



Full wwPDB EM Validation Report ⓘ

Oct 22, 2025 – 02:55 pm BST

PDB ID : 9RTU / pdb_00009rtu
EMDB ID : EMD-54253
Title : Structure of the 70S-EF-G(P610L)-GDP-Pi ribosome complex with tRNAs in hybrid state 1 (H1-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 : 3.00 Å(reported)
Based on initial model : 7PJV

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

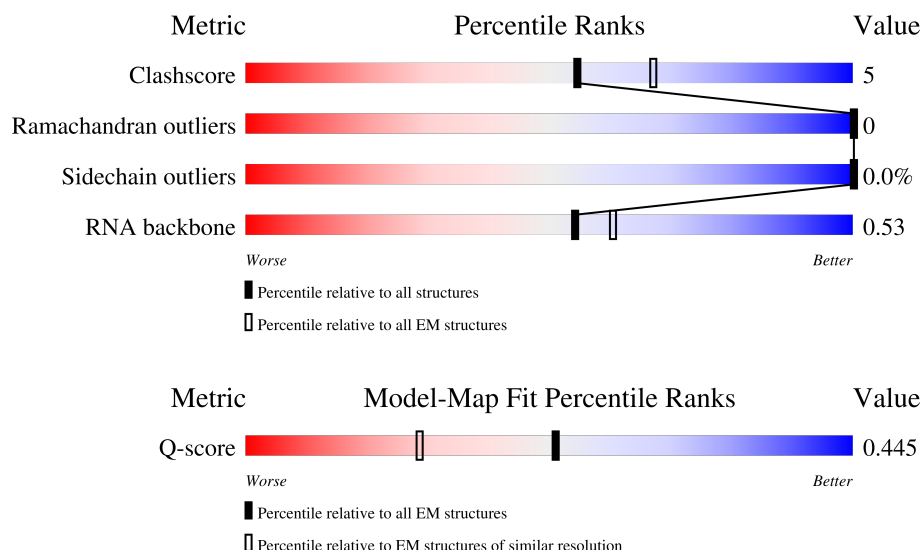
EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up 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 3.00 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	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	0	57	












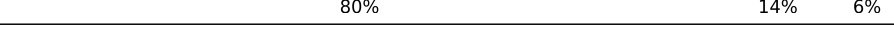







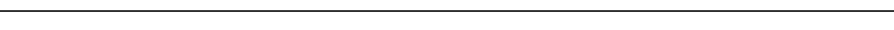

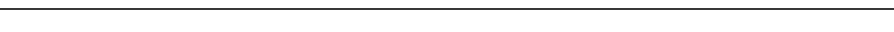
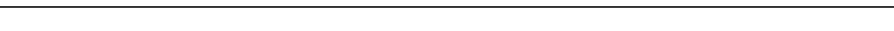


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Mol	Chain	Length	Quality of chain
2	1	55	
3	2	46	
4	3	65	
5	4	38	
6	5	165	
7	6	70	
8	A	2903	
9	B	120	
10	C	273	
11	D	209	
12	E	201	
13	F	179	
14	G	177	
15	H	149	
16	I	142	
17	J	142	
18	K	123	
19	L	144	
20	M	136	
21	N	127	
22	O	117	
23	P	115	
24	Q	118	
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	
53	t	87	
54	u	71	
55	v	77	
56	w	76	
57	x	704	
58	y	2	
59	z	33	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
64	PO4	x	802	-	-	X	-

2 Entry composition [i](#)

There are 65 unique types of molecules in this entry. The entry contains 256907 atoms, of which 103761 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	H	N	O	S	0	0
			904	269	460	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	H	N	O	0	0
			849	263	440	75	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
3	2	46	Total	C	H	N	O	S	0	0
			796	228	419	90	57	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	3	64	Total	C	H	N	O	S	0	0
			1076	323	572	105	74	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4	38	Total	C	H	N	O	S	0	0
			642	185	340	65	48	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	131	Total	C	H	N	O	0	0
			983	385	336	131	131		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	6	66	Total	C	H	N	O	S	0	0
			1042	323	520	99	94	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	A	2903	Total	C	H	N	O	P	0	0
			93694	27816	31356	11471	20148	2903		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	B	120	Total	C	H	N	O	P	0	0
			3871	1144	1301	468	838	120		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	C	271	Total	C	H	N	O	S	0	0
			4237	1288	2155	423	364	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	D	209	Total	C	H	N	O	S	0	0
			3183	979	1618	288	294	4		

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
14	G	176	Total	C	H	N	O	S	0	0
			2695	832	1372	243	246	2		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
16	I	141	Total	C	H	N	O		0	0
			1038	411	345	141	141			

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
19	L	143	Total	C	H	N	O	S	0	0
			2162	649	1117	206	189	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
20	M	136	Total	C	H	N	O	S	0	0
			2231	686	1157	205	177	6		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
22	O	116	Total	C	H	N	O		0	0
			1815	552	923	178	162			

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Q	117	Total	C	H	N	O		0	0
			1967	604	1020	192	151			

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

Mol	Chain	Residues	Atoms						AltConf	Trace
25	R	103	Total	C	H	N	O	S	0	0
			1655	516	839	153	145	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
26	S	110	Total	C	H	N	O	S	0	0
			1779	532	922	166	156	3		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
30	W	75	Total	C	H	N	O	S	0	0
			1169	356	594	116	102	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
31	X	77	Total	C	H	N	O	S	0	0
			1279	388	654	129	106	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
32	Y	63	Total	C	H	N	O	S	0	0
			1052	313	543	99	95	2		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
34	a	1540	Total	C	H	N	O	P	0	0
			49687	14748	16637	6057	10705	1540		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
35	b	218	Total	C	H	N	O	S	0	0
			3437	1081	1733	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	H	N	O	S	0	0
			3322	1028	1698	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	H	N	O	S	0	0
			3351	1026	1708	315	298	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
38	e	157	Total	C	H	N	O	S	0	0
			2311	709	1170	218	208	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
39	f	100	Total	C	H	N	O	S	0	0
			1626	515	809	148	148	6		

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
42	i	127	Total	C	H	N	O	S	0	0
			2092	634	1070	206	179	3		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
44	k	116	Total	C	H	N	O	S	0	0
			1748	535	879	173	158	3		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
46	m	114	Total	C	H	N	O	S	0	0
			1825	546	942	178	156	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
47	n	101	Total	C	H	N	O	S	0	0
			1638	498	839	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	H	N	O	S	0	0
			1451	439	737	144	130	1		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
50	q	80	Total	C	H	N	O	S	0	0
			1340	411	692	121	113	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
51	r	65	Total	C	H	N	O	S	0	0
			1087	339	552	100	95	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
52	s	82	Total	C	H	N	O	S	0	0
			1343	421	685	125	110	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
53	t	85	Total	C	H	N	O	S	0	0
			1381	411	716	137	114	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
54	u	65	Total	C	H	N	O	S	0	0
			1008	313	502	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	H	N	O	P	S	0	0
			2449	724	827	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	H	N	O	P	S	0	0
			2462	731	831	291	531	76	2		

- Molecule 57 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms							AltConf	Trace
57	x	703	Total	C	H	N	O	S		0	0
			10865	3430	5420	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	H	N	O	S		0	0
			40	15	19	2	3	1			

- Molecule 59 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms							AltConf	Trace
59	z	11	Total	C	H	N	O	P		0	0
			345	103	115	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	262	Total	Mg	0
			262	262	
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	N	1	Total 1	Mg 1	0
60	O	1	Total 1	Mg 1	0
60	P	1	Total 1	Mg 1	0
60	Z	1	Total 1	Mg 1	0
60	a	84	Total 84	Mg 84	0
60	m	2	Total 2	Mg 2	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	2	Total 2	Mg 2	0
60	z	1	Total 1	Mg 1	0

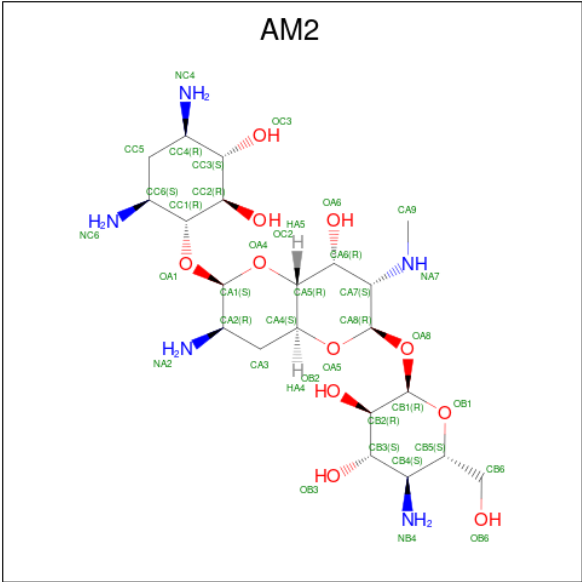
- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

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).

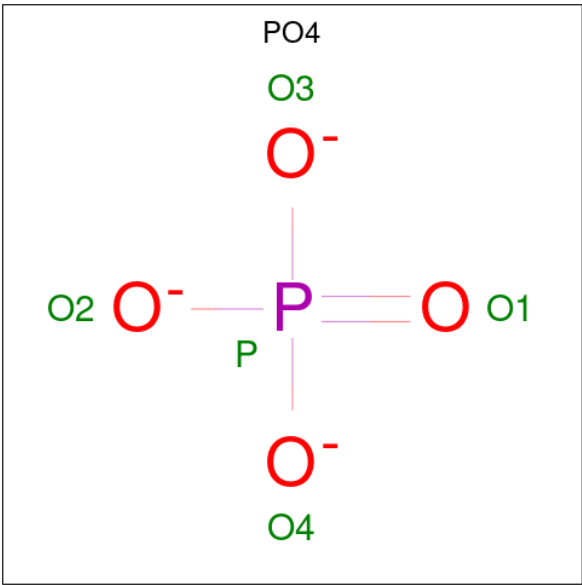
Mol	Chain	Residues	Atoms		AltConf
62	A	1	Total 1	Na 1	0
62	B	1	Total 1	Na 1	0

- Molecule 63 is APRAMYCIN (CCD ID: AM2) (formula: C₂₁H₄₁N₅O₁₁).



Mol	Chain	Residues	Atoms					AltConf
63	a	1	Total	C	H	N	O	0
			78	21	41	5	11	
63	a	1	Total	C	H	N	O	0
			78	21	41	5	11	
63	a	1	Total	C	H	N	O	0
			79	21	42	5	11	

- Molecule 64 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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


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- The image displays the chemical structure of GDP (Guanosine Diphosphate). It consists of a guanine base (a purine ring system with an amino group at C2 and a carbonyl group at C6) linked to a ribose sugar via a glycosidic bond. The ribose sugar is further linked to two phosphate groups (diphosphate) via a pyrophosphate bridge. The structure is labeled with atom names (N1, N2, N3, N7, N9, C2, C4, C5, C6, C8, C9, O1, O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100) and bond types (single, double, triple, aromatic, coordinate). The structure is shown in a 3D representation with wedge and dash bonds indicating stereochemistry.

Mol	Chain	Residues	Atoms					AltConf	
65	x	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	

3 Residue-property plots

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

- Molecule 1: 50S ribosomal protein L32

Chain 0: 



- Molecule 2: Large ribosomal subunit protein bL33

Chain 1: 



- Molecule 3: Large ribosomal subunit protein bL34

Chain 2: 



- Molecule 4: 50S ribosomal protein L35

Chain 3: 

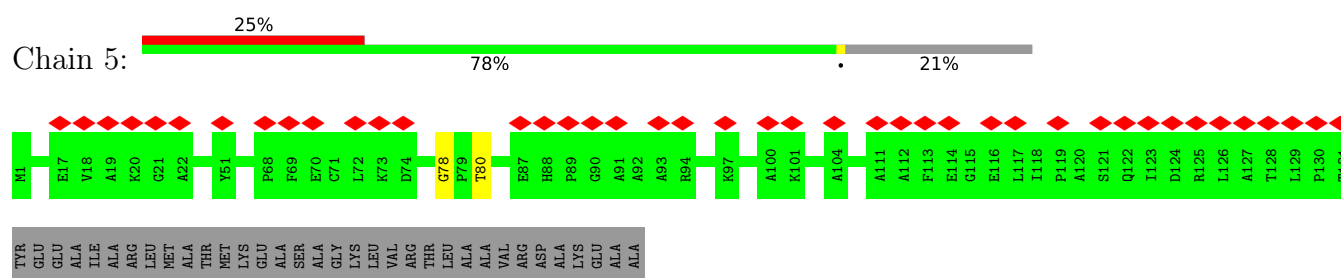


- Molecule 5: 50S ribosomal protein L36

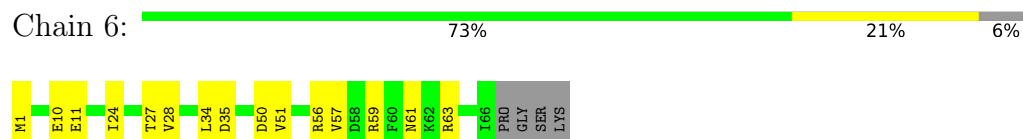
Chain 4: 



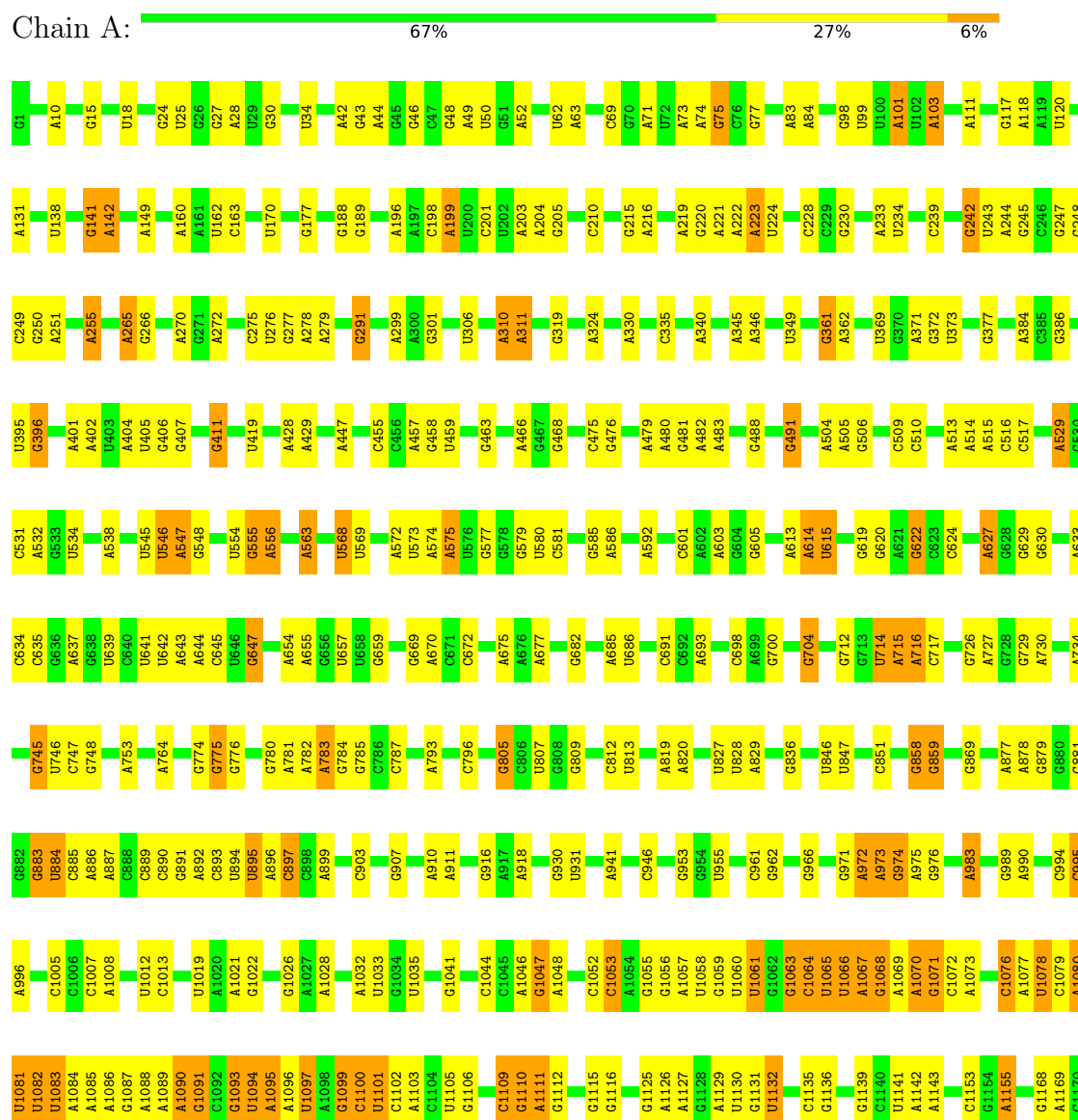
- Molecule 6: 50S ribosomal protein L10



• Molecule 7: 50S ribosomal protein L31



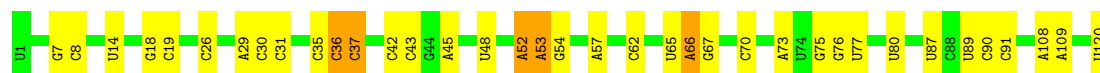
• Molecule 8: 23S ribosomal RNA




G2819	U2690	A2572	A2469	G2369	A2268	U2155	G2069	C1958	A1808	A1668	C1557	G1432	C1315	G1171
A2820	G2702	G2576	C2475	A2369	G2271	G2156	A2070	G1964	A1809	U1671	C1558	G1432	C1322	C1172
G2822	A2577	G2578	A2476	C2374	G2275	A2158	A2071	G1967	G1811	A1672	U1563	C1437	C1323	U1173
A2823	A2705	G2579	U2477	G2379	G2279	G2160	U2079	C1967	U1812	G1673	C1564	C1437	C1323	U1174
A2826	U2707	U2580	A2478	C2380	G2279	C2161	U2092	A1970	G1813	G1674	C1565	G1445	U1329	U1176
G2839	G2714	U2585	G2481	G2383	G2283	G2162	U2092	U1971	G1814		A1566	G1446	C1330	
G2848	G2715	G2595	G2484	C2385	A2284	A2163	G2093	G1972	A1815		G1567	C1447	G1331	G1179
U2849	G2716	G2598	G2488	C2386	A2287	C2165	G2100	G1980	G1817		G1568	C1447	G1332	U1180
G2718	G2717	U2596	U2491	U2391	A2288	U2167	C2103	U1982	U1818		A1569	C1451	G1333	U1187
G2719	U2720	A2602	U2495	C2394	U2291	G2168	G2104	U1982	G1826		A1572	U1453	G1334	U1188
G2723	U2604	G2603	G2494	U2402	A2297	A2170	U2105	U1991	G1827		U1578	U1453	G1338	U1199
A2860	U2605	U2605	A2496	U2402	A2298	A2171	G2107	G1992	A1829		U1584	C1461	C1340	U1206
			A2497	U2405	U2299	A2172	G2110	C1996	G1835		G1585	U1466	G1341	
				A2406	U2302	A2173	U2111	C1997	G1836		G1587	U1474	U1352	U1209
				A2406	U2302	A2175	U2112	A2005	G1837				A1353	
				A2406	U2302	A2176	U2113	G2012	G1857		A1591	G1478		
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
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				A2406	U2302	A2176	U2113	G2012	G1857					
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				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
				A2406	U2302	A2176	U2113	G2012	G1857					
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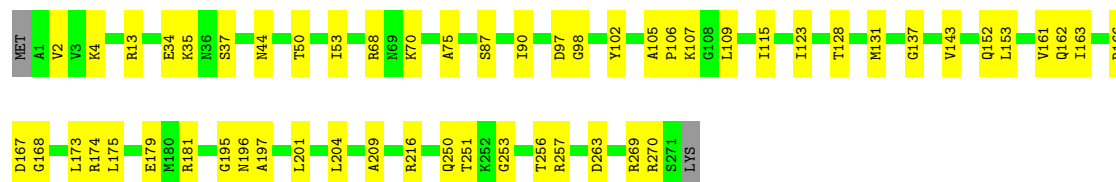
- Molecule 9: 5S ribosomal RNA

Chain B:  69% 27%




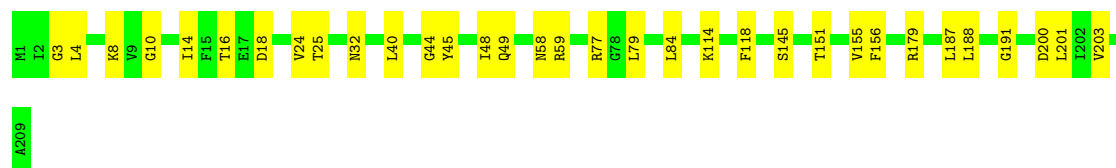
- Molecule 10: 50S ribosomal protein L2

Chain C:  79% 20%




- Molecule 11: 50S ribosomal protein L3

Chain D:  84% 16%




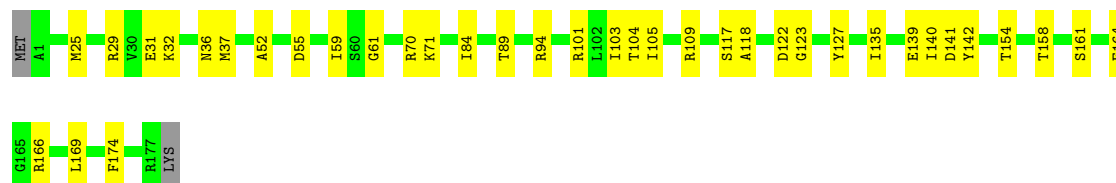
- Molecule 12: 50S ribosomal protein L4

Chain E:  84% 16%



- Molecule 13: 50S ribosomal protein L5

Chain F:  78% 21%

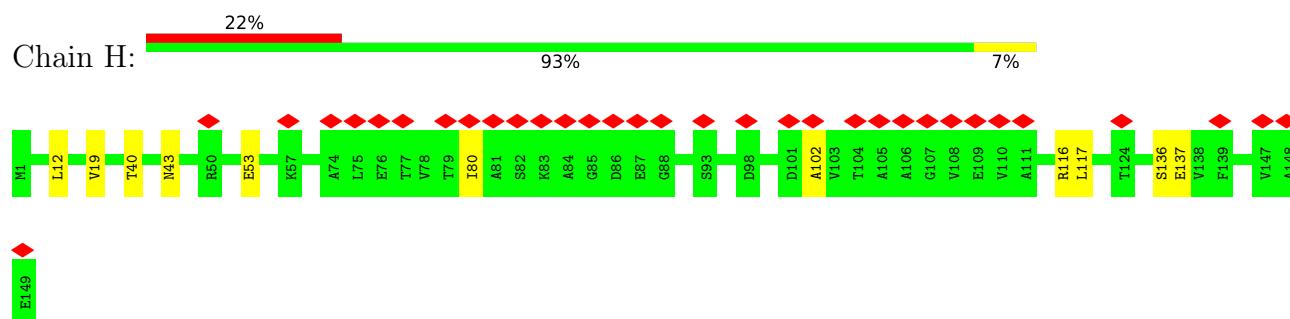


- Molecule 14: 50S ribosomal protein L6

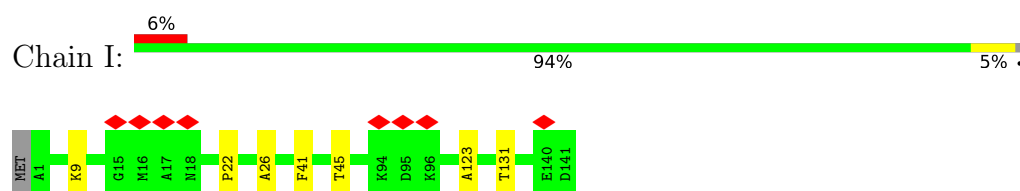
Chain G:  90% 10%



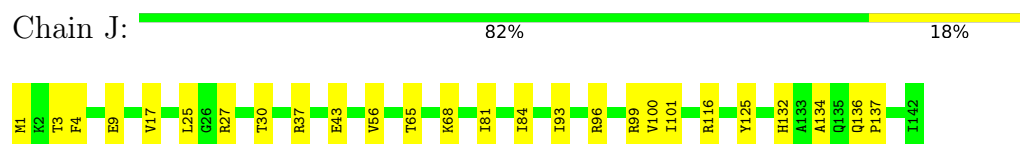
- Molecule 15: 50S ribosomal protein L9



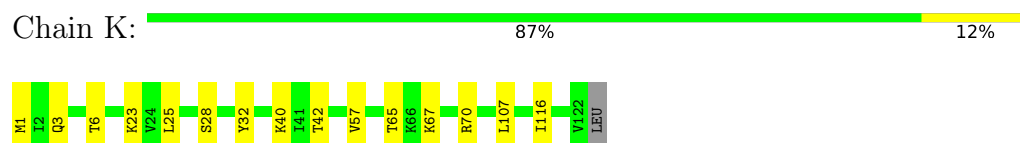
- Molecule 16: 50S ribosomal protein L11



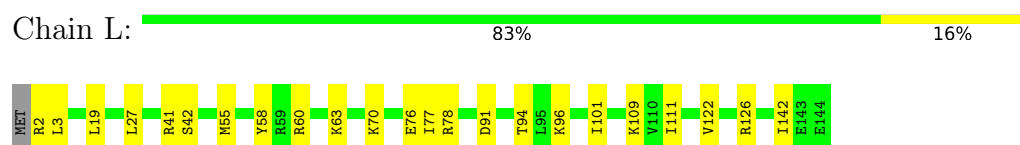
- Molecule 17: 50S ribosomal protein L13



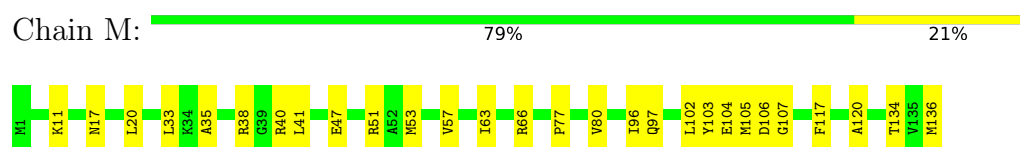
- Molecule 18: 50S ribosomal protein L14



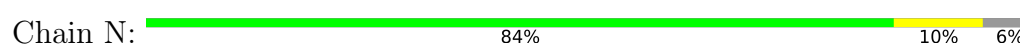
- Molecule 19: 50S ribosomal protein L15

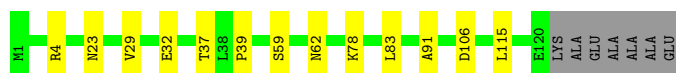


- Molecule 20: 50S ribosomal protein L16

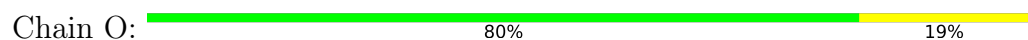


- Molecule 21: 50S ribosomal protein L17

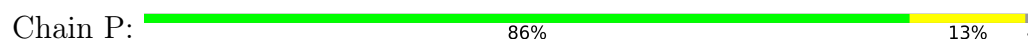




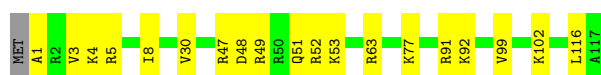
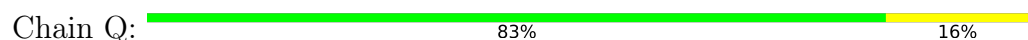
- Molecule 22: 50S ribosomal protein L18



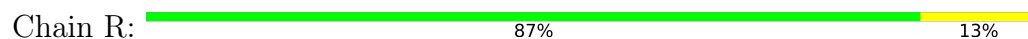
- Molecule 23: 50S ribosomal protein L19



- Molecule 24: 50S ribosomal protein L20



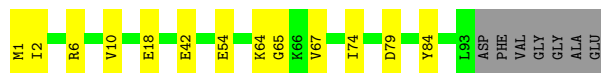
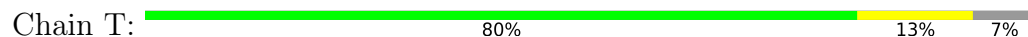
- Molecule 25: 50S ribosomal protein L21



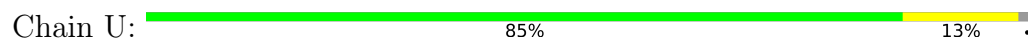
- Molecule 26: 50S ribosomal protein L22



- Molecule 27: 50S ribosomal protein L23



- Molecule 28: 50S ribosomal protein L24





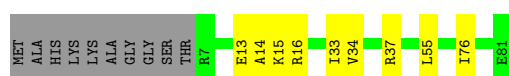
- Molecule 29: 50S ribosomal protein L25

Chain V: 83% 17%



- Molecule 30: Large ribosomal subunit protein bL27

Chain W: 78% 11% 12%



- Molecule 31: 50S ribosomal protein L28

Chain X: 86% 13%



- Molecule 32: 50S ribosomal protein L29

Chain Y: 90% 10%



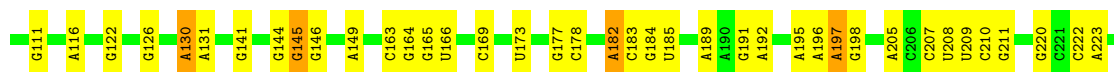
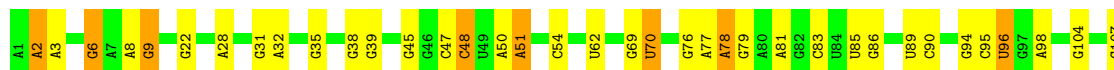
- Molecule 33: 50S ribosomal protein L30

