



## Full wwPDB EM Validation Report ⓘ

Oct 1, 2024 – 01:03 AM JST

PDB ID : 5IMR  
EMDB ID : EMD-6585  
Title : Structure of ribosome bound to cofactor at 5.7 angstrom resolution  
Authors : Kumar, V.; Ero, R.; Jian, G.K.; Ahmed, T.; Zhan, Y.; Bhushan, S.; Gao, Y.G.  
Deposited on : 2016-03-06  
Resolution : 5.70 Å(reported)  
Based on initial models : 4W2E, 5AA0

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

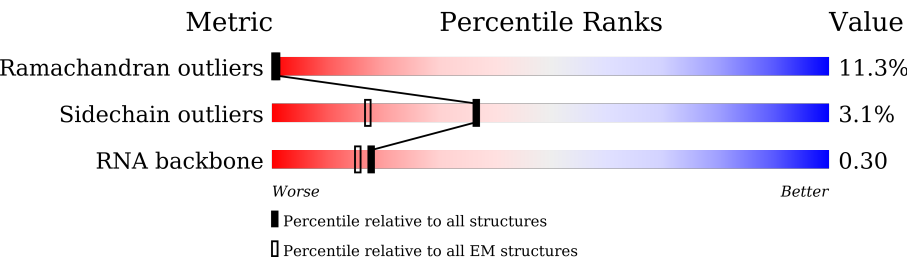
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 5.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	1522	<div><div>11%</div><div>55%</div><div>44%</div><div>.</div></div>
2	F	256	<div><div>56%</div><div>84%</div><div>7%</div><div>9%</div></div>
3	G	239	<div><div>54%</div><div>80%</div><div>6%</div><div>14%</div></div>
4	H	209	<div><div>49%</div><div>91%</div><div>9%</div></div>
5	I	162	<div><div>36%</div><div>88%</div><div>.</div><div>7%</div></div>
6	J	101	<div><div>51%</div><div>97%</div><div>.</div></div>
7	K	156	<div><div>62%</div><div>95%</div><div>.</div><div>.</div></div>
8	L	138	<div><div>42%</div><div>91%</div><div>9%</div></div>

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Mol	Chain	Length	Quality of chain
9	M	128	
10	N	105	
11	O	129	
12	P	132	
13	Q	126	
14	R	61	
15	S	89	
16	T	88	
17	U	105	
18	V	88	
19	W	93	
20	X	106	
21	Y	27	
22	C	610	
23	D	2893	
24	E	123	
25	Z	229	
26	a	276	
27	b	206	
28	c	210	
29	d	182	
30	e	180	
31	f	140	
32	g	122	
33	h	150	

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Mol	Chain	Length	Quality of chain
34	i	141	
35	j	118	
36	k	112	
37	l	146	
38	m	118	
39	n	101	
40	o	113	
41	p	96	
42	q	110	
43	r	206	
44	s	85	
45	t	67	
46	u	60	
47	v	71	
48	w	60	
49	x	54	
50	y	49	
51	z	65	
52	1	37	
53	2	173	
54	3	147	
55	4	77	
56	5	76	

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 152879 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1515	Total	C	N	O	P	0	0
			32554	14490	6022	10527	1515		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	234	Total	C	N	O	S	0	0
			1900	1213	341	341	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	206	Total	C	N	O	S	0	0
			1612	1016	314	281	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	208	Total	C	N	O	S	0	0
			1703	1066	339	291	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	150	Total	C	N	O	S	0	0
			1146	724	217	201	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	101	Total	C	N	O	S	0	0
			843	531	155	154	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	155	Total	C	N	O	S	0	0
			1257	781	252	218	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	138	Total	C	N	O	S	0	0
			1116	705	215	193	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	M	127	Total	C	N	O	0	0
			1010	639	197	174		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	98	Total	C	N	O	S	0	0
			794	499	156	138	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	119	Total	C	N	O	S	0	0
			885	549	168	165	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	124	Total	C	N	O	S	0	0
			970	611	195	163	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	114	Total	C	N	O	S	0	0
			914	565	189	158	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	88	Total	C	N	O	S	0	0
			734	459	147	126	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	83	Total	C	N	O	S	0	0
			700	443	139	117	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	104	Total	C	N	O	S	0	0
			857	547	161	147	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	V	73	Total	C	N	O	0	0
			597	380	118	99		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	80	Total	C	N	O	S	0	0
			647	414	119	112	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	99	Total	C	N	O	S	0	0
			763	470	162	129	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Y	24	Total	C	N	O	0	0
			208	128	50	30		

- Molecule 22 is a protein called Elongation factor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	C	570	Total	C	N	O	S	0	0
			4461	2858	768	826	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	D	2889	Total	C	N	O	P	0	0
			62218	27691	11629	20009	2889		

- Molecule 24 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	E	123	Total	C	N	O	P	0	0
			2641	1175	488	855	123		

- Molecule 25 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	228	Total	C	N	O	S	0	0
			1742	1102	318	319	3		

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	272	Total	C	N	O	S	0	0
			2124	1339	424	358	3		

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	206	Total	C	N	O	S	0	0
			1578	997	302	273	6		

- Molecule 28 is a protein called 50S ribosomal protein L4.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	208	Total	C	N	O	S	0	0
			1625	1034	303	286	2		

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	182	Total	C	N	O	S	0	0
			1482	947	269	261	5		

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	174	Total	C	N	O	S	0	0
			1328	844	248	235	1		

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	139	Total	C	N	O	S	0	0
			1113	717	207	186	3		

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	122	Total	C	N	O	S	0	0
			932	587	171	170	4		

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	145	Total	C	N	O	S	0	0
			1106	688	226	190	2		

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	136	Total	C	N	O	S	0	0
			1080	688	204	183	5		

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	j	117	Total	C	N	O	0	0
			960	599	202	159		

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	k	110	Total	C	N	O	0	0
			877	553	175	149		

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	117	Total	C	N	O	S	0	0
			976	614	197	164	1		

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	117	Total	C	N	O	S	0	0
			964	610	202	151	1		

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	101	Total	C	N	O	S	0	0
			779	501	142	135	1		

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	110	Total	C	N	O	S	0	0
			876	552	171	151	2		

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	p	94	Total	C	N	O	0	0
			742	483	133	126		

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	110	Total	C	N	O	S	0	0
			844	539	158	141	6		

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	180	Total	C	N	O	S	0	0
			1435	916	256	260	3		

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	79	Total	C	N	O	S	0	0
			625	387	131	106	1		

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	t	67	Total	C	N	O	S	0	0
			567	350	116	99	2		

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	u	59	Total	C	N	O	0	0
			469	298	90	81		

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	v	71	Total	C	N	O	S	0	0
			581	364	108	104	5		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	w	57	Total	C	N	O	S	0	0
			445	279	87	74	5		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	49	Total	C	N	O	S	0	0
			426	265	87	70	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	y	49	Total	C	N	O	S	0	0
			430	263	108	57	2		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	z	64	Total	C	N	O	S	0	0
			515	331	102	79	3		

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	37	Total	C	N	O	S	0	0
			307	188	68	47	4		

- Molecule 53 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	2	130	Total	C	N	O	0	0
			641	381	130	130		

- Molecule 54 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	134	Total	C	N	O	S	0	0
			993	632	175	181	5		

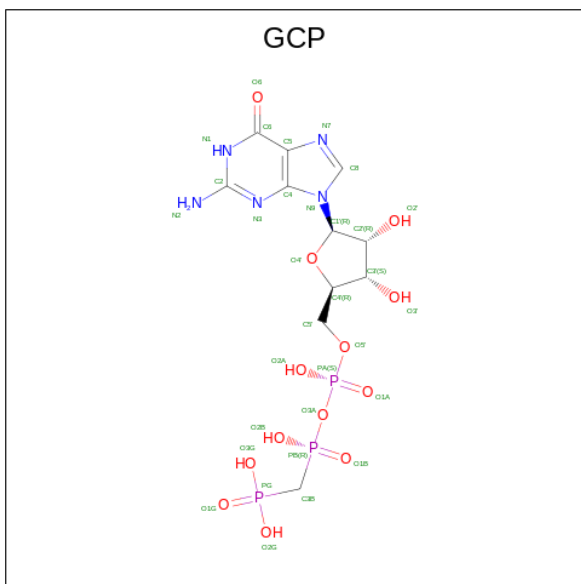
- Molecule 55 is a RNA chain called P site- tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

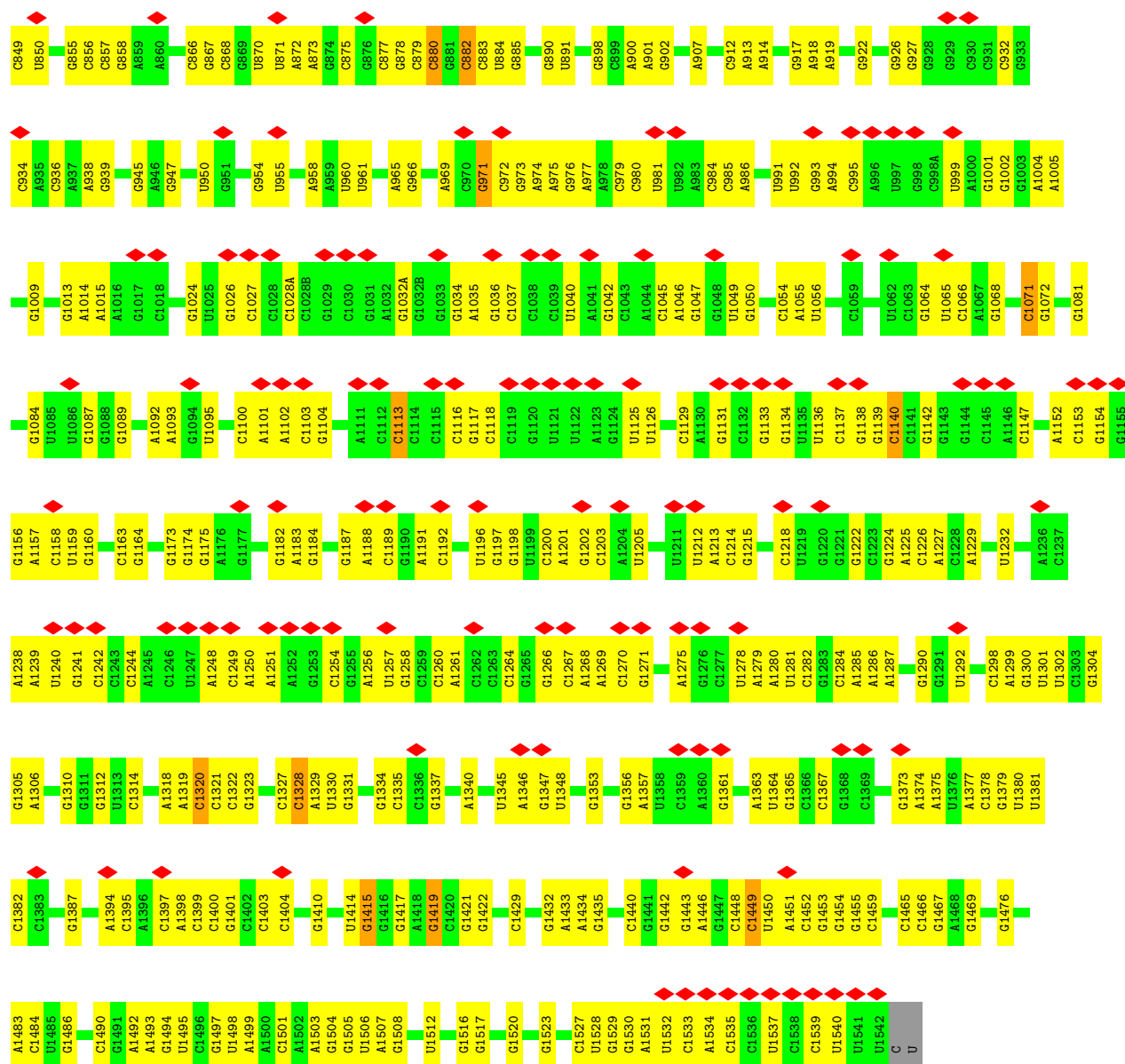
- Molecule 56 is a RNA chain called E site- tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	5	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

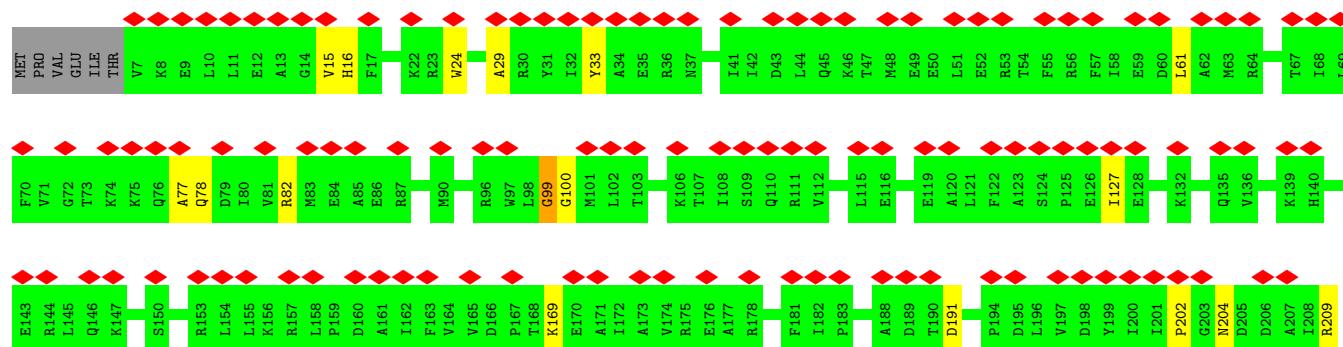
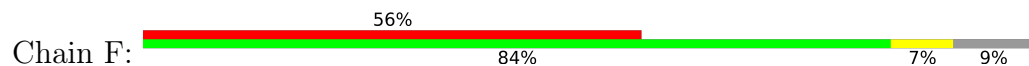
- Molecule 57 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula:  $C_{11}H_{18}N_5O_{13}P_3$ ).

