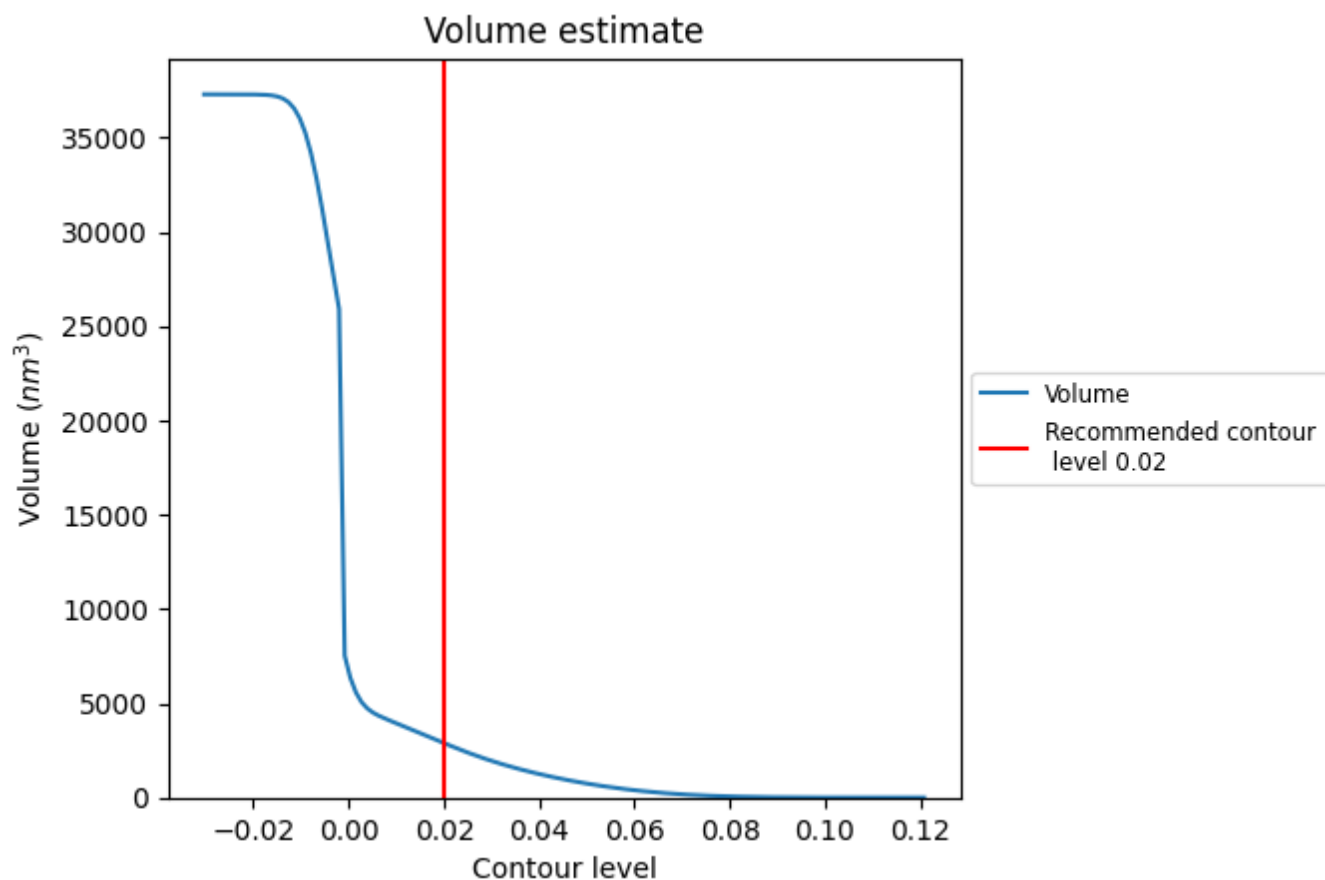
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