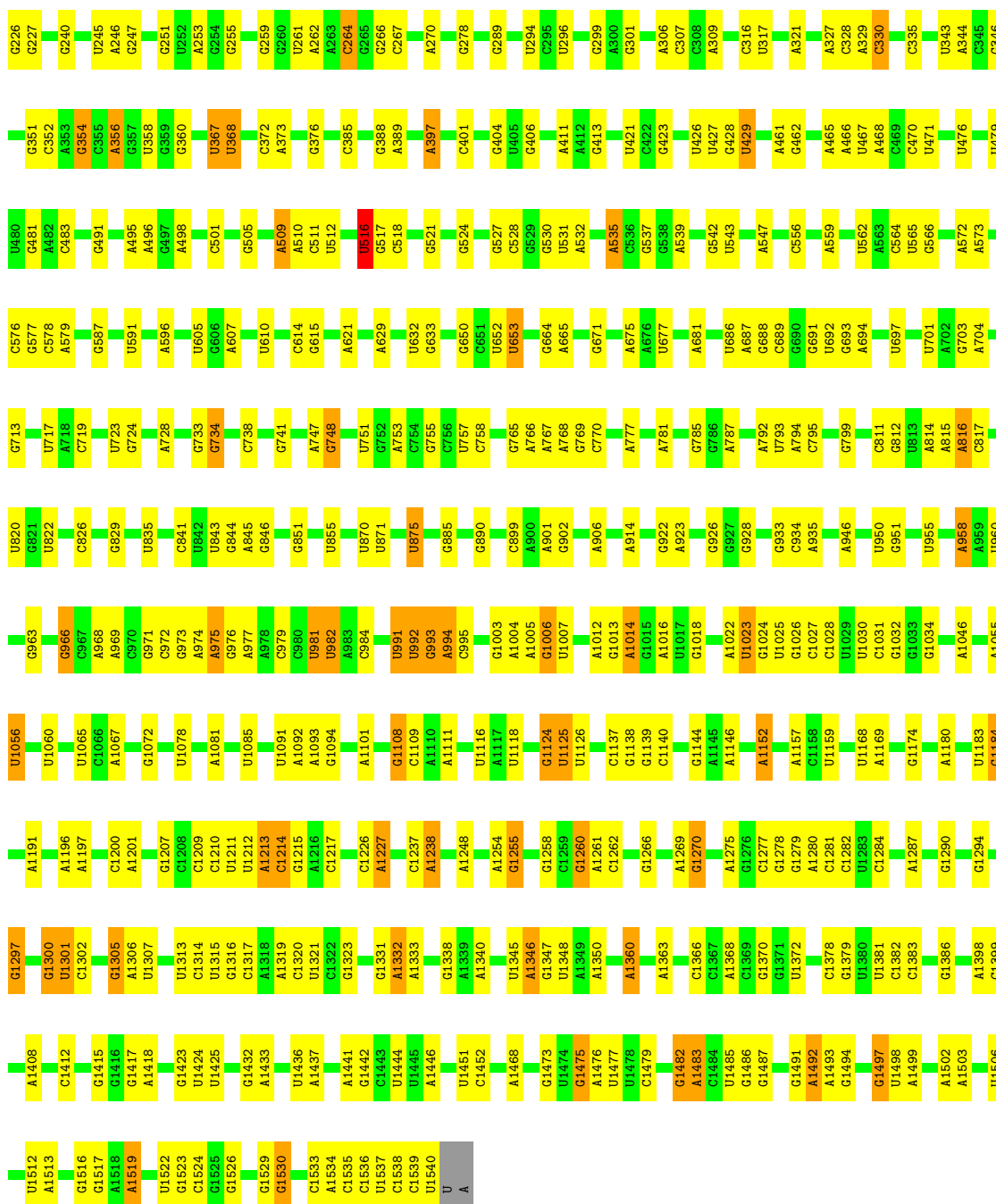
Chain Z: 76% 22%



- Molecule 34: 16S ribosomal RNA

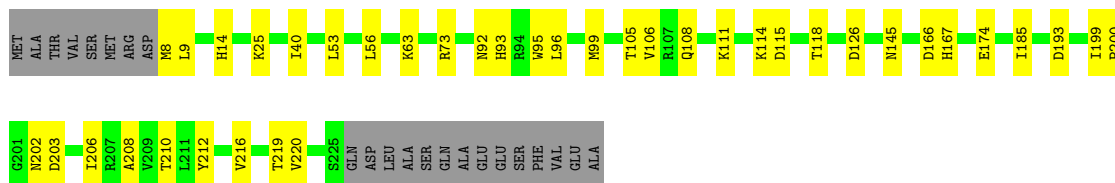
Chain a: 67% 29%






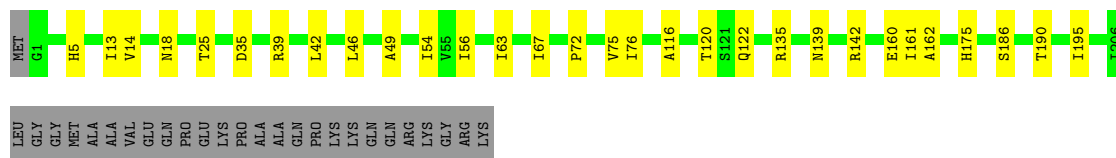
• Molecule 35: 30S ribosomal protein S2

Chain b: 75% 16% 9%




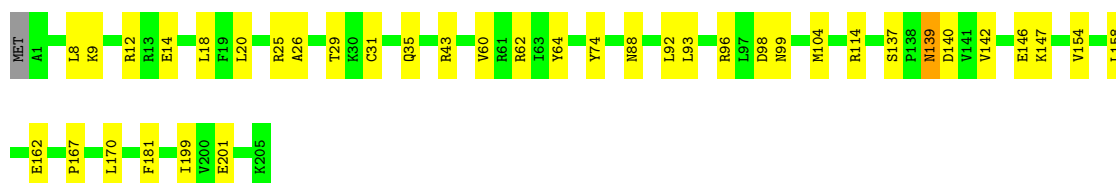
• Molecule 36: Small ribosomal subunit protein uS3

Chain c:  76% 13% 12%




- Molecule 37: Small ribosomal subunit protein uS4

Chain d:  81% 18%



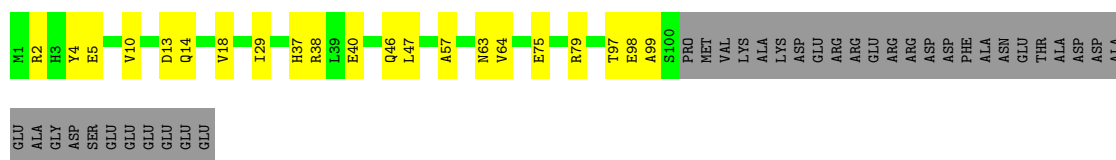
- Molecule 38: 30S ribosomal protein S5

Chain e:  80% 14% 6%



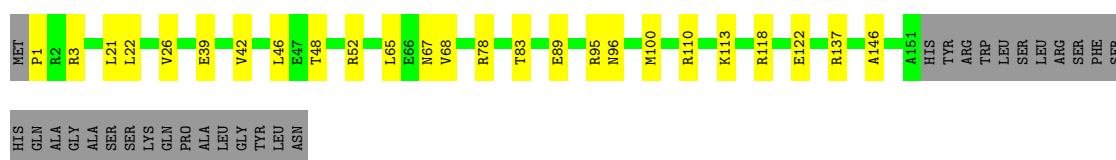
- Molecule 39: 30S ribosomal protein S6

Chain f:  59% 16% 26%




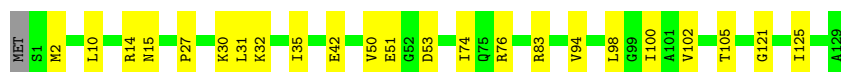
- Molecule 40: 30S ribosomal protein S7

Chain g:  70% 14% 16%




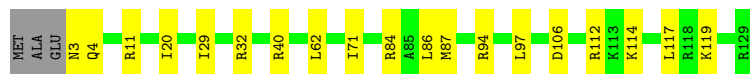
- Molecule 41: 30S ribosomal protein S8

Chain h:  82% 18%



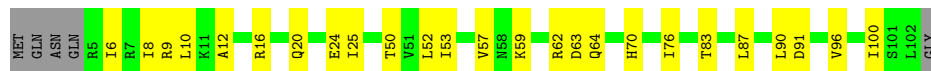
- Molecule 42: 30S ribosomal protein S9

Chain i:  83% 15%



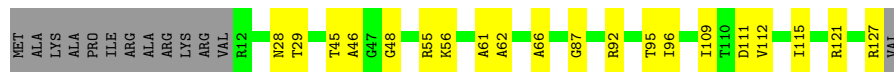
- Molecule 43: 30S ribosomal protein S10

Chain j:  71% 24% 5%




- Molecule 44: 30S ribosomal protein S11

Chain k:  74% 16% 10%




- Molecule 45: 30S ribosomal protein S12

Chain l:  85% 14%




- Molecule 46: 30S ribosomal protein S13

Chain m:  81% 15%



- Molecule 47: 30S ribosomal protein S14

Chain n:  79% 20%



- Molecule 48: Small ribosomal subunit protein uS15

Chain o:  90% 9%




- Molecule 49: 30S ribosomal protein S16

Chain p:  91% 9%




- Molecule 50: 30S ribosomal protein S17

Chain q:  80% 15% 5%



- Molecule 51: 30S ribosomal protein S18

Chain r:  79% 8% 13%




- Molecule 52: 30S ribosomal protein S19

Chain s:  66% 23% 11%




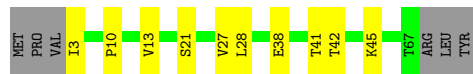
- Molecule 53: 30S ribosomal protein S20

Chain t:  84% 14% 2%



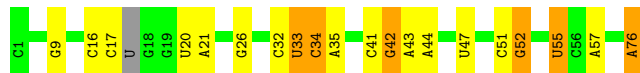
- Molecule 54: 30S ribosomal protein S21

Chain u:  77% 14% 8%




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

Chain v:  73% 18% 8% 1%




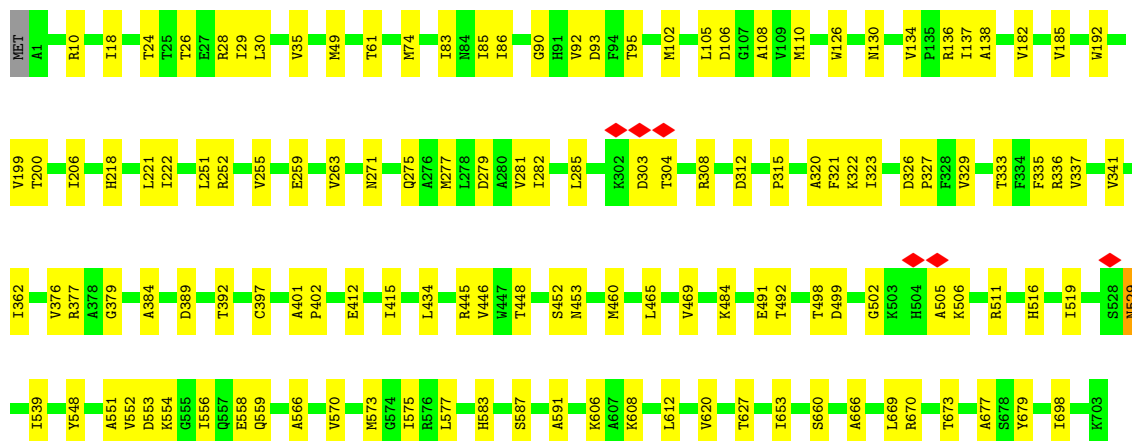
- Molecule 56: A/P-site tRNA(Phe)

Chain w:  66% 26% 8%



• Molecule 57: Elongation factor G

Chain x:  81% 18%



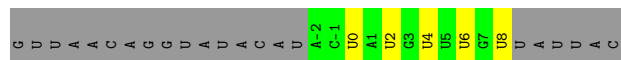
• Molecule 58: Dipeptide (FME-PHE)

Chain y:  50% 50%



• Molecule 59: mRNA

Chain z:  18% 15% 67%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	106477	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	0.130	Depositor
Minimum map value	-0.029	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.01	Depositor
Map size (\AA)	334.08, 334.08, 334.08	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: 5MC, 5MU, MG, G7M, 3TD, OMC, MA6, OMG, MIA, FME, NA, 2MA, AM2, 6MZ, PSU, PO4, OMU, H2U, 4OC, ZN, 1MG, GDP, UR3, 2MG, 4SU

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	0.17	0/450	0.35	0/599
2	1	0.18	0/416	0.37	0/554
3	2	0.16	0/380	0.31	0/498
4	3	0.17	0/513	0.42	0/676
5	4	0.16	0/303	0.40	0/397
6	5	0.13	0/646	0.36	0/898
7	6	0.19	0/531	0.43	0/709
8	A	0.17	0/69266	0.30	0/108055
9	B	0.13	0/2873	0.27	0/4478
10	C	0.18	0/2121	0.40	0/2852
11	D	0.18	0/1586	0.37	0/2134
12	E	0.16	0/1571	0.33	0/2113
13	F	0.19	0/1434	0.43	0/1926
14	G	0.15	0/1343	0.34	0/1816
15	H	0.15	0/1122	0.38	0/1515
16	I	0.14	0/692	0.37	0/960
17	J	0.19	0/1152	0.35	0/1551
18	K	0.16	0/947	0.35	0/1268
19	L	0.17	0/1054	0.40	0/1403
20	M	0.18	0/1093	0.41	0/1460
21	N	0.16	0/973	0.36	0/1301
22	O	0.15	0/902	0.36	0/1209
23	P	0.17	0/929	0.37	0/1242
24	Q	0.19	0/960	0.34	0/1278
25	R	0.19	0/829	0.42	0/1107
26	S	0.18	0/864	0.40	0/1156
27	T	0.17	0/744	0.36	0/994
28	U	0.16	0/787	0.37	0/1051
29	V	0.17	0/766	0.42	0/1025
30	W	0.16	0/582	0.38	0/769
31	X	0.19	0/635	0.37	0/848

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Y	0.18	0/510	0.45	0/677
33	Z	0.17	0/453	0.33	0/605
34	a	0.15	0/36725	0.29	0/57285
35	b	0.17	0/1735	0.40	0/2338
36	c	0.16	0/1651	0.34	0/2225
37	d	0.16	0/1665	0.35	0/2227
38	e	0.16	0/1154	0.42	0/1554
39	f	0.17	0/835	0.43	0/1128
40	g	0.92	5/1195 (0.4%)	0.99	5/1602 (0.3%)
41	h	0.18	0/989	0.42	0/1326
42	i	0.16	0/1034	0.41	0/1375
43	j	0.17	0/796	0.46	0/1077
44	k	0.19	0/885	0.39	0/1195
45	l	0.18	0/969	0.42	0/1300
46	m	0.19	0/892	0.47	0/1193
47	n	0.19	0/811	0.45	0/1081
48	o	0.16	0/722	0.37	0/964
49	p	0.16	0/659	0.37	0/884
50	q	0.16	0/657	0.40	0/881
51	r	0.15	0/544	0.36	0/731
52	s	0.16	0/675	0.39	0/908
53	t	0.16	0/671	0.33	0/888
54	u	0.18	0/512	0.41	0/683
55	v	0.17	0/1722	0.27	0/2678
56	w	0.22	0/1650	0.32	0/2569
57	x	0.18	0/5546	0.44	0/7503
58	y	0.14	0/11	0.33	0/13
59	z	0.14	0/255	0.23	0/394
All	All	0.18	5/164387 (0.0%)	0.34	5/245126 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	g	1	PRO	CB-CG	24.33	2.71	1.49
40	g	1	PRO	CG-CD	-16.38	0.95	1.50
40	g	1	PRO	CA-CB	-7.65	1.38	1.53
40	g	1	PRO	N-CA	-5.20	1.39	1.47
40	g	1	PRO	N-CD	5.00	1.54	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	g	1	PRO	CB-CG-CD	-29.23	12.56	106.10
40	g	1	PRO	N-CA-CB	-12.90	88.81	103.00
40	g	1	PRO	CA-CB-CG	-10.79	84.00	104.50
40	g	1	PRO	N-CD-CG	-8.00	91.20	103.20
40	g	1	PRO	CA-N-CD	-7.39	101.66	112.00

There are no chirality outliers.

There are no planarity outliers.

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	460	461	7	0
2	1	409	440	440	8	0
3	2	377	419	418	7	0
4	3	504	572	574	18	0
5	4	302	340	340	9	0
6	5	647	336	336	1	0
7	6	522	520	520	11	0
8	A	62338	31356	31371	387	0
9	B	2570	1301	1301	20	0
10	C	2082	2155	2157	39	0
11	D	1565	1618	1616	24	0
12	E	1552	1620	1619	23	0
13	F	1410	1445	1447	28	0
14	G	1323	1372	1374	11	0
15	H	1111	1148	1148	7	0
16	I	693	345	347	6	0
17	J	1129	1162	1162	26	0
18	K	938	1012	1012	13	0
19	L	1045	1117	1117	20	0
20	M	1074	1157	1157	19	0
21	N	960	1001	1000	10	0
22	O	892	923	923	16	0
23	P	917	963	965	9	0
24	Q	947	1020	1022	16	0
25	R	816	839	839	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	S	857	922	922	21	0
27	T	738	808	807	11	0
28	U	779	832	834	11	0
29	V	753	781	780	13	0
30	W	575	594	592	7	0
31	X	625	654	655	10	0
32	Y	509	543	543	5	0
33	Z	449	489	491	10	0
34	a	33050	16637	16653	210	0
35	b	1704	1733	1732	27	0
36	c	1624	1698	1699	23	0
37	d	1643	1708	1710	28	0
38	e	1141	1170	1170	17	0
39	f	817	809	808	17	0
40	g	1181	1238	1240	18	0
41	h	979	1032	1034	18	0
42	i	1022	1070	1070	14	0
43	j	786	829	828	22	0
44	k	869	879	878	18	0
45	l	955	1017	1019	14	0
46	m	883	942	944	15	0
47	n	799	839	841	21	0
48	o	714	737	737	7	0
49	p	649	666	666	6	0
50	q	648	692	691	8	0
51	r	535	552	552	7	0
52	s	658	685	685	19	0
53	t	665	716	714	10	0
54	u	506	502	502	7	0
55	v	1622	827	831	9	0
56	w	1631	831	837	4	0
57	x	5445	5420	5422	95	0
58	y	21	19	19	1	0
59	z	230	115	116	5	0
60	0	1	0	0	0	0
60	A	262	0	0	0	0
60	B	7	0	0	0	0
60	C	3	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	Z	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	a	84	0	0	0	0
60	m	2	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	2	0	0	0	0
60	z	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	124	123	6	0
64	x	5	0	0	2	0
65	x	28	10	12	1	0
All	All	153146	103761	103823	1189	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 5.