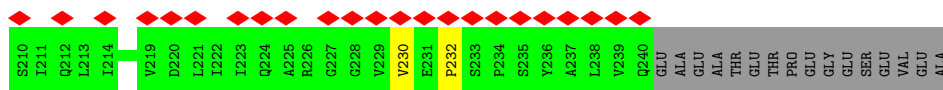




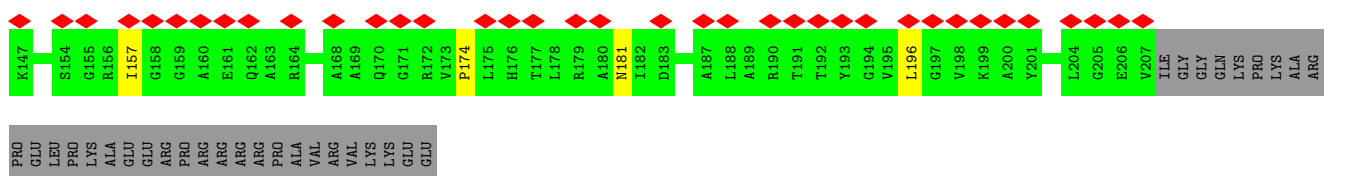
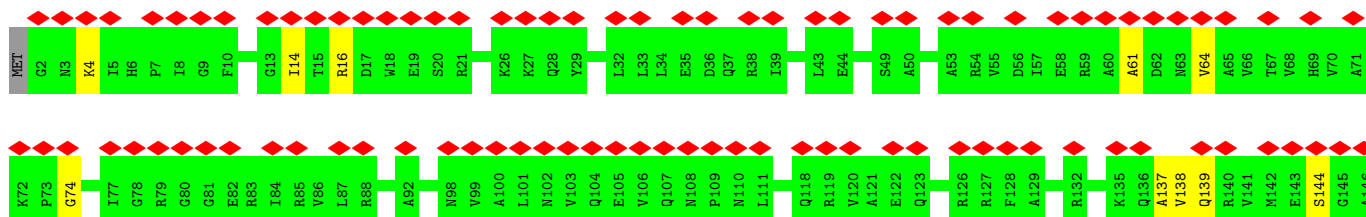
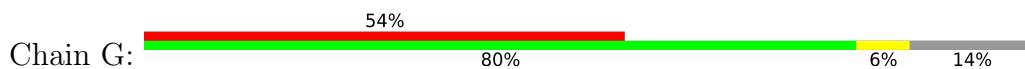


• Molecule 2: 30S ribosomal protein S2

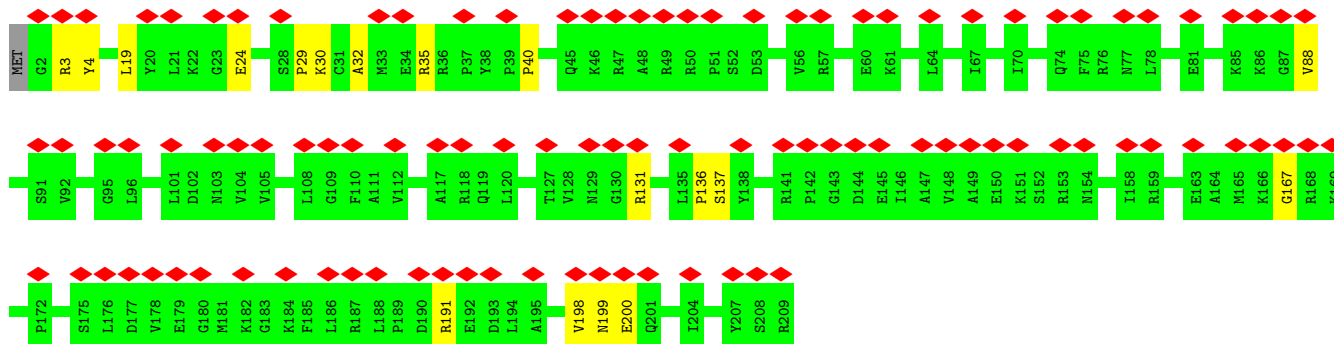




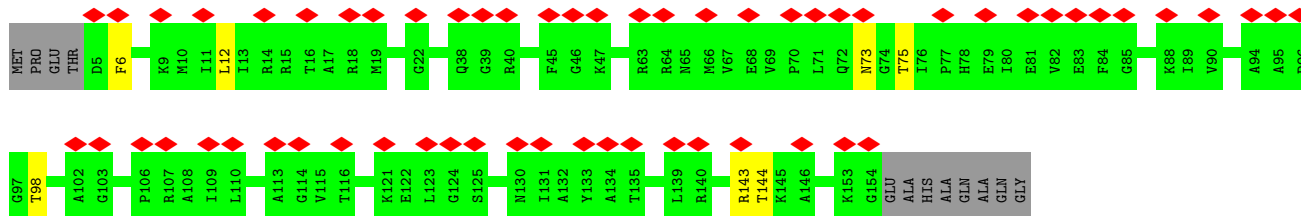
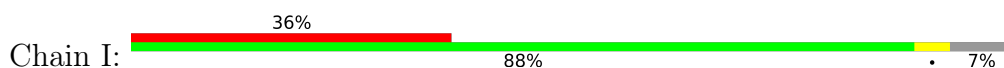
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4



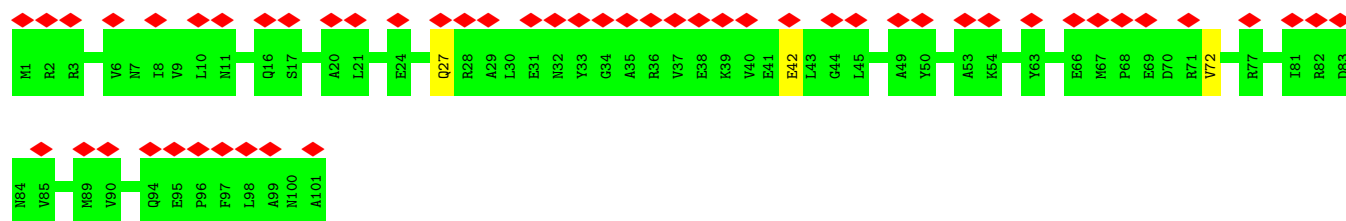
• Molecule 5: 30S ribosomal protein S5



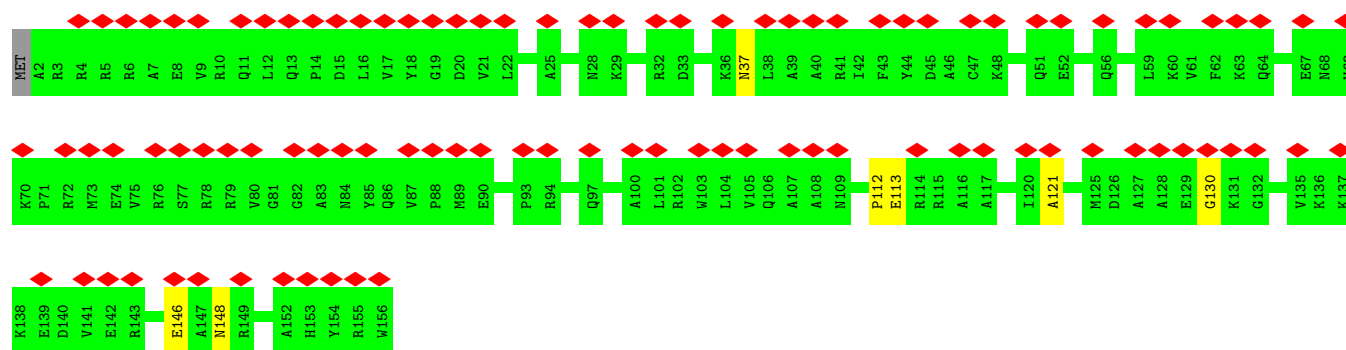
• Molecule 6: 30S ribosomal protein S6



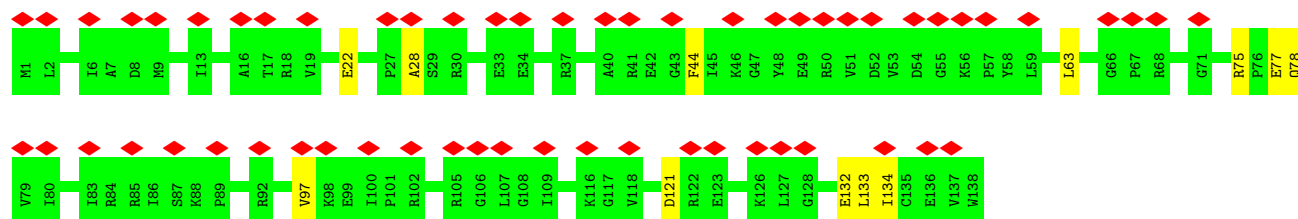
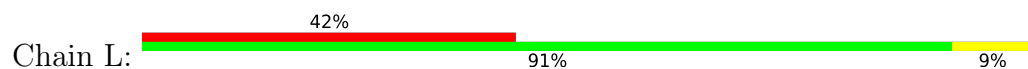




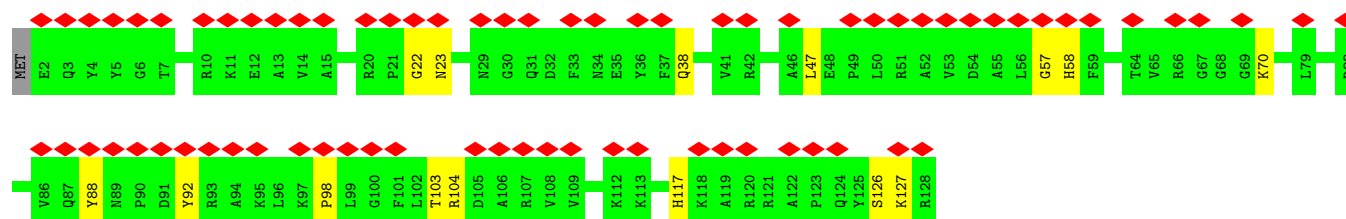
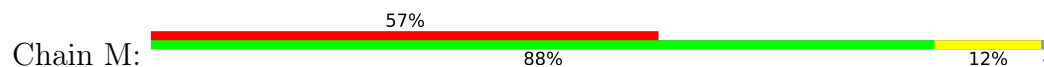
• Molecule 7: 30S ribosomal protein S7



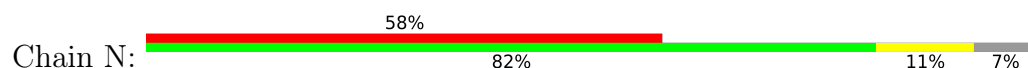
• Molecule 8: 30S ribosomal protein S8

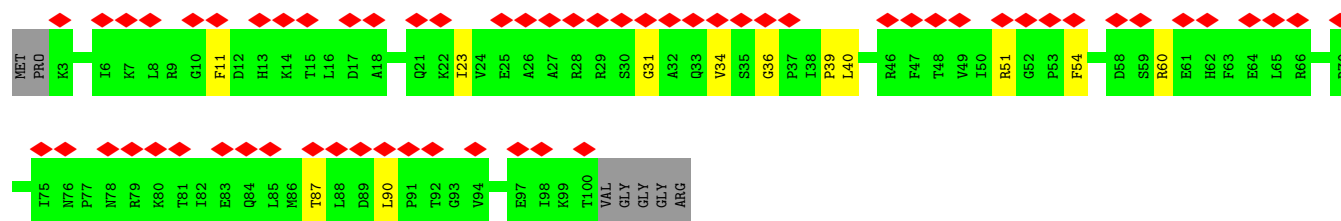


• Molecule 9: 30S ribosomal protein S9

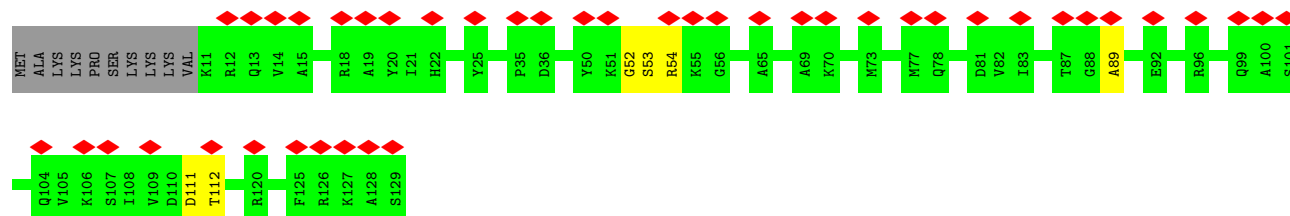
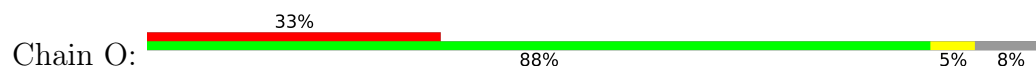


• Molecule 10: 30S ribosomal protein S10

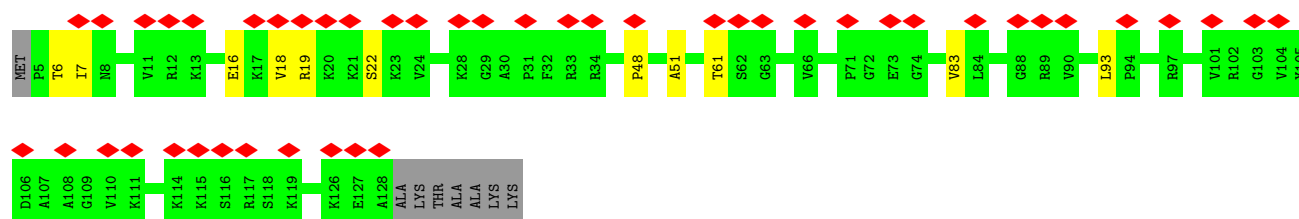
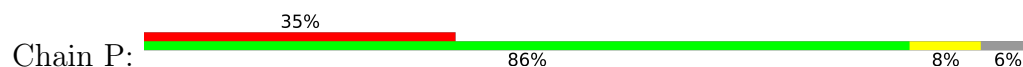




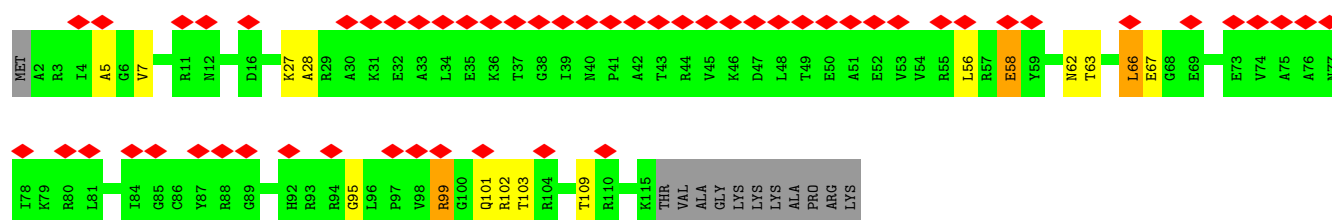
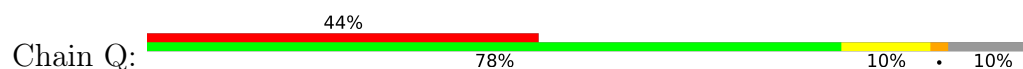
• Molecule 11: 30S ribosomal protein S11



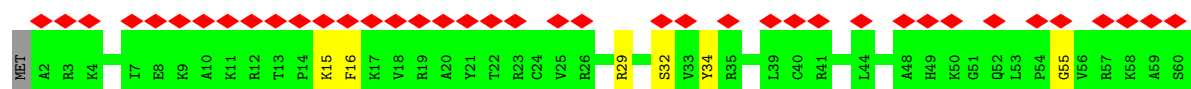
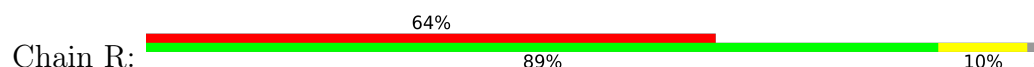
• Molecule 12: 30S ribosomal protein S12



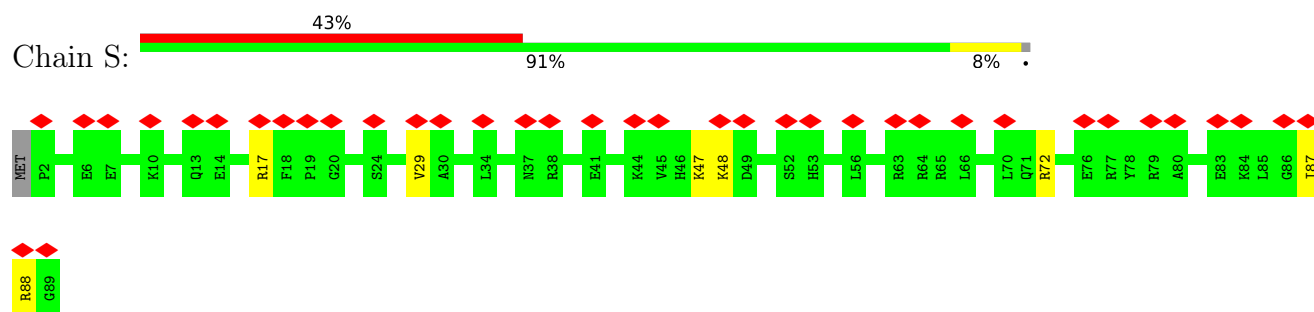
• Molecule 13: 30S ribosomal protein S13