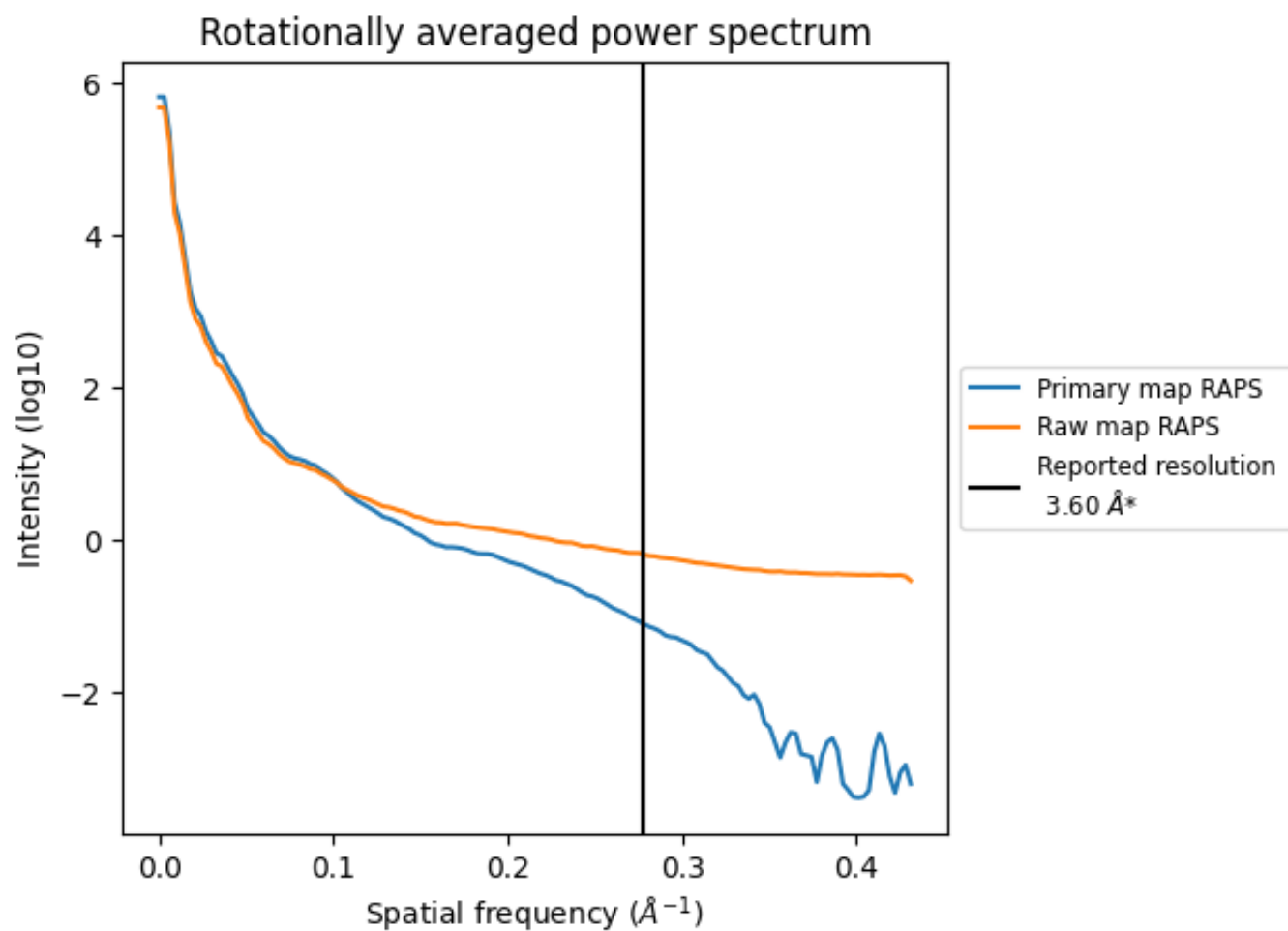
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2889 nm<sup>3</sup>; this corresponds to an approximate mass of 2610 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 ⓘ