All (1189) 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)
8:A:1071:G:H21	8:A:1089:A:N6	1.68	0.90
8:A:2386:A:O2'	30:W:37:ARG:NH2	2.06	0.87
40:g:21:LEU:HD21	40:g:65:LEU:HD11	1.57	0.85
8:A:1361:G:HO2'	8:A:2215:C:HO2'	1.07	0.84
8:A:1508:A:O2'	8:A:1509:A:O4'	1.95	0.82
34:a:1297:G:N2	40:g:113:LYS:O	2.12	0.82
8:A:1071:G:H21	8:A:1089:A:H61	1.27	0.81
8:A:2564:A:OP1	8:A:2648:G:O2'	1.98	0.81
8:A:1417:C:HO2'	8:A:1587:G:HO2'	1.21	0.81
34:a:28:A:O2'	34:a:296:U:OP1	1.99	0.81
8:A:1779:U:OP2	8:A:1784:A:N6	2.13	0.81
8:A:2013:A:O2'	26:S:94:ASP:OD2	1.98	0.80
8:A:796:C:OP1	12:E:57:LYS:NZ	2.15	0.79
8:A:25:U:O2	8:A:515:A:N6	2.14	0.79
34:a:501:C:OP1	45:l:113:ARG:NH2	2.16	0.79
8:A:1125:G:OP2	8:A:1126:A:O2'	2.00	0.78
13:F:117:SER:O	13:F:127:TYR:OH	2.00	0.78
34:a:261:U:OP2	53:t:73:ARG:NH2	2.16	0.78
57:x:673:THR:HG21	57:x:677:ALA:HB3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:75:G:HO2'	29:V:88:HIS:HE2	1.32	0.77
8:A:1071:G:N2	8:A:1089:A:H61	1.83	0.77
40:g:26:VAL:HG22	40:g:42:VAL:HG11	1.67	0.77
8:A:1053:C:O2	8:A:1106:G:N2	2.14	0.77
8:A:1660:G:N2	8:A:2689:U:O4	2.18	0.77
34:a:8:A:N6	37:d:201:GLU:O	2.17	0.77
38:e:156:ARG:NH2	41:h:42:GLU:OE2	2.17	0.77
8:A:249:C:OP2	8:A:2394:C:O2'	2.03	0.76
34:a:1300:G:O2'	34:a:1301:U:O5'	2.02	0.76
8:A:1093:G:O2'	8:A:1094:U:OP1	2.03	0.76
5:4:8:LYS:NZ	8:A:2467:C:OP1	2.17	0.76
32:Y:9:LYS:O	32:Y:60:LYS:NZ	2.19	0.76
8:A:569:U:O2'	8:A:983:A:N1	2.18	0.75
8:A:242:G:N2	8:A:255:A:OP2	2.19	0.75
8:A:629:G:N3	8:A:639:U:O2'	2.19	0.75
8:A:1799:G:OP1	10:C:257:ARG:NH1	2.19	0.75
34:a:1494:G:OP2	63:a:1633:AM2:NC6	2.18	0.75
52:s:78:THR:OG1	52:s:80:ARG:NH1	2.18	0.75
8:A:1538:G:O2'	8:A:1539:U:O4'	2.00	0.75
13:F:161:SER:OG	13:F:164:GLU:OE1	2.03	0.75
8:A:247:G:OP2	8:A:249:C:N4	2.20	0.74
8:A:1019:U:OP1	8:A:1035:U:O2'	2.03	0.74
8:A:1385:A:O2'	8:A:1396:U:O2	2.05	0.74
8:A:1916:A:O2'	8:A:1917:PSU:O4'	2.05	0.74
34:a:50:A:O2'	34:a:360:G:N2	2.20	0.74
8:A:475:C:O2	8:A:479:A:N6	2.20	0.74
8:A:2646:C:OP2	8:A:2732:G:O2'	2.03	0.74
57:x:138:ALA:HB3	57:x:263:VAL:HG12	1.70	0.74
8:A:1992:G:N2	8:A:1996:C:O2'	2.21	0.74
8:A:1070:A:H61	16:I:26:ALA:HB3	1.52	0.74
8:A:1791:A:O2'	10:C:204:LEU:O	2.05	0.74
57:x:548:TYR:OH	57:x:587:SER:O	2.05	0.74
8:A:2319:G:O2'	8:A:2320:U:O5'	2.06	0.73
8:A:1067:A:O2'	16:I:22:PRO:O	2.06	0.73
34:a:427:U:OP2	34:a:428:G:O2'	2.04	0.73
8:A:534:U:O2'	24:Q:48:ASP:OD2	2.04	0.73
8:A:514:A:N3	8:A:581:C:O2'	2.21	0.73
8:A:635:C:OP2	19:L:126:ARG:NH1	2.21	0.73
8:A:793:A:OP2	8:A:2071:A:O2'	2.05	0.73
8:A:310:A:O2'	8:A:311:A:O5'	2.04	0.73
34:a:426:U:OP1	37:d:35:GLN:NE2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:56:ARG:NH2	52:s:62:THR:O	2.21	0.73
34:a:1226:C:OP2	46:m:101:THR:OG1	2.03	0.73
44:k:87:GLY:O	44:k:92:ARG:NH1	2.21	0.73
8:A:1447:C:O2'	8:A:1544:A:N3	2.21	0.73
34:a:691:G:O6	44:k:56:LYS:NZ	2.20	0.73
8:A:1365:A:O2'	31:X:10:ARG:NH1	2.22	0.73
8:A:2469:A:N6	8:A:2481:G:O2'	2.22	0.72
8:A:994:C:OP1	24:Q:52:ARG:NH2	2.22	0.72
8:A:2705:A:O2'	8:A:2852:G:OP1	2.06	0.72
34:a:1237:C:O2'	34:a:1300:G:N2	2.19	0.72
34:a:1493:A:O2'	59:z:4:U:O2'	2.06	0.72
8:A:1093:G:N2	8:A:1097:U:OP2	2.23	0.72
8:A:704:G:O2'	8:A:727:A:N6	2.23	0.72
8:A:1818:U:O2'	10:C:152:GLN:O	2.08	0.72
23:P:61:ARG:NH1	23:P:70:GLU:OE2	2.23	0.72
8:A:2125:G:N2	8:A:2172:U:OP1	2.23	0.72
23:P:87:ARG:NH2	23:P:109:ILE:O	2.22	0.72
34:a:826:C:O2	41:h:15:ASN:ND2	2.22	0.72
34:a:1055:A:O2'	36:c:160:GLU:O	2.08	0.72
8:A:1419:A:O2'	8:A:1421:G:N7	2.22	0.71
18:K:42:THR:HG22	18:K:57:VAL:HG22	1.72	0.71
1:0:49:ARG:NH1	8:A:2884:U:O4'	2.23	0.71
2:1:20:TYR:HH	8:A:2347:C:HO2'	1.35	0.71
8:A:971:G:OP1	8:A:974:G:O2'	2.04	0.71
8:A:2100:G:O6	8:A:2189:U:O2	2.09	0.71
20:M:47:GLU:OE1	20:M:51:ARG:NH1	2.23	0.71
8:A:1826:G:O2'	8:A:1971:U:OP2	2.09	0.71
8:A:447:A:OP1	24:Q:4:LYS:NZ	2.24	0.71
8:A:1044:C:O2'	8:A:1111:A:N1	2.24	0.71
15:H:136:SER:OG	15:H:137:GLU:OE1	2.05	0.71
36:c:25:THR:OG1	47:n:76:LYS:NZ	2.22	0.71
8:A:2032:G:N2	11:D:151:THR:OG1	2.24	0.71
36:c:122:GLN:OE1	36:c:135:ARG:NH2	2.24	0.71
34:a:1116:U:O2	34:a:1184:G:O6	2.08	0.70
38:e:104:ILE:O	38:e:111:ARG:NH2	2.24	0.70
17:J:17:VAL:HG23	17:J:137:PRO:HB2	1.73	0.70
1:0:12:ARG:NH2	8:A:517:C:OP1	2.25	0.70
34:a:1315:U:O2'	34:a:1360:A:N3	2.23	0.70
8:A:324:A:OP2	8:A:1205:A:N6	2.24	0.70
34:a:591:U:OP2	41:h:30:LYS:NZ	2.16	0.70
54:u:3:ILE:N	54:u:21:SER:HG	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:v:16:C:OP1	55:v:17:C:N4	2.25	0.70
8:A:1715:G:N2	8:A:1744:A:OP2	2.25	0.70
37:d:139:ASN:ND2	37:d:139:ASN:O	2.24	0.70
57:x:252:ARG:NH2	57:x:285:LEU:O	2.25	0.70
34:a:972:C:OP2	43:j:59:LYS:NZ	2.21	0.70
34:a:1522:U:OP1	44:k:127:ARG:NH1	2.25	0.70
8:A:813:U:O2'	8:A:1225:G:O2'	2.08	0.69
13:F:61:GLY:O	13:F:94:ARG:NH2	2.25	0.69
34:a:890:G:O2'	34:a:906:A:N6	2.25	0.69
8:A:1649:G:O2'	21:N:106:ASP:OD2	2.10	0.69
34:a:404:G:OP2	37:d:114:ARG:NH2	2.24	0.69
36:c:190:THR:HG21	36:c:195:ILE:HD12	1.73	0.69
8:A:1700:A:N6	34:a:1475:G:OP1	2.22	0.69
34:a:491:G:OP1	37:d:147:LYS:NZ	2.24	0.69
8:A:643:A:N1	8:A:2369:A:O2'	2.25	0.69
10:C:179:GLU:OE1	10:C:269:ARG:NH2	2.25	0.69
8:A:974:G:O2'	8:A:989:G:N2	2.26	0.69
10:C:4:LYS:NZ	10:C:13:ARG:O	2.25	0.69
34:a:686:U:O2'	34:a:687:A:O4'	2.10	0.69
34:a:1314:C:OP2	52:s:3:SER:OG	2.06	0.69
11:D:14:ILE:HD11	11:D:188:LEU:HD13	1.74	0.69
24:Q:47:ARG:NE	24:Q:51:GLN:OE1	2.25	0.69
33:Z:2:LYS:NZ	33:Z:39:ASP:O	2.26	0.69
34:a:259:G:OP1	53:t:35:TYR:OH	2.09	0.69
34:a:1210:C:OP2	57:x:583:HIS:ND1	2.25	0.69
57:x:506:LYS:O	57:x:511:ARG:NE	2.26	0.69
8:A:2291:U:OP1	8:A:2380:C:O2'	2.10	0.69
8:A:1667:G:O2'	8:A:1991:U:O4	2.10	0.69
57:x:669:LEU:O	57:x:673:THR:HG22	1.93	0.69
22:O:93:ASP:OD2	22:O:95:SER:OG	2.09	0.68
9:B:8:C:O2'	22:O:25:ARG:NH2	2.26	0.68
34:a:182:A:N1	34:a:223:A:O2'	2.26	0.68
57:x:412:GLU:OE2	57:x:445:ARG:NH2	2.26	0.68
55:v:41:C:O2'	55:v:42:G:OP1	2.09	0.68
50:q:63:CYS:SG	50:q:73:THR:OG1	2.41	0.68
22:O:10:ARG:NH1	22:O:96:GLY:O	2.26	0.68
46:m:15:VAL:O	46:m:19:THR:HG23	1.92	0.68
8:A:251:A:OP1	19:L:58:TYR:OH	2.08	0.68
34:a:993:G:O2'	34:a:994:A:N7	2.26	0.68
39:f:47:LEU:HD21	39:f:57:ALA:HB3	1.75	0.68
8:A:1315:C:O2'	8:A:1392:A:N3	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1305:G:N2	34:a:1332:A:OP2	2.27	0.68
43:j:16:ARG:O	43:j:20:GLN:NE2	2.27	0.68
38:e:9:GLU:N	38:e:9:GLU:OE1	2.28	0.67
8:A:1926:U:O2'	8:A:1927:A:OP1	2.11	0.67
54:u:10:PRO:HB2	54:u:13:VAL:HG22	1.76	0.67
8:A:310:A:HO2'	8:A:311:A:P	2.17	0.67
8:A:627:A:OP1	19:L:78:ARG:NH1	2.27	0.67
34:a:542:G:OP1	37:d:9:LYS:NZ	2.26	0.67
38:e:156:ARG:NH1	41:h:98:LEU:O	2.27	0.67
8:A:2439:A:N6	8:A:2585:U:O2'	2.28	0.67
34:a:811:C:O2'	34:a:901:A:N1	2.26	0.67
1:O:39:ARG:NH2	8:A:2885:G:OP2	2.27	0.67
8:A:335:C:O2	28:U:67:SER:OG	2.13	0.67
11:D:25:THR:OG1	11:D:191:GLY:O	2.12	0.67
20:M:17:ASN:O	20:M:38:ARG:NH1	2.27	0.67
8:A:714:U:OP2	48:o:88:ARG:NH1	2.28	0.67
8:A:895:U:C4	8:A:897:C:N4	2.63	0.67
37:d:104:MET:HE1	37:d:142:VAL:HB	1.74	0.67
8:A:1340:U:OP1	27:T:84:TYR:OH	2.13	0.66
34:a:1200:C:OP1	34:a:1201:A:O2'	2.06	0.66
11:D:14:ILE:HD12	11:D:24:VAL:HG11	1.76	0.66
13:F:118:ALA:O	13:F:166:ARG:NH1	2.28	0.66
57:x:106:ASP:OD2	57:x:336:ARG:NH2	2.28	0.66
36:c:139:ASN:OD1	36:c:142:ARG:NH2	2.28	0.66
57:x:182:VAL:HG21	57:x:206:ILE:HD12	1.78	0.66
4:3:44:ARG:NH1	8:A:2350:C:OP2	2.29	0.66
34:a:652:U:O2'	34:a:653:U:O5'	2.12	0.66
34:a:1072:G:H21	35:b:105:THR:HG21	1.60	0.66
39:f:75:GLU:OE2	39:f:79:ARG:NH2	2.28	0.66
13:F:101:ARG:NE	13:F:139:GLU:OE2	2.28	0.66
33:Z:36:GLU:O	33:Z:37:ARG:NH1	2.29	0.66
34:a:1530:G:N7	54:u:45:LYS:NZ	2.43	0.66
37:d:14:GLU:OE2	37:d:62:ARG:NH1	2.29	0.66
8:A:291:G:O6	8:A:349:U:O2	2.14	0.66
55:v:33:U:O2'	55:v:34:C:O5'	2.13	0.66
34:a:197:A:N1	34:a:220:G:O2'	2.25	0.66
34:a:1152:A:OP1	43:j:70:HIS:ND1	2.29	0.66
8:A:411:G:OP2	8:A:2406:A:O2'	2.11	0.65
8:A:1366:A:OP1	31:X:1:SER:OG	2.14	0.65
57:x:548:TYR:HB2	57:x:551:ALA:HB3	1.77	0.65
8:A:781:A:OP1	10:C:216:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1279:G:OP1	43:j:9:ARG:NH2	2.28	0.65
4:3:44:ARG:NH2	8:A:2349:G:OP1	2.29	0.65
8:A:2200:C:OP2	31:X:36:ARG:NH1	2.28	0.65
35:b:25:LYS:NZ	35:b:193:ASP:OD2	2.26	0.65
8:A:1341:G:OP2	8:A:1394:U:O2'	2.09	0.65
9:B:75:G:O2'	29:V:88:HIS:NE2	2.30	0.65
34:a:294:U:OP1	34:a:610:U:O2'	2.10	0.65
26:S:20:VAL:HG21	26:S:43:ALA:HB3	1.77	0.65
34:a:1321:U:O2'	52:s:77:ARG:NH2	2.29	0.65
53:t:43:LYS:NZ	53:t:82:ILE:O	2.29	0.65
8:A:203:A:OP2	8:A:204:A:O2'	2.12	0.65
8:A:698:C:O2'	8:A:734:A:N6	2.28	0.65
10:C:35:LYS:NZ	10:C:37:SER:OG	2.18	0.65
34:a:481:G:O2'	34:a:483:C:N4	2.29	0.65
34:a:1013:G:N2	34:a:1016:A:OP2	2.21	0.65
35:b:99:MET:HA	35:b:106:VAL:HG21	1.78	0.65
43:j:52:LEU:O	47:n:81:ARG:NH1	2.30	0.65
8:A:614:A:O2'	8:A:615:U:OP2	2.13	0.65
33:Z:57:GLU:N	33:Z:57:GLU:OE1	2.30	0.65
8:A:2287:A:O2'	8:A:2288:A:O5'	2.13	0.65
8:A:2636:C:O2'	11:D:45:TYR:OH	2.12	0.65
17:J:125:TYR:OH	17:J:132:HIS:NE2	2.23	0.65
8:A:1954:G:O2'	8:A:1956:U:O4	2.07	0.65
34:a:1026:G:O6	34:a:1034:G:N1	2.30	0.65
34:a:1270:G:O2'	34:a:1313:U:O2'	1.97	0.65
8:A:577:G:O2'	8:A:1254:A:OP1	2.14	0.64
8:A:774:G:N2	8:A:787:C:O2'	2.30	0.64
34:a:820:U:O4	63:a:1618:AM2:HA2	1.97	0.64
8:A:219:A:N3	8:A:234:U:O2'	2.27	0.64
8:A:1076:C:N4	8:A:1078:U:O4	2.30	0.64
36:c:39:ARG:NH1	36:c:54:ILE:O	2.30	0.64
40:g:67:ASN:O	40:g:137:ARG:NH2	2.30	0.64
34:a:509:A:N3	34:a:543:U:O2'	2.26	0.64
56:w:68:C:N4	56:w:69:G:O6	2.31	0.64
5:4:2:LYS:NZ	5:4:32:LYS:O	2.26	0.64
8:A:2079:U:O2'	31:X:22:ASN:OD1	2.15	0.64
8:A:2468:A:O2'	8:A:2469:A:O5'	2.13	0.64
9:B:30:C:O2'	9:B:57:A:N1	2.28	0.64
26:S:3:THR:HG21	26:S:58:ALA:N	2.13	0.64
8:A:2313:C:O4'	13:F:36:ASN:ND2	2.30	0.64
22:O:111:ARG:NE	22:O:117:PHE:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1491:G:N2	63:a:1633:AM2:OB6	2.30	0.64
8:A:1007:C:OP1	17:J:37:ARG:NH1	2.30	0.64
34:a:816:A:OP1	34:a:1526:G:O2'	2.16	0.64
34:a:1412:C:OP1	45:l:53:ARG:NH1	2.30	0.64
8:A:239:C:O2'	8:A:622:G:O2'	2.16	0.64
8:A:1565:C:O2'	8:A:1567:G:N7	2.24	0.64
13:F:55:ASP:O	13:F:59:ILE:HD12	1.96	0.64
8:A:529:A:OP2	17:J:116:ARG:NH2	2.31	0.64
8:A:2618:G:H21	11:D:155:VAL:HG21	1.63	0.64
36:c:161:ILE:HD11	59:z:8:U:H2'	1.80	0.64
8:A:84:A:N1	8:A:98:G:O2'	2.28	0.63
8:A:585:G:N7	24:Q:5:ARG:NH2	2.45	0.63
9:B:76:G:O2'	29:V:78:GLN:OE1	2.09	0.63
46:m:16:ILE:O	46:m:19:THR:OG1	2.15	0.63
34:a:401:C:O2'	34:a:621:A:N3	2.30	0.63
8:A:2566:A:N1	18:K:28:SER:OG	2.24	0.63
34:a:1492:A:N6	45:l:46:SER:OG	2.31	0.63
4:3:11:LYS:NZ	8:A:249:C:O2	2.30	0.63
23:P:67:GLU:N	23:P:67:GLU:OE1	2.31	0.63
34:a:376:G:O2'	49:p:5:ARG:NH1	2.32	0.63
37:d:8:LEU:HD13	37:d:31:CYS:HB3	1.81	0.63
34:a:527:G7M:O2'	34:a:535:A:N1	2.30	0.63
34:a:45:G:OP1	34:a:307:C:O2'	2.17	0.63
8:A:1814:G:OP2	8:A:1815:A:O2'	2.13	0.62
8:A:2431:U:O2'	8:A:2433:A:N7	2.29	0.62
8:A:265:A:O2'	8:A:428:A:N6	2.32	0.62
8:A:396:G:OP2	31:X:9:LYS:NZ	2.32	0.62
8:A:1654:A:O2'	11:D:118:PHE:O	2.14	0.62
17:J:56:VAL:HG11	17:J:101:ILE:HD13	1.81	0.62
8:A:574:A:N6	8:A:2034:U:OP1	2.31	0.62
34:a:738:C:OP1	39:f:4:TYR:OH	2.18	0.62
57:x:130:ASN:OD1	57:x:136:ARG:NH2	2.32	0.62
7:6:10:GLU:N	7:6:10:GLU:OE1	2.32	0.62
8:A:1601:G:OP1	27:T:64:LYS:NZ	2.30	0.62
34:a:31:G:O2'	34:a:48:C:N4	2.33	0.62
34:a:751:U:OP1	48:o:16:ARG:NH2	2.32	0.62
34:a:1255:G:O2'	34:a:1258:G:N3	2.26	0.62
40:g:78:ARG:HD3	40:g:83:THR:HG22	1.80	0.62
57:x:90:GLY:N	64:x:802:PO4:O4	2.32	0.62
8:A:1061:U:O2'	16:I:9:LYS:O	2.16	0.62
8:A:2139:U:C4	8:A:2152:G:O6	2.51	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2250:G:O2'	8:A:2496:C:OP1	2.10	0.62
34:a:1217:C:OP2	47:n:8:ARG:NH2	2.33	0.62
8:A:641:U:O2'	8:A:2350:C:OP1	2.18	0.62
34:a:1317:C:OP1	47:n:23:ARG:NH1	2.33	0.62
8:A:2528:U:O2'	8:A:2530:A:OP1	2.06	0.62
1:0:8:THR:OG1	8:A:2021:C:OP1	2.13	0.62
34:a:565:U:OP2	34:a:566:G:O2'	2.17	0.62
34:a:1006:G:N2	34:a:1023:U:O4'	2.33	0.61
34:a:757:U:OP1	34:a:822:U:O2'	2.18	0.61
4:3:32:LEU:HD12	4:3:40:LYS:HD3	1.81	0.61
7:6:59:ARG:O	7:6:63:ARG:NE	2.31	0.61
8:A:2505:G:O2'	8:A:2506:U:O5'	2.17	0.61
10:C:166:ARG:NH1	10:C:168:GLY:O	2.34	0.61
4:3:38:LYS:NZ	8:A:2365:G:N7	2.37	0.61
57:x:434:LEU:HB3	57:x:446:VAL:HG21	1.82	0.61
28:U:2:ALA:O	28:U:5:ARG:NE	2.28	0.61
35:b:216:VAL:O	35:b:220:VAL:HG22	2.00	0.61
25:R:27:ILE:HD13	25:R:33:VAL:HG22	1.82	0.61
43:j:8:ILE:HG12	43:j:100:ILE:HG22	1.82	0.61
8:A:483:A:O2'	28:U:56:GLY:N	2.34	0.61
8:A:579:G:O2'	8:A:2019:A:OP1	2.18	0.61
34:a:1290:G:N3	42:i:40:ARG:NH2	2.48	0.61
46:m:82:LEU:HD11	52:s:64:GLU:OE1	2.00	0.61
17:J:43:GLU:OE2	24:Q:102:LYS:NZ	2.31	0.61
48:o:16:ARG:NH1	48:o:20:ASP:OD2	2.34	0.61
8:A:2314:A:H1'	13:F:154:THR:HG21	1.83	0.60
33:Z:23:LEU:HD11	33:Z:53:MET:CE	2.30	0.60
34:a:770:C:O2'	34:a:899:C:N3	2.32	0.60
34:a:1417:G:O2'	34:a:1483:A:N6	2.34	0.60
45:l:34:THR:N	45:l:53:ARG:O	2.34	0.60
8:A:859:G:O2'	8:A:916:G:O6	2.15	0.60
8:A:1323:C:OP1	26:S:98:LYS:NZ	2.32	0.60
34:a:404:G:O2'	34:a:498:A:N1	2.27	0.60
8:A:1754:A:N1	8:A:2716:C:O2'	2.34	0.60
11:D:77:ARG:NH1	11:D:200:ASP:OD1	2.34	0.60
13:F:135:ILE:HD13	13:F:140:ILE:HG21	1.84	0.60
34:a:343:U:O2'	34:a:346:G:O6	2.10	0.60
8:A:2092:U:OP1	8:A:2199:A:O2'	2.09	0.60
12:E:199:MET:HG3	12:E:200:LEU:HD12	1.83	0.60
52:s:48:ILE:HD11	52:s:70:LEU:HD22	1.82	0.60
4:3:32:LEU:O	4:3:33:THR:OG1	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1916:A:O2'	8:A:1917:PSU:O5'	2.19	0.60
8:A:84:A:O2'	28:U:6:ARG:NH2	2.34	0.60
10:C:106:PRO:HG2	10:C:109:LEU:HD13	1.83	0.60
34:a:995:C:N3	34:a:1046:A:O2'	2.34	0.60
35:b:56:LEU:HD13	35:b:216:VAL:HG23	1.82	0.60
8:A:2014:A:O2'	26:S:92:ARG:NH2	2.35	0.60
10:C:70:LYS:NZ	10:C:97:ASP:OD2	2.21	0.60
34:a:429:U:H3'	37:d:8:LEU:HD12	1.82	0.60
8:A:224:U:O4	8:A:419:U:O2'	2.20	0.60
8:A:2684:U:O4'	18:K:70:ARG:NH1	2.35	0.60
8:A:1964:G:O2'	8:A:1967:C:OP2	2.13	0.59
34:a:975:A:N1	34:a:1366:C:O2'	2.24	0.59
48:o:38:LEU:HD23	48:o:42:PHE:HE2	1.66	0.59
57:x:415:ILE:HD11	57:x:666:ALA:HB3	1.83	0.59
9:B:7:G:OP1	22:O:4:LYS:NZ	2.19	0.59
11:D:179:ARG:HB3	11:D:188:LEU:HD12	1.84	0.59
8:A:672:C:OP2	19:L:42:SER:OG	2.18	0.59
8:A:1022:G:O6	17:J:68:LYS:NZ	2.27	0.59
8:A:1131:G:N2	8:A:1132:U:O4	2.31	0.59
8:A:2796:U:O2'	8:A:2797:U:OP1	2.21	0.59
37:d:18:LEU:HB2	37:d:20:LEU:HD13	1.83	0.59
8:A:270:A:N1	8:A:369:U:O2'	2.31	0.59
34:a:933:G:OP1	40:g:3:ARG:NH2	2.34	0.59
40:g:89:GLU:OE1	40:g:95:ARG:NH2	2.35	0.59
46:m:70:ARG:HG2	46:m:74:MET:HE2	1.84	0.59
8:A:2013:A:OP2	26:S:99:ARG:NH1	2.35	0.59
34:a:429:U:OP1	37:d:12:ARG:NH2	2.36	0.59
42:i:40:ARG:NH1	42:i:71:ILE:HG21	2.18	0.59
8:A:1081:U:C2	16:I:123:ALA:HB1	2.38	0.59
8:A:1322:A:N1	8:A:1333:G:O2'	2.33	0.59
8:A:1538:G:O2'	8:A:1539:U:O5'	2.20	0.59
8:A:1913:A:N1	56:w:37:MIA:O2'	2.34	0.59
34:a:35:G:N3	45:l:114:SER:OG	2.35	0.59
34:a:512:U:OP1	37:d:43:ARG:NH1	2.35	0.59
34:a:1338:G:O2'	55:v:42:G:OP1	2.19	0.59
8:A:1668:A:O2'	8:A:1674:G:N7	2.25	0.59
8:A:2788:C:O2'	8:A:2809:A:N3	2.33	0.59
34:a:719:C:O2'	51:r:38:ILE:O	2.21	0.59
1:O:9:ARG:NH2	8:A:516:C:OP1	2.35	0.59
8:A:659:G:O2'	12:E:95:LYS:O	2.20	0.59
8:A:1607:C:N4	8:A:1622:G:OP2	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:358:U:O2'	57:x:327:PRO:O	2.22	0.58
34:a:1260:G:OP1	34:a:1284:C:O2'	2.16	0.58
57:x:620:VAL:HG12	57:x:679:TYR:CB	2.33	0.58
15:H:53:GLU:N	15:H:53:GLU:OE1	2.36	0.58
8:A:2645:G:OP2	8:A:2645:G:N2	2.19	0.58
26:S:59:GLU:OE2	26:S:66:ILE:HD11	2.03	0.58
42:i:20:ILE:HG22	42:i:62:LEU:HG	1.86	0.58
54:u:38:GLU:OE2	54:u:42:THR:OG1	2.19	0.58
5:4:1:MET:N	8:A:2526:G:N3	2.52	0.58
12:E:147:LEU:HD11	12:E:170:ARG:HG3	1.84	0.58
42:i:86:LEU:HD22	42:i:97:LEU:HD11	1.86	0.58
42:i:114:LYS:HB2	42:i:117:LEU:HD12	1.85	0.58
56:w:60:U:O2'	56:w:61:C:OP1	2.19	0.58
57:x:134:VAL:O	57:x:136:ARG:NH1	2.36	0.58
27:T:65:GLY:N	27:T:79:ASP:OD1	2.36	0.58
5:4:19:ARG:NE	8:A:2756:U:OP2	2.32	0.58
10:C:167:ASP:OD1	34:a:681:A:O2'	2.20	0.58
12:E:1:MET:N	12:E:14:VAL:O	2.37	0.58
19:L:96:LYS:HG3	19:L:101:ILE:HD11	1.85	0.58
30:W:33:ILE:HG21	30:W:76:ILE:HG21	1.84	0.58
37:d:146:GLU:N	37:d:146:GLU:OE1	2.34	0.58
8:A:546:U:O2'	8:A:547:A:O4'	2.21	0.58
8:A:1008:A:OP2	17:J:37:ARG:NH2	2.36	0.58
9:B:37:C:O2	9:B:48:U:O2'	2.21	0.58
57:x:620:VAL:HG12	57:x:679:TYR:HB2	1.85	0.58
8:A:1063:G:N2	16:I:131:THR:O	2.35	0.57
8:A:1266:G:O2'	8:A:2012:G:O6	2.18	0.57
34:a:692:U:O2'	34:a:694:A:N7	2.27	0.57
35:b:14:HIS:CE1	35:b:212:TYR:HH	2.22	0.57
57:x:673:THR:HG21	57:x:677:ALA:CB	2.32	0.57
22:O:79:ALA:HB1	22:O:115:LEU:HD13	1.87	0.57
8:A:2865:U:OP2	8:A:2866:U:O2'	2.10	0.57
34:a:95:C:O2'	34:a:96:U:OP1	2.20	0.57
34:a:195:A:O2'	34:a:196:A:O4'	2.19	0.57
34:a:427:U:OP1	37:d:12:ARG:NH2	2.37	0.57
55:v:51:C:O2'	55:v:52:G:OP1	2.23	0.57
57:x:337:VAL:O	57:x:379:GLY:N	2.36	0.57
8:A:1490:A:O2'	8:A:1491:G:OP1	2.19	0.57
30:W:55:LEU:HD12	30:W:76:ILE:HD12	1.87	0.57
34:a:1415:G:O6	34:a:1485:U:O2	2.23	0.57
10:C:75:ALA:HB3	10:C:115:ILE:HG13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:116:ARG:C	15:H:117:LEU:HD12	2.30	0.57
33:Z:23:LEU:HD11	33:Z:53:MET:HE2	1.85	0.57
34:a:991:U:O2'	34:a:992:U:O5'	2.20	0.57
37:d:139:ASN:N	37:d:181:PHE:O	2.36	0.57
44:k:46:ALA:HB1	44:k:61:ALA:HB1	1.87	0.57
8:A:2149:U:O2'	8:A:2150:C:OP1	2.23	0.57
8:A:2299:U:OP2	13:F:70:ARG:NH1	2.37	0.57
34:a:537:G:OP1	45:l:109:ARG:NH2	2.37	0.57
34:a:1432:G:O2'	34:a:1468:A:N6	2.38	0.57
57:x:24:THR:OG1	65:x:804:GDP:O1A	2.14	0.57
8:A:1064:C:O2'	8:A:1065:U:OP1	2.21	0.56
8:A:1090:A:O2'	8:A:1091:G:OP1	2.18	0.56
8:A:2522:U:O2'	8:A:2647:U:OP1	2.11	0.56
8:A:2661:G:O6	14:G:176:LYS:NZ	2.37	0.56
25:R:14:VAL:HG11	25:R:20:VAL:HG21	1.86	0.56
8:A:726:G:O5'	8:A:1432:G:O2'	2.23	0.56
11:D:58:ASN:OD1	11:D:59:ARG:N	2.38	0.56
12:E:46:GLN:O	12:E:88:ARG:NH2	2.37	0.56
17:J:1:MET:SD	24:Q:92:LYS:NZ	2.71	0.56
38:e:114:LEU:HD13	38:e:122:VAL:HG11	1.87	0.56
57:x:529:ASN:C	57:x:529:ASN:HD22	2.12	0.56
8:A:1322:A:OP1	26:S:11:ARG:NH1	2.38	0.56
8:A:2723:C:OP1	11:D:114:LYS:NZ	2.37	0.56
45:l:49:ARG:CB	45:l:89:LEU:HD11	2.36	0.56
8:A:1532:A:N6	8:A:1540:G:O6	2.38	0.56
12:E:10:SER:OG	12:E:11:ALA:N	2.38	0.56
15:H:80:ILE:HD13	15:H:102:ALA:HB2	1.87	0.56
57:x:498:THR:HG22	57:x:499:ASP:H	1.70	0.56
8:A:1109:C:O2'	8:A:1110:G:O4'	2.20	0.56
14:G:1:SER:OG	14:G:2:ARG:N	2.38	0.56
29:V:45:ASP:OD1	29:V:46:LYS:N	2.38	0.56
8:A:2299:U:OP1	13:F:71:LYS:NZ	2.30	0.56
20:M:20:LEU:HD13	29:V:81:PRO:HG2	1.88	0.56
40:g:22:LEU:O	40:g:26:VAL:HG23	2.06	0.56
19:L:122:VAL:CG2	19:L:142:ILE:HG23	2.35	0.56
37:d:154:VAL:O	37:d:158:LEU:HD23	2.05	0.56
57:x:415:ILE:CD1	57:x:666:ALA:HB3	2.35	0.56
44:k:112:VAL:HG12	51:r:72:ARG:NH2	2.20	0.56
8:A:99:U:O2	28:U:6:ARG:NH1	2.39	0.55
57:x:397:CYS:SG	57:x:401:ALA:HB3	2.46	0.55
3:2:29:GLN:NE2	8:A:210:C:OP1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:642:U:O2'	8:A:644:A:N7	2.31	0.55
24:Q:77:LYS:O	24:Q:116:LEU:HD11	2.05	0.55
34:a:675:A:O2'	44:k:115:ILE:O	2.23	0.55
49:p:48:GLU:OE2	49:p:51:ARG:NH2	2.38	0.55
8:A:1082:U:O2'	8:A:1083:U:OP1	2.23	0.55
9:B:8:C:O3'	22:O:25:ARG:NH2	2.38	0.55
9:B:36:C:O2'	9:B:37:C:OP1	2.22	0.55
10:C:250:GLN:NE2	10:C:251:THR:O	2.40	0.55
20:M:41:LEU:HD13	20:M:96:ILE:HG13	1.88	0.55