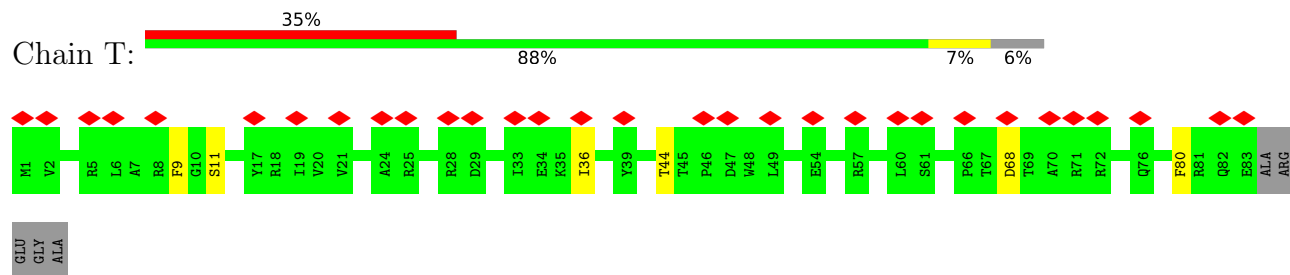
• Molecule 14: 30S ribosomal protein S14 type Z



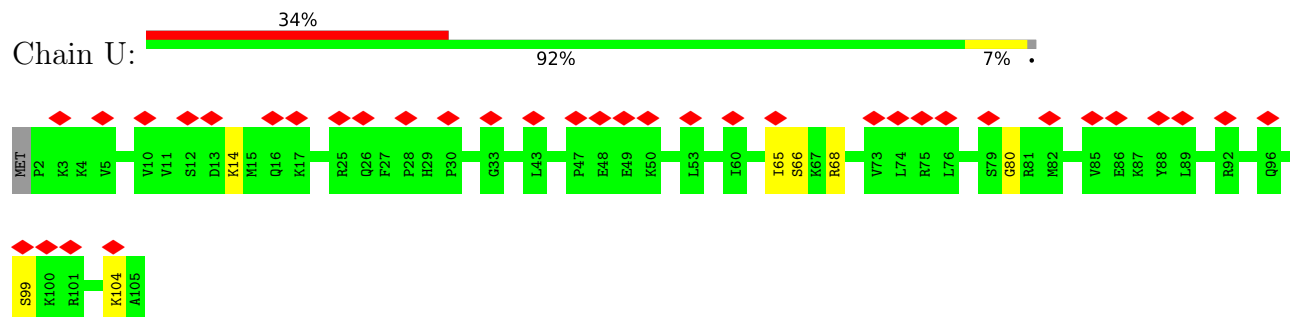
• Molecule 15: 30S ribosomal protein S15



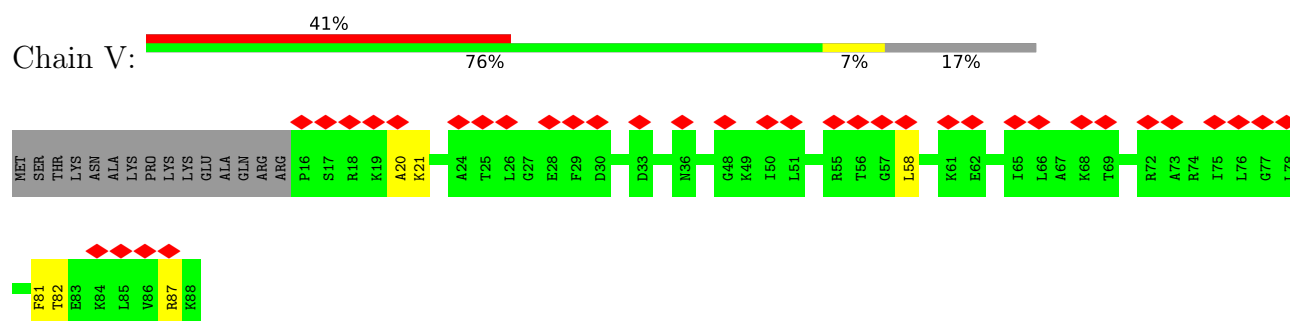
- Molecule 16: 30S ribosomal protein S16



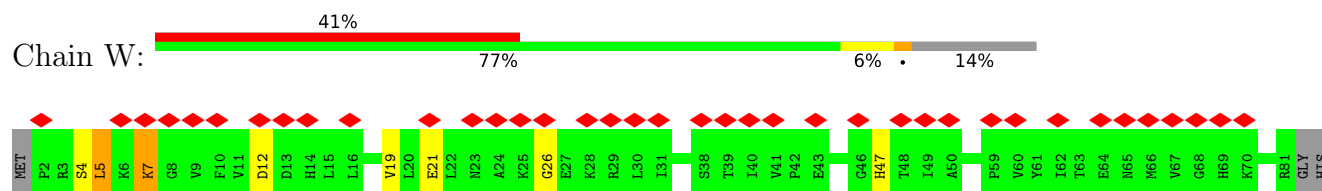
- Molecule 17: 30S ribosomal protein S17



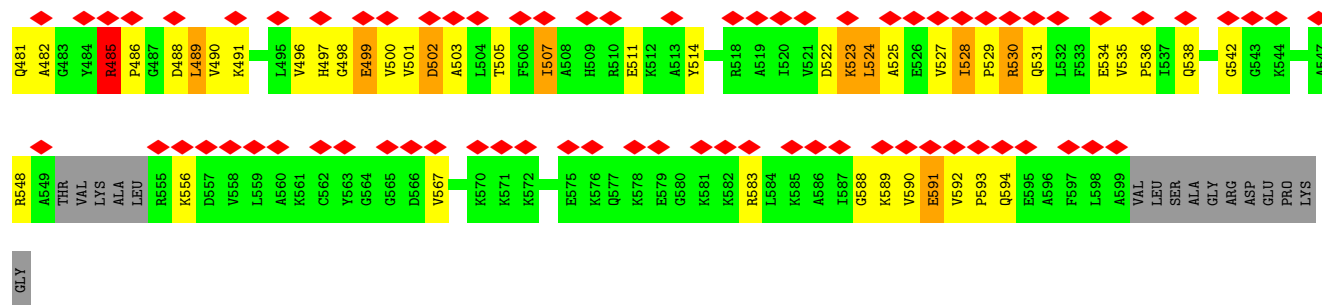
- Molecule 18: 30S ribosomal protein S18



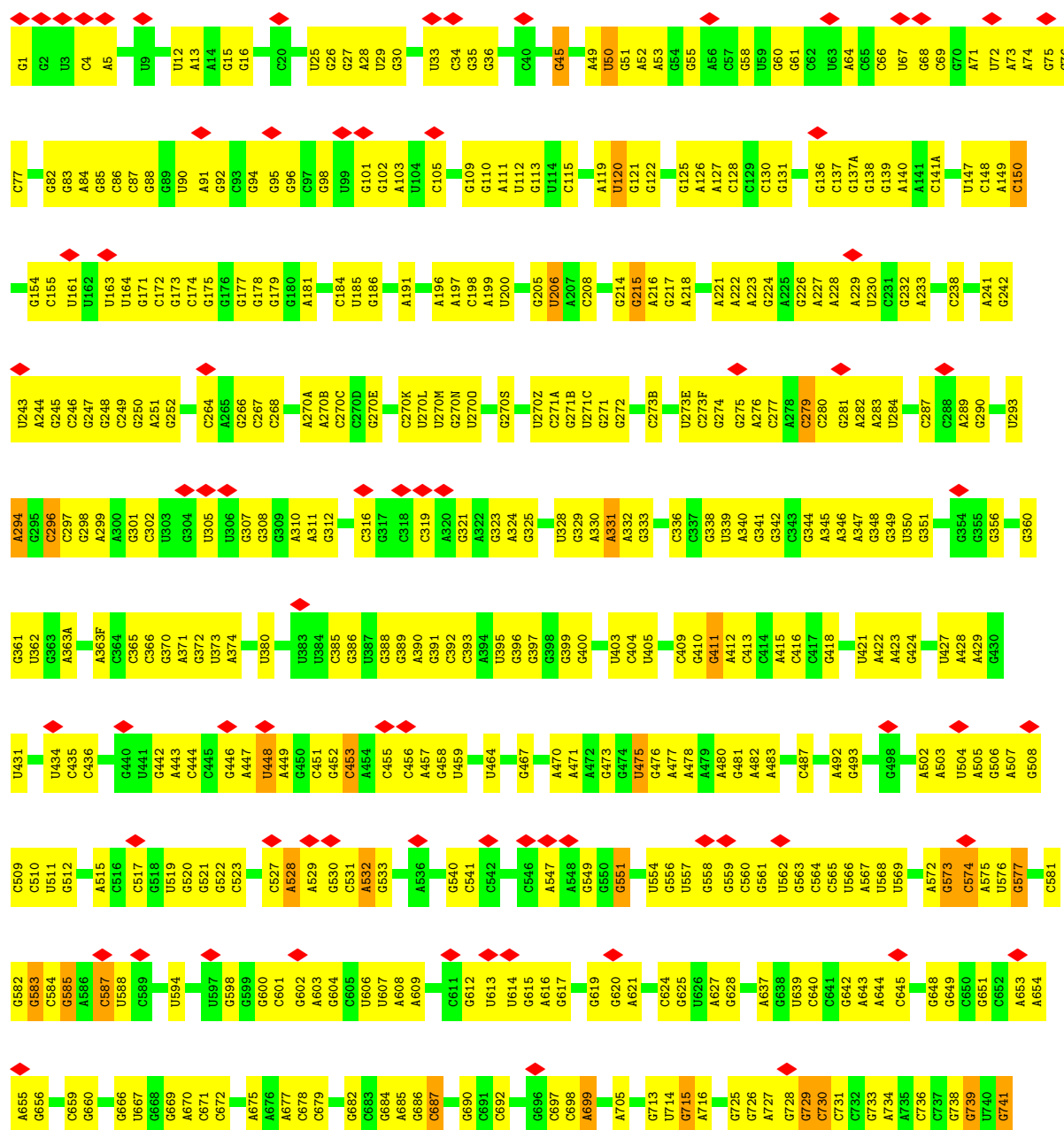
- Molecule 19: 30S ribosomal protein S19





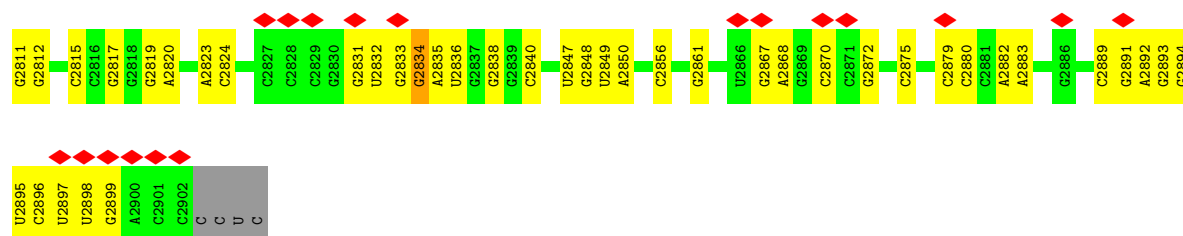


• Molecule 23: 23S ribosomal RNA

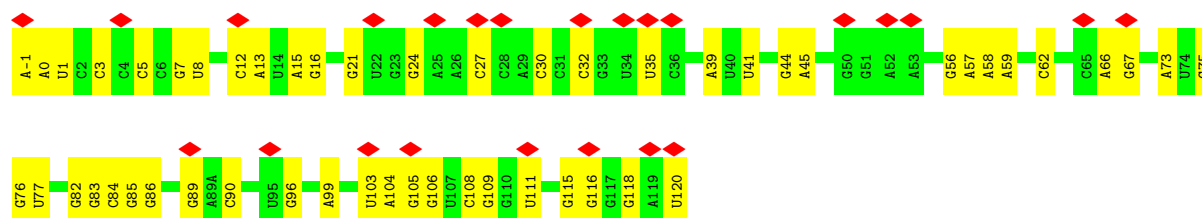




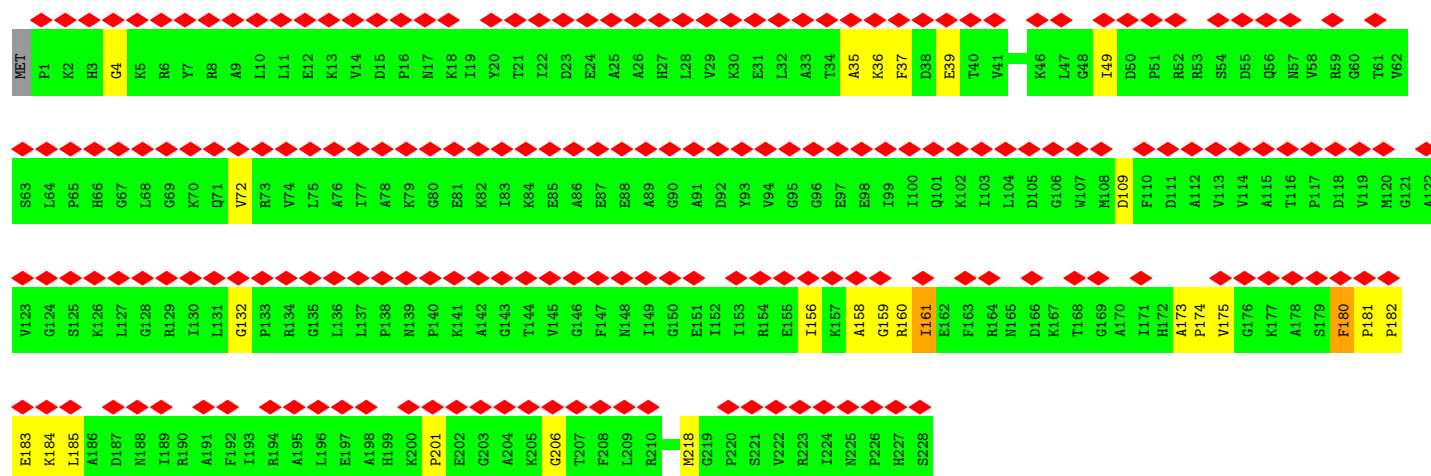
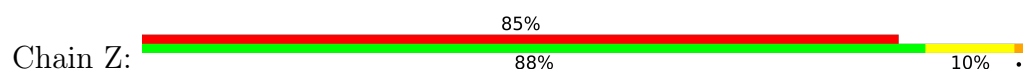
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	U1915		C2065	G2146		G2242	U2406		G2487				
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G1816	G1817		C2067	G2148		U2244	U2408		A2489				
G1817	A1919		U2068			U2245	G2409		U2491				
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A1819	G1921		G2070			A2247	C2417		U2493				
U1820				G2151		G2250	C2418						
A1821	C1924		G2003	G2152		G2251	C2419		C2496				
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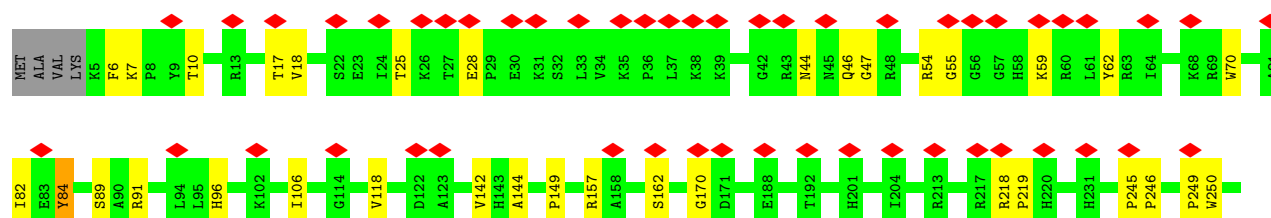
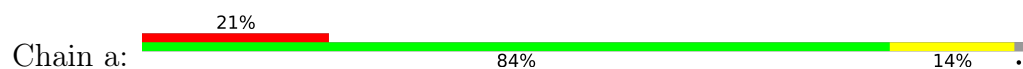
• Molecule 24: 5S ribosomal RNA