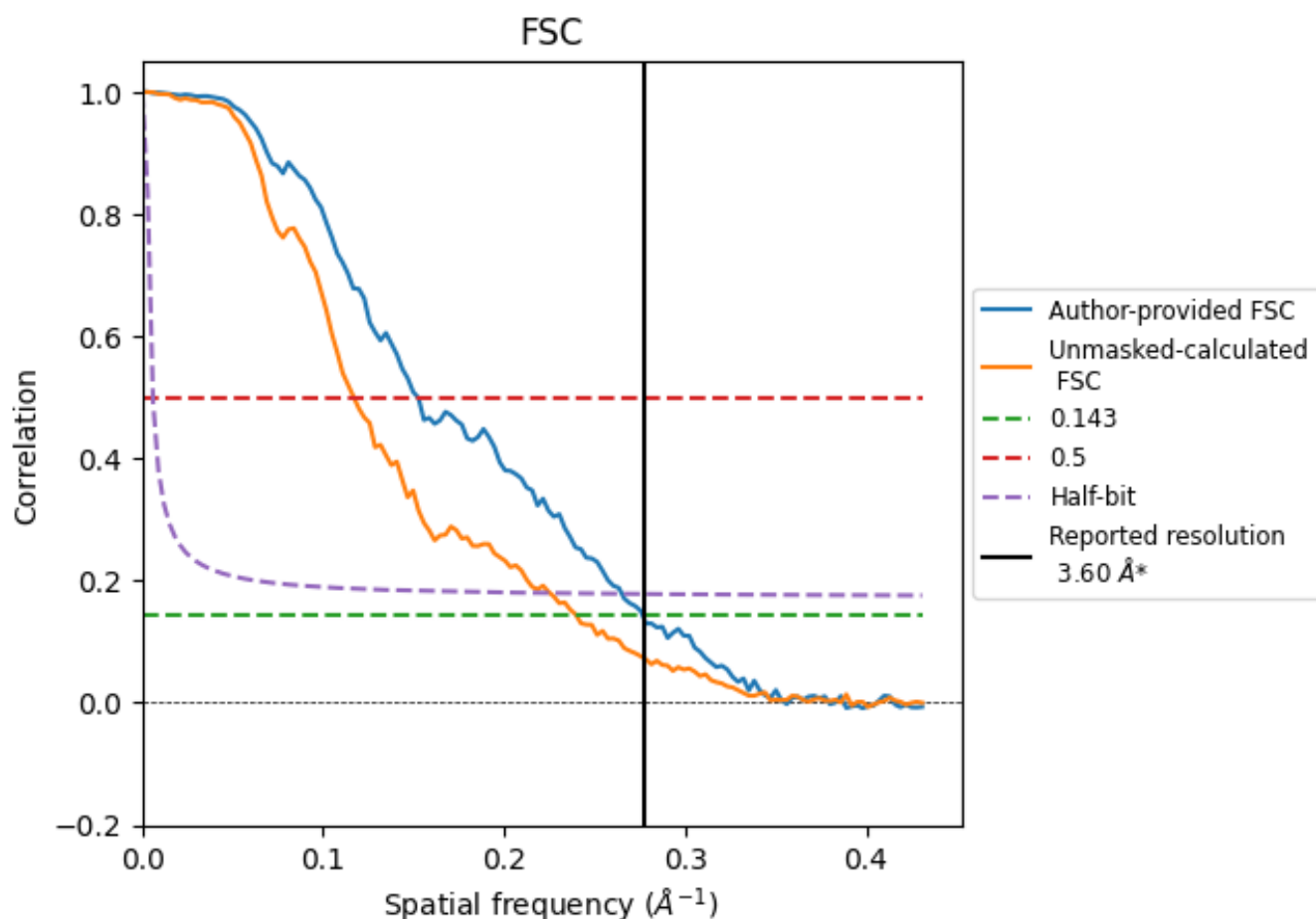


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 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  $0.278 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