38:e:71:ILE:HD11	38:e:140:ILE:CG2	2.37	0.55
42:i:87:MET:SD	42:i:94:ARG:NH2	2.80	0.55
47:n:88:ALA:HB2	47:n:96:LEU:HD23	1.89	0.55
8:A:1064:C:N3	8:A:1068:G:O2'	2.38	0.55
8:A:1080:A:O2'	8:A:1082:U:O4	2.25	0.55
8:A:1521:G:OP2	8:A:1522:A:O2'	2.21	0.55
9:B:77:U:OP1	29:V:21:ARG:NH2	2.38	0.55
17:J:25:LEU:HD13	17:J:100:VAL:HG12	1.88	0.55
57:x:199:VAL:HG23	57:x:200:THR:HG23	1.88	0.55
2:1:5:ARG:NH2	2:1:23:THR:O	2.39	0.55
8:A:299:A:N3	8:A:319:G:O2'	2.29	0.55
11:D:156:PHE:CE1	17:J:81:ILE:HD13	2.41	0.55
40:g:78:ARG:CD	40:g:83:THR:HG22	2.36	0.55
4:3:28:LEU:HD11	4:3:43:LEU:HB2	1.89	0.55
8:A:976:G:O2'	8:A:1155:A:O2'	2.21	0.55
8:A:2154:A:O2'	8:A:2155:U:O4'	2.24	0.55
25:R:27:ILE:O	25:R:66:HIS:NE2	2.36	0.55
33:Z:58:GLU:OE1	33:Z:58:GLU:N	2.39	0.55
13:F:103:ILE:HG23	13:F:104:THR:HG23	1.89	0.55
20:M:106:ASP:OD1	20:M:107:GLY:N	2.39	0.55
9:B:48:U:OP2	22:O:30:ARG:NH2	2.40	0.55
12:E:112:LEU:HD13	12:E:186:VAL:HG21	1.89	0.55
21:N:29:VAL:O	21:N:78:LYS:NZ	2.40	0.55
45:l:52:CYS:SG	45:l:64:SER:OG	2.65	0.55
8:A:1248:G:OP1	24:Q:1:ALA:N	2.39	0.55
57:x:566:ALA:HA	57:x:698:ILE:HD13	1.89	0.54
8:A:245:G:O2'	8:A:384:A:N1	2.31	0.54
8:A:781:A:O2'	8:A:1788:C:O2	2.25	0.54
34:a:677:U:H3	34:a:713:G:H22	1.55	0.54
34:a:1270:G:HO2'	34:a:1313:U:HO2'	1.15	0.54
34:a:1408:A:N1	63:a:1633:AM2:OA6	2.32	0.54
35:b:73:ARG:NH2	35:b:92:ASN:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:h:2:MET:HE2	41:h:2:MET:HA	1.89	0.54
35:b:115:ASP:O	35:b:118:THR:OG1	2.22	0.54
57:x:362:ILE:HG21	57:x:376:VAL:HG23	1.90	0.54
34:a:253:A:O2'	50:q:16:MET:SD	2.64	0.54
8:A:2356:U:O2'	30:W:16:ARG:NH1	2.41	0.54
12:E:151:GLY:O	12:E:195:GLN:NE2	2.41	0.54
13:F:29:ARG:N	13:F:158:THR:OG1	2.40	0.54
34:a:356:A:N3	34:a:368:U:O2'	2.39	0.54
8:A:619:G:OP2	8:A:620:G:N2	2.40	0.54
34:a:979:C:O2	47:n:59:ARG:NH1	2.40	0.54
48:o:13:GLU:O	48:o:83:ARG:NH2	2.40	0.54
57:x:484:LYS:NZ	57:x:660:SER:O	2.35	0.54
8:A:69:C:O2	8:A:73:A:O2'	2.25	0.54
32:Y:18:LEU:HD11	32:Y:54:LYS:HE3	1.88	0.54
35:b:166:ASP:OD1	35:b:167:HIS:N	2.40	0.54
39:f:13:ASP:OD2	39:f:14:GLN:N	2.41	0.54
57:x:519:ILE:HG22	57:x:577:LEU:HG	1.89	0.54
8:A:2450:A:OP1	8:A:2497:A:O2'	2.09	0.54
12:E:73:ILE:HD12	12:E:78:TRP:CZ3	2.42	0.54
28:U:33:VAL:HG13	28:U:66:VAL:HG22	1.90	0.54
2:l:24:LYS:NZ	2:l:29:LYS:O	2.21	0.54
8:A:1614:A:N6	26:S:92:ARG:O	2.28	0.54
8:A:2005:A:O2'	8:A:2049:G:OP1	2.21	0.54
34:a:1227:A:OP1	52:s:79:TYR:OH	2.15	0.54
8:A:1067:A:H2'	8:A:1068:G:H21	1.73	0.54
8:A:2391:G:H2'	8:A:2424:C:H41	1.73	0.54
57:x:551:ALA:HB1	57:x:554:LYS:HE2	1.89	0.54
4:3:7:ARG:NH2	8:A:244:A:OP2	2.40	0.53
14:G:117:PRO:HG2	14:G:120:ILE:HD12	1.88	0.53
34:a:192:A:N3	53:t:54:GLN:NE2	2.55	0.53
39:f:10:VAL:HG21	39:f:18:VAL:CG2	2.39	0.53
47:n:19:TYR:CD1	47:n:51:LEU:HD22	2.44	0.53
8:A:2291:U:O2'	8:A:2374:C:O2	2.25	0.53
10:C:97:ASP:OD1	10:C:98:GLY:N	2.41	0.53
34:a:356:A:O2'	34:a:367:U:O2'	2.20	0.53
10:C:163:ILE:HA	10:C:173:LEU:HD23	1.89	0.53
19:L:122:VAL:HG23	19:L:142:ILE:HG23	1.90	0.53
39:f:46:GLN:NE2	39:f:47:LEU:O	2.41	0.53
40:g:146:ALA:O	44:k:55:ARG:NH1	2.41	0.53
41:h:35:ILE:HG13	41:h:102:VAL:HG11	1.90	0.53
57:x:502:GLY:O	57:x:516:HIS:ND1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1209:U:O2'	8:A:1237:A:N1	2.36	0.53
8:A:2391:G:O2'	8:A:2429:G:N2	2.41	0.53
34:a:126:G:OP1	34:a:605:U:O2'	2.23	0.53
34:a:982:U:OP2	47:n:63:ARG:NH2	2.39	0.53
57:x:606:LYS:O	57:x:608:LYS:NZ	2.42	0.53
9:B:54:G:N2	13:F:25:MET:SD	2.81	0.53
27:T:10:VAL:HG21	27:T:42:GLU:HG3	1.90	0.53
2:1:31:GLU:N	2:1:31:GLU:OE1	2.42	0.53
8:A:714:U:O2'	8:A:716:A:N7	2.34	0.53
8:A:1437:C:HO2'	8:A:1516:G:HO2'	1.21	0.53
57:x:570:VAL:HG11	57:x:573:MET:SD	2.49	0.53
35:b:202:ASN:OD1	35:b:203:ASP:N	2.40	0.53
57:x:10:ARG:NH2	57:x:282:ILE:O	2.40	0.53
4:3:31:ILE:HG22	4:3:31:ILE:O	2.09	0.53
8:A:1129:A:N1	8:A:2569:G:O2'	2.38	0.53
9:B:30:C:H1'	9:B:57:A:H61	1.74	0.53
8:A:575:A:OP2	8:A:2055:C:N4	2.42	0.52
40:g:68:VAL:HG12	40:g:68:VAL:O	2.09	0.52
12:E:113:VAL:CG2	12:E:118:LEU:HD23	2.40	0.52
3:2:1:MET:HE3	8:A:753:A:OP1	2.10	0.52
8:A:189:G:OP2	31:X:13:THR:HG21	2.09	0.52
8:A:1799:G:O2'	10:C:179:GLU:OE2	2.26	0.52
34:a:835:U:OP1	51:r:52:ARG:NH2	2.43	0.52
23:P:28:LYS:HB3	23:P:39:LEU:HD21	1.91	0.52
34:a:1060:U:OP1	47:n:85:ARG:NH2	2.40	0.52
8:A:463:G:N2	8:A:466:A:OP2	2.38	0.52
8:A:2468:A:O5'	8:A:2476:A:N6	2.42	0.52
8:A:2839:G:N2	21:N:91:ALA:O	2.42	0.52
57:x:218:HIS:NE2	57:x:222:ILE:HD11	2.24	0.52
8:A:83:A:O2'	8:A:103:A:N6	2.43	0.52
8:A:111:A:O3'	32:Y:58:ASN:ND2	2.42	0.52
8:A:1796:U:O2'	10:C:253:GLY:N	2.42	0.52
12:E:7:ASP:OD1	12:E:7:ASP:N	2.43	0.52
38:e:44:ARG:HG2	38:e:70:MET:HE2	1.92	0.52
47:n:19:TYR:HD1	47:n:51:LEU:HD22	1.74	0.52
57:x:61:THR:N	64:x:802:PO4:O2	2.42	0.52
57:x:102:MET:HE3	57:x:134:VAL:HG21	1.92	0.52
8:A:24:G:O2'	26:S:78:GLU:O	2.28	0.52
8:A:586:A:N1	8:A:809:G:O2'	2.37	0.52
34:a:335:C:O2'	34:a:1433:A:N3	2.41	0.52
34:a:1368:A:OP1	43:j:64:GLN:NE2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:l:99:GLY:N	45:l:103:CYS:O	2.39	0.52
57:x:303:ASP:OD1	57:x:304:THR:N	2.41	0.52
8:A:2452:C:O4'	58:y:101:FME:HE2	2.09	0.52
9:B:66:A:O5'	9:B:108:A:N6	2.43	0.52
11:D:4:LEU:HD12	11:D:32:ASN:OD1	2.10	0.52
17:J:4:PHE:O	24:Q:63:ARG:NH1	2.40	0.52
29:V:32:GLY:O	29:V:93:ARG:NH1	2.43	0.52
36:c:56:ILE:CG2	36:c:63:ILE:HD11	2.40	0.52
46:m:18:LEU:HD22	46:m:33:LEU:CD2	2.39	0.52
57:x:29:ILE:HD11	57:x:277:MET:CE	2.40	0.52
4:3:3:ILE:HD11	8:A:592:A:C2	2.44	0.52
8:A:1047:G:N2	8:A:1110:G:O2'	2.43	0.52
39:f:40:GLU:N	39:f:40:GLU:OE1	2.43	0.52
8:A:2595:G:N2	8:A:2598:A:OP2	2.35	0.52
34:a:1277:C:O2'	34:a:1279:G:N3	2.39	0.52
34:a:1345:U:O2'	34:a:1346:A:OP2	2.26	0.52
39:f:10:VAL:HG21	39:f:18:VAL:HG22	1.91	0.52
8:A:2319:G:HO2'	8:A:2320:U:P	2.32	0.51
8:A:475:C:N3	8:A:479:A:N7	2.58	0.51
8:A:624:C:O2'	8:A:657:U:OP1	2.25	0.51
47:n:88:ALA:CB	47:n:96:LEU:HD23	2.41	0.51
34:a:354:G:O2'	34:a:389:A:OP1	2.27	0.51
8:A:995:C:O2	17:J:3:THR:OG1	2.28	0.51
34:a:539:A:OP2	45:l:111:GLN:NE2	2.42	0.51
8:A:1127:A:N7	8:A:2488:G:O2'	2.43	0.51
27:T:6:ARG:O	27:T:10:VAL:HG23	2.10	0.51
34:a:787:A:N1	34:a:795:C:N4	2.57	0.51
10:C:50:THR:OG1	10:C:53:ILE:HD12	2.10	0.51
14:G:80:GLU:OE1	14:G:80:GLU:N	2.44	0.51
37:d:98:ASP:OD1	37:d:99:ASN:N	2.44	0.51
8:A:715:A:O2'	8:A:716:A:OP1	2.29	0.51
34:a:195:A:N3	34:a:222:C:O2'	2.44	0.51
34:a:1418:A:N6	34:a:1482:G:O2'	2.44	0.51
42:i:86:LEU:CD2	42:i:97:LEU:HD11	2.41	0.51
8:A:1980:G:O2'	8:A:1982:U:OP2	2.29	0.51
16:I:41:PHE:O	16:I:45:THR:CB	2.59	0.51
34:a:107:G:N7	53:t:9:ARG:NH1	2.59	0.51
40:g:42:VAL:O	40:g:46:LEU:HD23	2.10	0.51
8:A:2134:A:N7	8:A:2157:G:O2'	2.44	0.51
26:S:17:VAL:HG12	26:S:76:VAL:HG21	1.93	0.51
34:a:38:G:H22	34:a:397:A:H5'	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:693:A:O2'	8:A:1353:A:N3	2.37	0.50
34:a:1072:G:N2	35:b:105:THR:HG21	2.24	0.50
9:B:52:A:O2'	9:B:53:A:O5'	2.29	0.50
30:W:34:VAL:HG22	30:W:55:LEU:HB2	1.94	0.50
37:d:64:TYR:CD2	37:d:93:LEU:HD13	2.47	0.50
8:A:605:G:OP1	12:E:99:LYS:NZ	2.44	0.50
8:A:1153:C:OP1	24:Q:91:ARG:NH1	2.41	0.50
10:C:153:LEU:CD1	10:C:175:LEU:HD22	2.41	0.50
10:C:257:ARG:NH2	10:C:263:ASP:OD1	2.45	0.50
11:D:16:THR:OG1	11:D:18:ASP:OD2	2.24	0.50
46:m:85:TYR:N	52:s:72:GLU:O	2.43	0.50
8:A:2720:U:OP1	23:P:52:ARG:NH2	2.44	0.50
34:a:556:C:OP1	45:l:13:ARG:NH2	2.44	0.50
34:a:875:U:O2'	41:h:14:ARG:NH1	2.44	0.50
35:b:108:GLN:OE1	35:b:111:LYS:NZ	2.39	0.50
41:h:31:LEU:O	41:h:35:ILE:HD12	2.10	0.50
7:6:27:THR:HG23	7:6:27:THR:O	2.12	0.50
8:A:805:G:N2	8:A:829:A:OP1	2.45	0.50
8:A:1953:A:O2'	8:A:2559:C:O2	2.30	0.50
13:F:36:ASN:OD1	13:F:37:MET:N	2.44	0.50
14:G:23:ILE:HG21	14:G:71:LEU:HD11	1.94	0.50
34:a:1014:A:OP2	52:s:17:LYS:NZ	2.31	0.50
55:v:33:U:O2'	55:v:35:A:OP2	2.17	0.50
10:C:143:VAL:HG21	10:C:161:VAL:HG11	1.94	0.50
14:G:136:ASP:HB3	14:G:139:VAL:HG22	1.93	0.50
34:a:1494:G:N7	63:a:1633:AM2:NC6	2.60	0.50
57:x:556:ILE:HD11	57:x:577:LEU:HD11	1.93	0.50
8:A:715:A:HO2'	8:A:716:A:P	2.35	0.50
3:2:39:ARG:NH2	8:A:468:G:N7	2.53	0.50
8:A:2306:C:OP2	8:A:2307:G:O2'	2.19	0.50
8:A:2640:G:H5'	17:J:96:ARG:HH12	1.77	0.50
57:x:192:TRP:NE1	57:x:275:GLN:OE1	2.41	0.50
57:x:401:ALA:HB1	57:x:402:PRO:HD2	1.93	0.50
8:A:1070:A:N6	8:A:1095:A:O2'	2.45	0.50
34:a:768:A:N3	34:a:1512:U:O2'	2.45	0.50
34:a:1366:C:O2'	43:j:62:ARG:NH2	2.44	0.50
49:p:36:VAL:O	49:p:36:VAL:HG23	2.12	0.50
57:x:505:ALA:O	57:x:511:ARG:NH2	2.45	0.50
8:A:1662:U:O2'	8:A:2687:U:OP1	2.29	0.49
9:B:14:U:OP2	9:B:70:C:O2'	2.27	0.49
10:C:68:ARG:HB3	10:C:128:THR:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:411:A:OP2	37:d:25:ARG:NH1	2.45	0.49
39:f:5:GLU:OE1	39:f:63:ASN:ND2	2.44	0.49
8:A:568:U:H1'	8:A:2030:6MZ:H9C1	1.93	0.49
8:A:1338:G:O2'	8:A:1393:A:N1	2.40	0.49
8:A:2898:U:O2	17:J:134:ALA:HB1	2.12	0.49
19:L:77:ILE:HD11	19:L:101:ILE:CG2	2.42	0.49
8:A:858:G:O2'	8:A:2268:A:O2'	2.25	0.49
8:A:1779:U:O2	8:A:1783:A:N6	2.45	0.49
18:K:107:LEU:HB2	18:K:116:ILE:HD11	1.94	0.49
21:N:59:SER:OG	21:N:62:ASN:OD1	2.28	0.49
34:a:855:U:OP1	63:a:1618:AM2:HB3	2.12	0.49
57:x:108:ALA:HB3	57:x:136:ARG:HG3	1.94	0.49
8:A:1199:U:H1'	24:Q:3:VAL:HG22	1.94	0.49
8:A:1837:C:O2'	8:A:1927:A:N3	2.41	0.49
8:A:2202:U:O2'	8:A:2204:G:OP1	2.21	0.49
20:M:17:ASN:OD1	20:M:97:GLN:NE2	2.46	0.49
20:M:53:MET:HE1	20:M:103:TYR:CD1	2.47	0.49
41:h:14:ARG:NH2	41:h:74:ILE:O	2.42	0.49
46:m:89:ARG:HH22	46:m:101:THR:HG21	1.77	0.49
46:m:95:PRO:HG2	46:m:101:THR:HG22	1.95	0.49
47:n:93:ILE:HG21	47:n:96:LEU:HD22	1.93	0.49
4:3:5:THR:HG23	4:3:61:LEU:HD23	1.95	0.49
8:A:601:C:O2'	8:A:605:G:OP1	2.28	0.49
8:A:780:G:C2'	8:A:783:A:H61	2.26	0.49
11:D:8:LYS:HB2	11:D:201:LEU:HD11	1.95	0.49
34:a:767:A:O2'	34:a:1524:C:O2	2.28	0.49
49:p:51:ARG:C	49:p:52:LEU:HD22	2.37	0.49
4:3:63:TYR:OH	8:A:592:A:O2'	2.26	0.49
8:A:745:1MG:O2'	8:A:748:G:O2'	2.29	0.49
8:A:1437:C:O2'	8:A:1516:G:O2'	1.99	0.49
44:k:62:ALA:HB1	44:k:95:THR:OG1	2.13	0.49
8:A:2512:C:O2	11:D:145:SER:OG	2.30	0.49
34:a:104:G:OP1	53:t:15:LYS:NZ	2.24	0.49
34:a:671:G:O2'	39:f:79:ARG:NH2	2.45	0.49
34:a:1081:A:OP2	38:e:51:LYS:NZ	2.41	0.49
8:A:807:U:OP2	19:L:41:ARG:NH2	2.46	0.49
8:A:2627:G:N2	8:A:2777:G:OP2	2.44	0.49
34:a:1320:C:OP1	52:s:69:LYS:NZ	2.31	0.49
7:6:11:GLU:OE2	7:6:24:ILE:N	2.46	0.49
8:A:962:G:HO2'	8:A:2496:C:HO2'	1.59	0.49
12:E:113:VAL:HG22	12:E:118:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:141:ASP:OD1	46:m:70:ARG:NH2	2.45	0.49
34:a:747:A:O2'	34:a:748:G:OP1	2.26	0.49
43:j:10:LEU:HD11	43:j:25:ILE:HD12	1.95	0.49
57:x:218:HIS:CE1	57:x:222:ILE:HD11	2.48	0.49
5:4:28:SER:O	14:G:169:ARG:NH2	2.46	0.49
8:A:488:G:O2'	26:S:49:LYS:NZ	2.28	0.49
8:A:2898:U:O2'	17:J:134:ALA:O	2.19	0.49
34:a:246:A:N1	34:a:278:G:O2'	2.44	0.49
34:a:1238:A:N7	34:a:1301:U:O4	2.46	0.49
57:x:304:THR:HG23	57:x:304:THR:O	2.12	0.49
57:x:389:ASP:O	57:x:389:ASP:OD2	2.31	0.49
8:A:563:A:OP2	25:R:79:ARG:NH1	2.41	0.48
8:A:774:G:O2'	8:A:775:G:O4'	2.30	0.48
8:A:1495:A:N3	8:A:1578:U:O2'	2.43	0.48
12:E:170:ARG:NH1	12:E:176:ASP:OD2	2.46	0.48
35:b:8:MET:SD	35:b:9:LEU:N	2.86	0.48
8:A:2653:U:O2	14:G:109:SER:OG	2.21	0.48
18:K:1:MET:N	18:K:65:THR:HG21	2.28	0.48
57:x:28:ARG:NE	57:x:271:ASN:OD1	2.45	0.48
57:x:322:LYS:O	57:x:323:ILE:HD13	2.13	0.48
8:A:201:C:O2'	8:A:251:A:N1	2.42	0.48
8:A:634:C:OP1	19:L:70:LYS:NZ	2.46	0.48
10:C:269:ARG:HE	10:C:270:ARG:H	1.61	0.48
19:L:76:GLU:HB2	19:L:111:ILE:HD13	1.96	0.48
34:a:145:G:N2	34:a:178:C:N3	2.61	0.48
34:a:1111:A:N6	36:c:175:HIS:O	2.46	0.48
37:d:162:GLU:N	37:d:162:GLU:OE1	2.47	0.48
43:j:50:THR:HG22	43:j:62:ARG:HD3	1.96	0.48
45:l:49:ARG:HB2	45:l:89:LEU:HD11	1.94	0.48
8:A:1712:U:OP2	8:A:1713:A:O2'	2.25	0.48
13:F:169:LEU:HD22	13:F:174:PHE:CZ	2.48	0.48
43:j:12:ALA:HB2	43:j:96:VAL:HG12	1.95	0.48
7:6:1:MET:HE1	13:F:94:ARG:HG3	1.95	0.48
8:A:1022:G:N2	8:A:1142:A:N1	2.61	0.48
8:A:2304:G:H22	8:A:2312:U:H3	1.62	0.48
13:F:37:MET:CE	13:F:52:ALA:HB1	2.43	0.48
14:G:120:ILE:HD13	14:G:143:VAL:HG11	1.94	0.48
35:b:40:ILE:HG21	35:b:200:PRO:O	2.13	0.48
20:M:41:LEU:HD13	20:M:96:ILE:CG1	2.44	0.48
21:N:32:GLU:OE1	21:N:115:LEU:HD12	2.14	0.48
34:a:717:U:O2'	34:a:734:G:O4'	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:b:93:HIS:ND1	35:b:145:ASN:O	2.47	0.48
37:d:104:MET:HG2	37:d:170:LEU:HD13	1.96	0.48
52:s:30:LEU:HB2	52:s:48:ILE:HG22	1.95	0.48
57:x:138:ALA:CB	57:x:263:VAL:HG12	2.43	0.48
57:x:320:ALA:HB1	57:x:333:THR:CG2	2.43	0.48
26:S:72:THR:HG21	26:S:108:SER:OG	2.14	0.48
29:V:75:GLN:HB2	29:V:92:VAL:HG23	1.94	0.48
34:a:981:U:OP1	47:n:8:ARG:NH1	2.46	0.48
52:s:55:GLN:OE1	52:s:55:GLN:N	2.46	0.48
57:x:92:VAL:O	57:x:95:THR:HG23	2.14	0.48
8:A:555:G:HO2'	8:A:556:A:P	2.37	0.48
20:M:134:THR:HG21	29:V:79:ARG:NH2	2.28	0.48
42:i:3:ASN:OD1	42:i:4:GLN:N	2.46	0.48
34:a:1526:G:OP2	54:u:41:THR:HG23	2.14	0.48
35:b:216:VAL:HA	35:b:219:THR:HG22	1.95	0.48
43:j:6:ILE:HG23	43:j:76:ILE:HB	1.95	0.48
3:2:44:VAL:HG23	3:2:44:VAL:O	2.13	0.48
8:A:1223:G:N2	8:A:1226:A:OP2	2.39	0.48
34:a:963:G:H21	43:j:57:VAL:HG21	1.77	0.48
34:a:1046:A:N6	34:a:1211:U:O2'	2.46	0.48
34:a:1217:C:OP1	47:n:8:ARG:NE	2.42	0.48
57:x:18:ILE:HD12	57:x:18:ILE:H	1.79	0.48
8:A:2167:U:N3	8:A:2170:A:OP2	2.44	0.47
57:x:529:ASN:O	57:x:529:ASN:ND2	2.37	0.47
8:A:198:C:O2'	8:A:199:A:O5'	2.32	0.47
26:S:29:VAL:HB	26:S:55:ILE:HD11	1.95	0.47
53:t:38:ILE:HD11	53:t:82:ILE:HG13	1.95	0.47
2:1:21:THR:OG1	4:3:33:THR:HG22	2.15	0.47
8:A:223:A:N1	8:A:407:G:O2'	2.41	0.47
20:M:66:ARG:NH1	20:M:104:GLU:OE2	2.46	0.47
34:a:95:C:HO2'	34:a:96:U:P	2.36	0.47
34:a:766:A:OP2	34:a:812:G:N2	2.45	0.47
8:A:2857:G:N2	8:A:2860:A:OP2	2.37	0.47
29:V:7:GLU:OE2	29:V:7:GLU:N	2.47	0.47
34:a:6:G:O6	38:e:99:SER:N	2.44	0.47
36:c:56:ILE:HG23	36:c:63:ILE:HD11	1.95	0.47
10:C:204:LEU:HB3	10:C:209:ALA:HB3	1.96	0.47
24:Q:8:ILE:HD12	24:Q:8:ILE:H	1.80	0.47
34:a:1116:U:C2	34:a:1184:G:O6	2.68	0.47
38:e:105:ILE:HB	38:e:123:LEU:HD23	1.96	0.47
2:1:7:LYS:NZ	4:3:33:THR:OG1	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:j:83:THR:O	43:j:87:LEU:HD23	2.14	0.47
8:A:49:A:OP1	8:A:50:U:O2'	2.25	0.47
8:A:1797:G:O2'	10:C:256:THR:OG1	2.28	0.47
12:E:181:ILE:CG2	19:L:3:LEU:HD13	2.45	0.47
30:W:13:GLU:O	30:W:15:LYS:NZ	2.48	0.47
34:a:255:G:OP1	50:q:70:LYS:NZ	2.48	0.47
34:a:1350:A:OP2	42:i:119:LYS:NZ	2.45	0.47
34:a:1382:C:O2'	40:g:78:ARG:NH2	2.47	0.47
36:c:72:PRO:O	36:c:76:ILE:HG22	2.14	0.47
41:h:50:VAL:HG12	41:h:50:VAL:O	2.15	0.47
57:x:86:ILE:CG2	57:x:105:LEU:HD11	2.45	0.47
5:4:3:VAL:HG21	8:A:2539:C:H5'	1.96	0.47
11:D:10:GLY:HA3	23:P:4:ILE:HD11	1.97	0.47
34:a:1067:A:N1	34:a:1108:G:O2'	2.40	0.47
48:o:38:LEU:HD23	48:o:42:PHE:CE2	2.48	0.47
8:A:1141:U:H2'	17:J:65:THR:HG21	1.97	0.47
8:A:1361:G:O2'	8:A:2215:C:O2'	1.97	0.47
22:O:51:ALA:HB3	22:O:78:VAL:HB	1.97	0.47
34:a:1524:C:OP1	44:k:121:ARG:NH2	2.48	0.47
44:k:29:THR:HG21	44:k:62:ALA:HB2	1.97	0.47
57:x:452:SER:OG	57:x:453:ASN:N	2.48	0.47
8:A:911:A:N6	20:M:11:LYS:O	2.45	0.47
8:A:2250:G:OP1	8:A:2275:C:O2'	2.27	0.47
34:a:769:G:H4'	34:a:1513:A:H4'	1.96	0.47
34:a:993:G:H2'	34:a:995:C:H41	1.78	0.47
57:x:627:THR:HG23	57:x:653:ILE:HD11	1.97	0.47
8:A:1550:C:OP1	8:A:1720:U:O2'	2.25	0.46
31:X:66:VAL:O	31:X:70:LEU:HD23	2.15	0.46
34:a:516:PSU:OP1	57:x:591:ALA:N	2.47	0.46
44:k:28:ASN:OD1	44:k:29:THR:N	2.48	0.46
8:A:30:G:O2'	8:A:1214:A:N3	2.40	0.46
44:k:66:ALA:HB2	44:k:95:THR:HG23	1.95	0.46
57:x:110:MET:HE1	57:x:126:TRP:HB2	1.97	0.46
57:x:308:ARG:NH2	57:x:315:PRO:O	2.47	0.46
14:G:151:ARG:O	14:G:161:VAL:N	2.48	0.46
8:A:142:A:O2'	27:T:1:MET:N	2.42	0.46
8:A:614:A:HO2'	8:A:615:U:P	2.34	0.46
8:A:2148:G:N2	8:A:2150:C:N3	2.63	0.46
8:A:2302:U:O2'	13:F:122:ASP:O	2.18	0.46
10:C:162:GLN:OE1	10:C:174:ARG:NH2	2.46	0.46
34:a:264:C:O2'	50:q:65:PRO:O	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:928:G:O2'	34:a:1533:C:OP1	2.34	0.46
52:s:48:ILE:HD11	52:s:70:LEU:CD2	2.45	0.46
57:x:326:ASP:OD2	57:x:329:VAL:HG12	2.15	0.46
8:A:990:A:N1	25:R:78:ARG:NH2	2.58	0.46
17:J:25:LEU:HD13	17:J:100:VAL:CG1	2.45	0.46
22:O:39:VAL:O	22:O:48:LEU:N	2.48	0.46
24:Q:49:ARG:O	24:Q:53:LYS:NZ	2.48	0.46
36:c:72:PRO:HA	36:c:75:VAL:HG12	1.98	0.46
51:r:31:TYR:HD1	51:r:44:THR:HG21	1.80	0.46
57:x:30:LEU:HD22	57:x:35:VAL:HG11	1.97	0.46
8:A:630:G:N2	8:A:633:A:OP2	2.42	0.46
13:F:122:ASP:OD1	13:F:123:GLY:N	2.48	0.46
22:O:55:GLU:OE2	22:O:81:ARG:NH2	2.49	0.46
34:a:2:A:O2'	34:a:3:A:O4'	2.29	0.46
36:c:161:ILE:HD11	59:z:8:U:C2'	2.46	0.46
38:e:40:ASP:N	38:e:40:ASP:OD1	2.49	0.46
8:A:2848:G:O2'	8:A:2849:U:O5'	2.32	0.46
53:t:34:VAL:HG21	53:t:53:MET:SD	2.56	0.46
8:A:1631:G:N1	8:A:1634:A:OP2	2.43	0.46
8:A:2898:U:O2'	17:J:136:GLN:NE2	2.47	0.46
25:R:28:ALA:HB3	25:R:31:GLU:OE1	2.16	0.46
34:a:1078:U:C2	38:e:89:THR:HG21	2.51	0.46
38:e:91:SER:OG	38:e:135:VAL:HG12	2.15	0.46
43:j:53:ILE:HG22	47:n:85:ARG:HD2	1.97	0.46
46:m:99:GLN:N	46:m:99:GLN:OE1	2.49	0.46
57:x:251:LEU:O	57:x:255:VAL:HG23	2.16	0.46
57:x:341:VAL:HG22	57:x:377:ARG:HD2	1.97	0.46
4:3:53:ASP:OD2	4:3:57:VAL:HG23	2.16	0.46
8:A:1392:A:N6	27:T:18:GLU:OE2	2.39	0.46
8:A:2312:U:H5'	13:F:84:ILE:HD11	1.96	0.46
8:A:2500:U:O2'	8:A:2504:PSU:OP1	2.32	0.46
34:a:69:G:HO2'	34:a:70:U:P	2.39	0.46
34:a:1266:G:N2	34:a:1269:A:OP2	2.38	0.46
44:k:96:ILE:HG12	44:k:109:ILE:HD12	1.98	0.46
57:x:492:THR:OG1	57:x:612:LEU:HD11	2.16	0.46
8:A:1992:G:N2	8:A:1996:C:HO2'	2.12	0.45
8:A:2532:G:N2	8:A:2663:G:O2'	2.49	0.45
19:L:77:ILE:N	19:L:109:LYS:O	2.45	0.45
34:a:530:G:O6	59:z:6:U:O2'	2.22	0.45
40:g:39:GLU:HA	40:g:42:VAL:HG12	1.97	0.45
57:x:552:VAL:HG12	57:x:552:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:105:ILE:HG22	13:F:109:ARG:HH12	1.81	0.45
20:M:33:LEU:HD13	20:M:117:PHE:HB3	1.98	0.45
20:M:35:ALA:HB2	20:M:102:LEU:HD11	1.98	0.45
34:a:974:A:O4'	47:n:71:HIS:ND1	2.50	0.45
36:c:42:LEU:HD22	36:c:67:ILE:HD11	1.97	0.45
8:A:277:G:O2'	8:A:361:G:O6	2.26	0.45
8:A:1769:U:O2'	8:A:1958:C:OP1	2.34	0.45
34:a:9:G:OP2	38:e:125:LYS:NZ	2.45	0.45
34:a:227:G:O2'	49:p:63:GLN:OE1	2.31	0.45
41:h:51:GLU:OE1	41:h:51:GLU:N	2.45	0.45
57:x:335:PHE:CE1	57:x:384:ALA:HB2	2.51	0.45
3:2:1:MET:HE2	3:2:1:MET:HA	1.98	0.45
8:A:1791:A:N6	8:A:1828:G:O2'	2.40	0.45
8:A:2627:G:O2'	8:A:2781:A:N1	2.48	0.45
35:b:95:TRP:NE1	35:b:174:GLU:OE1	2.47	0.45
43:j:8:ILE:CD1	43:j:87:LEU:HD12	2.46	0.45
8:A:2245:U:O2'	8:A:2436:G:OP2	2.34	0.45
11:D:187:LEU:CD2	11:D:203:VAL:HG11	2.46	0.45
19:L:55:MET:O	19:L:60:ARG:NH1	2.49	0.45
28:U:8:ASP:OD2	28:U:71:ILE:HG22	2.16	0.45
35:b:14:HIS:HB3	35:b:208:ALA:HB2	1.96	0.45
25:R:68:ARG:O	25:R:90:ARG:NH2	2.49	0.45
26:S:43:ALA:O	26:S:47:VAL:HG23	2.16	0.45
57:x:259:GLU:OE1	57:x:259:GLU:N	2.48	0.45
8:A:340:A:O2'	12:E:162:ARG:NH2	2.49	0.45
9:B:76:G:OP1	29:V:9:ARG:NH1	2.46	0.45
11:D:40:LEU:HD13	11:D:44:GLY:C	2.42	0.45
34:a:1012:A:N6	34:a:1018:G:O6	2.49	0.45
34:a:1279:G:O2'	34:a:1281:C:OP2	2.21	0.45
40:g:110:ARG:HH21	40:g:122:GLU:HG2	1.82	0.45
5:4:23:ILE:HD13	8:A:1032:A:H1'	1.97	0.45
8:A:2874:C:OP1	21:N:4:ARG:NH2	2.48	0.45
11:D:3:GLY:C	11:D:4:LEU:HD22	2.42	0.45
27:T:10:VAL:HG21	27:T:42:GLU:CG	2.47	0.45
34:a:578:C:O2'	34:a:728:A:N3	2.47	0.45