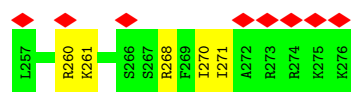
• Molecule 25: 50S ribosomal protein L1



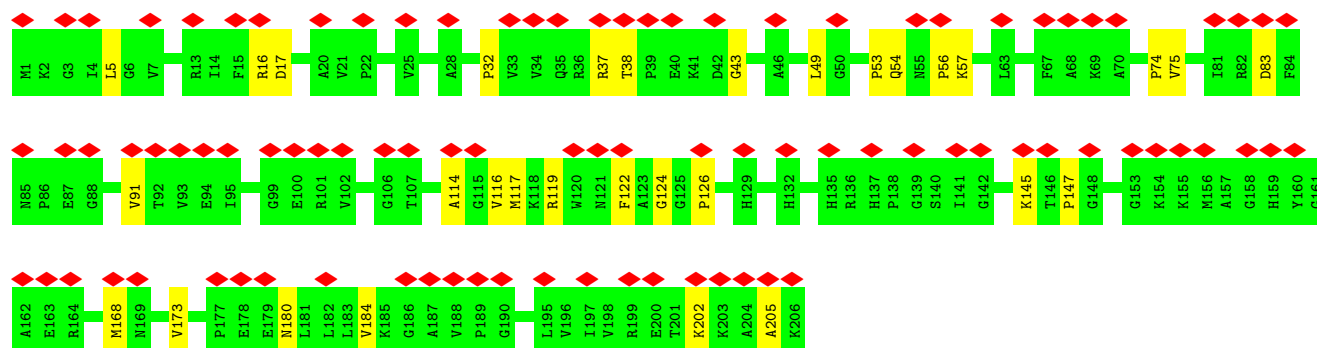
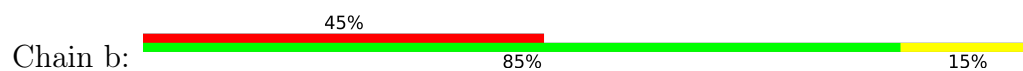
• Molecule 26: 50S ribosomal protein L2



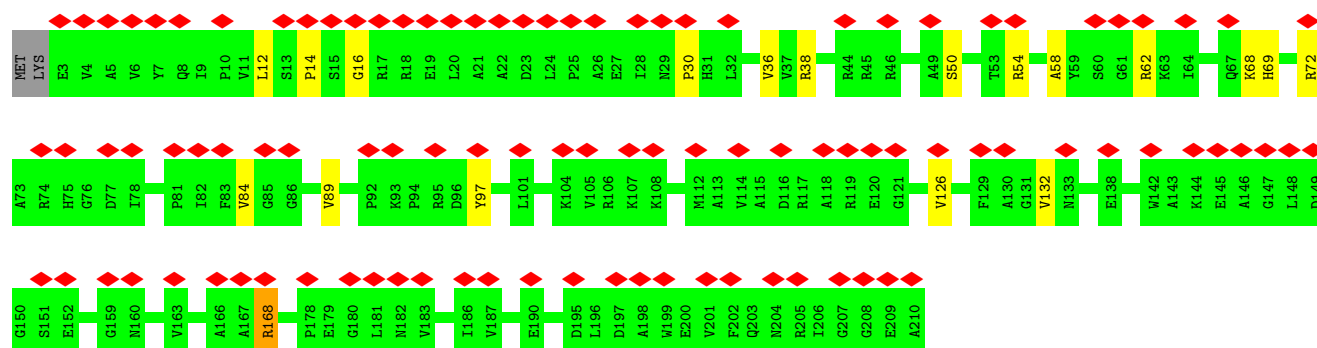
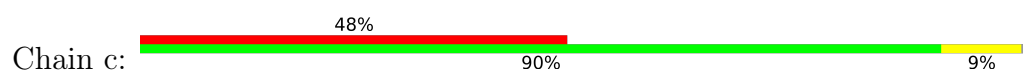




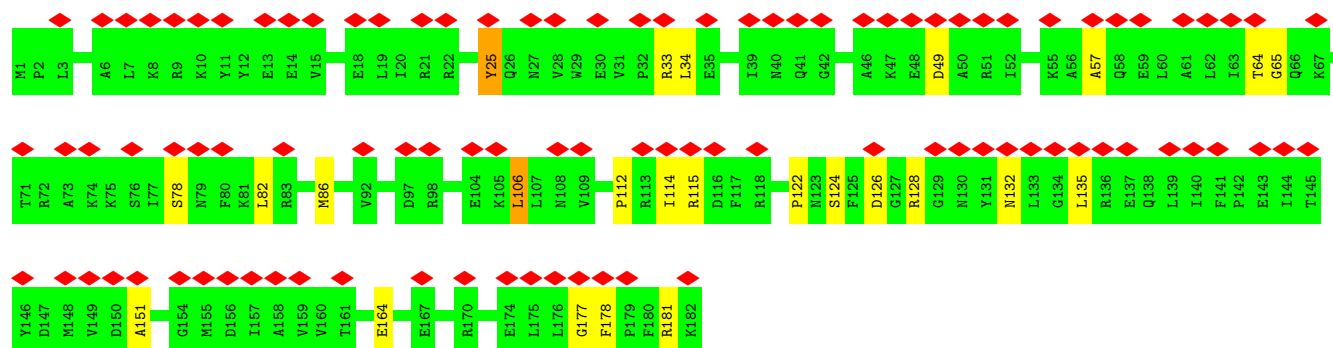
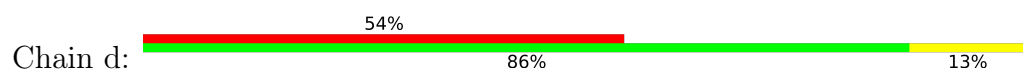
• Molecule 27: 50S ribosomal protein L3




• Molecule 28: 50S ribosomal protein L4

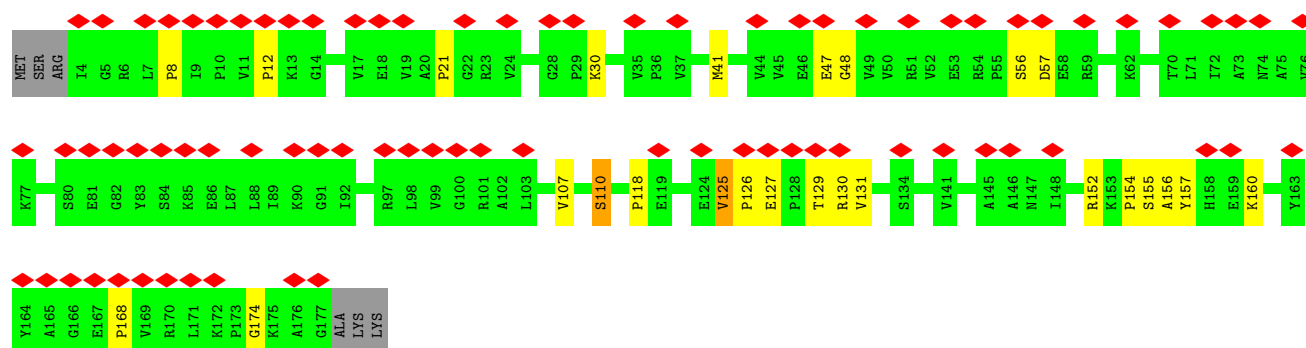


• Molecule 29: 50S ribosomal protein L5




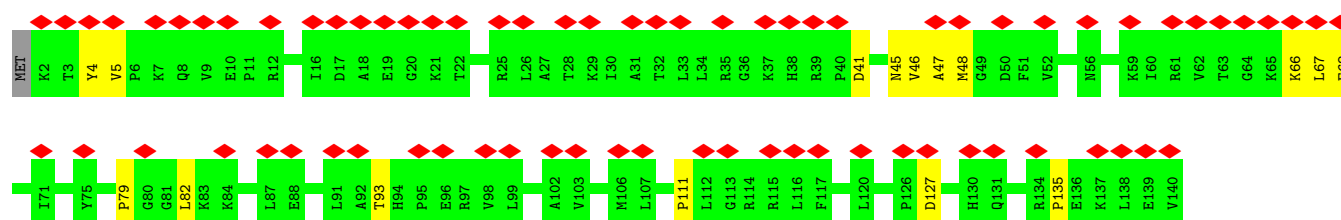
• Molecule 30: 50S ribosomal protein L6

Chain e: 

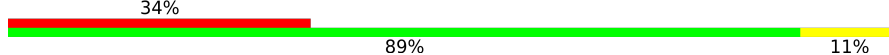


• Molecule 31: 50S ribosomal protein L13

Chain f: 




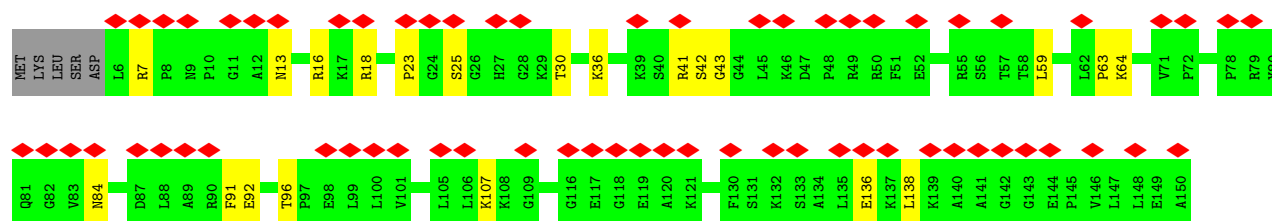
• Molecule 32: 50S ribosomal protein L14

Chain g: 




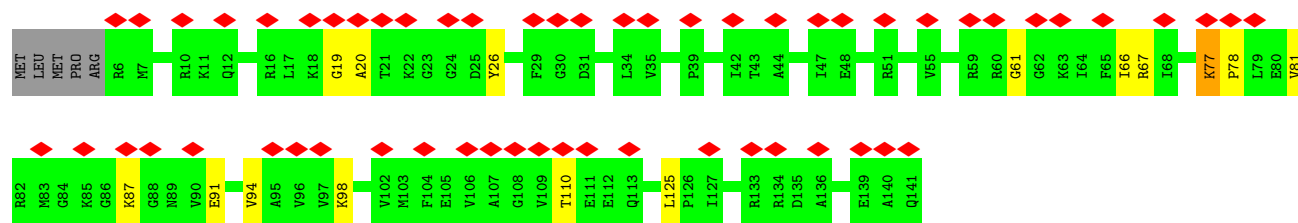
• Molecule 33: 50S ribosomal protein L15

Chain h: 

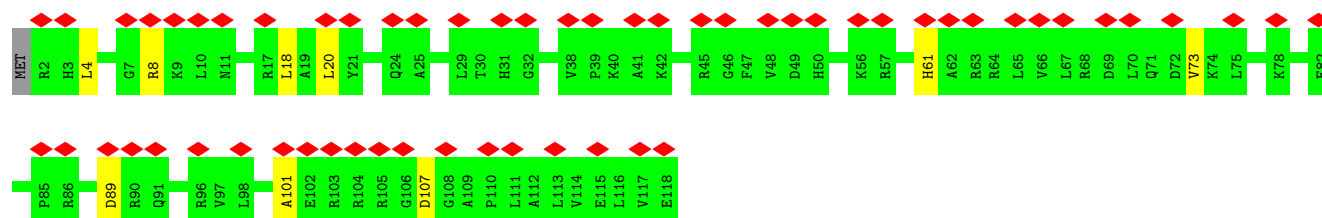
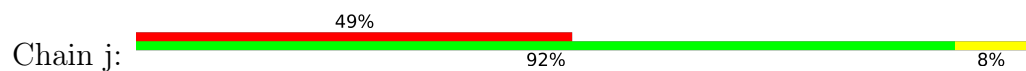


• Molecule 34: 50S ribosomal protein L16

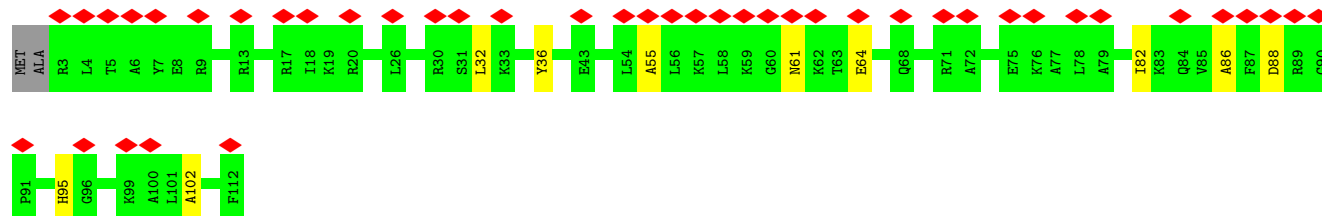
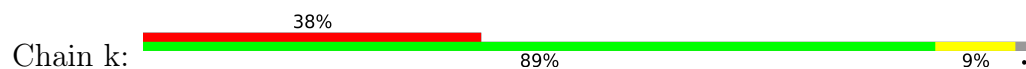
Chain i: 



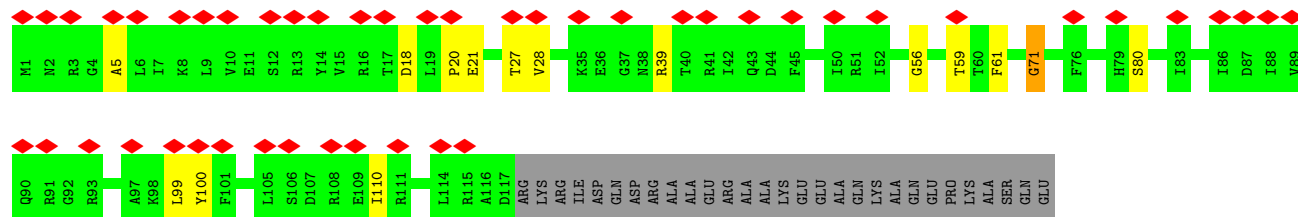
• Molecule 35: 50S ribosomal protein L17