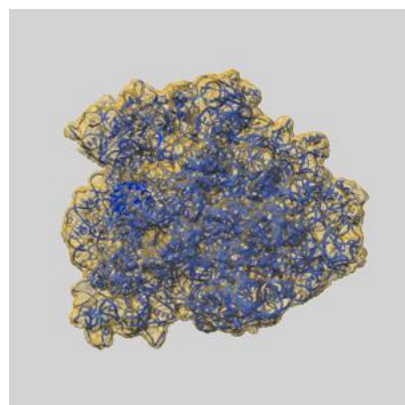
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.62	6.57	3.77
Unmasked-calculated*	4.17	8.55	4.44

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.17 differs from the reported value 3.6 by more than 10 %

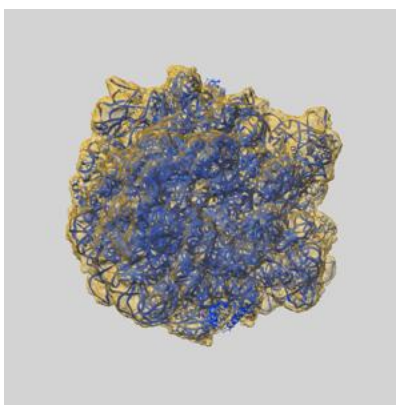
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54254 and PDB model 9RTV. Per-residue inclusion information can be found in section 3 on page 18.

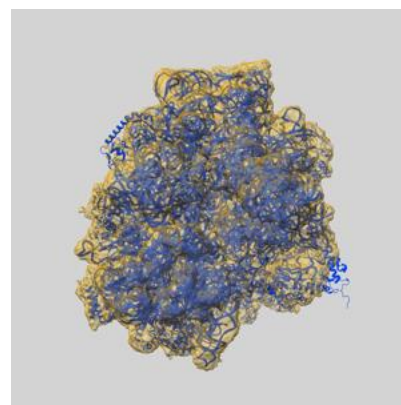
### 9.1 Map-model overlay [i](#)