34:a:687:A:N7	34:a:701:U:N3	2.64	0.45
34:a:923:A:O2'	34:a:1399:C:OP2	2.29	0.45
35:b:14:HIS:NE2	35:b:212:TYR:OH	2.39	0.45
36:c:35:ASP:OD1	36:c:56:ILE:HG21	2.17	0.45
10:C:107:LYS:NZ	10:C:197:ALA:HB2	2.32	0.45
25:R:14:VAL:HG11	25:R:20:VAL:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:689:C:OP1	44:k:28:ASN:ND2	2.50	0.45
44:k:112:VAL:HG12	51:r:72:ARG:CZ	2.46	0.45
8:A:52:A:OP2	8:A:117:G:N1	2.50	0.45
8:A:476:G:N1	8:A:479:A:OP2	2.45	0.45
8:A:700:G:O2'	8:A:1632:A:N3	2.39	0.45
8:A:930:G:H1'	33:Z:24:LEU:HD21	1.99	0.45
43:j:63:ASP:OD1	43:j:64:GLN:N	2.50	0.45
43:j:64:GLN:O	47:n:99:ALA:N	2.49	0.45
44:k:45:THR:OG1	44:k:48:GLY:N	2.46	0.45
57:x:321:PHE:O	57:x:392:THR:HG23	2.17	0.45
8:A:306:U:H3	8:A:310:A:H62	1.64	0.44
8:A:807:U:O2'	8:A:2060:A:N1	2.48	0.44
10:C:87:SER:O	10:C:196:ASN:ND2	2.50	0.44
21:N:83:LEU:CD2	21:N:115:LEU:HD13	2.47	0.44
28:U:71:ILE:CD1	28:U:82:VAL:HG22	2.47	0.44
34:a:111:G:H1	34:a:330:C:H41	1.65	0.44
34:a:1368:A:OP1	42:i:112:ARG:NH2	2.49	0.44
34:a:1436:U:O4	34:a:1437:A:N6	2.50	0.44
57:x:448:THR:O	57:x:448:THR:HG23	2.17	0.44
8:A:918:A:N3	9:B:80:U:O2'	2.48	0.44
34:a:146:G:N2	34:a:177:G:N7	2.65	0.44
36:c:13:ILE:HG22	36:c:14:VAL:HG13	1.98	0.44
36:c:120:THR:HG1	36:c:186:SER:HG	1.53	0.44
43:j:52:LEU:HD23	43:j:62:ARG:HG2	1.98	0.44
57:x:312:ASP:OD2	57:x:377:ARG:NH1	2.50	0.44
57:x:460:MET:HE3	57:x:460:MET:HA	1.97	0.44
8:A:77:G:OP1	32:Y:52:ARG:NE	2.49	0.44
8:A:691:C:OP1	10:C:216:ARG:NH1	2.50	0.44
8:A:1099:G:HO2'	8:A:1100:C:P	2.39	0.44
11:D:40:LEU:HD13	11:D:44:GLY:O	2.18	0.44
34:a:955:U:O2'	52:s:82:HIS:ND1	2.44	0.44
37:d:26:ALA:O	37:d:29:THR:OG1	2.30	0.44
43:j:57:VAL:HG12	43:j:57:VAL:O	2.18	0.44
8:A:84:A:H62	8:A:101:A:H2	1.65	0.44
8:A:2723:C:P	11:D:114:LYS:HZ3	2.40	0.44
8:A:2796:U:HO2'	8:A:2797:U:P	2.41	0.44
27:T:2:ILE:HG21	27:T:42:GLU:OE2	2.18	0.44
57:x:539:ILE:HG23	57:x:539:ILE:O	2.18	0.44
12:E:127:GLU:HG2	12:E:133:LEU:HD13	1.99	0.44
12:E:184:ASP:OD1	19:L:2:ARG:NH2	2.49	0.44
34:a:309:A:O2'	34:a:607:A:N1	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:f:47:LEU:HD22	51:r:65:SER:HB2	2.00	0.44
8:A:883:G:H21	8:A:884:U:H2'	1.82	0.44
8:A:2154:A:O2'	8:A:2155:U:O5'	2.26	0.44
9:B:29:A:OP2	22:O:31:THR:HG23	2.18	0.44
9:B:31:C:C2'	9:B:53:A:H61	2.30	0.44
11:D:49:GLN:NE2	11:D:79:LEU:HD13	2.33	0.44
34:a:1124:G:N2	34:a:1125:U:O4	2.25	0.44
34:a:1211:U:O2'	34:a:1213:A:N1	2.49	0.44
49:p:21:VAL:HG13	49:p:21:VAL:O	2.18	0.44
57:x:552:VAL:HG11	57:x:577:LEU:CD2	2.48	0.44
7:6:35:ASP:OD1	7:6:35:ASP:N	2.51	0.44
17:J:27:ARG:O	17:J:30:THR:OG1	2.33	0.44
26:S:4:ILE:HG12	26:S:106:VAL:HG22	2.00	0.44
26:S:20:VAL:HG11	26:S:44:ALA:HA	1.99	0.44
34:a:1498:UR3:O2'	59:z:2:U:OP1	2.31	0.44
37:d:60:VAL:HG21	37:d:199:ILE:HD11	1.99	0.44
38:e:45:VAL:HG23	38:e:116:VAL:HG23	1.98	0.44
54:u:27:VAL:HG23	54:u:28:LEU:HD22	1.99	0.44
19:L:91:ASP:HB2	19:L:94:THR:HG23	2.00	0.44
19:L:91:ASP:N	19:L:94:THR:OG1	2.46	0.44
34:a:51:A:HO2'	34:a:116:A:C1'	2.30	0.44
34:a:1316:G:H22	34:a:1319:A:H5'	1.83	0.44
35:b:96:LEU:H	35:b:99:MET:HE3	1.83	0.44
40:g:48:THR:HG22	40:g:52:ARG:HD3	2.00	0.44
52:s:10:ILE:HG21	52:s:15:LEU:HD21	1.98	0.44
57:x:362:ILE:HG21	57:x:376:VAL:CG2	2.47	0.44
8:A:2548:U:O2	18:K:23:LYS:NZ	2.50	0.44
18:K:3:GLN:O	18:K:6:THR:OG1	2.30	0.44
28:U:96:LYS:O	28:U:97:SER:OG	2.29	0.44
34:a:1118:U:O3'	42:i:84:ARG:NH2	2.51	0.44
8:A:1047:G:O2'	8:A:1110:G:N1	2.50	0.43
23:P:26:GLU:OE2	23:P:41:ALA:HB1	2.18	0.43
34:a:177:G:OP2	34:a:177:G:N2	2.45	0.43
37:d:74:TYR:OH	37:d:96:ARG:NH1	2.46	0.43
50:q:24:ILE:CD1	50:q:43:LEU:HD12	2.48	0.43
57:x:83:ILE:HD11	57:x:282:ILE:HD11	1.99	0.43
57:x:465:LEU:O	57:x:469:VAL:HG23	2.17	0.43
1:0:3:GLN:O	8:A:2016:U:O2'	2.36	0.43
7:6:57:VAL:O	7:6:61:ASN:N	2.48	0.43
8:A:820:A:H4'	8:A:836:G:H22	1.83	0.43
8:A:1099:G:O2'	8:A:1100:C:OP1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:123:ILE:O	10:C:123:ILE:HG22	2.17	0.43
15:H:40:THR:HG22	15:H:43:ASN:OD1	2.18	0.43
20:M:77:PRO:O	20:M:80:VAL:HG12	2.18	0.43
34:a:62:U:OP1	34:a:385:C:O2'	2.36	0.43
41:h:10:LEU:HD12	41:h:76:ARG:HB2	2.00	0.43
57:x:137:ILE:HD11	57:x:281:VAL:HG22	2.00	0.43
8:A:2066:C:H2'	8:A:2067:G:H5'	1.99	0.43
8:A:2683:C:O2	18:K:70:ARG:NH2	2.51	0.43
10:C:153:LEU:HD12	10:C:175:LEU:HD22	2.01	0.43
12:E:12:LEU:HD23	12:E:193:VAL:HG11	2.00	0.43
45:l:53:ARG:HE	45:l:61:GLU:HG3	1.84	0.43
52:s:52:ASN:ND2	52:s:75:PRO:O	2.48	0.43
8:A:1294:U:O2	21:N:23:ASN:ND2	2.51	0.43
8:A:1614:A:C2	26:S:93:ALA:HB2	2.53	0.43
8:A:2271:G:OP1	30:W:14:ALA:HB1	2.18	0.43
34:a:1006:G:N2	34:a:1007:U:O4	2.51	0.43
52:s:10:ILE:HD13	52:s:15:LEU:CD2	2.48	0.43
8:A:48:G:N1	8:A:177:G:OP2	2.50	0.43
8:A:704:G:H2'	8:A:726:G:H22	1.83	0.43
8:A:966:G:O4'	8:A:2267:A:N6	2.51	0.43
8:A:2139:U:O4	8:A:2152:G:O6	2.36	0.43
36:c:5:HIS:HB3	47:n:89:MET:HE3	2.00	0.43
37:d:88:ASN:O	37:d:92:LEU:HD13	2.18	0.43
38:e:37:VAL:HG11	38:e:113:VAL:HG22	2.01	0.43
20:M:40:ARG:C	20:M:41:LEU:HD12	2.44	0.43
21:N:37:THR:HG22	21:N:39:PRO:HD2	2.01	0.43
54:u:38:GLU:CD	54:u:42:THR:HG1	2.25	0.43
7:6:50:ASP:OD1	7:6:51:VAL:N	2.51	0.43
17:J:4:PHE:HB3	24:Q:99:VAL:HG21	2.00	0.43
18:K:65:THR:HG22	18:K:67:LYS:H	1.83	0.43
34:a:1209:C:O2'	34:a:1214:C:N4	2.48	0.43
36:c:46:LEU:HB3	36:c:49:ALA:HB3	2.00	0.43
43:j:24:GLU:OE2	43:j:90:LEU:HD21	2.18	0.43
8:A:2577:A:O4'	8:A:2612:C:N4	2.52	0.43
22:O:31:THR:O	22:O:102:ARG:NH1	2.47	0.43
34:a:950:U:OP2	46:m:100:ARG:NE	2.52	0.43
44:k:92:ARG:NH2	44:k:111:ASP:OD2	2.52	0.43
57:x:83:ILE:HG22	57:x:85:ILE:HG23	2.01	0.43
4:3:3:ILE:HD11	8:A:592:A:H2	1.82	0.43
8:A:675:A:N3	8:A:2443:C:O2'	2.47	0.43
8:A:1187:G:N2	8:A:1188:U:O4	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:946:A:O2'	34:a:1333:A:N3	2.47	0.43
34:a:1497:G:H21	34:a:1519:MA6:C2	2.30	0.43
47:n:30:ILE:HD12	47:n:45:VAL:HG23	2.01	0.43
8:A:301:G:OP2	28:U:81:ARG:NH2	2.52	0.43
8:A:1807:G:N2	8:A:1810:A:OP2	2.49	0.43
8:A:2047:C:O2'	8:A:2823:A:N1	2.50	0.43
20:M:53:MET:HG3	20:M:120:ALA:HB2	2.01	0.43
40:g:96:ASN:HB3	40:g:100:MET:HE1	2.01	0.43
8:A:491:G:O6	26:S:49:LYS:NZ	2.45	0.42
8:A:538:A:O2'	17:J:9:GLU:OE1	2.37	0.42
8:A:580:U:O3'	24:Q:30:VAL:HG13	2.19	0.42
33:Z:50:VAL:O	33:Z:54:VAL:HG22	2.19	0.42
34:a:517:G:HO2'	34:a:531:U:H5	1.64	0.42
40:g:110:ARG:NH2	40:g:118:ARG:O	2.51	0.42
50:q:59:GLU:OE1	50:q:76:ARG:NE	2.52	0.42
55:v:32:C:N4	55:v:33:U:O4	2.52	0.42
3:2:30:VAL:HG22	3:2:33:ARG:NH2	2.34	0.42
8:A:1365:A:OP1	31:X:27:ARG:NH2	2.49	0.42
11:D:48:ILE:HG23	11:D:84:LEU:HD21	2.01	0.42
17:J:93:ILE:HD11	17:J:100:VAL:HG21	2.00	0.42
34:a:664:G:H22	34:a:741:G:H1	1.67	0.42
34:a:1279:G:O2'	34:a:1282:C:N4	2.52	0.42
57:x:74:MET:HE2	57:x:279:ASP:OD2	2.19	0.42
7:6:34:LEU:HD13	13:F:105:ILE:HG23	2.02	0.42
8:A:83:A:OP1	28:U:1:ALA:HB2	2.18	0.42
8:A:188:G:O2'	8:A:1365:A:N6	2.52	0.42
10:C:137:GLY:N	10:C:163:ILE:O	2.48	0.42
34:a:958:A:N6	52:s:76:THR:O	2.52	0.42
47:n:52:PRO:O	47:n:55:SER:OG	2.34	0.42
57:x:548:TYR:O	57:x:552:VAL:HG23	2.19	0.42
8:A:189:G:P	31:X:13:THR:HG21	2.60	0.42
8:A:1671:U:O2'	8:A:1673:G:N7	2.41	0.42
12:E:157:LEU:HG	12:E:169:VAL:HG21	2.01	0.42
34:a:54:C:OP1	34:a:351:G:N2	2.46	0.42
42:i:40:ARG:HH12	42:i:71:ILE:HG21	1.82	0.42
57:x:29:ILE:HD11	57:x:277:MET:HE1	2.00	0.42
3:2:30:VAL:HG22	3:2:33:ARG:HH22	1.84	0.42
8:A:1386:C:H2'	8:A:1387:A:C8	2.54	0.42
13:F:32:LYS:HD2	13:F:89:THR:HG23	2.02	0.42
25:R:4:VAL:O	25:R:39:LEU:N	2.48	0.42
34:a:738:C:OP1	39:f:2:ARG:NH1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:q:6:THR:C	50:q:7:LEU:HD12	2.44	0.42
57:x:86:ILE:HG21	57:x:105:LEU:HD11	2.01	0.42
8:A:2821:A:O2'	8:A:2826:A:N1	2.52	0.42
10:C:105:ALA:O	10:C:195:GLY:N	2.44	0.42
15:H:12:LEU:CD1	15:H:19:VAL:HG11	2.49	0.42
26:S:71:VAL:HA	26:S:107:VAL:HG12	2.01	0.42
35:b:14:HIS:CD2	35:b:212:TYR:HH	2.35	0.42
8:A:291:G:O6	8:A:349:U:C2	2.73	0.42
8:A:1372:U:O2'	8:A:2212:A:N3	2.46	0.42
8:A:1604:C:O2'	8:A:1610:A:N1	2.34	0.42
8:A:1996:C:N4	18:K:32:TYR:OH	2.51	0.42
8:A:2123:G:N2	8:A:2175:C:H41	2.17	0.42
8:A:2394:C:O2	55:v:76:A:O3'	2.38	0.42
18:K:25:LEU:HD11	18:K:40:LYS:HB2	2.01	0.42
35:b:185:ILE:HD13	35:b:199:ILE:HB	2.01	0.42
37:d:167:PRO:HB2	37:d:170:LEU:HD12	2.02	0.42
42:i:29:ILE:N	42:i:32:ARG:O	2.44	0.42
46:m:4:ALA:HB2	46:m:59:VAL:HG11	2.02	0.42
55:v:26:G:H22	55:v:44:A:H2	1.67	0.42
5:4:16:ILE:HD13	5:4:25:VAL:HG22	2.01	0.42
8:A:2839:G:O6	8:A:2878:U:O2	2.37	0.42
12:E:196:VAL:HG13	12:E:200:LEU:HD13	2.02	0.42
35:b:114:LYS:O	35:b:118:THR:HG23	2.20	0.42
39:f:37:HIS:N	39:f:63:ASN:O	2.52	0.42
39:f:97:THR:O	39:f:97:THR:HG23	2.20	0.42
7:6:28:VAL:HG12	13:F:139:GLU:HA	2.02	0.42
13:F:31:GLU:OE1	13:F:158:THR:HG22	2.20	0.42
18:K:1:MET:H2	18:K:65:THR:HG21	1.84	0.42
31:X:5:GLN:O	31:X:70:LEU:HD11	2.20	0.42
33:Z:4:ILE:HG22	33:Z:58:GLU:HA	2.01	0.42
48:o:42:PHE:CD2	48:o:55:LEU:HD22	2.55	0.42
57:x:185:VAL:HG13	57:x:221:LEU:HD21	2.01	0.42
5:4:3:VAL:HG12	5:4:36:ARG:HD2	2.02	0.42
6:5:78:GLY:O	6:5:80:THR:N	2.52	0.42
8:A:1426:G:O2'	8:A:1572:A:N6	2.53	0.42
8:A:1490:A:HO2'	8:A:1491:G:P	2.39	0.42
10:C:90:ILE:HD12	10:C:102:TYR:CD1	2.55	0.42
19:L:19:LEU:HD22	19:L:27:LEU:HD12	2.02	0.42
20:M:53:MET:O	20:M:57:VAL:HG12	2.19	0.42
29:V:86:LEU:HD13	29:V:89:ILE:HD11	2.02	0.42
34:a:185:U:O2	53:t:75:LYS:NZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:951:G:OP2	46:m:100:ARG:NH2	2.53	0.42
39:f:29:ILE:HD13	39:f:64:VAL:HG11	2.01	0.42
4:3:32:LEU:HD12	4:3:40:LYS:CD	2.47	0.41
8:A:851:C:O2'	33:Z:42:ALA:O	2.37	0.41
57:x:498:THR:HG22	57:x:499:ASP:N	2.33	0.41
8:A:1445:G:O6	8:A:1466:U:O2	2.38	0.41
8:A:2320:U:O2'	8:A:2322:A:N7	2.44	0.41
20:M:63:ILE:HD13	20:M:105:MET:HB3	2.02	0.41
41:h:102:VAL:O	41:h:125:ILE:N	2.53	0.41
50:q:68:LYS:HG3	50:q:69:THR:HG23	2.02	0.41
2:1:24:LYS:NZ	2:1:31:GLU:O	2.35	0.41
8:A:1452:G:N2	8:A:1452:G:OP2	2.53	0.41
8:A:1816:C:H41	10:C:34:GLU:CD	2.28	0.41
34:a:130:A:O2'	34:a:131:A:O5'	2.27	0.41
42:i:11:ARG:NH1	42:i:106:ASP:OD2	2.53	0.41
45:l:42:LYS:N	45:l:88:ASP:O	2.52	0.41
8:A:75:G:H22	8:A:111:A:H2	1.68	0.41
8:A:2450:A:N6	8:A:2501:C:O2	2.54	0.41
34:a:1399:C:O2	34:a:1502:A:N6	2.53	0.41
43:j:91:ASP:OD1	43:j:91:ASP:N	2.52	0.41
8:A:972:A:OP2	8:A:973:A:O2'	2.35	0.41
8:A:2379:G:H4'	22:O:21:LEU:HD11	2.01	0.41
17:J:84:ILE:HG23	17:J:84:ILE:O	2.19	0.41
27:T:54:GLU:OE1	27:T:54:GLU:N	2.53	0.41
34:a:765:G:N1	34:a:812:G:O2'	2.42	0.41
35:b:63:LYS:HD2	35:b:63:LYS:O	2.20	0.41
36:c:120:THR:OG1	36:c:186:SER:OG	2.11	0.41
57:x:491:GLU:HB2	57:x:570:VAL:HG13	2.01	0.41
57:x:556:ILE:HD13	57:x:575:ILE:HG21	2.01	0.41
8:A:1666:G:O2'	18:K:3:GLN:NE2	2.53	0.41
8:A:1730:C:O2'	8:A:1731:G:O5'	2.36	0.41
34:a:77:A:O2'	34:a:78:A:OP1	2.34	0.41
34:a:1277:C:O2	34:a:1279:G:N2	2.53	0.41
41:h:94:VAL:HG21	41:h:100:ILE:O	2.20	0.41
8:A:18:U:O2'	8:A:554:U:OP1	2.27	0.41
8:A:27:G:O2'	8:A:28:A:OP2	2.28	0.41
8:A:138:U:O2'	8:A:141:G:O6	2.20	0.41
8:A:220:G:O2'	8:A:233:A:N3	2.52	0.41
8:A:645:C:H2'	8:A:647:G:C8	2.55	0.41
8:A:1093:G:HO2'	8:A:1094:U:P	2.31	0.41
10:C:131:MET:CE	10:C:173:LEU:HD21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:135:ILE:HD12	13:F:142:TYR:HD1	1.85	0.41
15:H:80:ILE:HD13	15:H:102:ALA:CB	2.51	0.41
23:P:21:PRO:HD3	23:P:49:ILE:HD12	2.03	0.41
27:T:67:VAL:HG12	27:T:74:ILE:HD11	2.02	0.41
34:a:1056:U:H4'	36:c:162:ALA:HB2	2.01	0.41
34:a:1523:G:OP1	44:k:127:ARG:NH2	2.54	0.41
38:e:133:ILE:H	38:e:133:ILE:HD12	1.84	0.41
57:x:558:GLU:OE2	57:x:559:GLN:NE2	2.53	0.41
12:E:181:ILE:HG23	19:L:3:LEU:HD13	2.02	0.41
36:c:18:ASN:O	36:c:39:ARG:NH2	2.46	0.41
39:f:98:GLU:OE1	39:f:98:GLU:N	2.53	0.41
41:h:105:THR:HG22	41:h:121:GLY:O	2.20	0.41
56:w:32:PSU:O2'	56:w:37:MIA:H161	2.21	0.41
57:x:102:MET:HE1	57:x:108:ALA:HB2	2.01	0.41
1:0:30:ASP:O	1:0:34:GLY:HA2	2.20	0.41
8:A:1100:C:N4	8:A:1101:U:O2	2.54	0.41
8:A:1800:C:OP2	10:C:181:ARG:NH2	2.53	0.41
8:A:2331:G:O2'	8:A:2336:A:N1	2.53	0.41
10:C:2:VAL:HG21	10:C:201:LEU:HD12	2.01	0.41
14:G:126:THR:OG1	14:G:127:GLN:N	2.53	0.41
17:J:96:ARG:NE	17:J:99:ARG:HG3	2.35	0.41
34:a:587:G:OP1	41:h:83:ARG:NH2	2.50	0.41
34:a:1091:U:O2'	34:a:1093:A:N7	2.25	0.41
41:h:53:ASP:OD1	41:h:53:ASP:N	2.52	0.41
46:m:21:ILE:HG23	46:m:65:GLU:OE2	2.21	0.41
47:n:46:LEU:HD13	52:s:12:LEU:HD13	2.02	0.41
51:r:31:TYR:CD1	51:r:44:THR:HG21	2.56	0.41
57:x:553:ASP:OD1	57:x:554:LYS:N	2.52	0.41
57:x:620:VAL:HG12	57:x:679:TYR:HB3	2.02	0.41
21:N:83:LEU:HD21	21:N:115:LEU:HD13	2.02	0.41
26:S:6:LYS:HG2	26:S:104:THR:HG23	2.03	0.41
34:a:1003:G:O3'	34:a:1024:G:N1	2.54	0.41
41:h:27:PRO:O	41:h:32:LYS:NZ	2.47	0.41
4:3:29:ARG:NH2	19:L:63:LYS:O	2.53	0.40
8:A:1066:U:O2'	8:A:1068:G:OP2	2.28	0.40
17:J:96:ARG:HE	17:J:99:ARG:HG3	1.85	0.40
57:x:26:THR:HG21	57:x:49:MET:HG3	2.02	0.40
8:A:1378:A:O2'	8:A:1380:G:N7	2.48	0.40
8:A:1682:G:OP2	8:A:1699:G:N2	2.54	0.40
8:A:1900:A:H1'	8:A:1970:A:H2'	2.03	0.40
8:A:2117:A:H61	8:A:2166:U:H3	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:49:VAL:HG21	22:O:81:ARG:HB3	2.03	0.40
34:a:697:U:O2'	34:a:785:G:O2'	2.35	0.40
35:b:53:LEU:HA	35:b:56:LEU:HD12	2.04	0.40
35:b:126:ASP:OD1	35:b:126:ASP:N	2.54	0.40
8:A:2050:C:H2'	8:A:2051:A:O4'	2.20	0.40
22:O:7:ARG:NH1	22:O:95:SER:O	2.48	0.40
34:a:77:A:HO2'	34:a:78:A:P	2.43	0.40
35:b:206:ILE:O	35:b:210:THR:HG23	2.21	0.40
36:c:116:ALA:O	36:c:120:THR:OG1	2.26	0.40
37:d:137:SER:N	37:d:140:ASP:OD2	2.51	0.40
57:x:93:ASP:OD1	57:x:670:ARG:NH1	2.54	0.40
8:A:2505:G:HO2'	8:A:2506:U:P	2.43	0.40
20:M:136:MET:HE1	29:V:77:VAL:HG22	2.02	0.40
23:P:90:ALA:N	23:P:110:LYS:O	2.52	0.40
34:a:1157:A:N7	34:a:1180:A:N6	2.69	0.40
34:a:1315:U:H2'	34:a:1316:G:O4'	2.22	0.40
39:f:38:ARG:NH1	39:f:99:ALA:O	2.55	0.40
53:t:30:PHE:O	53:t:34:VAL:HG23	2.21	0.40
2:1:4:ILE:N	8:A:2284:A:OP1	2.54	0.40
8:A:111:A:O2'	32:Y:58:ASN:ND2	2.45	0.40
8:A:1812:U:O4'	10:C:44:ASN:ND2	2.54	0.40
8:A:1929:G:OP2	8:A:1929:G:N2	2.44	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
2	1	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
3	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	3	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
5	4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
6	5	129/165 (78%)	106 (82%)	23 (18%)	0	100	100
7	6	64/70 (91%)	55 (86%)	9 (14%)	0	100	100
10	C	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
11	D	207/209 (99%)	195 (94%)	12 (6%)	0	100	100
12	E	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
13	F	175/179 (98%)	161 (92%)	14 (8%)	0	100	100
14	G	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
15	H	147/149 (99%)	137 (93%)	10 (7%)	0	100	100
16	I	139/142 (98%)	125 (90%)	14 (10%)	0	100	100
17	J	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
18	K	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
19	L	141/144 (98%)	131 (93%)	10 (7%)	0	100	100
20	M	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
21	N	118/127 (93%)	113 (96%)	5 (4%)	0	100	100
22	O	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
23	P	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
24	Q	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
25	R	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
26	S	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
27	T	91/100 (91%)	85 (93%)	6 (7%)	0	100	100
28	U	100/104 (96%)	95 (95%)	5 (5%)	0	100	100
29	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
30	W	73/85 (86%)	73 (100%)	0	0	100	100
31	X	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
32	Y	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
33	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
35	b	216/240 (90%)	199 (92%)	17 (8%)	0	100	100
36	c	204/233 (88%)	199 (98%)	5 (2%)	0	100	100
37	d	203/206 (98%)	193 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	e	155/167 (93%)	151 (97%)	4 (3%)	0	100	100
39	f	98/135 (73%)	87 (89%)	11 (11%)	0	100	100
40	g	149/179 (83%)	138 (93%)	11 (7%)	0	100	100
41	h	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
42	i	125/130 (96%)	111 (89%)	14 (11%)	0	100	100
43	j	96/103 (93%)	88 (92%)	8 (8%)	0	100	100
44	k	114/129 (88%)	108 (95%)	6 (5%)	0	100	100
45	l	121/124 (98%)	111 (92%)	10 (8%)	0	100	100
46	m	112/118 (95%)	102 (91%)	10 (9%)	0	100	100
47	n	99/102 (97%)	93 (94%)	6 (6%)	0	100	100
48	o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
49	p	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
50	q	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
51	r	63/75 (84%)	61 (97%)	2 (3%)	0	100	100
52	s	80/92 (87%)	71 (89%)	9 (11%)	0	100	100
53	t	83/87 (95%)	79 (95%)	4 (5%)	0	100	100
54	u	63/71 (89%)	61 (97%)	2 (3%)	0	100	100
57	x	701/704 (100%)	652 (93%)	49 (7%)	0	100	100
All	All	6551/6924 (95%)	6175 (94%)	376 (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%)	47 (100%)	0	100	100
2	1	45/49 (92%)	45 (100%)	0	100	100
3	2	38/38 (100%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3	51/52 (98%)	51 (100%)	0	100	100
5	4	34/34 (100%)	34 (100%)	0	100	100
7	6	59/62 (95%)	59 (100%)	0	100	100
10	C	216/218 (99%)	216 (100%)	0	100	100
11	D	164/164 (100%)	164 (100%)	0	100	100
12	E	165/165 (100%)	165 (100%)	0	100	100
13	F	148/150 (99%)	148 (100%)	0	100	100
14	G	137/138 (99%)	137 (100%)	0	100	100
15	H	114/114 (100%)	114 (100%)	0	100	100
17	J	116/116 (100%)	116 (100%)	0	100	100
18	K	103/104 (99%)	103 (100%)	0	100	100
19	L	102/103 (99%)	102 (100%)	0	100	100
20	M	109/109 (100%)	109 (100%)	0	100	100
21	N	100/103 (97%)	100 (100%)	0	100	100
22	O	86/87 (99%)	86 (100%)	0	100	100
23	P	99/100 (99%)	99 (100%)	0	100	100
24	Q	89/90 (99%)	89 (100%)	0	100	100
25	R	84/84 (100%)	84 (100%)	0	100	100
26	S	93/93 (100%)	93 (100%)	0	100	100
27	T	80/84 (95%)	80 (100%)	0	100	100
28	U	83/85 (98%)	83 (100%)	0	100	100
29	V	78/78 (100%)	78 (100%)	0	100	100
30	W	57/63 (90%)	57 (100%)	0	100	100
31	X	67/68 (98%)	67 (100%)	0	100	100
32	Y	55/55 (100%)	55 (100%)	0	100	100
33	Z	48/49 (98%)	48 (100%)	0	100	100
35	b	180/198 (91%)	180 (100%)	0	100	100
36	c	170/190 (90%)	170 (100%)	0	100	100
37	d	172/173 (99%)	171 (99%)	1 (1%)	84	93
38	e	114/126 (90%)	114 (100%)	0	100	100
39	f	87/116 (75%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	g	124/147 (84%)	124 (100%)	0	100	100
41	h	104/105 (99%)	104 (100%)	0	100	100
42	i	105/107 (98%)	105 (100%)	0	100	100
43	j	86/90 (96%)	86 (100%)	0	100	100
44	k	89/99 (90%)	89 (100%)	0	100	100
45	l	103/104 (99%)	103 (100%)	0	100	100
46	m	92/96 (96%)	92 (100%)	0	100	100
47	n	79/84 (94%)	79 (100%)	0	100	100
48	o	76/77 (99%)	76 (100%)	0	100	100
49	p	65/65 (100%)	65 (100%)	0	100	100
50	q	74/78 (95%)	74 (100%)	0	100	100
51	r	56/65 (86%)	56 (100%)	0	100	100
52	s	72/79 (91%)	72 (100%)	0	100	100
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%)	576 (100%)	1 (0%)	92	97
58	y	1/1 (100%)	1 (100%)	0	100	100
All	All	5204/5408 (96%)	5202 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
37	d	139	ASN
57	x	529	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	42	HIS
11	D	42	ASN
13	F	51	ASN
14	G	19	ASN
14	G	29	ASN
14	G	87	GLN
23	P	55	HIS