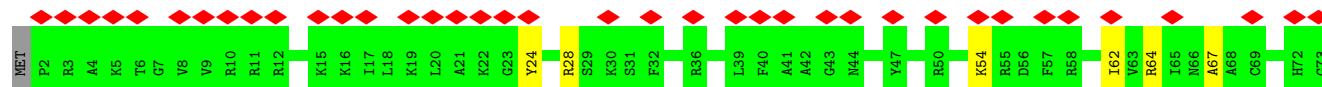
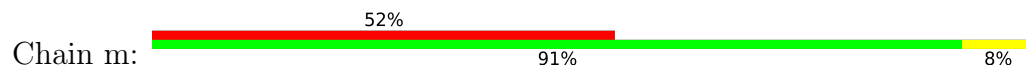
• Molecule 36: 50S ribosomal protein L18



• Molecule 37: 50S ribosomal protein L19

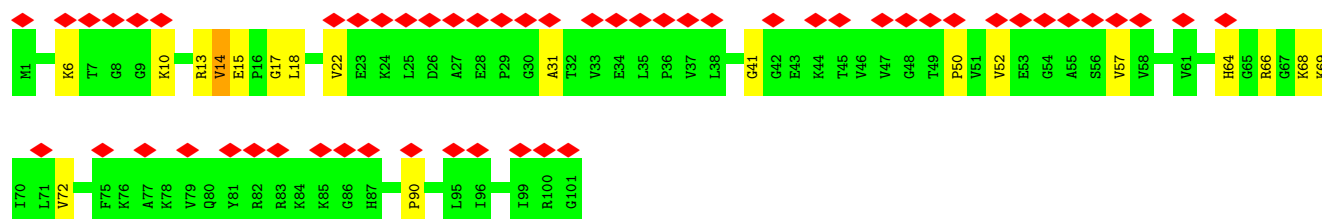
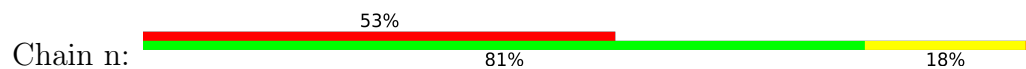


• Molecule 38: 50S ribosomal protein L20

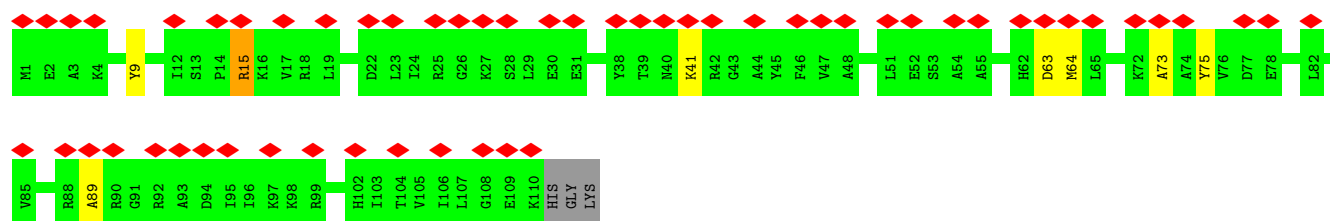
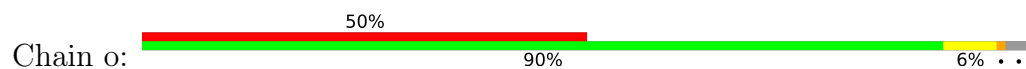




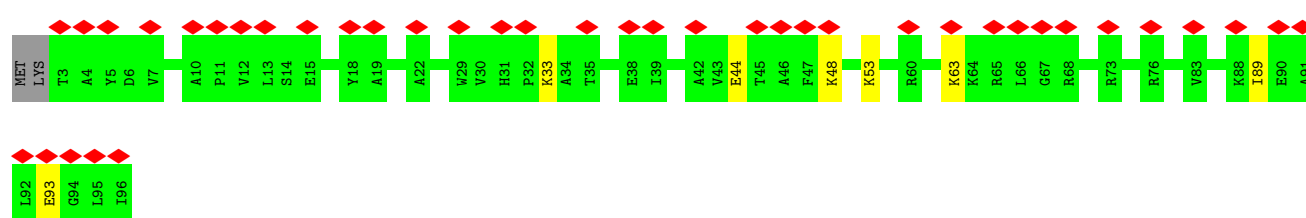
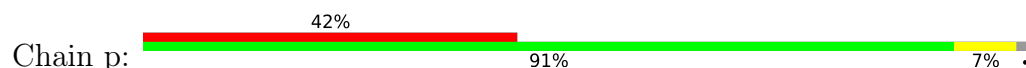
- Molecule 39: 50S ribosomal protein L21



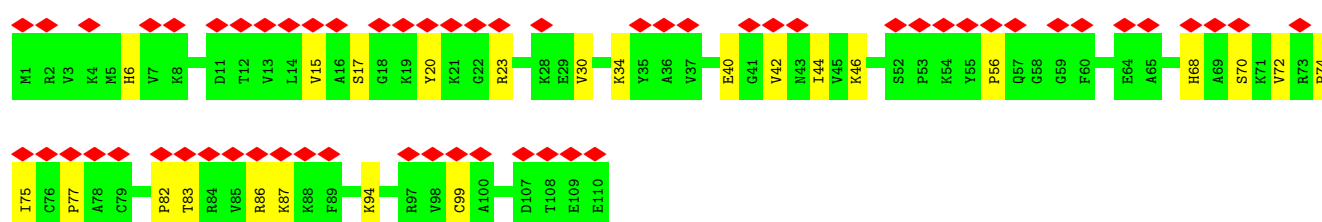
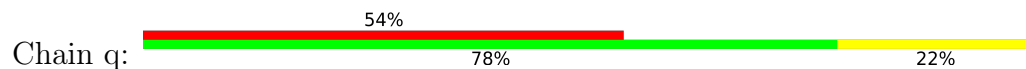
- Molecule 40: 50S ribosomal protein L22



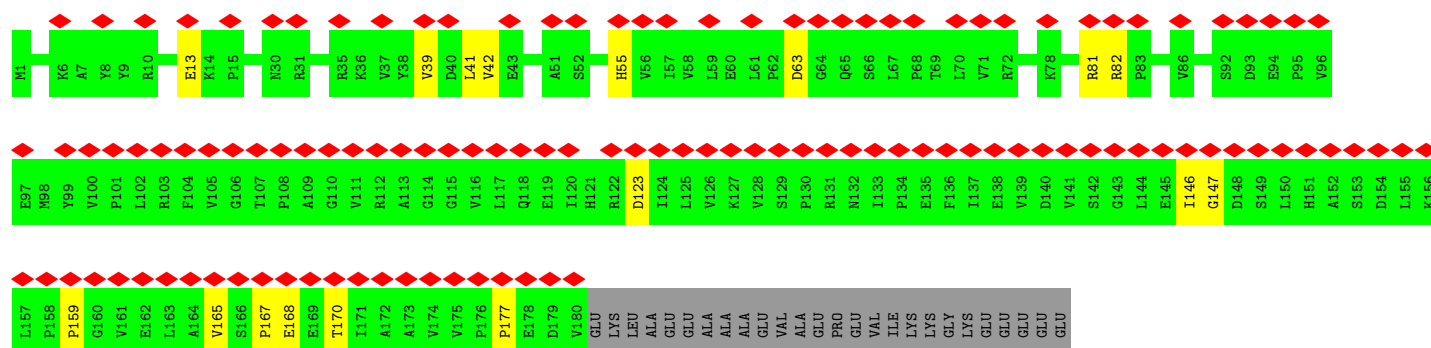
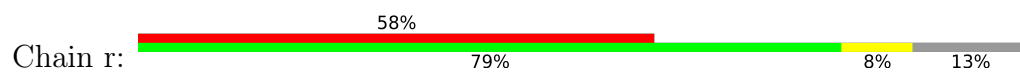
- Molecule 41: 50S ribosomal protein L23



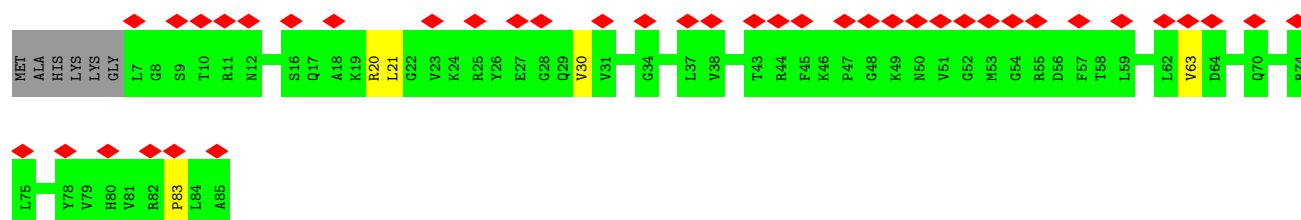
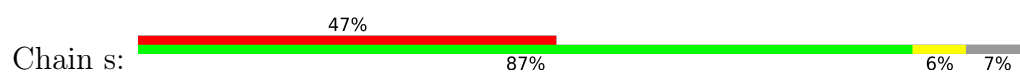
- Molecule 42: 50S ribosomal protein L24



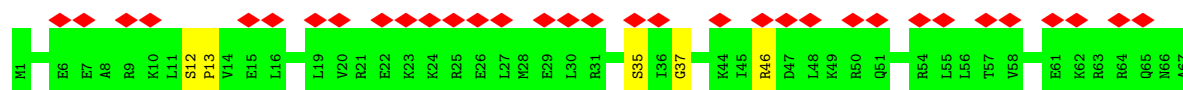
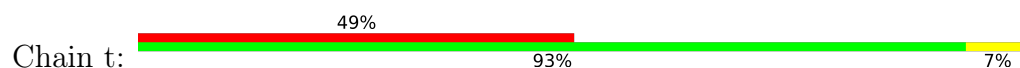
- Molecule 43: 50S ribosomal protein L25



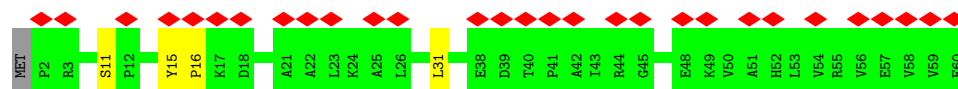
• Molecule 44: 50S ribosomal protein L27



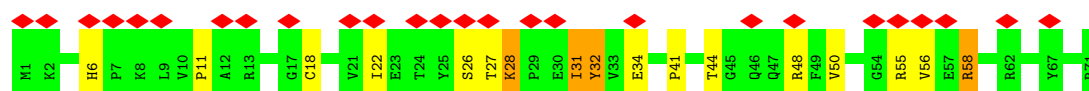
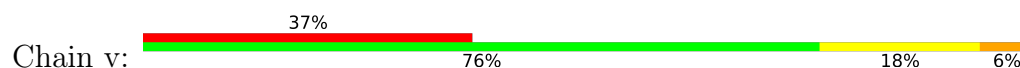
• Molecule 45: 50S ribosomal protein L29



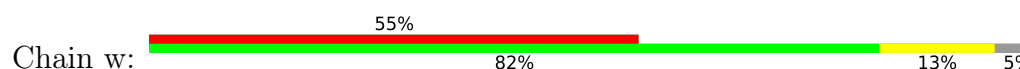
• Molecule 46: 50S ribosomal protein L30



• Molecule 47: 50S ribosomal protein L31

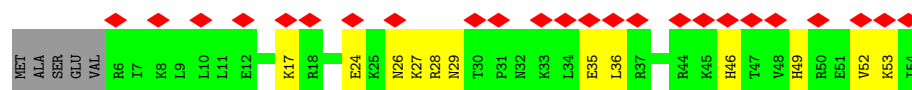


• Molecule 48: 50S ribosomal protein L32

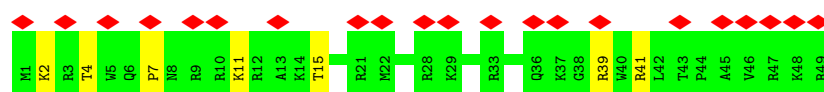
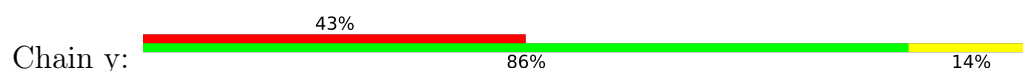




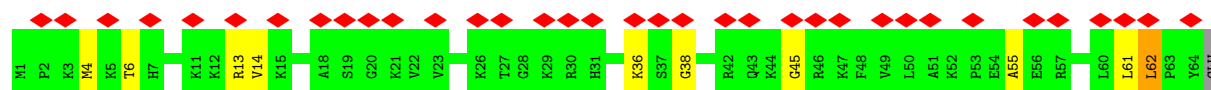
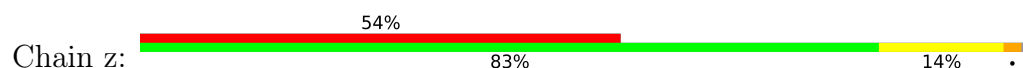
- Molecule 49: 50S ribosomal protein L33



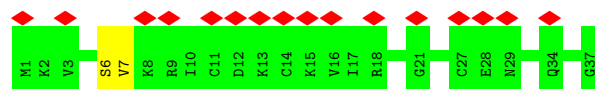
- Molecule 50: 50S ribosomal protein L34



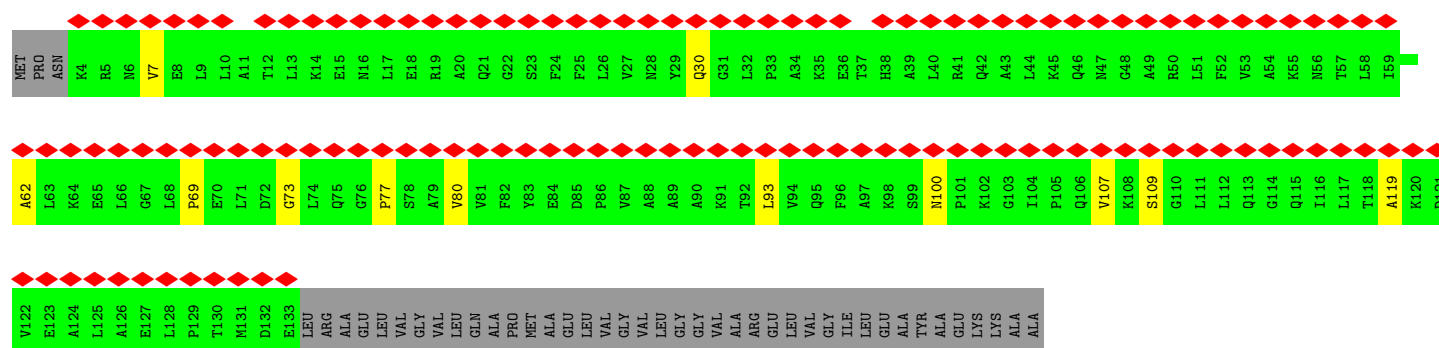
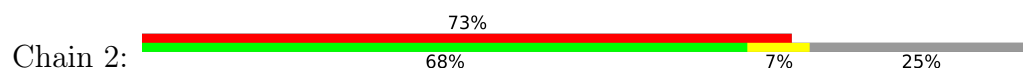
- Molecule 51: 50S ribosomal protein L35