X



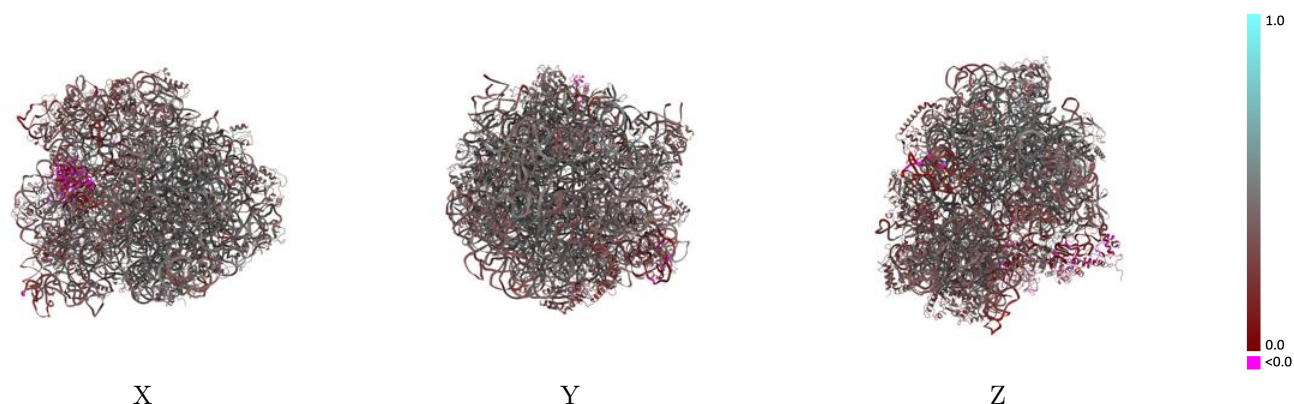
Y



Z

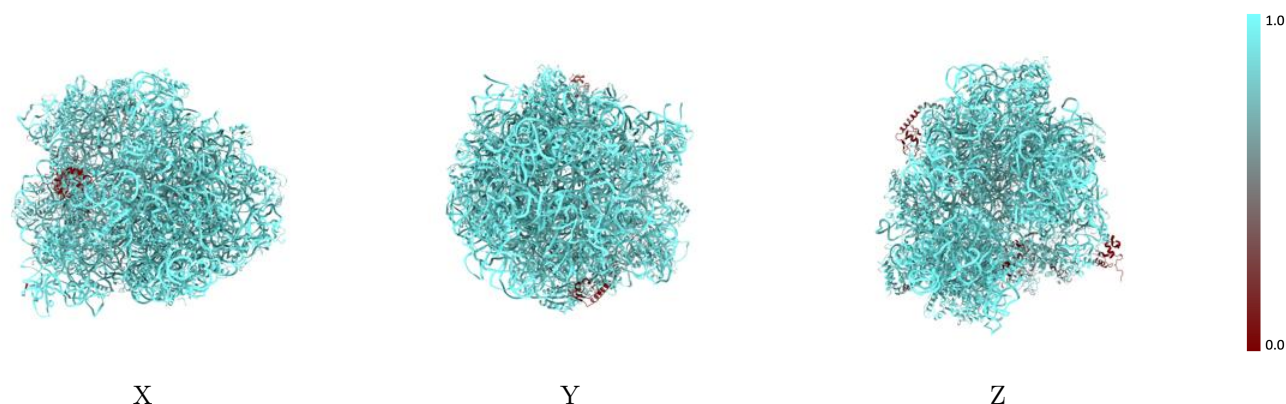
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

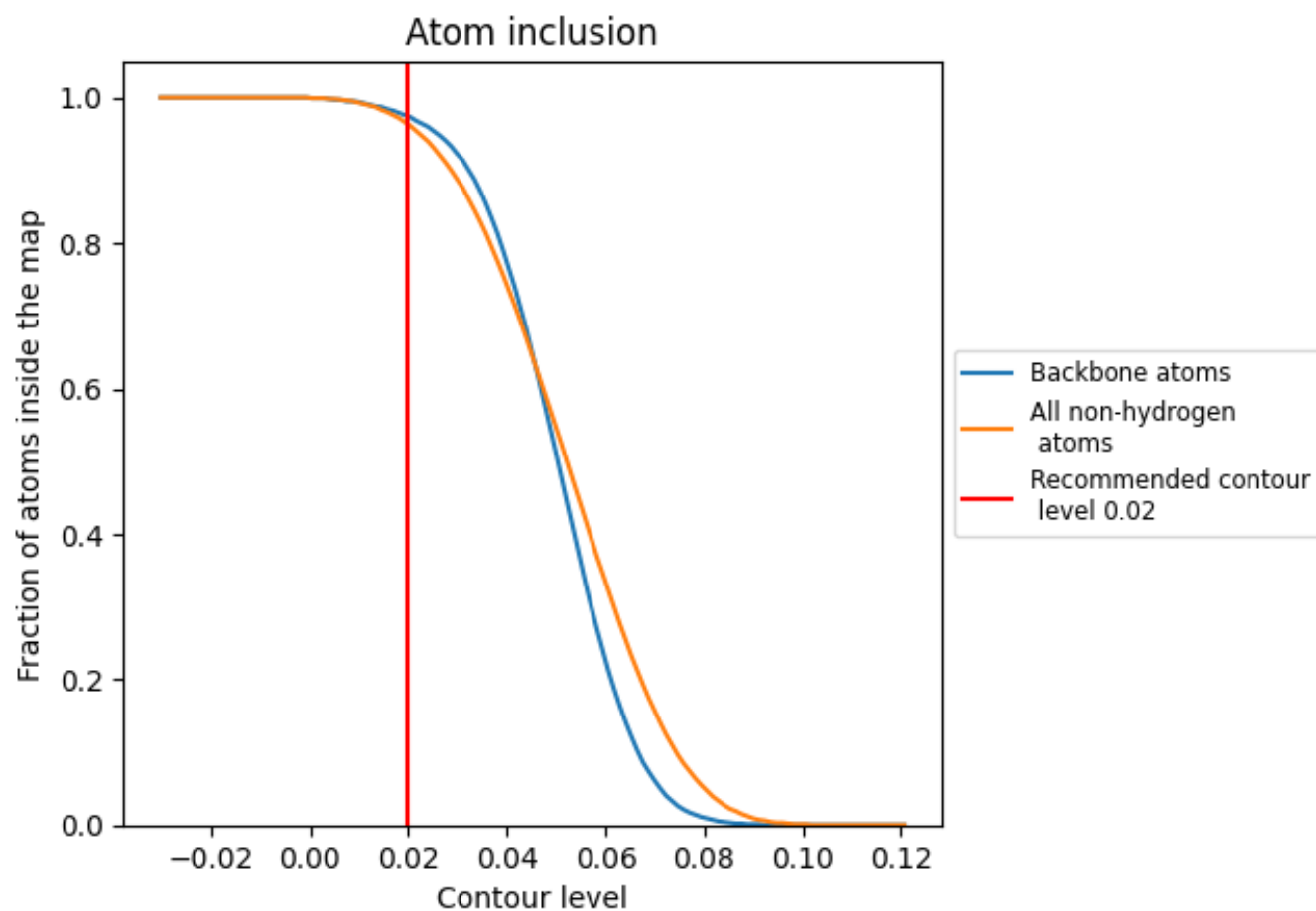
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ



















