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Mol	Chain	Res	Type
25	R	86	GLN
36	c	99	GLN
37	d	58	GLN
37	d	88	ASN
38	e	88	HIS
39	f	17	GLN
40	g	96	ASN
45	l	95	HIS
53	t	60	GLN
57	x	350	ASN
57	x	454	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	a	1539/1542 (99%)	295 (19%)	0
55	v	74/77 (96%)	12 (16%)	0
56	w	75/76 (98%)	22 (29%)	0
59	z	10/33 (30%)	1 (10%)	0
8	A	2902/2903 (99%)	560 (19%)	38 (1%)
9	B	119/120 (99%)	19 (15%)	3 (2%)
All	All	4719/4751 (99%)	909 (19%)	41 (0%)

All (909) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	10	A
8	A	15	G
8	A	34	U
8	A	42	A
8	A	43	G
8	A	44	A
8	A	46	G
8	A	62	U
8	A	63	A
8	A	71	A
8	A	74	A
8	A	75	G
8	A	101	A
8	A	103	A
8	A	118	A

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Mol	Chain	Res	Type
8	A	120	U
8	A	131	A
8	A	141	G
8	A	142	A
8	A	149	A
8	A	160	A
8	A	162	U
8	A	163	C
8	A	170	U
8	A	196	A
8	A	199	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	248	G
8	A	250	G
8	A	255	A
8	A	265	A
8	A	266	G
8	A	272	A
8	A	275	C
8	A	276	U
8	A	278	A
8	A	279	A
8	A	291	G
8	A	311	A
8	A	330	A
8	A	345	A
8	A	346	A
8	A	361	G
8	A	362	A
8	A	371	A
8	A	372	G
8	A	373	U
8	A	377	G

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Mol	Chain	Res	Type
8	A	386	G
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	429	A
8	A	455	C
8	A	457	A
8	A	458	G
8	A	459	U
8	A	480	A
8	A	481	G
8	A	482	A
8	A	491	G
8	A	504	A
8	A	505	A
8	A	506	G
8	A	509	C
8	A	510	C
8	A	513	A
8	A	529	A
8	A	531	C
8	A	532	A
8	A	545	U
8	A	546	U
8	A	547	A
8	A	548	G
8	A	556	A
8	A	563	A
8	A	568	U
8	A	572	A
8	A	573	U
8	A	575	A
8	A	603	A
8	A	613	A
8	A	614	A
8	A	615	U
8	A	622	G

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Mol	Chain	Res	Type
8	A	627	A
8	A	637	A
8	A	647	G
8	A	654	A
8	A	655	A
8	A	669	G
8	A	670	A
8	A	677	A
8	A	682	G
8	A	685	A
8	A	686	U
8	A	704	G
8	A	712	G
8	A	714	U
8	A	716	A
8	A	717	C
8	A	729	G
8	A	730	A
8	A	747	5MC
8	A	764	A
8	A	775	G
8	A	776	G
8	A	782	A
8	A	783	A
8	A	784	G
8	A	785	G
8	A	805	G
8	A	812	C
8	A	819	A
8	A	827	U
8	A	828	U
8	A	846	U
8	A	847	U
8	A	858	G
8	A	859	G
8	A	869	G
8	A	877	A
8	A	878	A
8	A	879	G
8	A	881	G
8	A	884	U
8	A	885	C

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Mol	Chain	Res	Type
8	A	886	A
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	895	U
8	A	896	A
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	941	A
8	A	946	C
8	A	953	G
8	A	961	C
8	A	972	A
8	A	973	A
8	A	974	G
8	A	975	A
8	A	983	A
8	A	995	C
8	A	996	A
8	A	1005	C
8	A	1012	U
8	A	1013	C
8	A	1021	A
8	A	1026	G
8	A	1028	A
8	A	1033	U
8	A	1041	G
8	A	1046	A
8	A	1047	G
8	A	1048	A
8	A	1052	C
8	A	1053	C
8	A	1055	G
8	A	1056	G
8	A	1057	A

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Mol	Chain	Res	Type
8	A	1058	U
8	A	1059	G
8	A	1060	U
8	A	1061	U
8	A	1063	G
8	A	1064	C
8	A	1065	U
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	1076	C
8	A	1077	A
8	A	1078	U
8	A	1079	C
8	A	1080	A
8	A	1081	U
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	1090	A
8	A	1091	G
8	A	1094	U
8	A	1095	A
8	A	1096	A
8	A	1097	U
8	A	1099	G
8	A	1100	C
8	A	1101	U
8	A	1102	C
8	A	1103	A
8	A	1105	U
8	A	1109	C
8	A	1110	G
8	A	1111	A

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Mol	Chain	Res	Type
8	A	1112	G
8	A	1115	G
8	A	1116	G
8	A	1130	U
8	A	1132	U
8	A	1135	C
8	A	1136	G
8	A	1139	G
8	A	1143	A
8	A	1155	A
8	A	1168	G
8	A	1169	A
8	A	1171	G
8	A	1173	U
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	1206	G
8	A	1212	G
8	A	1225	G
8	A	1227	G
8	A	1236	G
8	A	1247	A
8	A	1250	G
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	1306	C
8	A	1329	U
8	A	1334	G
8	A	1340	U
8	A	1352	U

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Mol	Chain	Res	Type
8	A	1359	A
8	A	1360	G
8	A	1365	A
8	A	1368	G
8	A	1378	A
8	A	1379	U
8	A	1383	A
8	A	1386	C
8	A	1387	A
8	A	1395	A
8	A	1415	U
8	A	1416	G
8	A	1417	C
8	A	1420	A
8	A	1421	G
8	A	1428	C
8	A	1429	G
8	A	1432	G
8	A	1452	G
8	A	1453	A
8	A	1460	U
8	A	1461	C
8	A	1474	U
8	A	1478	G
8	A	1482	G
8	A	1490	A
8	A	1491	G
8	A	1493	C
8	A	1494	A
8	A	1497	U
8	A	1509	A
8	A	1515	A
8	A	1524	G
8	A	1532	A
8	A	1534	U
8	A	1536	C
8	A	1539	U
8	A	1554	U
8	A	1557	C
8	A	1558	C
8	A	1563	U
8	A	1566	A

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Mol	Chain	Res	Type
8	A	1569	A
8	A	1578	U
8	A	1584	U
8	A	1585	C
8	A	1591	A
8	A	1608	A
8	A	1610	A
8	A	1626	A
8	A	1634	A
8	A	1635	A
8	A	1646	C
8	A	1647	U
8	A	1648	U
8	A	1649	G
8	A	1651	G
8	A	1674	G
8	A	1693	U
8	A	1715	G
8	A	1716	U
8	A	1726	C
8	A	1729	U
8	A	1730	C
8	A	1731	G
8	A	1732	C
8	A	1738	G
8	A	1744	A
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
8	A	1809	A
8	A	1816	C
8	A	1829	A
8	A	1857	G
8	A	1869	G
8	A	1884	G
8	A	1901	A

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Mol	Chain	Res	Type
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	1925	C
8	A	1926	U
8	A	1927	A
8	A	1930	G
8	A	1937	A
8	A	1939	5MU
8	A	1955	U
8	A	1964	G
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
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	2055	C
8	A	2056	G
8	A	2060	A
8	A	2061	G
8	A	2062	A
8	A	2069	G7M
8	A	2093	G
8	A	2101	A
8	A	2102	G

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Mol	Chain	Res	Type
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	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
8	A	2137	U
8	A	2138	G
8	A	2139	U
8	A	2140	G
8	A	2143	C
8	A	2145	C
8	A	2146	C
8	A	2148	G
8	A	2149	U
8	A	2150	C
8	A	2151	U
8	A	2153	C
8	A	2155	U
8	A	2157	G
8	A	2159	G
8	A	2161	C
8	A	2162	G
8	A	2164	C
8	A	2169	A
8	A	2170	A
8	A	2171	A

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Mol	Chain	Res	Type
8	A	2172	U
8	A	2173	A
8	A	2174	C
8	A	2175	C
8	A	2176	A
8	A	2180	U
8	A	2183	A
8	A	2184	A
8	A	2186	G
8	A	2190	G
8	A	2193	G
8	A	2204	G
8	A	2211	A
8	A	2225	A
8	A	2226	C
8	A	2238	G
8	A	2239	G
8	A	2279	G
8	A	2283	C
8	A	2287	A
8	A	2288	A
8	A	2297	A
8	A	2305	U
8	A	2309	A
8	A	2312	U
8	A	2320	U
8	A	2325	G
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	2361	G
8	A	2383	G
8	A	2385	C
8	A	2402	U
8	A	2406	A
8	A	2410	G
8	A	2419	U
8	A	2423	U
8	A	2425	A

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Mol	Chain	Res	Type
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
8	A	2476	A
8	A	2478	A
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	2504	PSU
8	A	2505	G
8	A	2506	U
8	A	2518	A
8	A	2535	G
8	A	2547	A
8	A	2554	U
8	A	2566	A
8	A	2567	G
8	A	2572	A
8	A	2576	G
8	A	2578	G
8	A	2585	U
8	A	2602	A
8	A	2608	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	2636	C
8	A	2646	C

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Mol	Chain	Res	Type
8	A	2655	G
8	A	2656	U
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	2714	G
8	A	2718	G
8	A	2726	A
8	A	2727	A
8	A	2729	G
8	A	2733	A
8	A	2744	G
8	A	2748	A
8	A	2751	G
8	A	2752	C
8	A	2755	C
8	A	2765	A
8	A	2769	U
8	A	2778	A
8	A	2779	U
8	A	2790	U
8	A	2797	U
8	A	2798	U
8	A	2799	A
8	A	2800	A
8	A	2808	G
8	A	2809	A
8	A	2818	U
8	A	2820	A
8	A	2821	A
8	A	2849	U
8	A	2867	G
8	A	2872	A
8	A	2879	A
8	A	2884	U
8	A	2886	A
8	A	2893	A
8	A	2899	A
9	B	18	G

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Mol	Chain	Res	Type
9	B	19	C
9	B	26	C
9	B	35	C
9	B	37	C
9	B	42	C
9	B	43	C
9	B	45	A
9	B	53	A
9	B	62	C
9	B	65	U
9	B	67	G
9	B	73	A
9	B	87	U
9	B	89	U
9	B	90	C
9	B	91	C
9	B	109	A
9	B	120	U
34	a	2	A
34	a	6	G
34	a	9	G
34	a	22	G
34	a	32	A
34	a	39	G
34	a	47	C
34	a	48	C
34	a	51	A
34	a	70	U
34	a	76	G
34	a	78	A
34	a	79	G
34	a	81	A
34	a	83	C
34	a	85	U
34	a	86	G
34	a	89	U
34	a	90	C
34	a	94	G
34	a	96	U
34	a	98	A
34	a	122	G
34	a	130	A

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Mol	Chain	Res	Type
34	a	141	G
34	a	144	G
34	a	145	G
34	a	149	A
34	a	163	C
34	a	164	G
34	a	165	G
34	a	166	U
34	a	169	C
34	a	173	U
34	a	182	A
34	a	183	C
34	a	184	G
34	a	189	A
34	a	191	G
34	a	197	A
34	a	198	G
34	a	205	A
34	a	207	C
34	a	208	U
34	a	209	U
34	a	210	C
34	a	211	G
34	a	226	G
34	a	240	G
34	a	245	U
34	a	247	G
34	a	251	G
34	a	262	A
34	a	264	C
34	a	266	G
34	a	267	C
34	a	270	A
34	a	289	G
34	a	299	G
34	a	301	G
34	a	306	A
34	a	316	C
34	a	317	U
34	a	321	A
34	a	327	A
34	a	328	C

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Mol	Chain	Res	Type
34	a	329	A
34	a	330	C
34	a	344	A
34	a	352	C
34	a	354	G
34	a	356	A
34	a	367	U
34	a	368	U
34	a	372	C
34	a	373	A
34	a	388	G
34	a	397	A
34	a	406	G
34	a	413	G
34	a	421	U
34	a	423	G
34	a	429	U
34	a	461	A
34	a	462	G
34	a	465	A
34	a	466	A
34	a	467	U
34	a	468	A
34	a	470	C
34	a	471	U
34	a	476	U
34	a	479	U
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	518	C
34	a	521	G
34	a	524	G
34	a	528	C
34	a	532	A
34	a	535	A
34	a	547	A
34	a	559	A

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Mol	Chain	Res	Type
34	a	562	U
34	a	564	C
34	a	572	A
34	a	573	A
34	a	576	C
34	a	577	G
34	a	579	A
34	a	596	A
34	a	614	C
34	a	615	G
34	a	629	A
34	a	632	U
34	a	633	G
34	a	650	G
34	a	653	U
34	a	665	A
34	a	688	G
34	a	693	G
34	a	703	G
34	a	704	A
34	a	723	U
34	a	724	G
34	a	733	G
34	a	734	G
34	a	748	G
34	a	753	A
34	a	755	G
34	a	758	C
34	a	777	A
34	a	781	A
34	a	792	A
34	a	793	U
34	a	794	A
34	a	799	G
34	a	814	A
34	a	815	A
34	a	816	A
34	a	817	C
34	a	829	G
34	a	841	C
34	a	843	U
34	a	844	G

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Mol	Chain	Res	Type
34	a	845	A
34	a	846	G
34	a	851	G
34	a	870	U
34	a	871	U
34	a	875	U
34	a	885	G
34	a	902	G
34	a	914	A
34	a	922	G
34	a	926	G
34	a	934	C
34	a	935	A
34	a	958	A
34	a	960	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	991	U
34	a	992	U
34	a	993	G
34	a	994	A
34	a	1004	A
34	a	1005	A
34	a	1006	G
34	a	1014	A
34	a	1022	A
34	a	1023	U
34	a	1025	U
34	a	1027	C
34	a	1028	C
34	a	1030	U
34	a	1031	C
34	a	1032	G

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Mol	Chain	Res	Type
34	a	1056	U
34	a	1065	U
34	a	1085	U
34	a	1092	A
34	a	1094	G
34	a	1101	A
34	a	1108	G
34	a	1109	C
34	a	1124	G
34	a	1125	U
34	a	1126	U
34	a	1137	C
34	a	1138	G
34	a	1139	G
34	a	1140	C
34	a	1144	G
34	a	1146	A
34	a	1152	A
34	a	1159	U
34	a	1168	U
34	a	1169	A
34	a	1174	G
34	a	1183	U
34	a	1184	G
34	a	1191	A
34	a	1196	A
34	a	1197	A
34	a	1212	U
34	a	1213	A
34	a	1214	C
34	a	1215	G
34	a	1227	A
34	a	1238	A
34	a	1248	A
34	a	1254	A
34	a	1255	G
34	a	1260	G
34	a	1261	A
34	a	1262	C
34	a	1270	G
34	a	1275	A
34	a	1278	G

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Mol	Chain	Res	Type
34	a	1280	A
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	1306	A
34	a	1307	U
34	a	1323	G
34	a	1331	G
34	a	1332	A
34	a	1340	A
34	a	1346	A
34	a	1347	G
34	a	1348	U
34	a	1360	A
34	a	1363	A
34	a	1370	G
34	a	1372	U
34	a	1378	C
34	a	1379	G
34	a	1381	U
34	a	1383	C
34	a	1386	G
34	a	1398	A
34	a	1423	G
34	a	1424	U
34	a	1425	U
34	a	1441	A
34	a	1442	G
34	a	1444	U
34	a	1446	A
34	a	1451	U
34	a	1452	C
34	a	1473	G
34	a	1475	G
34	a	1476	A
34	a	1477	U
34	a	1479	C
34	a	1482	G

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Mol	Chain	Res	Type
34	a	1483	A
34	a	1486	G
34	a	1487	G
34	a	1492	A
34	a	1497	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	20	H2U
55	v	21	A
55	v	33	U
55	v	34	C
55	v	42	G
55	v	43	A
55	v	47	U
55	v	52	G
55	v	55	PSU
55	v	57	A
55	v	76	A
56	w	13	C
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	39	PSU
56	w	45	U
56	w	46	G7M

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Mol	Chain	Res	Type
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	73	A
56	w	74	C
56	w	75	C
59	z	0	U

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	242	G
8	A	310	A
8	A	458	G
8	A	481	G
8	A	555	G
8	A	715	A
8	A	784	G
8	A	883	G
8	A	894	U
8	A	1064	C
8	A	1082	U
8	A	1086	A
8	A	1090	A
8	A	1093	G
8	A	1099	G
8	A	1300	G
8	A	1331	G
8	A	1358	G
8	A	1415	U
8	A	1451	C
8	A	1490	A
8	A	1538	G
8	A	1715	G
8	A	1730	C
8	A	1907	G
8	A	1926	U

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Mol	Chain	Res	Type
8	A	2149	U
8	A	2192	U
8	A	2287	A
8	A	2319	G
8	A	2324	U
8	A	2405	G
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	$\# Z > 2$
56	G7M	w	46	56	20,26,27	0.51	0	17,39,42	0.41	0
56	PSU	w	55	56	18,21,22	1.08	1 (5%)	22,30,33	1.79	5 (22%)
56	PSU	w	39	56	18,21,22	1.09	1 (5%)	22,30,33	1.68	4 (18%)
8	5MU	A	1939	8	19,22,23	0.29	0	28,32,35	0.40	0
55	PSU	v	55	55	18,21,22	1.08	1 (5%)	22,30,33	1.72	4 (18%)
8	PSU	A	2604	8	18,21,22	1.05	1 (5%)	22,30,33	1.86	5 (22%)
8	PSU	A	1911	8	18,21,22	1.05	1 (5%)	22,30,33	1.80	5 (22%)
8	PSU	A	955	8	18,21,22	1.09	1 (5%)	22,30,33	1.84	5 (22%)
8	6MZ	A	2030	8,60	18,25,26	0.76	0	16,36,39	0.77	1 (6%)
34	PSU	a	516	34	18,21,22	1.01	1 (5%)	22,30,33	1.84	5 (22%)
8	2MG	A	2445	8	18,26,27	1.02	3 (16%)	16,38,41	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	5MC	A	747	8	18,22,23	0.30	0	26,32,35	0.41	0
8	PSU	A	2605	8	18,21,22	1.04	1 (5%)	22,30,33	1.78	4 (18%)
8	5MC	A	1962	8	18,22,23	0.28	0	26,32,35	0.42	0
34	G7M	a	527	34	20,26,27	0.59	0	17,39,42	0.42	0
8	6MZ	A	1618	8	18,25,26	0.73	0	16,36,39	0.77	1 (6%)
34	4OC	a	1402	34	20,23,24	0.31	0	26,32,35	0.46	0
56	MIA	w	37	56	24,31,32	0.61	0	26,44,47	0.89	2 (7%)
34	2MG	a	1516	34	18,26,27	0.97	2 (11%)	16,38,41	0.69	0
8	PSU	A	746	8,60	18,21,22	1.09	1 (5%)	22,30,33	1.65	4 (18%)
34	2MG	a	966	34	18,26,27	0.97	2 (11%)	16,38,41	0.67	0
56	PSU	w	32	56	18,21,22	1.07	1 (5%)	22,30,33	1.65	4 (18%)
34	UR3	a	1498	34	19,22,23	0.31	0	26,32,35	0.45	0
34	2MG	a	1207	34	18,26,27	0.94	1 (5%)	16,38,41	0.67	0
34	MA6	a	1519	34	18,26,27	0.76	0	19,38,41	0.69	0
55	4SU	v	8	55	18,21,22	0.30	0	26,30,33	0.37	0
8	OMG	A	2251	8,56	18,26,27	0.96	2 (11%)	19,38,41	0.55	0
34	MA6	a	1518	34	18,26,27	0.76	0	19,38,41	0.62	0
8	OMU	A	2552	8	19,22,23	0.33	0	26,31,34	0.45	0
8	3TD	A	1915	8	18,22,23	0.48	0	22,32,35	0.62	0
8	PSU	A	2580	8	18,21,22	1.10	2 (11%)	22,30,33	1.95	6 (27%)
55	H2U	v	20	55	18,21,22	0.37	0	21,30,33	0.34	0
8	2MA	A	2503	8,60	19,25,26	1.03	2 (10%)	21,37,40	3.12	5 (23%)
34	5MC	a	967	34	18,22,23	0.28	0	26,32,35	0.42	0
8	PSU	A	1917	8	18,21,22	1.01	1 (5%)	22,30,33	1.78	4 (18%)
56	5MU	w	54	56	19,22,23	0.31	0	28,32,35	0.30	0
8	PSU	A	2504	8	18,21,22	1.06	1 (5%)	22,30,33	1.79	4 (18%)
8	PSU	A	2457	8	18,21,22	0.99	1 (5%)	22,30,33	2.01	6 (27%)
34	5MC	a	1407	34	18,22,23	0.33	0	26,32,35	0.48	0
55	5MU	v	54	55	19,22,23	0.29	0	28,32,35	0.29	0
8	G7M	A	2069	8	20,26,27	0.60	0	17,39,42	0.49	0
8	2MG	A	1835	8	18,26,27	0.95	2 (11%)	16,38,41	0.67	0
58	FME	y	101	58	8,9,10	0.97	0	7,9,11	0.79	0
8	1MG	A	745	8	18,26,27	0.94	2 (11%)	19,39,42	0.55	0
56	4SU	w	8	56	18,21,22	0.31	0	26,30,33	0.37	0
8	OMC	A	2498	8,60	19,22,23	0.30	0	26,31,34	0.44	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
56	G7M	w	46	56	-	1/3/25/26	0/3/3/3
56	PSU	w	55	56	-	0/7/25/26	0/2/2/2
56	PSU	w	39	56	-	5/7/25/26	0/2/2/2
8	5MU	A	1939	8	-	1/7/25/26	0/2/2/2
55	PSU	v	55	55	-	3/7/25/26	0/2/2/2
8	PSU	A	2604	8	-	0/7/25/26	0/2/2/2
8	PSU	A	1911	8	-	0/7/25/26	0/2/2/2
8	PSU	A	955	8	-	0/7/25/26	0/2/2/2
8	6MZ	A	2030	8,60	-	2/5/27/28	0/3/3/3
34	PSU	a	516	34	-	0/7/25/26	0/2/2/2
8	2MG	A	2445	8	-	0/5/27/28	0/3/3/3
8	5MC	A	747	8	-	0/7/25/26	0/2/2/2
8	PSU	A	2605	8	-	0/7/25/26	0/2/2/2
8	5MC	A	1962	8	-	0/7/25/26	0/2/2/2
34	G7M	a	527	34	-	3/3/25/26	0/3/3/3
8	6MZ	A	1618	8	-	0/5/27/28	0/3/3/3
34	4OC	a	1402	34	-	0/9/29/30	0/2/2/2
56	MIA	w	37	56	-	0/11/33/34	0/3/3/3
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
8	PSU	A	746	8,60	-	1/7/25/26	0/2/2/2
34	2MG	a	966	34	-	0/5/27/28	0/3/3/3
56	PSU	w	32	56	-	3/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
34	2MG	a	1207	34	-	2/5/27/28	0/3/3/3
34	MA6	a	1519	34	-	2/7/29/30	0/3/3/3
55	4SU	v	8	55	-	0/7/25/26	0/2/2/2
8	OMG	A	2251	8,56	-	0/5/27/28	0/3/3/3
34	MA6	a	1518	34	-	0/7/29/30	0/3/3/3
8	OMU	A	2552	8	-	2/9/27/28	0/2/2/2
8	3TD	A	1915	8	-	3/7/25/26	0/2/2/2
8	PSU	A	2580	8	-	0/7/25/26	0/2/2/2
55	H2U	v	20	55	-	2/7/38/39	0/2/2/2
8	2MA	A	2503	8,60	-	1/3/25/26	0/3/3/3
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
8	PSU	A	1917	8	-	0/7/25/26	0/2/2/2
56	5MU	w	54	56	-	0/7/25/26	0/2/2/2
8	PSU	A	2504	8	-	2/7/25/26	0/2/2/2
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
8	G7M	A	2069	8	-	1/3/25/26	0/3/3/3
8	2MG	A	1835	8	-	0/5/27/28	0/3/3/3
58	FME	y	101	58	-	3/7/9/11	-
8	1MG	A	745	8	-	0/3/25/26	0/3/3/3
56	4SU	w	8	56	-	0/7/25/26	0/2/2/2
8	OMC	A	2498	8,60	-	0/9/27/28	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	32	PSU	C6-C5	3.65	1.39	1.35
56	w	39	PSU	C6-C5	3.64	1.39	1.35
55	v	55	PSU	C6-C5	3.61	1.39	1.35
8	A	746	PSU	C6-C5	3.52	1.39	1.35
56	w	55	PSU	C6-C5	3.48	1.39	1.35
8	A	955	PSU	C6-C5	3.41	1.39	1.35
8	A	1911	PSU	C6-C5	3.37	1.39	1.35
8	A	2504	PSU	C6-C5	3.37	1.39	1.35
8	A	1917	PSU	C6-C5	3.28	1.39	1.35
8	A	2604	PSU	C6-C5	3.27	1.39	1.35
8	A	2580	PSU	C6-C5	3.22	1.39	1.35
8	A	2605	PSU	C6-C5	3.22	1.39	1.35
34	a	516	PSU	C6-C5	3.18	1.39	1.35
8	A	2457	PSU	C6-C5	2.75	1.38	1.35
8	A	2445	2MG	C5-C6	-2.55	1.42	1.47
34	a	966	2MG	C5-C6	-2.53	1.42	1.47
8	A	745	1MG	C5-C4	-2.48	1.36	1.43
8	A	2251	OMG	C5-C6	-2.42	1.42	1.47
8	A	1835	2MG	C5-C6	-2.42	1.42	1.47
34	a	1516	2MG	C5-C6	-2.33	1.42	1.47
8	A	2503	2MA	C6-N6	-2.27	1.25	1.34
34	a	1207	2MG	C5-C6	-2.27	1.42	1.47
8	A	2580	PSU	O4'-C1'	-2.19	1.40	1.43
8	A	745	1MG	C8-N7	-2.12	1.31	1.35
8	A	2503	2MA	C6-N1	2.10	1.37	1.33
8	A	2445	2MG	C5-C4	-2.06	1.37	1.43
8	A	1835	2MG	C8-N7	-2.05	1.31	1.35
8	A	2251	OMG	C8-N7	-2.05	1.31	1.35
34	a	966	2MG	C8-N7	-2.04	1.31	1.35
8	A	2445	2MG	C8-N7	-2.04	1.31	1.35
34	a	1516	2MG	C5-C4	-2.00	1.38	1.43

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2503	2MA	C5-C6-N1	-12.57	112.76	121.01
8	A	2457	PSU	C4-N3-C2	-5.22	118.82	126.34
8	A	2457	PSU	N1-C2-N3	5.03	120.83	115.13
34	a	516	PSU	C4-N3-C2	-4.84	119.36	126.34
8	A	2605	PSU	C4-N3-C2	-4.82	119.39	126.34
8	A	1917	PSU	C4-N3-C2	-4.79	119.44	126.34
8	A	2580	PSU	N1-C2-N3	4.77	120.54	115.13
8	A	2580	PSU	C4-N3-C2	-4.76	119.47	126.34
8	A	955	PSU	C4-N3-C2	-4.70	119.56	126.34
8	A	2604	PSU	C4-N3-C2	-4.67	119.60	126.34
56	w	55	PSU	C4-N3-C2	-4.66	119.62	126.34
8	A	2604	PSU	N1-C2-N3	4.66	120.41	115.13
8	A	1911	PSU	C4-N3-C2	-4.64	119.65	126.34
8	A	955	PSU	N1-C2-N3	4.64	120.39	115.13
8	A	2504	PSU	C4-N3-C2	-4.61	119.70	126.34
8	A	2504	PSU	N1-C2-N3	4.59	120.33	115.13
8	A	1911	PSU	N1-C2-N3	4.57	120.31	115.13
8	A	2605	PSU	N1-C2-N3	4.53	120.26	115.13
8	A	746	PSU	C4-N3-C2	-4.51	119.84	126.34
34	a	516	PSU	N1-C2-N3	4.50	120.22	115.13
56	w	55	PSU	N1-C2-N3	4.49	120.22	115.13
55	v	55	PSU	C4-N3-C2	-4.45	119.92	126.34
56	w	39	PSU	N1-C2-N3	4.45	120.18	115.13
8	A	1917	PSU	N1-C2-N3	4.45	120.17	115.13
56	w	39	PSU	C4-N3-C2	-4.42	119.97	126.34
55	v	55	PSU	N1-C2-N3	4.36	120.07	115.13
8	A	746	PSU	N1-C2-N3	4.35	120.06	115.13
56	w	32	PSU	C4-N3-C2	-4.30	120.15	126.34
56	w	32	PSU	N1-C2-N3	4.27	119.97	115.13
8	A	2503	2MA	C2-N1-C6	4.02	124.35	118.08
8	A	2503	2MA	C2-N3-C4	-3.85	112.39	115.52
8	A	2457	PSU	O2-C2-N1	-3.14	119.34	122.79
8	A	2580	PSU	O2-C2-N1	-2.88	119.62	122.79
34	a	516	PSU	O2-C2-N1	-2.83	119.67	122.79
8	A	1917	PSU	O2-C2-N1	-2.80	119.71	122.79
56	w	37	MIA	C2-N3-C4	-2.73	111.56	115.32
8	A	2504	PSU	O2-C2-N1	-2.70	119.82	122.79
8	A	2604	PSU	O2-C2-N1	-2.68	119.84	122.79
8	A	2457	PSU	C6-C5-C4	2.66	120.06	118.20
55	v	55	PSU	O2-C2-N1	-2.65	119.87	122.79
8	A	2580	PSU	O4'-C1'-C2'	2.62	108.84	105.14
8	A	1911	PSU	O2-C2-N1	-2.61	119.92	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	37	MIA	C5-C6-N1	-2.60	118.65	120.81
8	A	746	PSU	O2-C2-N1	-2.57	119.96	122.79
8	A	955	PSU	O2-C2-N1	-2.55	119.99	122.79
56	w	32	PSU	O2-C2-N1	-2.54	119.99	122.79
56	w	55	PSU	O2-C2-N1	-2.51	120.03	122.79
8	A	2605	PSU	O2-C2-N1	-2.47	120.07	122.79
8	A	2604	PSU	C6-C5-C4	2.41	119.88	118.20
8	A	2503	2MA	N6-C6-N1	2.40	123.60	117.07
8	A	955	PSU	C6-C5-C4	2.28	119.79	118.20
8	A	2580	PSU	C6-N1-C2	-2.25	120.38	122.68
8	A	2580	PSU	C6-C5-C4	2.25	119.77	118.20
8	A	2604	PSU	C6-N1-C2	-2.25	120.39	122.68
56	w	39	PSU	C6-N1-C2	-2.24	120.39	122.68
56	w	39	PSU	O2-C2-N1	-2.24	120.33	122.79
56	w	32	PSU	C6-N1-C2	-2.20	120.44	122.68
8	A	746	PSU	C6-N1-C2	-2.19	120.44	122.68
8	A	2504	PSU	C6-N1-C2	-2.19	120.45	122.68
8	A	955	PSU	C6-N1-C2	-2.18	120.46	122.68
8	A	2605	PSU	C6-N1-C2	-2.18	120.46	122.68
8	A	1911	PSU	C6-C5-C4	2.17	119.71	118.20
8	A	2503	2MA	C5-C6-N6	2.16	123.64	120.35
34	a	516	PSU	C6-C5-C4	2.13	119.69	118.20
55	v	55	PSU	C6-N1-C2	-2.13	120.51	122.68
8	A	1911	PSU	C6-N1-C2	-2.12	120.51	122.68
56	w	55	PSU	C6-N1-C2	-2.12	120.51	122.68
8	A	2457	PSU	C6-N1-C2	-2.11	120.53	122.68
8	A	2457	PSU	O4'-C1'-C2'	2.09	108.09	105.14
8	A	1618	6MZ	C2-N1-C6	2.09	118.38	116.59
8	A	2030	6MZ	C2-N1-C6	2.08	118.37	116.59
56	w	55	PSU	C6-C5-C4	2.07	119.65	118.20
8	A	1917	PSU	C6-N1-C2	-2.02	120.61	122.68
34	a	516	PSU	O4'-C1'-C2'	2.01	107.98	105.14

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	a	1207	2MG	N1-C2-N2-CM2
34	a	1207	2MG	N3-C2-N2-CM2
34	a	1498	UR3	O4'-C1'-N1-C2
55	v	55	PSU	O4'-C1'-C5-C4
55	v	55	PSU	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
8	A	1915	3TD	O4'-C1'-C5-C4
8	A	1915	3TD	C2'-C1'-C5-C6
8	A	1915	3TD	O4'-C1'-C5-C6
8	A	1939	5MU	O4'-C4'-C5'-O5'
8	A	2504	PSU	O4'-C4'-C5'-O5'
8	A	2552	OMU	O4'-C1'-N1-C2
8	A	2552	OMU	O4'-C1'-N1-C6
56	w	32	PSU	C2'-C1'-C5-C4
56	w	32	PSU	O4'-C1'-C5-C4
56	w	32	PSU	O4'-C1'-C5-C6
56	w	39	PSU	C2'-C1'-C5-C4
56	w	39	PSU	O4'-C1'-C5-C4
56	w	39	PSU	O4'-C1'-C5-C6
56	w	39	PSU	C3'-C4'-C5'-O5'
58	y	101	FME	O1-CN-N-CA
58	y	101	FME	CB-CA-N-CN
58	y	101	FME	CA-CB-CG-SD
8	A	2030	6MZ	O4'-C4'-C5'-O5'
8	A	2030	6MZ	C3'-C4'-C5'-O5'
56	w	39	PSU	O4'-C4'-C5'-O5'
34	a	1498	UR3	O4'-C1'-N1-C6
8	A	2504	PSU	C3'-C4'-C5'-O5'
55	v	20	H2U	C3'-C4'-C5'-O5'
34	a	527	G7M	C3'-C4'-C5'-O5'
55	v	20	H2U	O4'-C4'-C5'-O5'
34	a	1519	MA6	C5-C6-N6-C10
8	A	2503	2MA	O4'-C4'-C5'-O5'
34	a	1519	MA6	C4'-C5'-O5'-P
55	v	55	PSU	C4'-C5'-O5'-P
34	a	527	G7M	O4'-C4'-C5'-O5'
8	A	746	PSU	O4'-C1'-C5-C6
56	w	46	G7M	C4'-C5'-O5'-P
8	A	2069	G7M	O4'-C4'-C5'-O5'
34	a	527	G7M	C4'-C5'-O5'-P

There are no ring outliers.