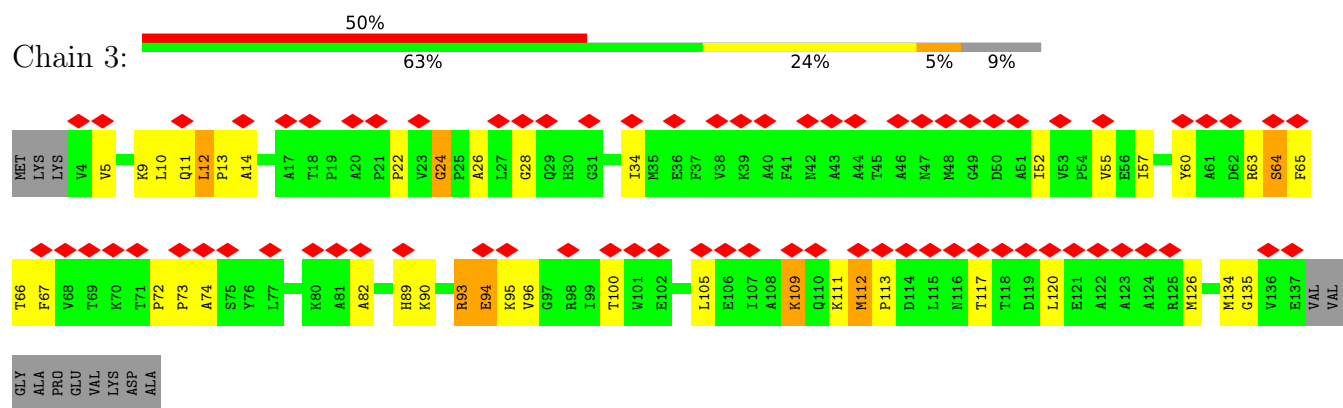
- Molecule 52: 50S ribosomal protein L36



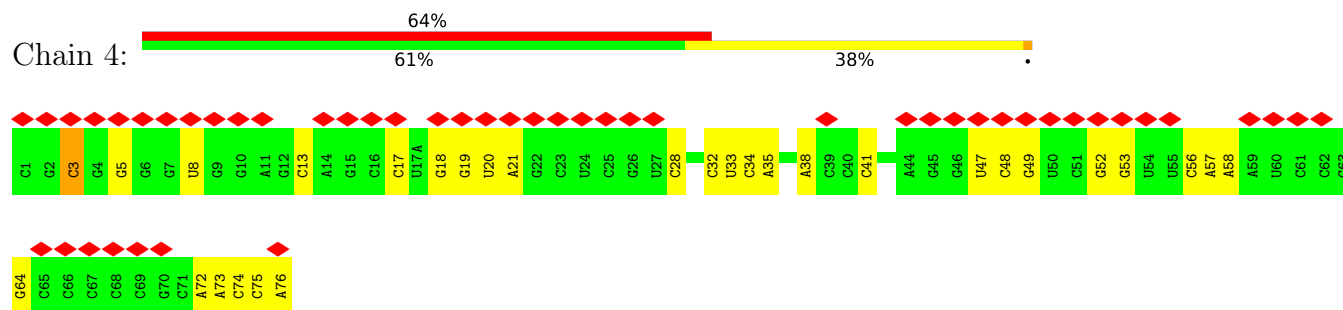
- Molecule 53: 50S ribosomal protein L10



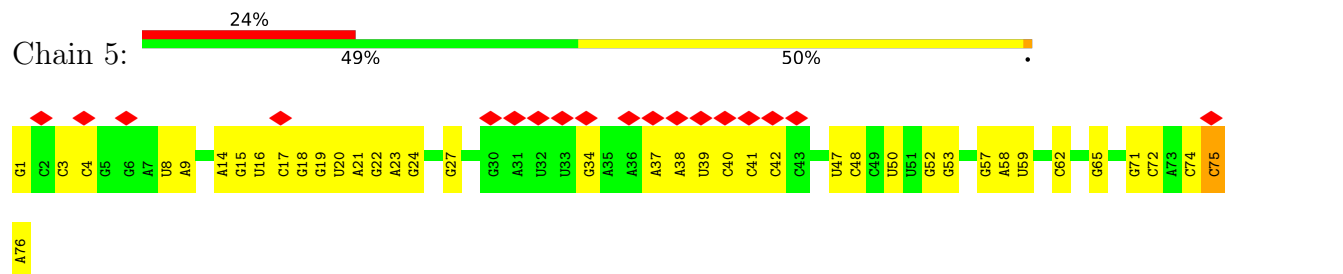
- Molecule 54: 50S ribosomal protein L11



- Molecule 55: P site- tRNA



- Molecule 56: E site- tRNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	22	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.959	Depositor
Minimum map value	-0.573	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.161	Depositor
Map size ( $\text{\AA}$ )	414.72, 414.72, 414.72	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.28, 1.28, 1.28	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GCP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.78	1/36438 (0.0%)	1.10	50/56869 (0.1%)
2	F	0.44	0/1935	0.72	1/2609 (0.0%)
3	G	0.42	0/1636	0.66	0/2205
4	H	0.49	0/1733	0.71	1/2318 (0.0%)
5	I	0.49	0/1162	0.76	0/1564
6	J	0.40	0/856	0.63	0/1154
7	K	0.38	0/1276	0.67	0/1709
8	L	0.48	0/1136	0.77	1/1527 (0.1%)
9	M	0.38	0/1029	0.65	0/1379
10	N	0.34	0/807	0.67	0/1085
11	O	0.39	0/900	0.63	0/1213
12	P	0.54	0/986	0.79	0/1320
13	Q	0.35	0/924	0.67	1/1238 (0.1%)
14	R	0.42	0/501	0.69	0/664
15	S	0.56	0/745	0.78	0/992
16	T	0.53	0/716	0.75	0/963
17	U	0.48	0/870	0.71	0/1159
18	V	0.41	0/603	0.72	1/799 (0.1%)
19	W	0.39	0/661	0.67	0/890
20	X	0.50	0/765	0.79	0/1007
21	Y	0.36	0/212	0.66	0/277
22	C	0.44	0/4545	0.57	25/6155 (0.4%)
23	D	0.97	10/69685 (0.0%)	1.24	293/108786 (0.3%)
24	E	0.82	1/2954 (0.0%)	1.09	2/4606 (0.0%)
25	Z	0.33	0/1775	0.58	2/2393 (0.1%)
26	a	0.57	1/2174 (0.0%)	0.80	1/2927 (0.0%)
27	b	0.54	0/1611	0.85	2/2171 (0.1%)
28	c	0.56	0/1660	0.78	0/2247
29	d	0.39	0/1507	0.73	2/2027 (0.1%)
30	e	0.47	0/1354	0.75	1/1831 (0.1%)
31	f	0.53	0/1140	0.79	2/1537 (0.1%)
32	g	0.52	0/942	0.80	0/1268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	h	0.48	0/1123	0.85	1/1493 (0.1%)
34	i	0.55	0/1100	0.81	1/1470 (0.1%)
35	j	0.52	0/974	0.73	0/1302
36	k	0.48	0/887	0.78	0/1180
37	l	0.52	0/990	0.81	1/1325 (0.1%)
38	m	0.60	0/982	0.79	0/1306
39	n	0.45	0/790	0.78	0/1057
40	o	0.52	0/886	0.71	0/1189
41	p	0.47	0/756	0.71	0/1015
42	q	0.43	0/857	0.78	0/1142
43	r	0.41	0/1467	0.70	0/1992
44	s	0.48	0/633	0.71	0/843
45	t	0.50	0/569	0.72	0/751
46	u	0.56	0/474	0.77	0/635
47	v	0.51	0/594	0.85	1/795 (0.1%)
48	w	0.56	0/459	0.76	0/621
49	x	0.49	0/433	0.87	0/576
50	y	0.58	0/438	0.78	0/575
51	z	0.57	0/523	0.83	0/690
52	1	0.46	0/310	0.72	0/407
53	2	0.23	0/640	0.45	0/889
54	3	0.43	0/1012	0.70	2/1373 (0.1%)
55	4	0.57	0/1832	0.96	1/2855 (0.0%)
56	5	1.93	7/1813 (0.4%)	1.02	3/2823 (0.1%)
All	All	0.81	20/165780 (0.0%)	1.07	395/247193 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1
8	L	0	1
26	a	0	5
28	c	0	3
30	e	0	1
31	f	0	1
32	g	0	1
37	l	0	2
38	m	0	1
39	n	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
40	o	0	1
41	p	0	1
42	q	0	1
46	u	0	1
47	v	0	1
49	x	0	1
51	z	0	1
54	3	0	2
All	All	0	26

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	5	75	C	N3-C4	39.72	1.61	1.33
56	5	75	C	N1-C6	36.95	1.59	1.37
56	5	75	C	C2-N3	36.64	1.65	1.35
56	5	75	C	C4-C5	26.84	1.64	1.43
56	5	75	C	N1-C2	25.86	1.66	1.40
56	5	75	C	C5-C6	24.77	1.54	1.34
24	E	-1	A	OP3-P	-10.77	1.48	1.61
23	D	1	G	OP3-P	-10.70	1.48	1.61
56	5	1	G	OP3-P	-10.68	1.48	1.61
23	D	1978	A	N9-C4	-6.54	1.33	1.37
23	D	2662	A	N9-C4	-5.91	1.34	1.37
26	a	250	TRP	CB-CG	-5.73	1.40	1.50
23	D	528	A	N9-C4	-5.45	1.34	1.37
23	D	515	A	N9-C4	-5.36	1.34	1.37
23	D	1681	G	N9-C4	-5.29	1.33	1.38
23	D	126	A	N9-C4	-5.26	1.34	1.37
1	A	120	A	N9-C4	-5.25	1.34	1.37
23	D	761	A	N9-C4	-5.18	1.34	1.37
23	D	699	A	N9-C4	-5.11	1.34	1.37
23	D	1206	G	N7-C5	-5.11	1.36	1.39