The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9630	 0.3920
0	 0.9490	 0.4050
1	 0.9750	 0.3960
2	 0.9720	 0.4440
3	 0.9490	 0.4360
4	 0.9900	 0.3960
5	 0.4190	 0.0850
6	 0.8910	 0.2610
A	 0.9960	 0.4190
B	 0.9960	 0.3960
C	 0.9500	 0.4390
D	 0.9440	 0.4310
E	 0.9380	 0.4000
F	 0.9210	 0.3100
G	 0.9360	 0.3520
H	 0.3470	 0.2300
I	 0.7600	 0.1020
J	 0.9740	 0.4180
K	 0.8590	 0.4260
L	 0.9580	 0.4280
M	 0.9370	 0.4160
N	 0.9840	 0.4290
O	 0.9910	 0.3680
P	 0.8930	 0.4080
Q	 0.9840	 0.4100
R	 0.9470	 0.4110
S	 0.9490	 0.4130
T	 0.9600	 0.3770
U	 0.9610	 0.3700
V	 0.9490	 0.3950
W	 0.9770	 0.4280
X	 0.9650	 0.4120
Y	 0.9660	 0.3390
Z	 0.9220	 0.4190
a	 0.9960	 0.3980



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Chain	Atom inclusion	Q-score
b	 0.8440	 0.3340
c	 0.9370	 0.3620
d	 0.9400	 0.3510
e	 0.9370	 0.3990
f	 0.9220	 0.3290
g	 0.8650	 0.2890
h	 0.9550	 0.4070
i	 0.9690	 0.3390
j	 0.9370	 0.3280
k	 0.9570	 0.3940
l	 0.9000	 0.4210
m	 0.9400	 0.3240
n	 0.9840	 0.3410
o	 0.9620	 0.3720
p	 0.9600	 0.4030
q	 0.9480	 0.3910
r	 0.9730	 0.3520
s	 0.9420	 0.3100
t	 0.9540	 0.3200
u	 0.9400	 0.3530
v	 0.9730	 0.3560
w	 0.9550	 0.2710
x	 0.7660	 0.2850
y	 0.9520	 0.3210
z	 1.0000	 0.3980