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2030	6MZ	1	0
34	a	516	PSU	1	0
34	a	527	G7M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	w	37	MIA	2	0
56	w	32	PSU	1	0
34	a	1498	UR3	1	0
34	a	1519	MA6	1	0
8	A	1917	PSU	2	0
8	A	2504	PSU	1	0
58	y	101	FME	1	0
8	A	745	1MG	1	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
65	GDP	x	804	60	24,30,30	0.85	1 (4%)	30,47,47	0.80	1 (3%)
64	PO4	x	802	-	4,4,4	0.99	0	6,6,6	0.41	0
63	AM2	a	1633	-	40,40,40	0.54	0	53,60,60	0.69	2 (3%)
63	AM2	a	1630	-	40,40,40	0.51	0	53,60,60	0.73	1 (1%)
63	AM2	a	1618	-	40,40,40	0.51	0	53,60,60	0.71	2 (3%)

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	1633	-	-	0/12/84/84	0/4/4/4
65	GDP	x	804	60	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	AM2	a	1630	-	-	3/12/84/84	0/4/4/4
63	AM2	a	1618	-	-	4/12/84/84	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	x	804	GDP	C5-C6	-2.08	1.43	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	x	804	GDP	PA-O3A-PB	3.05	143.28	132.83
63	a	1618	AM2	OA1-CA1-CA2	2.45	112.33	108.23
63	a	1618	AM2	OA4-CA1-CA2	2.43	115.66	110.25
63	a	1633	AM2	OA4-CA1-CA2	2.38	115.55	110.25
63	a	1633	AM2	OA1-CA1-CA2	2.33	112.14	108.23
63	a	1630	AM2	OA1-CA1-CA2	2.23	111.97	108.23

There are no chirality outliers.

All (8) torsion outliers are listed below:

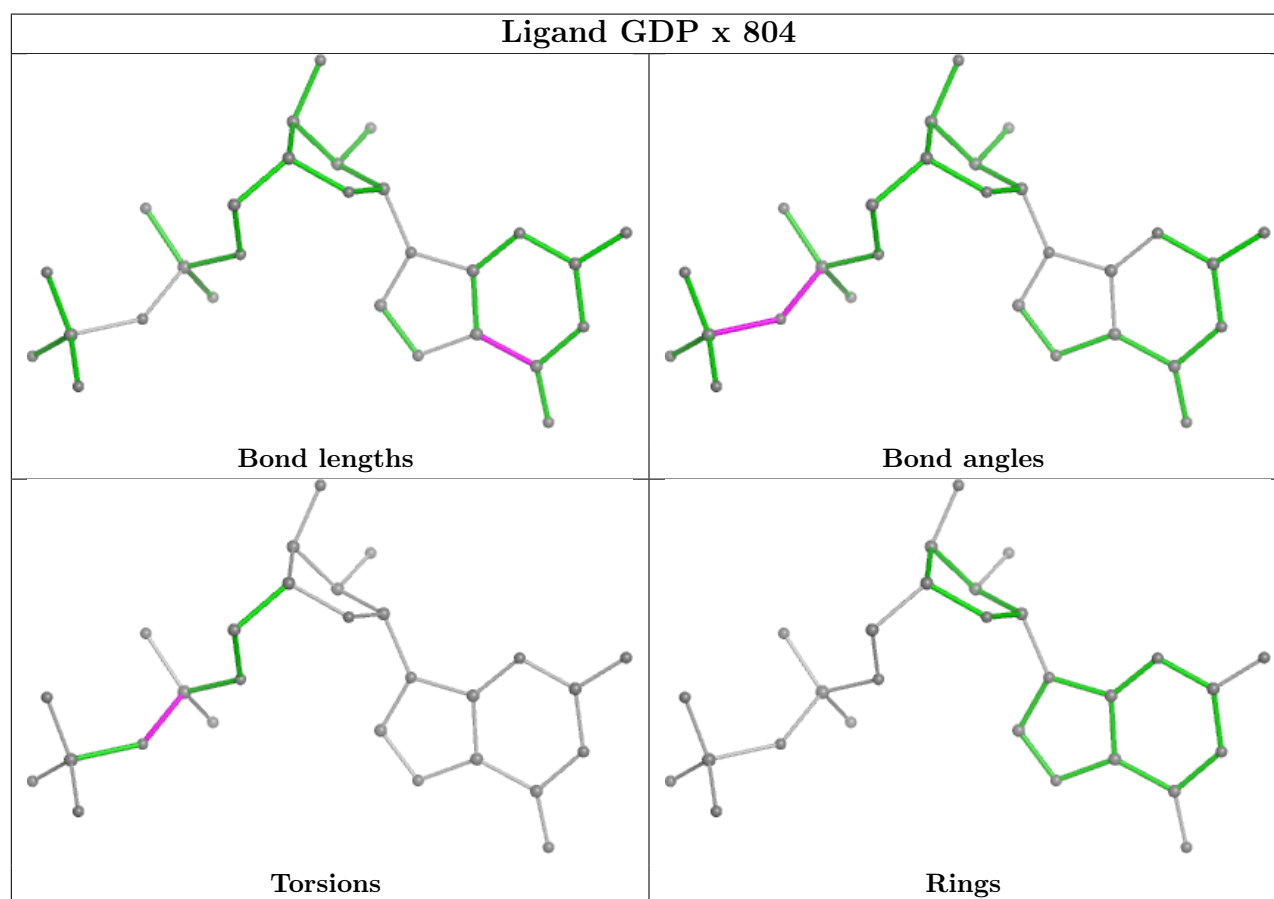
Mol	Chain	Res	Type	Atoms
63	a	1630	AM2	OA5-CA8-OA8-CB1
63	a	1630	AM2	OA4-CA1-OA1-CC1
63	a	1618	AM2	OB1-CB5-CB6-OB6
63	a	1618	AM2	OB1-CB1-OA8-CA8
63	a	1618	AM2	CB2-CB1-OA8-CA8
63	a	1630	AM2	CC2-CC1-OA1-CA1
65	x	804	GDP	PB-O3A-PA-O2A
63	a	1618	AM2	CC2-CC1-OA1-CA1

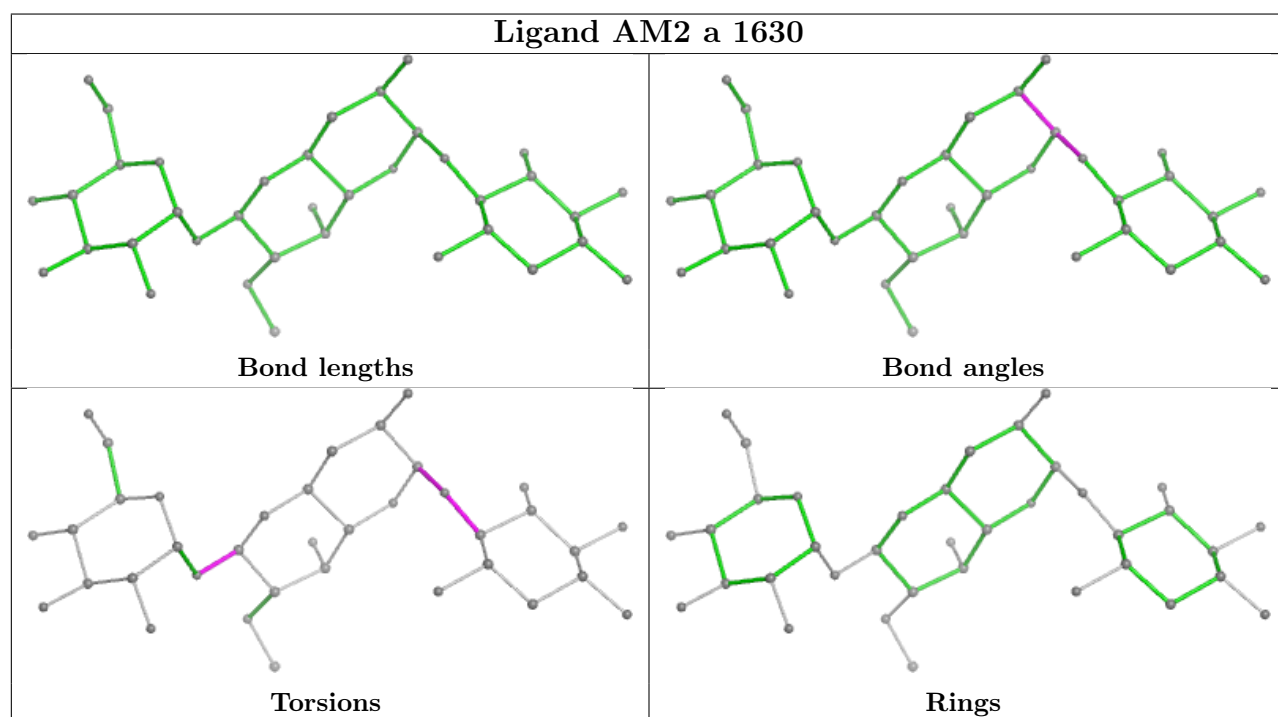
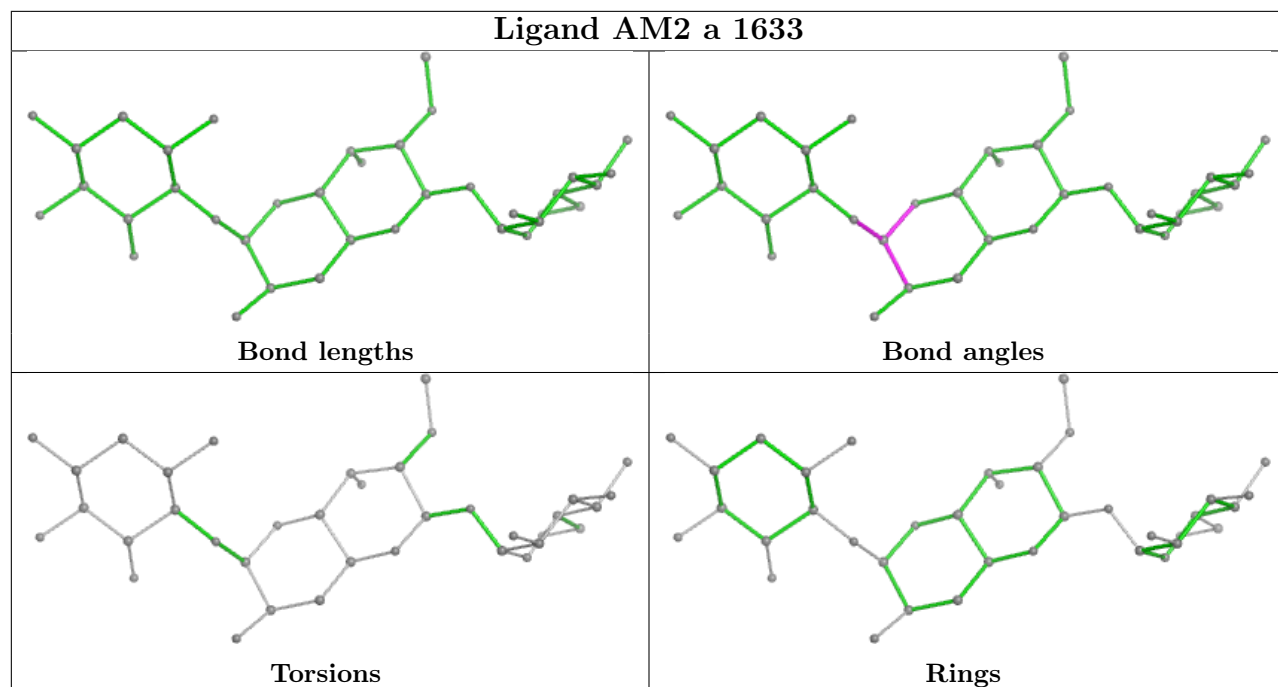
There are no ring outliers.

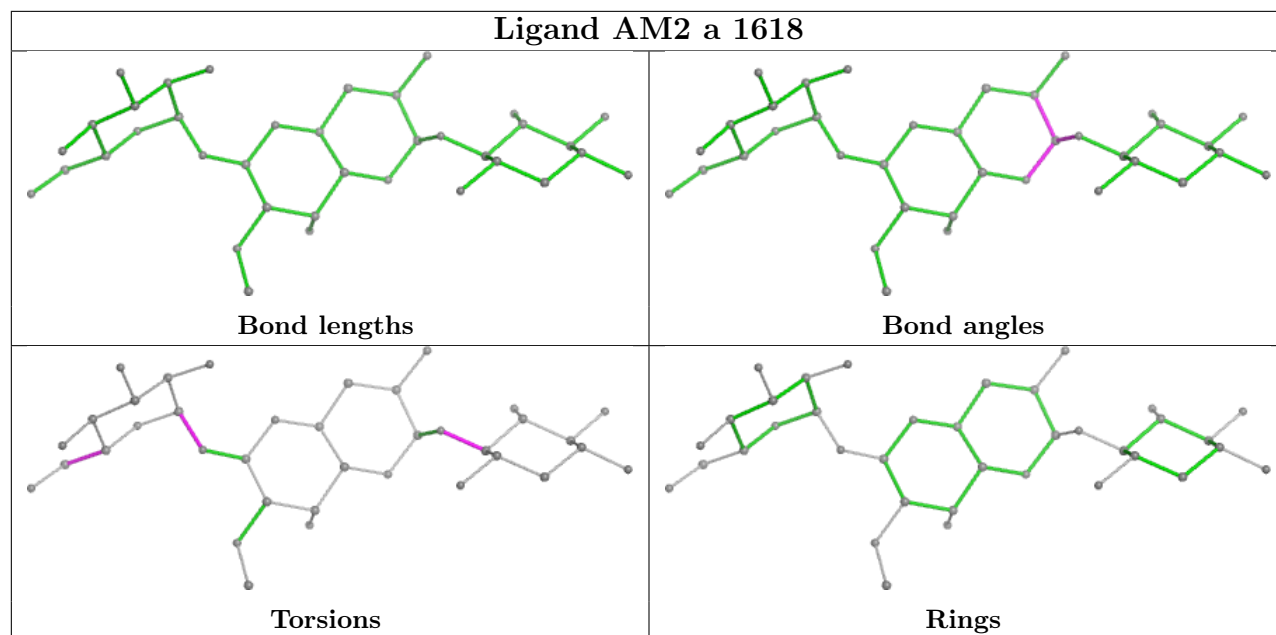
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
65	x	804	GDP	1	0
64	x	802	PO4	2	0
63	a	1633	AM2	4	0
63	a	1618	AM2	2	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

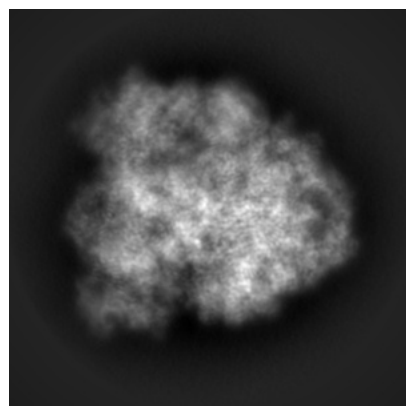
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54253. These allow visual inspection of the internal detail of the map and identification of artifacts.

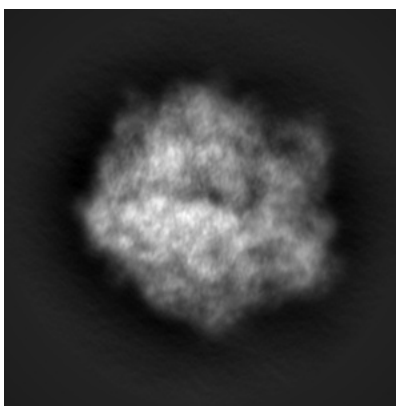
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

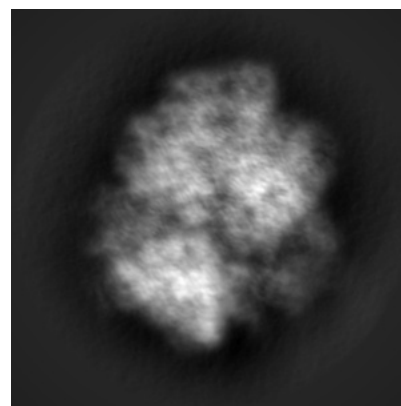
6.1.1 Primary map



X

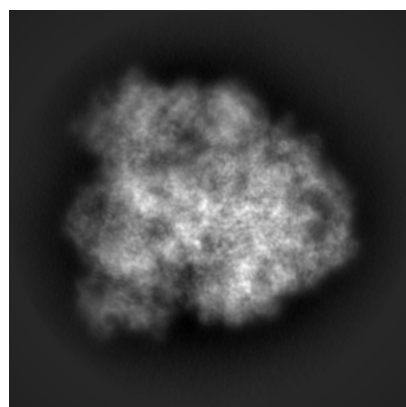


Y

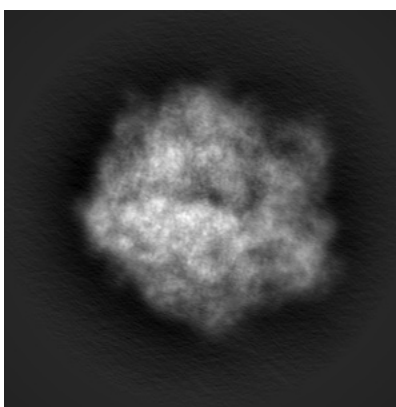


Z

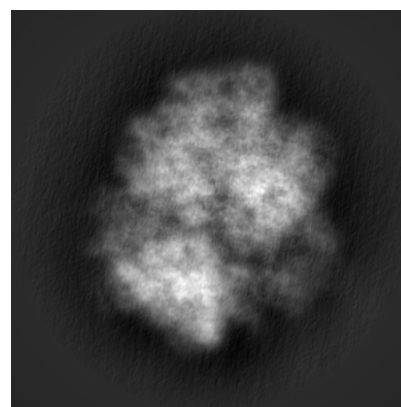
6.1.2 Raw map



X



Y

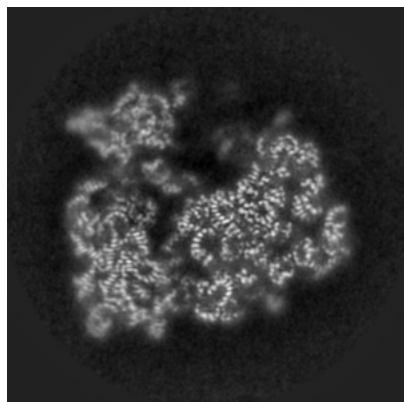


Z

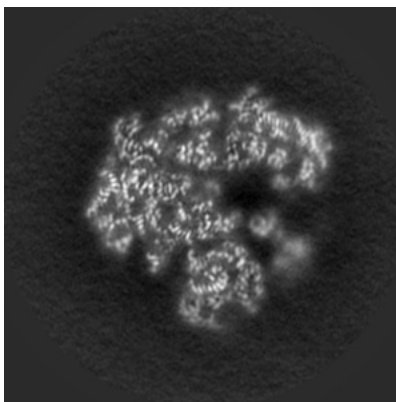
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

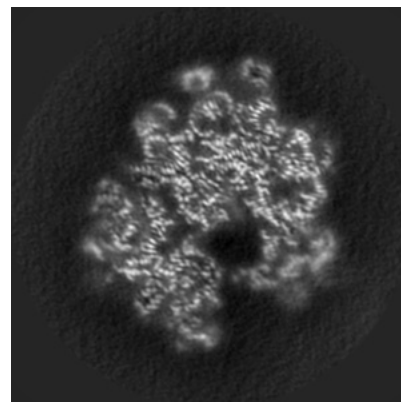
6.2.1 Primary map



X Index: 144

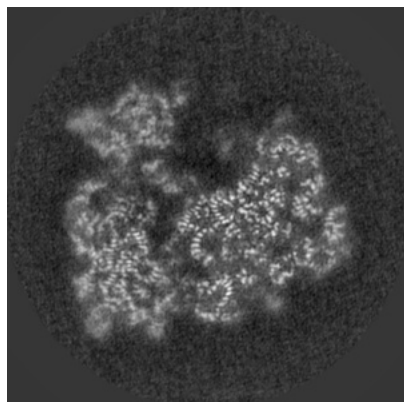


Y Index: 144

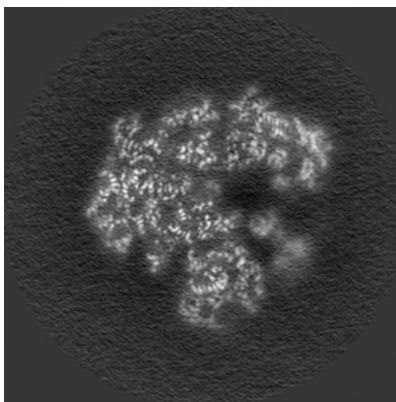


Z Index: 144

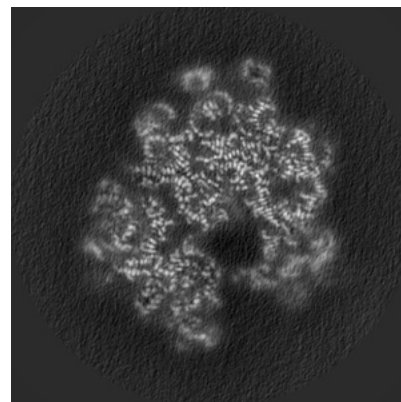
6.2.2 Raw map



X Index: 144



Y Index: 144

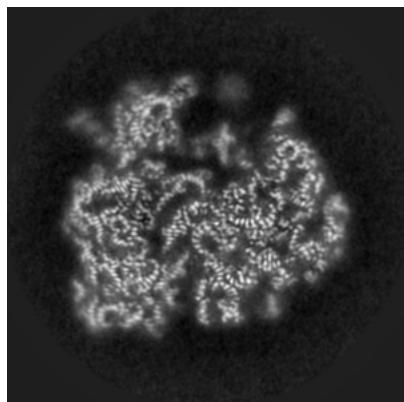


Z Index: 144

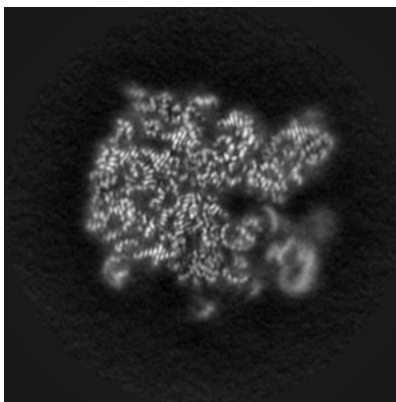
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

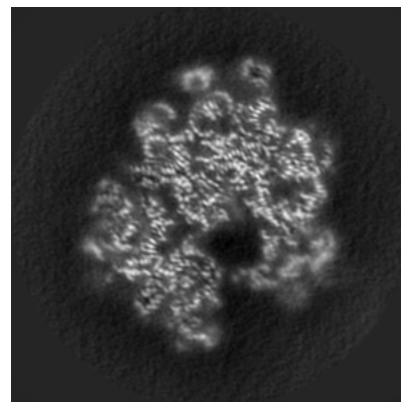
6.3.1 Primary map



X Index: 138

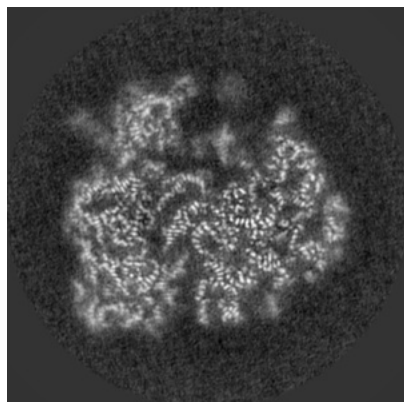


Y Index: 161

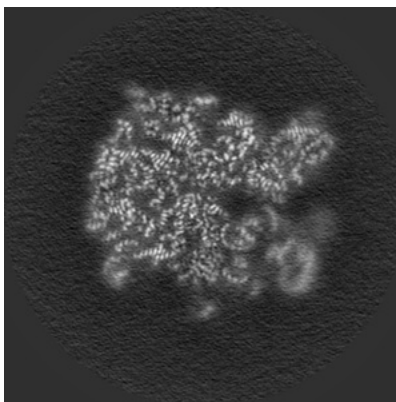


Z Index: 144

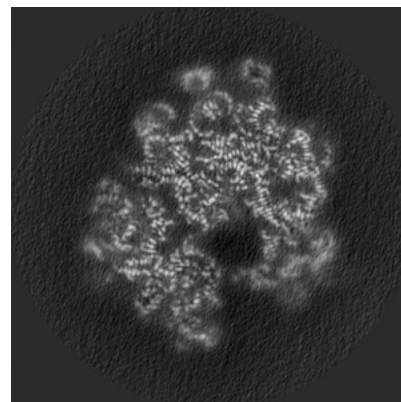
6.3.2 Raw map



X Index: 138



Y Index: 161

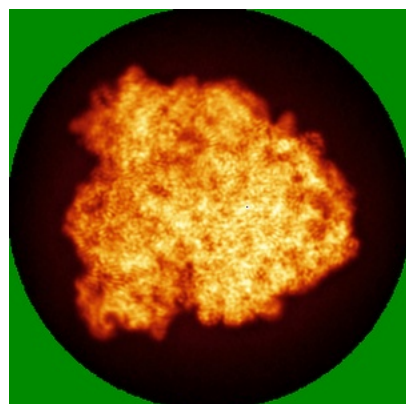


Z Index: 144

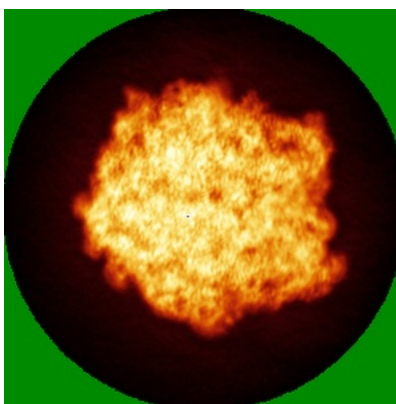
The images above show the largest variance slices of the map in three orthogonal directions.