All (395) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	2075	U	N1-C2-O2	10.51	130.16	122.80
23	D	1498	C	C2-N1-C1'	10.33	130.16	118.80
23	D	2498	C	N1-C2-O2	9.67	124.70	118.90
23	D	2498	C	N3-C2-O2	-9.54	115.22	121.90
23	D	1937	A	N1-C6-N6	-9.37	112.98	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	576	U	N1-C2-O2	9.06	129.14	122.80
23	D	1498	C	N1-C2-O2	9.04	124.32	118.90
23	D	150	C	N1-C2-O2	9.01	124.31	118.90
23	D	453	C	N1-C2-O2	8.95	124.27	118.90
23	D	1955	U	C2-N1-C1'	8.89	128.37	117.70
23	D	2258	C	C2-N1-C1'	8.85	128.53	118.80
1	A	1328	C	N1-C2-O2	8.57	124.04	118.90
23	D	1498	C	C6-N1-C1'	-8.54	110.55	120.80
23	D	1638	C	C6-N1-C2	8.43	123.67	120.30
23	D	908	C	C2-N1-C1'	8.39	128.03	118.80
23	D	453	C	C2-N1-C1'	8.27	127.90	118.80
1	A	1113	C	C2-N1-C1'	8.08	127.69	118.80
23	D	2075	U	C2-N1-C1'	7.96	127.25	117.70
23	D	1978	A	C8-N9-C4	7.95	108.98	105.80
23	D	1258	C	C6-N1-C2	7.93	123.47	120.30
27	b	49	LEU	CA-CB-CG	7.93	133.55	115.30
23	D	2586	C	C2-N1-C1'	7.89	127.48	118.80
23	D	2499	C	N1-C2-O2	7.88	123.63	118.90
23	D	954	G	C8-N9-C4	7.86	109.55	106.40
23	D	908	C	N1-C2-O2	7.84	123.60	118.90
23	D	150	C	N3-C2-O2	-7.69	116.52	121.90
23	D	448	U	N1-C2-O2	7.67	128.17	122.80
1	A	1328	C	N3-C2-O2	-7.64	116.55	121.90
23	D	889	C	N1-C2-O2	7.40	123.34	118.90
23	D	1937	A	C6-C5-N7	7.38	137.46	132.30
23	D	2498	C	C2-N1-C1'	7.29	126.81	118.80
23	D	453	C	N3-C2-O2	-7.26	116.82	121.90
23	D	1920	C	C6-N1-C2	-7.25	117.40	120.30
23	D	2680	C	C6-N1-C2	7.21	123.18	120.30
23	D	1937	A	N9-C4-C5	7.11	108.65	105.80
23	D	138	G	N3-C4-C5	-7.08	125.06	128.60
23	D	150	C	O4'-C1'-N1	7.07	113.86	108.20
23	D	1498	C	N3-C2-O2	-7.06	116.96	121.90
2	F	100	GLY	N-CA-C	-7.05	95.46	113.10
23	D	409	C	C2-N1-C1'	6.98	126.48	118.80
1	A	808	C	C6-N1-C2	6.98	123.09	120.30
23	D	1604	C	C2-N1-C1'	6.92	126.42	118.80
23	D	1784	A	O4'-C1'-N9	6.89	113.71	108.20
23	D	1937	A	N3-C4-N9	-6.88	121.90	127.40
23	D	775	G	N3-C4-C5	-6.86	125.17	128.60
23	D	2682	U	N1-C2-O2	6.85	127.59	122.80
23	D	741	G	C8-N9-C4	-6.79	103.69	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	1493	C	O5'-P-OP2	-6.78	99.59	105.70
23	D	296	C	O4'-C1'-N1	6.75	113.60	108.20
23	D	2258	C	N1-C2-O2	6.75	122.95	118.90
23	D	1605	C	C6-N1-C2	-6.73	117.61	120.30
23	D	50	U	C5-C6-N1	6.72	126.06	122.70
23	D	208	C	C6-N1-C2	6.71	122.98	120.30
37	I	71	GLY	N-CA-C	-6.70	96.36	113.10
1	A	1320	C	C5-C6-N1	6.69	124.34	121.00
23	D	2258	C	C6-N1-C1'	-6.68	112.78	120.80
1	A	1320	C	C6-N1-C2	-6.68	117.63	120.30
23	D	749	C	C6-N1-C2	6.68	122.97	120.30
23	D	448	U	N3-C2-O2	-6.67	117.53	122.20
23	D	2682	U	N3-C2-O2	-6.67	117.53	122.20
1	A	48	C	N1-C2-O2	6.64	122.88	118.90
23	D	576	U	N3-C2-O2	-6.62	117.57	122.20
1	A	1113	C	N1-C2-O2	6.61	122.87	118.90
23	D	2075	U	N3-C2-O2	-6.60	117.58	122.20
23	D	889	C	C2-N1-C1'	6.60	126.06	118.80
1	A	308	C	N1-C2-O2	6.59	122.86	118.90
23	D	773	U	N3-C2-O2	-6.59	117.59	122.20
1	A	390	C	C6-N1-C2	6.59	122.94	120.30
23	D	1352	U	C5-C6-N1	-6.58	119.41	122.70
23	D	2605	U	N1-C2-N3	6.57	118.84	114.90
23	D	487	C	C2-N1-C1'	6.55	126.01	118.80
1	A	1320	C	C2-N1-C1'	6.55	126.00	118.80
23	D	1559	G	C2-N3-C4	6.54	115.17	111.90
23	D	1914	C	C2-N1-C1'	6.54	125.99	118.80
23	D	1681	G	N3-C4-C5	6.53	131.87	128.60
23	D	453	C	C6-N1-C1'	-6.53	112.96	120.80
23	D	2591	C	N3-C2-O2	-6.48	117.37	121.90
56	5	75	C	N1-C2-N3	-6.47	114.67	119.20
23	D	1914	C	N1-C2-O2	6.47	122.78	118.90
23	D	1955	U	C5-C6-N1	6.46	125.93	122.70
23	D	1131	G	O4'-C1'-N9	6.44	113.35	108.20
23	D	1493	C	C2-N1-C1'	6.41	125.86	118.80
23	D	573	G	C8-N9-C4	-6.40	103.84	106.40
23	D	2075	U	C2-N3-C4	6.40	130.84	127.00
1	A	308	C	N3-C2-O2	-6.38	117.43	121.90
23	D	908	C	C6-N1-C1'	-6.37	113.16	120.80
23	D	1990	C	N3-C4-C5	6.37	124.45	121.90
23	D	678	C	C6-N1-C2	6.35	122.84	120.30
23	D	1298	C	N3-C2-O2	-6.35	117.45	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	2432	A	O4'-C1'-N9	6.35	113.28	108.20
1	A	713	G	O4'-C1'-N9	6.33	113.26	108.20
56	5	75	C	N1-C2-O2	6.32	122.69	118.90
23	D	1937	A	C5-C6-N6	6.31	128.75	123.70
23	D	991	C	C6-N1-C2	6.28	122.81	120.30
23	D	2772	C	N1-C2-O2	6.25	122.65	118.90
1	A	308	C	C2-N1-C1'	6.25	125.67	118.80
23	D	2589	A	C6-N1-C2	-6.25	114.85	118.60
1	A	868	C	N3-C2-O2	-6.24	117.53	121.90
23	D	582	G	N9-C4-C5	-6.24	102.91	105.40
23	D	2308	G	N3-C4-C5	-6.23	125.48	128.60
23	D	1616	A	C8-N9-C4	6.22	108.29	105.80
23	D	2680	C	N3-C4-C5	6.22	124.39	121.90
23	D	1681	G	N3-C4-N9	-6.19	122.29	126.00
26	a	47	GLY	N-CA-C	-6.19	97.62	113.10
23	D	2772	C	N3-C2-O2	-6.19	117.57	121.90
23	D	787	U	O4'-C1'-N1	6.18	113.14	108.20
23	D	2433	A	C8-N9-C4	-6.18	103.33	105.80
23	D	1888	G	C4-N9-C1'	6.17	134.52	126.50
23	D	1626	G	O4'-C1'-N9	-6.16	103.27	108.20
23	D	319	C	C6-N1-C2	-6.16	117.84	120.30
23	D	1955	U	C6-N1-C1'	-6.15	112.60	121.20
23	D	587	C	C6-N1-C2	6.14	122.76	120.30
23	D	1947	C	N3-C2-O2	-6.14	117.60	121.90
23	D	137	C	N1-C2-O2	6.14	122.58	118.90
23	D	2834	G	C8-N9-C4	-6.13	103.95	106.40
23	D	2586	C	C6-N1-C1'	-6.12	113.45	120.80
23	D	1571	A	C2-N3-C4	6.12	113.66	110.60
23	D	1604	C	C6-N1-C2	-6.10	117.86	120.30
23	D	659	C	C6-N1-C2	6.10	122.74	120.30
23	D	1559	G	N3-C4-C5	-6.09	125.55	128.60
23	D	2075	U	C6-N1-C1'	-6.08	112.68	121.20
23	D	409	C	N1-C2-O2	6.07	122.54	118.90
23	D	2196	C	N3-C2-O2	-6.05	117.66	121.90
23	D	2607	G	C8-N9-C1'	-6.05	119.13	127.00
23	D	1778	U	N1-C2-N3	6.05	118.53	114.90
23	D	739	G	O4'-C1'-N9	6.03	113.02	108.20
23	D	1206	G	C6-C5-N7	-6.01	126.79	130.40
23	D	2605	U	O4'-C1'-N1	6.00	113.00	108.20
23	D	409	C	C6-N1-C1'	-5.99	113.61	120.80
23	D	1947	C	C2-N1-C1'	5.99	125.39	118.80
23	D	850	C	C6-N1-C2	5.99	122.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	838	C	C6-N1-C2	5.97	122.69	120.30
23	D	294	A	O4'-C1'-N9	5.95	112.96	108.20
23	D	1815	A	O4'-C1'-N9	5.95	112.96	108.20
23	D	1221	C	N1-C2-O2	5.94	122.47	118.90
1	A	1113	C	C6-N1-C1'	-5.93	113.69	120.80
23	D	1199	U	N1-C2-O2	5.93	126.95	122.80
23	D	2289	G	C8-N9-C4	5.92	108.77	106.40
23	D	773	U	N1-C2-O2	5.92	126.94	122.80
23	D	992	C	C6-N1-C2	5.90	122.66	120.30
23	D	2591	C	C6-N1-C2	-5.89	117.94	120.30
23	D	1785	A	N7-C8-N9	5.89	116.75	113.80
1	A	48	C	N3-C2-O2	-5.89	117.78	121.90
23	D	2447	G	C8-N9-C4	-5.89	104.05	106.40
23	D	2605	U	N3-C2-O2	-5.88	118.08	122.20
23	D	206	U	C2-N1-C1'	-5.88	110.64	117.70
23	D	889	C	N3-C2-O2	-5.88	117.79	121.90
23	D	1771	C	C2-N3-C4	-5.87	116.97	119.90
23	D	1974	C	C5-C6-N1	-5.87	118.07	121.00
23	D	2499	C	N3-C2-O2	-5.86	117.80	121.90
23	D	1656	C	C5-C6-N1	-5.86	118.07	121.00
23	D	582	G	C4-C5-N7	5.83	113.13	110.80
23	D	2433	A	O4'-C1'-N9	5.82	112.86	108.20
23	D	1807	G	N3-C4-N9	-5.82	122.51	126.00
56	5	75	C	N3-C4-C5	-5.82	119.57	121.90
23	D	1816	G	C8-N9-C4	5.81	108.72	106.40
23	D	1836	C	C5-C6-N1	-5.79	118.10	121.00
55	4	3	C	C2-N1-C1'	5.79	125.17	118.80
23	D	736	C	C6-N1-C2	5.78	122.61	120.30
23	D	2067	G	C8-N9-C4	5.78	108.71	106.40
23	D	573	G	N7-C8-N9	5.76	115.98	113.10
23	D	2787	C	C6-N1-C2	-5.76	118.00	120.30
23	D	576	U	C2-N1-C1'	5.75	124.60	117.70
23	D	1774	C	N3-C4-C5	5.75	124.20	121.90
23	D	2196	C	N1-C2-O2	5.75	122.35	118.90
23	D	2586	C	N1-C2-O2	5.75	122.35	118.90
23	D	1320	C	C5-C6-N1	-5.75	118.13	121.00
23	D	1980	G	N3-C4-N9	5.74	129.44	126.00
23	D	2308	G	N3-C4-N9	5.73	129.44	126.00
23	D	577	G	O4'-C1'-N9	5.73	112.78	108.20
23	D	1559	G	N3-C4-N9	5.72	129.43	126.00
23	D	1937	A	C8-N9-C1'	5.71	137.99	127.70
23	D	954	G	N7-C8-N9	-5.71	110.24	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1173	G	C5-C6-O6	-5.71	125.17	128.60
23	D	1667	G	C4-N9-C1'	5.71	133.92	126.50
23	D	279	C	N3-C4-N4	-5.70	114.01	118.00
23	D	1634	A	C8-N9-C4	5.70	108.08	105.80
1	A	651	C	C2-N1-C1'	5.70	125.07	118.80
23	D	1903	G	N3-C4-N9	5.70	129.42	126.00
23	D	206	U	N1-C2-O2	-5.69	118.82	122.80
1	A	295	C	C6-N1-C2	5.68	122.57	120.30
23	D	741	G	O4'-C1'-N9	5.68	112.74	108.20
23	D	540	G	N3-C4-C5	5.67	131.44	128.60
23	D	1605	C	N3-C2-O2	-5.67	117.93	121.90
1	A	821	G	C8-N9-C4	5.67	108.67	106.40
1	A	689	C	C5-C6-N1	5.66	123.83	121.00
23	D	2787	C	C2-N1-C1'	5.66	125.02	118.80
23	D	45	G	C4-N9-C1'	-5.65	119.16	126.50
23	D	2714	G	C8-N9-C4	5.64	108.66	106.40
23	D	1667	G	C8-N9-C1'	-5.63	119.67	127.00
23	D	697	C	C6-N1-C2	5.62	122.55	120.30
23	D	2787	C	N3-C2-O2	-5.61	117.97	121.90
23	D	908	C	N3-C2-O2	-5.61	117.98	121.90
23	D	1667	G	N3-C4-N9	5.59	129.35	126.00
23	D	2582	G	N3-C4-C5	-5.59	125.81	128.60
23	D	1947	C	N1-C2-O2	5.58	122.25	118.90
23	D	1937	A	C4-C5-C6	-5.58	114.21	117.00
23	D	2767	C	N1-C2-O2	5.58	122.25	118.90
23	D	729	G	C8-N9-C4	-5.58	104.17	106.40
23	D	1656	C	C6-N1-C2	5.58	122.53	120.30
23	D	1778	U	O4'-C1'-N1	5.58	112.66	108.20
23	D	730	C	C6-N1-C2	-5.57	118.07	120.30
31	f	67	LEU	CA-CB-CG	5.57	128.11	115.30
1	A	670	G	N3-C4-N9	5.54	129.32	126.00
23	D	1978	A	N7-C8-N9	-5.54	111.03	113.80
23	D	1616	A	N9-C4-C5	-5.54	103.58	105.80
23	D	2517	C	N3-C2-O2	-5.54	118.02	121.90
23	D	2782	G	N1-C6-O6	5.54	123.22	119.90
23	D	974	G	N1-C6-O6	5.54	123.22	119.90
23	D	2607	G	C4-N9-C1'	5.53	133.69	126.50
23	D	2729	G	C8-N9-C4	5.52	108.61	106.40
23	D	2572	A	P-O3'-C3'	5.52	126.33	119.70
23	D	2682	U	C2-N1-C1'	5.52	124.32	117.70
23	D	2580	U	N1-C2-O2	5.51	126.66	122.80
1	A	295	C	C5-C6-N1	-5.50	118.25	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	1351	C	C5-C6-N1	-5.49	118.25	121.00
23	D	1627	G	N3-C4-N9	-5.49	122.70	126.00
23	D	487	C	C6-N1-C1'	-5.49	114.21	120.80
23	D	741	G	N3-C4-C5	-5.49	125.86	128.60
1	A	1469	G	C8-N9-C4	5.48	108.59	106.40
23	D	576	U	C6-N1-C1'	-5.48	113.53	121.20
23	D	2027	G	O4'-C1'-N9	5.48	112.58	108.20
23	D	2785	C	N3-C4-C5	5.48	124.09	121.90
23	D	738	G	C4-N9-C1'	5.47	133.62	126.50
1	A	651	C	N1-C2-O2	5.47	122.18	118.90
23	D	238	C	N3-C2-O2	-5.47	118.07	121.90
23	D	297	C	C2-N1-C1'	5.46	124.81	118.80
23	D	1809	A	N1-C6-N6	-5.46	115.32	118.60
25	Z	173	ALA	C-N-CD	-5.46	108.58	120.60
23	D	418	G	C8-N9-C4	5.46	108.58	106.40
23	D	1627	G	N3-C4-C5	5.46	131.33	128.60
23	D	532	A	O4'-C1'-N9	5.45	112.56	108.20
23	D	448	U	C2-N1-C1'	5.45	124.24	117.70
23	D	2258	C	C5-C6-N1	5.45	123.73	121.00
23	D	1937	A	C4-N9-C1'	-5.45	116.50	126.30
33	h	43	GLY	N-CA-C	-5.43	99.52	113.10
23	D	2576	G	C4-N9-C1'	5.43	133.56	126.50
23	D	397	G	C8-N9-C4	5.42	108.57	106.40
1	A	1415	G	N3-C4-N9	-5.41	122.75	126.00
23	D	2158	A	P-O3'-C3'	5.40	126.18	119.70
1	A	1113	C	N3-C2-O2	-5.39	118.13	121.90
23	D	2586	C	N3-C2-O2	-5.39	118.13	121.90
23	D	738	G	N3-C4-N9	5.38	129.23	126.00
23	D	741	G	N7-C8-N9	5.38	115.79	113.10
23	D	777	A	N1-C2-N3	5.38	131.99	129.30
23	D	585	G	C8-N9-C4	-5.36	104.26	106.40
23	D	487	C	N1-C2-O2	5.36	122.11	118.90
23	D	787	U	C2-N1-C1'	-5.36	111.27	117.70
23	D	583	G	C4-N9-C1'	-5.36	119.54	126.50
23	D	238	C	O4'-C1'-N1	5.34	112.48	108.20
23	D	2308	G	C2-N3-C4	5.34	114.57	111.90
1	A	880	C	O4'-C1'-N1	5.33	112.46	108.20
23	D	551	G	N3-C4-N9	5.32	129.19	126.00
23	D	2662	A	C8-N9-C4	5.32	107.93	105.80
23	D	1888	G	C8-N9-C1'	-5.32	120.08	127.00
23	D	348	G	C4-N9-C1'	5.32	133.41	126.50
23	D	775	G	C8-N9-C4	-5.31	104.28	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	846	C	C6-N1-C2	5.31	122.42	120.30
23	D	814	C	C6-N1-C2	5.31	122.42	120.30
1	A	736	C	N1-C2-O2	5.30	122.08	118.90
23	D	137	C	N3-C2-O2	-5.30	118.19	121.90
23	D	584	C	N1-C2-O2	5.30	122.08	118.90
1	A	23	C	N3-C2-O2	-5.29	118.19	121.90
23	D	2633	G	C8-N9-C4	5.29	108.51	106.40
23	D	2607	G	O4'-C1'-N9	-5.28	103.97	108.20
23	D	319	C	N3-C2-O2	-5.28	118.20	121.90
23	D	779	U	N3-C2-O2	-5.28	118.50	122.20
23	D	1199	U	C2-N1-C1'	5.28	124.04	117.70
23	D	1565	C	C6-N1-C2	5.26	122.41	120.30
23	D	551	G	C8-N9-C1'	-5.26	120.16	127.00
23	D	120	U	C2-N1-C1'	5.26	124.01	117.70
23	D	1861	G	C8-N9-C4	5.25	108.50	106.40
23	D	2440	C	C6-N1-C2	5.25	122.40	120.30
23	D	1668	A	C8-N9-C4	-5.25	103.70	105.80
23	D	475	U	C2-N1-C1'	5.25	124.00	117.70
23	D	2583	G	C6-C5-N7	-5.25	127.25	130.40
31	f	82	LEU	CA-CB-CG	-5.24	103.24	115.30
23	D	2500	U	P-O3'-C3'	5.23	125.97	119.70
13	Q	56	LEU	CA-CB-CG	5.23	127.32	115.30
23	D	1836	C	C2-N1-C1'	-5.22	113.05	118.80
27	b	43	GLY	N-CA-C	-5.22	100.05	113.10
1	A	912	C	N1-C2-O2	5.21	122.03	118.90
34	i	77	LYS	C-N-CA	-5.21	100.11	122.00
1	A	882	C	N3-C2-O2	-5.21	118.25	121.90
23	D	2010	G	C8-N9-C4	5.21	108.48	106.40
1	A	123	C	C6-N1-C2	5.20	122.38	120.30
23	D	1497	U	N1-C2-O2	5.20	126.44	122.80
23	D	331	A	C8-N9-C4	5.20	107.88	105.80
23	D	2444	G	N9-C4-C5	-5.20	103.32	105.40
22	C	373	ALA	C-N-CD	5.19	139.31	128.40
1	A	1071	C	N1-C2-O2	5.19	122.02	118.90
23	D	1234	U	N3-C2-O2	-5.19	118.57	122.20
23	D	574	C	C6-N1-C2	5.19	122.38	120.30
23	D	58	G	N3-C4-N9	5.18	129.11	126.00
18	V	58	LEU	CA-CB-CG	-5.17	103.40	115.30
23	D	16	G	C8-N9-C4	5.17	108.47	106.40
23	D	2723	C	C5-C6-N1	-5.17	118.41	121.00
23	D	2767	C	C2-N1-C1'	5.17	124.49	118.80
23	D	2576	G	C6-C5-N7	-5.17	127.30	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	2428	G	C4-N9-C1'	-5.16	119.79	126.50
22	C	485	ARG	C-N-CD	5.16	139.24	128.40
23	D	58	G	C6-C5-N7	-5.16	127.31	130.40
29	d	82	LEU	CB-CG-CD2	-5.16	102.23	111.00
1	A	1419	G	N9-C4-C5	5.16	107.46	105.40
23	D	2580	U	N3-C2-O2	-5.15	118.59	122.20
23	D	787	U	C5-C6-N1	-5.15	120.12	122.70
23	D	1156	A	C5-C6-N6	-5.15	119.58	123.70
1	A	314	C	N3-C2-O2	-5.15	118.30	121.90
23	D	2498	C	C6-N1-C1'	-5.14	114.63	120.80
29	d	106	LEU	CA-CB-CG	5.14	127.12	115.30
23	D	1476	C	C6-N1-C2	-5.13	118.25	120.30
23	D	991	C	C5-C6-N1	-5.13	118.43	121.00
24	E	82	G	C8-N9-C4	5.13	108.45	106.40
23	D	502	A	N1-C2-N3	5.13	131.86	129.30
1	A	1449	C	C6-N1-C1'	-5.13	114.65	120.80
23	D	1376	C	N1-C2-O2	5.13	121.98	118.90
25	Z	181	PRO	C-N-CD	5.12	139.16	128.40
23	D	1914	C	N3-C2-O2	-5.12	118.31	121.90
23	D	45	G	N3-C4-N9	-5.12	122.93	126.00
23	D	2591	C	O4'-C1'-N1	5.12	112.29	108.20
22	C	187	PRO	C-N-CD	5.11	139.14	128.40
23	D	2767	C	N3-C2-O2	-5.11	118.32	121.90
1	A	357	G	C8-N9-C4	5.11	108.44	106.40
1	A	1140	C	N1-C2-O2	5.11	121.96	118.90
23	D	1638	C	C5-C6-N1	-5.11	118.45	121.00
23	D	738	G	N3-C4-C5	-5.10	126.05	128.60
22	C	186	PRO	C-N-CD	5.10	139.11	128.40
1	A	1449	C	C2-N1-C1'	5.10	124.41	118.80
23	D	411	G	N3-C4-N9	5.10	129.06	126.00
23	D	138	G	N3-C4-N9	5.09	129.06	126.00
1	A	1415	G	C8-N9-C1'	5.09	133.62	127.00
23	D	186	G	N3-C4-N9	5.09	129.05	126.00
23	D	1778	U	C6-N1-C1'	5.09	128.32	121.20
23	D	600	G	C8-N9-C4	5.08	108.43	106.40
4	H	19	LEU	CA-CB-CG	-5.08	103.61	115.30
23	D	1645	G	O4'-C1'-N9	5.08	112.27	108.20
23	D	2433	A	N1-C2-N3	5.08	131.84	129.30
22	C	83	THR	C-N-CD	5.08	139.07	128.40
1	A	148	G	C8-N9-C4	5.08	108.43	106.40
22	C	144	ARG	C-N-CD	5.08	139.06	128.40
22	C	158	LEU	C-N-CD	5.08	139.06	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	1237	A	P-O3'-C3'	5.08	125.79	119.70
1	A	689	C	C2-N1-C1'	5.07	124.38	118.80
23	D	1493	C	OP1-P-O3'	5.07	116.36	105.20
1	A	737	A	C8-N9-C4	5.07	107.83	105.80
1	A	1512	U	N3-C2-O2	-5.07	118.65	122.20
22	C	333	GLU	C-N-CD	5.07	139.05	128.40
22	C	441	LEU	C-N-CD	5.07	139.05	128.40
22	C	212	ILE	C-N-CD	5.07	139.04	128.40
1	A	578	C	N1-C2-O2	5.07	121.94	118.90
22	C	223	ARG	C-N-CD	5.06	139.03	128.40
22	C	592	VAL	C-N-CD	5.06	139.03	128.40
23	D	1771	C	N3-C2-O2	-5.06	118.36	121.90
54	3	24	GLY	C-N-CD	5.06	139.03	128.40
22	C	454	ALA	C-N-CD	5.06	139.03	128.40
23	D	1376	C	N3-C2-O2	-5.06	118.36	121.90
22	C	398	ASP	C-N-CD	5.06	139.02	128.40
23	D	2782	G	C5-C6-O6	-5.06	125.57	128.60
22	C	132	ILE	C-N-CD	5.06	139.02	128.40
22	C	416	THR	C-N-CD	5.06	139.02	128.40
22	C	298	LYS	C-N-CD	5.05	139.02	128.40
22	C	528	ILE	C-N-CD	5.05	139.01	128.40
22	C	295	ARG	C-N-CD	5.05	139.01	128.40
22	C	407	GLU	C-N-CD	5.05	139.01	128.40
54	3	12	LEU	C-N-CD	5.05	139.01	128.40
22	C	185	ILE	C-N-CD	5.05	139.00	128.40
22	C	246	THR	C-N-CD	5.05	139.00	128.40
22	C	289	SER	C-N-CD	5.05	139.00	128.40
23	D	1557	C	C5-C6-N1	-5.05	118.47	121.00
23	D	1955	U	N1-C2-O2	5.05	126.33	122.80
22	C	535	VAL	C-N-CD	5.05	139.00	128.40
23	D	715	G	N1-C6-O6	-5.05	116.87	119.90
23	D	1251	C	N3-C4-N4	-5.05	114.47	118.00
30	e	125	VAL	C-N-CD	5.05	139.00	128.40
23	D	1758	G	C6-C5-N7	-5.04	127.37	130.40
22	C	392	ASN	C-N-CD	5.04	138.99	128.40
23	D	409	C	N3-C2-O2	-5.04	118.37	121.90
47	v	28	LYS	C-N-CD	5.04	138.99	128.40
23	D	1980	G	N9-C4-C5	-5.04	103.38	105.40
23	D	1214	A	C8-N9-C4	5.03	107.81	105.80
8	L	63	LEU	CA-CB-CG	5.03	126.87	115.30
23	D	2661	G	C4-N9-C1'	5.03	133.04	126.50
23	D	215	G	P-O3'-C3'	5.03	125.74	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	908	C	C5-C6-N1	5.03	123.51	121.00
23	D	1351	C	C2-N3-C4	-5.03	117.39	119.90
23	D	2681	C	C6-N1-C2	-5.03	118.29	120.30
1	A	971	G	C8-N9-C4	5.02	108.41	106.40
1	A	1415	G	C4-N9-C1'	-5.02	119.97	126.50
23	D	889	C	C6-N1-C1'	-5.02	114.77	120.80
23	D	336	C	C5-C6-N1	-5.02	118.49	121.00
23	D	687	C	N3-C2-O2	-5.02	118.39	121.90
23	D	2487	G	N3-C4-N9	5.01	129.01	126.00
1	A	320	C	N3-C2-O2	-5.01	118.39	121.90
23	D	1221	C	C2-N1-C1'	5.00	124.31	118.80
24	E	106	G	C8-N9-C4	5.00	108.40	106.40