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

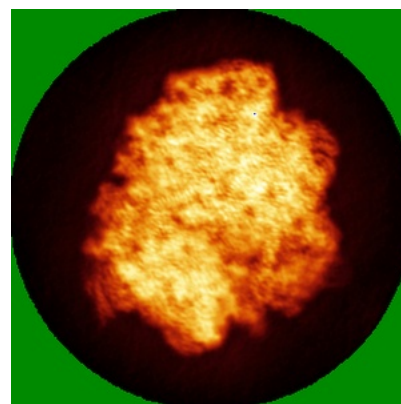
6.4.1 Primary map



X

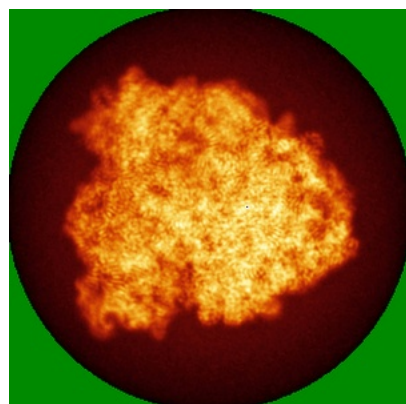


Y

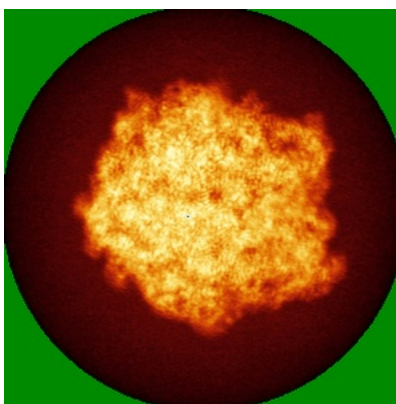


Z

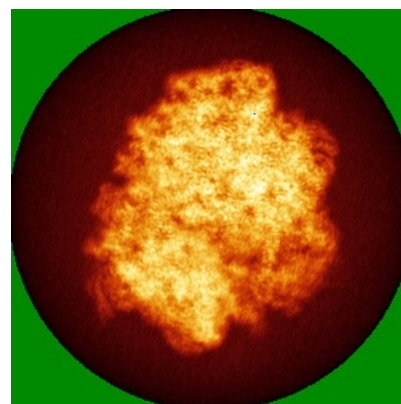
6.4.2 Raw map



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



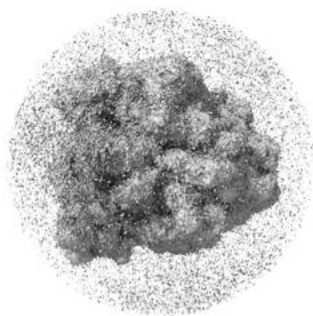
Y



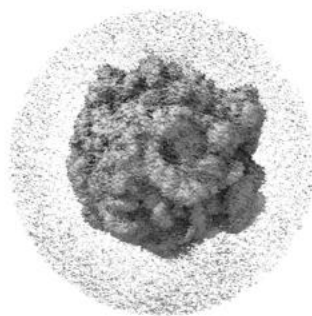
Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

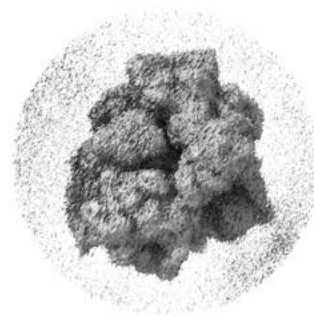
6.5.2 Raw map



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.

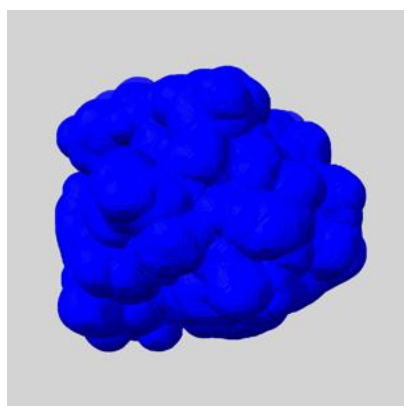
6.6 Mask visualisation [i](#)

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

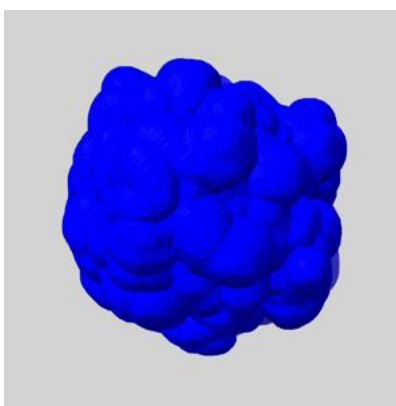
A mask typically either:

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

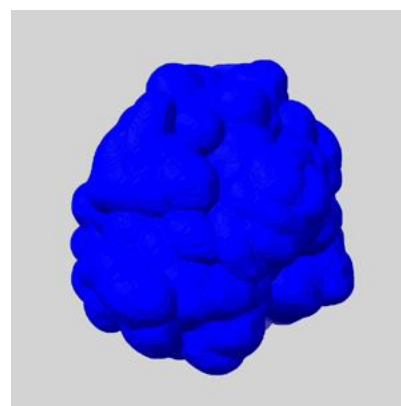
6.6.1 emd_54253_msk_1.map [i](#)



X



Y

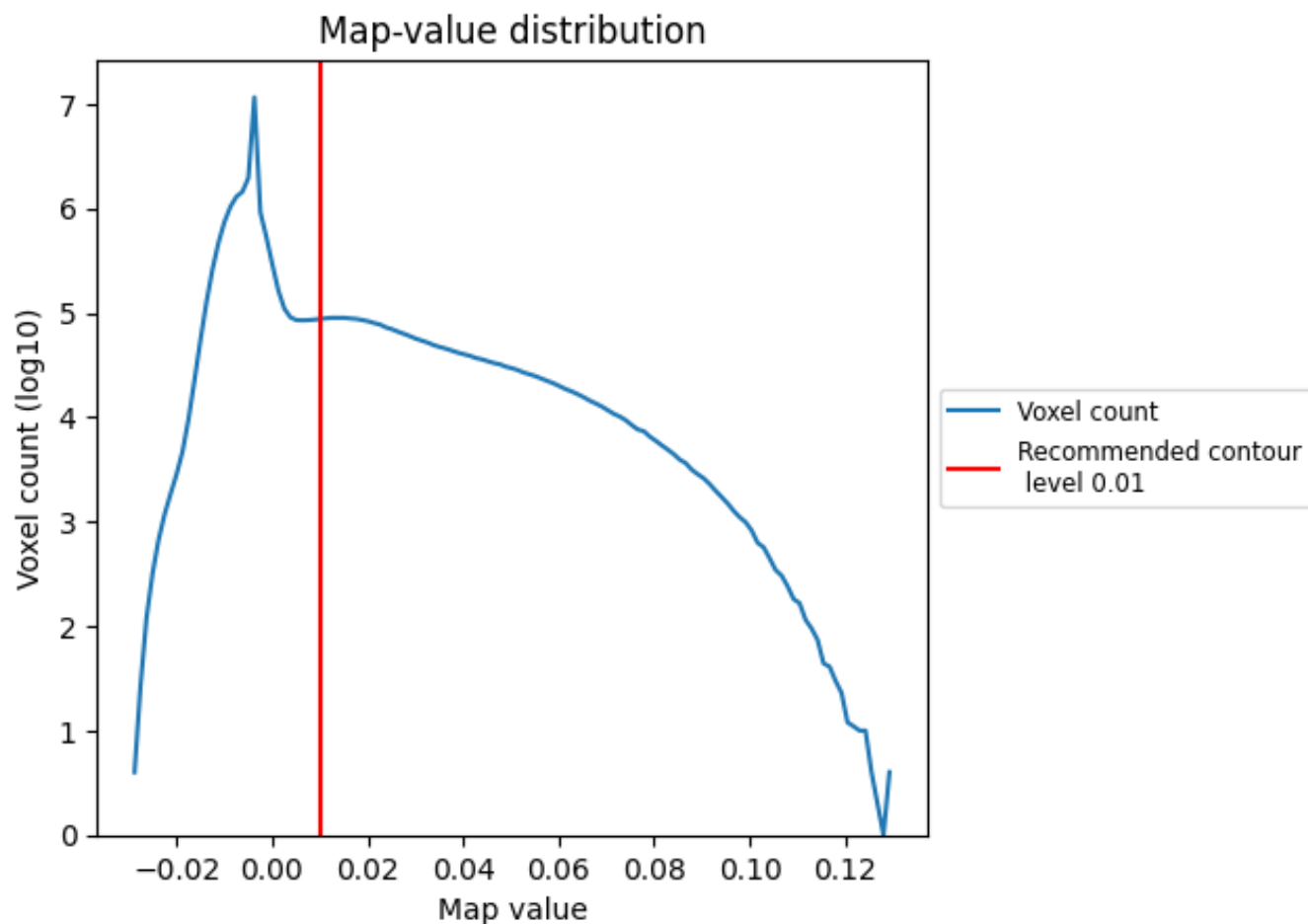


Z

7 Map analysis [i](#)

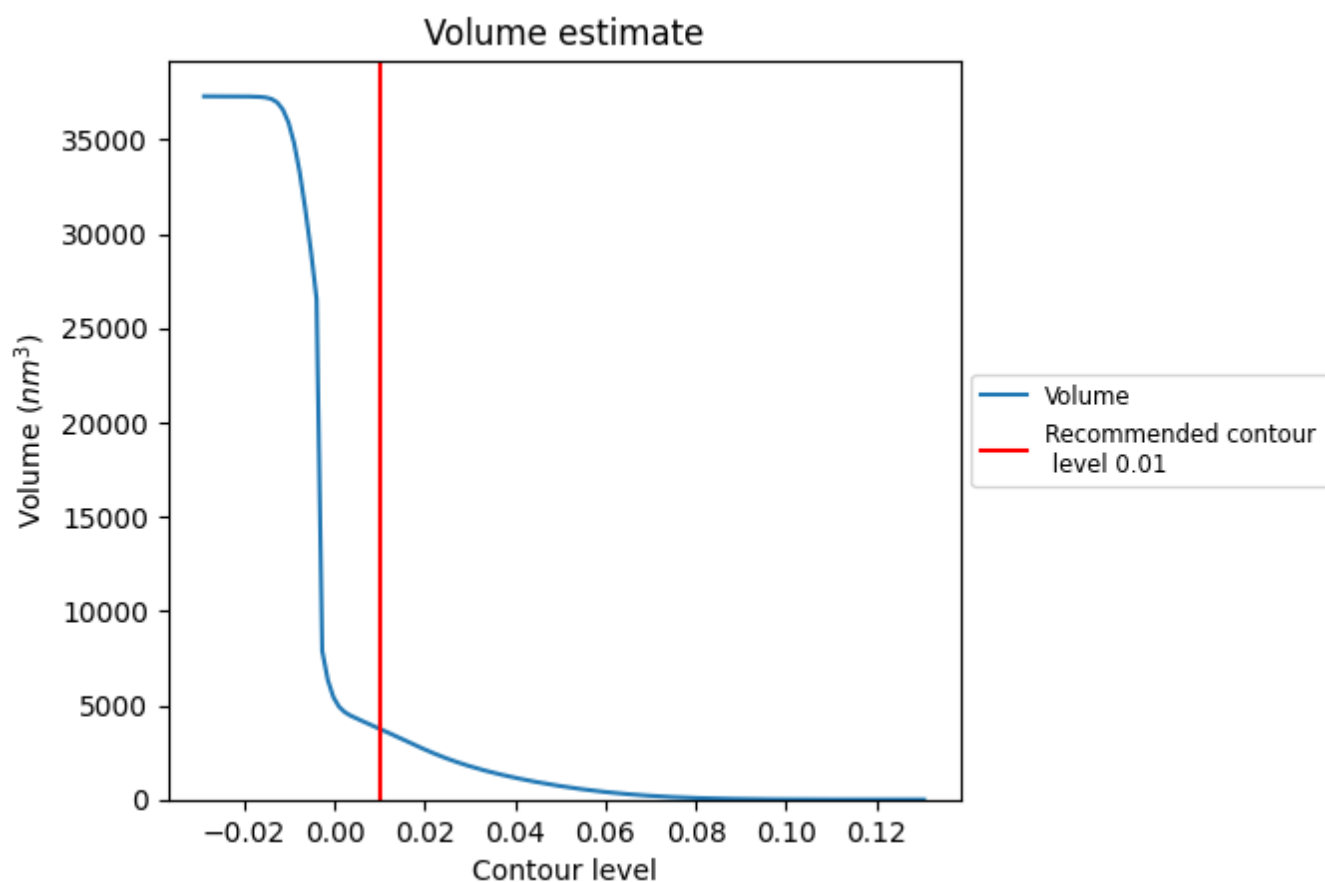
This section contains the results of statistical analysis of the map.

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.

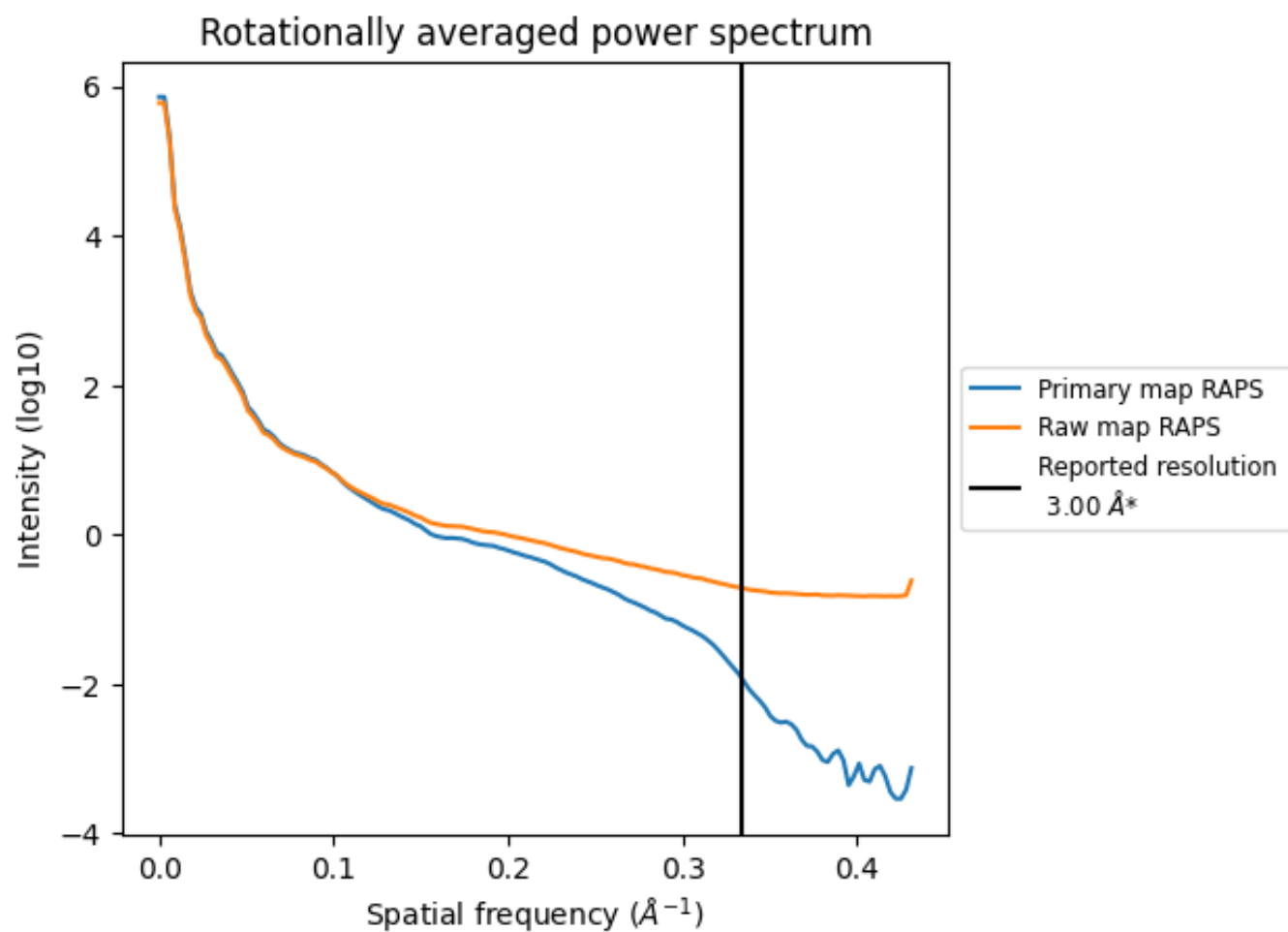
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3762 nm³; this corresponds to an approximate mass of 3398 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

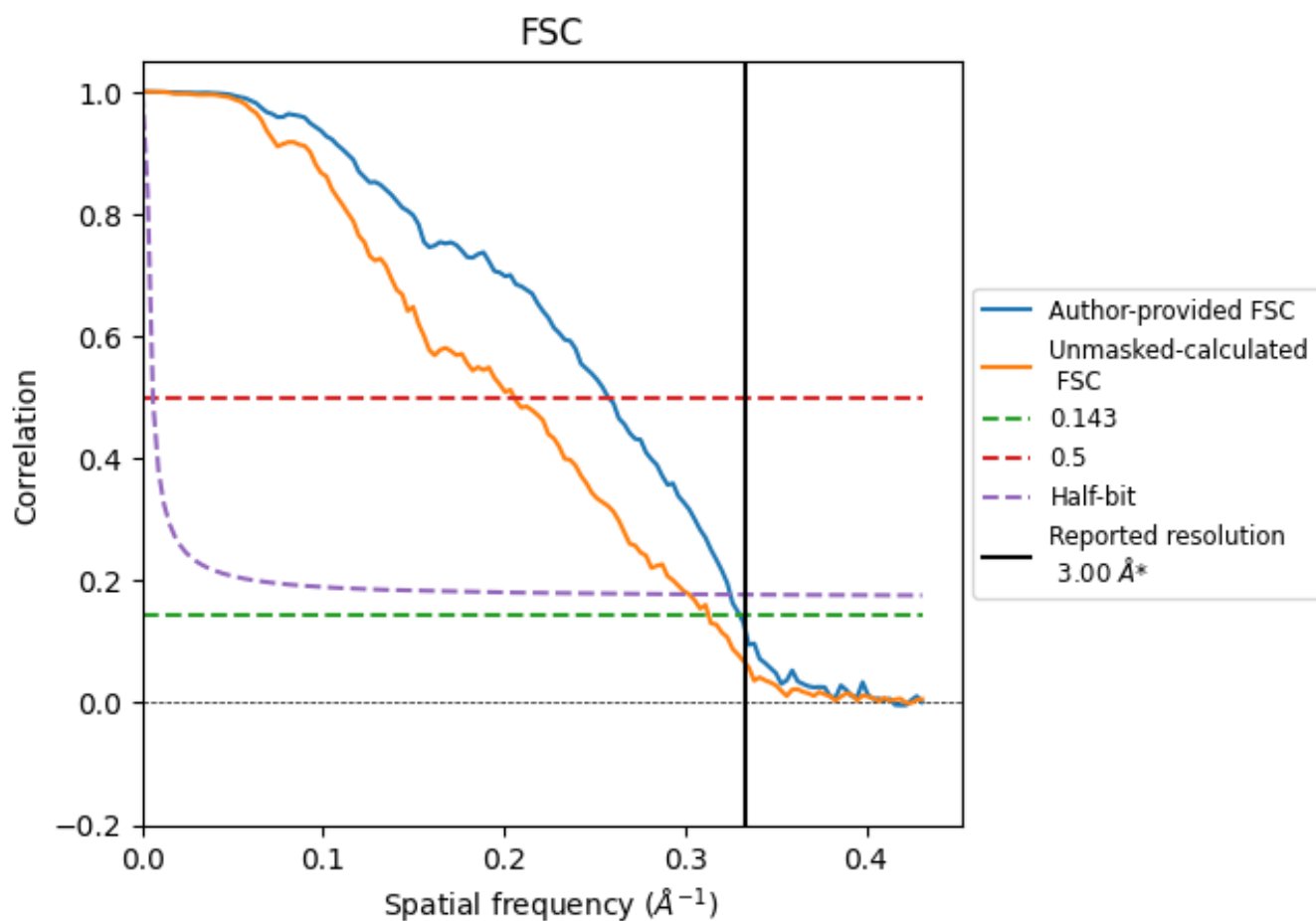


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

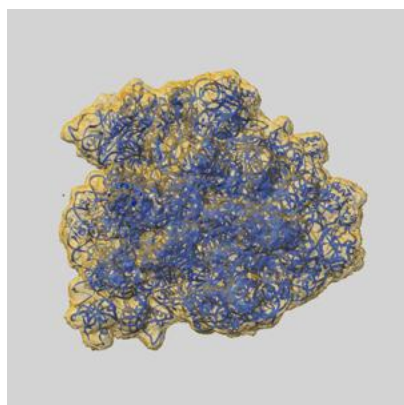
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.03	3.89	3.08
Unmasked-calculated*	3.19	4.86	3.31

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

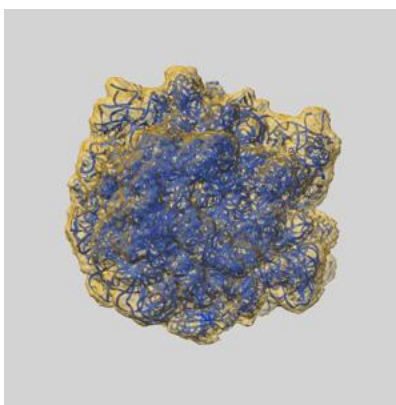
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54253 and PDB model 9RTU. Per-residue inclusion information can be found in section 3 on page 18.

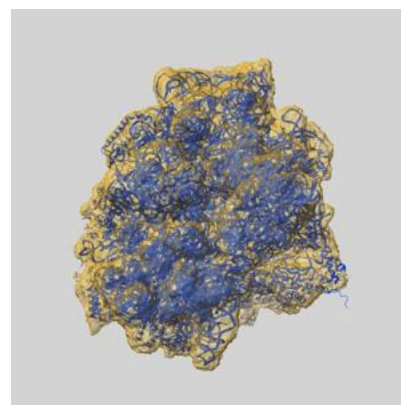
9.1 Map-model overlay [i](#)



X



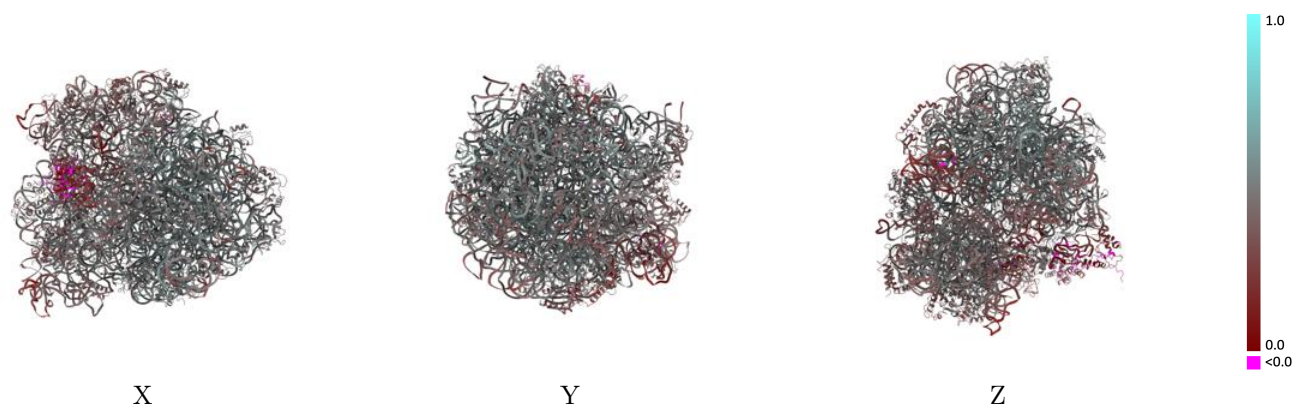
Y



Z

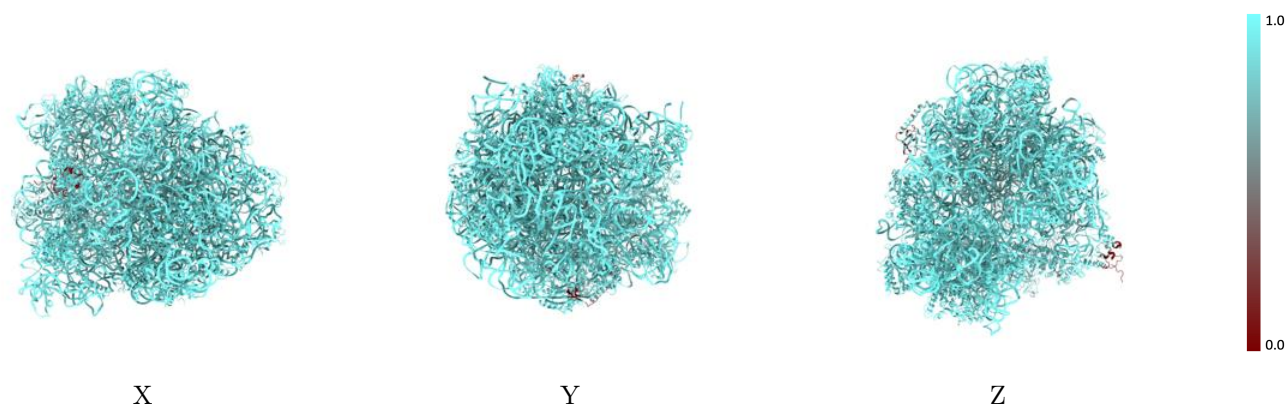
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



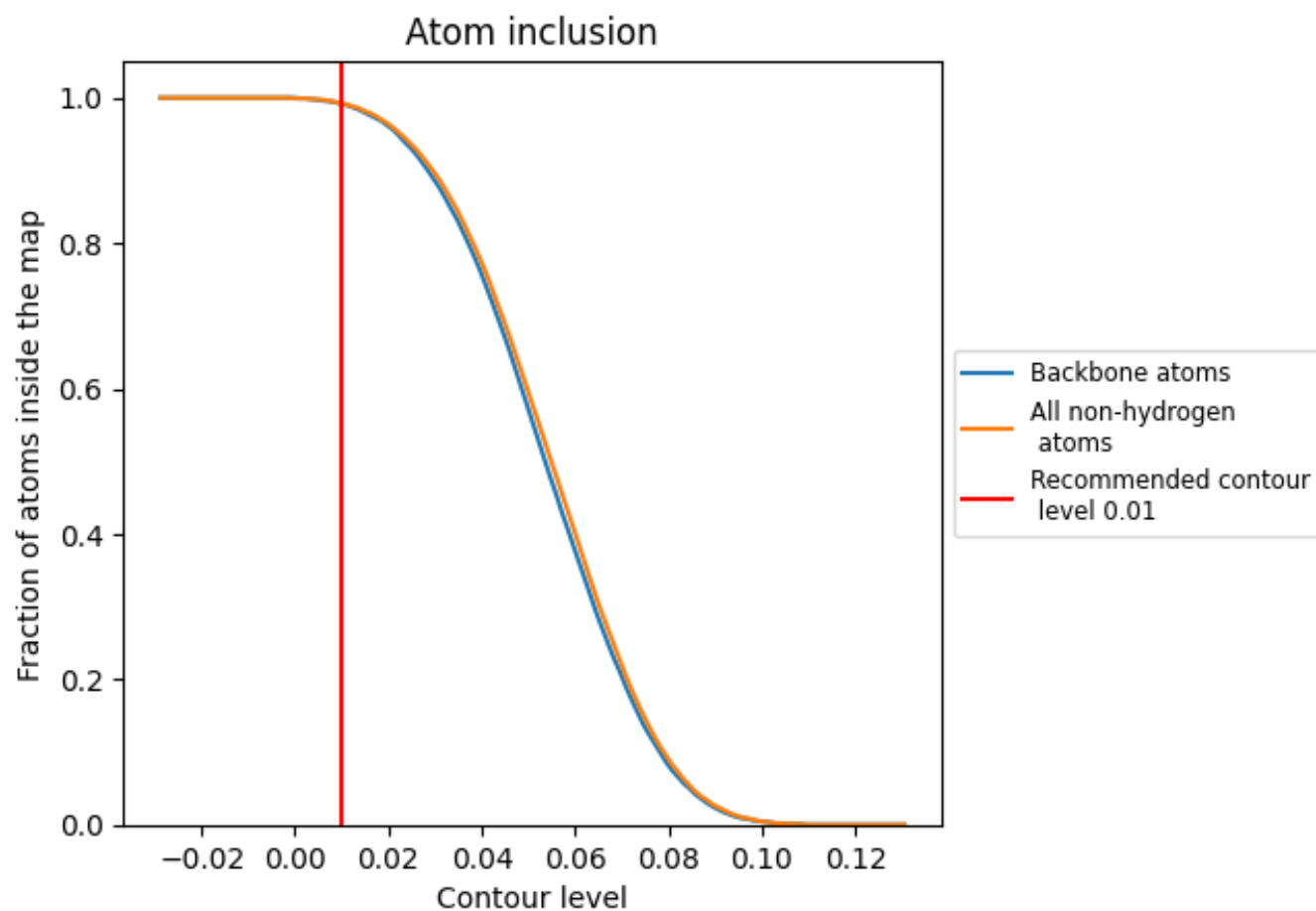
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9920	 0.4450
0	 0.9950	 0.4820
1	 1.0000	 0.4590
2	 1.0000	 0.5030
3	 0.9960	 0.5070
4	 1.0000	 0.4540
5	 0.6600	 0.1080
6	 0.9900	 0.3190
A	 0.9990	 0.4690
B	 1.0000	 0.4470
C	 0.9960	 0.4960
D	 0.9940	 0.4860
E	 0.9940	 0.4650
F	 0.9880	 0.3600
G	 0.9850	 0.4090
H	 0.6930	 0.3110
I	 0.9260	 0.1700
J	 0.9970	 0.4780
K	 0.9830	 0.4830
L	 0.9960	 0.4850
M	 0.9940	 0.4780
N	 0.9990	 0.4820
O	 0.9990	 0.4240
P	 0.9920	 0.4700
Q	 0.9990	 0.4830
R	 0.9940	 0.4760
S	 0.9960	 0.4730
T	 1.0000	 0.4550
U	 0.9910	 0.4320
V	 0.9910	 0.4520
W	 0.9950	 0.4870
X	 0.9930	 0.4680
Y	 0.9960	 0.3870
Z	 0.9890	 0.4740
a	 0.9990	 0.4480



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	 0.9740	 0.3870
c	 0.9910	 0.4190
d	 0.9970	 0.4110
e	 0.9980	 0.4590
f	 0.9750	 0.3830
g	 0.9870	 0.3470
h	 0.9970	 0.4670
i	 0.9940	 0.3970
j	 0.9960	 0.3860
k	 0.9950	 0.4410
l	 0.9860	 0.4810
m	 0.9910	 0.3700
n	 1.0000	 0.4080
o	 0.9960	 0.4240
p	 0.9950	 0.4520
q	 0.9970	 0.4520
r	 0.9960	 0.4240
s	 0.9890	 0.3690
t	 0.9950	 0.3860
u	 0.9940	 0.4010
v	 0.9960	 0.4080
w	 0.9960	 0.3600
x	 0.9640	 0.3450
y	 1.0000	 0.3420
z	 1.0000	 0.4660