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
54	3	55	VAL	Peptide
54	3	72	PRO	Peptide
2	F	99	GLY	Peptide
8	L	28	ALA	Peptide
26	a	218	ARG	Peptide
26	a	261	LYS	Peptide
26	a	46	GLN	Peptide
26	a	82	ILE	Peptide
26	a	96	HIS	Peptide
28	c	168	ARG	Peptide
28	c	38	ARG	Peptide
28	c	50	SER	Peptide
30	e	110	SER	Peptide
31	f	5	VAL	Peptide
32	g	61	VAL	Peptide
37	l	21	GLU	Peptide
37	l	71	GLY	Peptide
38	m	28	ARG	Peptide
39	n	14	VAL	Peptide
40	o	15	ARG	Peptide
41	p	93	GLU	Peptide
42	q	70	SER	Peptide
46	u	15	TYR	Peptide
47	v	58	ARG	Peptide
49	x	26	ASN	Peptide

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Mol	Chain	Res	Type	Group
51	z	62	LEU	Peptide

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	232/256 (91%)	181 (78%)	33 (14%)	18 (8%)	1	9
3	G	204/239 (85%)	157 (77%)	33 (16%)	14 (7%)	1	11
4	H	206/209 (99%)	168 (82%)	21 (10%)	17 (8%)	0	9
5	I	148/162 (91%)	122 (82%)	19 (13%)	7 (5%)	2	16
6	J	99/101 (98%)	85 (86%)	11 (11%)	3 (3%)	3	22
7	K	153/156 (98%)	130 (85%)	16 (10%)	7 (5%)	2	16
8	L	136/138 (99%)	107 (79%)	19 (14%)	10 (7%)	1	10
9	M	125/128 (98%)	96 (77%)	14 (11%)	15 (12%)	0	4
10	N	96/105 (91%)	73 (76%)	11 (12%)	12 (12%)	0	4
11	O	117/129 (91%)	96 (82%)	15 (13%)	6 (5%)	1	15
12	P	122/132 (92%)	79 (65%)	33 (27%)	10 (8%)	1	9
13	Q	112/126 (89%)	80 (71%)	19 (17%)	13 (12%)	0	5
14	R	58/61 (95%)	40 (69%)	12 (21%)	6 (10%)	0	6
15	S	86/89 (97%)	70 (81%)	9 (10%)	7 (8%)	1	9
16	T	81/88 (92%)	65 (80%)	10 (12%)	6 (7%)	1	10
17	U	102/105 (97%)	82 (80%)	13 (13%)	7 (7%)	1	11
18	V	71/88 (81%)	57 (80%)	9 (13%)	5 (7%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	W	78/93 (84%)	53 (68%)	17 (22%)	8 (10%)	0	6
20	X	97/106 (92%)	85 (88%)	7 (7%)	5 (5%)	1	15
21	Y	22/27 (82%)	17 (77%)	2 (9%)	3 (14%)	0	4
22	C	562/610 (92%)	244 (43%)	187 (33%)	131 (23%)	0	1
25	Z	226/229 (99%)	180 (80%)	26 (12%)	20 (9%)	0	8
26	a	270/276 (98%)	188 (70%)	51 (19%)	31 (12%)	0	5
27	b	204/206 (99%)	147 (72%)	29 (14%)	28 (14%)	0	4
28	c	206/210 (98%)	160 (78%)	29 (14%)	17 (8%)	0	9
29	d	180/182 (99%)	119 (66%)	39 (22%)	22 (12%)	0	4
30	e	172/180 (96%)	121 (70%)	27 (16%)	24 (14%)	0	3
31	f	137/140 (98%)	106 (77%)	18 (13%)	13 (10%)	0	8
32	g	120/122 (98%)	86 (72%)	22 (18%)	12 (10%)	0	7
33	h	143/150 (95%)	98 (68%)	25 (18%)	20 (14%)	0	3
34	i	134/141 (95%)	89 (66%)	30 (22%)	15 (11%)	0	6
35	j	115/118 (98%)	93 (81%)	13 (11%)	9 (8%)	1	9
36	k	108/112 (96%)	78 (72%)	20 (18%)	10 (9%)	0	8
37	l	115/146 (79%)	70 (61%)	32 (28%)	13 (11%)	0	5
38	m	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	9
39	n	99/101 (98%)	59 (60%)	21 (21%)	19 (19%)	0	2
40	o	108/113 (96%)	82 (76%)	18 (17%)	8 (7%)	1	10
41	p	92/96 (96%)	74 (80%)	12 (13%)	6 (6%)	1	12
42	q	108/110 (98%)	61 (56%)	24 (22%)	23 (21%)	0	2
43	r	178/206 (86%)	128 (72%)	33 (18%)	17 (10%)	0	7
44	s	77/85 (91%)	60 (78%)	12 (16%)	5 (6%)	1	12
45	t	65/67 (97%)	58 (89%)	2 (3%)	5 (8%)	1	9
46	u	57/60 (95%)	43 (75%)	11 (19%)	3 (5%)	1	14
47	v	69/71 (97%)	39 (56%)	14 (20%)	16 (23%)	0	1
48	w	55/60 (92%)	35 (64%)	12 (22%)	8 (14%)	0	3
49	x	47/54 (87%)	21 (45%)	15 (32%)	11 (23%)	0	1
50	y	47/49 (96%)	30 (64%)	10 (21%)	7 (15%)	0	3
51	z	62/65 (95%)	38 (61%)	14 (23%)	10 (16%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	1	35/37 (95%)	25 (71%)	8 (23%)	2 (6%)	1	14
53	2	128/173 (74%)	95 (74%)	21 (16%)	12 (9%)	0	8
54	3	132/147 (90%)	82 (62%)	20 (15%)	30 (23%)	0	1
All	All	6511/6972 (93%)	4639 (71%)	1137 (18%)	735 (11%)	1	5

All (735) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	191	ASP
2	F	209	ARG
3	G	64	VAL
4	H	30	LYS
4	H	191	ARG
5	I	98	THR
5	I	143	ARG
6	J	42	GLU
7	K	113	GLU
7	K	146	GLU
8	L	77	GLU
8	L	121	ASP
9	M	38	GLN
9	M	98	PRO
9	M	103	THR
9	M	126	SER
10	N	39	PRO
11	O	53	SER
12	P	18	VAL
13	Q	5	ALA
13	Q	99	ARG
16	T	36	ILE
16	T	44	THR
16	T	80	PHE
17	U	104	LYS
18	V	81	PHE
19	W	4	SER
19	W	5	LEU
19	W	12	ASP
19	W	21	GLU
20	X	14	LYS
20	X	24	LEU
20	X	25	ARG

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Mol	Chain	Res	Type
20	X	73	HIS
21	Y	9	ARG
22	C	4	MET
22	C	9	ILE
22	C	36	VAL
22	C	49	LEU
22	C	69	ARG
22	C	71	LYS
22	C	138	ILE
22	C	160	ALA
22	C	205	TYR
22	C	208	TYR
22	C	246	THR
22	C	271	ILE
22	C	284	ASP
22	C	296	PRO
22	C	297	ALA
22	C	315	LYS
22	C	323	LEU
22	C	329	ALA
22	C	339	ALA
22	C	341	GLY
22	C	351	LEU
22	C	373	ALA
22	C	435	LEU
22	C	437	ASN
22	C	485	ARG
22	C	489	LEU
22	C	490	VAL
22	C	497	HIS
22	C	502	ASP
22	C	523	LYS
22	C	524	LEU
22	C	525	ALA
25	Z	180	PHE
25	Z	182	PRO
25	Z	201	PRO
26	a	44	ASN
26	a	70	TRP
26	a	106	ILE
26	a	157	ARG
26	a	249	PRO

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Mol	Chain	Res	Type
27	b	38	THR
27	b	53	PRO
27	b	56	PRO
27	b	74	PRO
27	b	180	ASN
27	b	205	ALA
28	c	14	PRO
28	c	132	VAL
29	d	25	TYR
29	d	57	ALA
29	d	78	SER
29	d	106	LEU
29	d	112	PRO
29	d	114	ILE
29	d	122	PRO
29	d	181	ARG
30	e	8	PRO
30	e	130	ARG
30	e	156	ALA
30	e	157	TYR
31	f	41	ASP
31	f	46	VAL
31	f	66	LYS
31	f	79	PRO
32	g	31	LYS
32	g	53	LYS
32	g	63	VAL
32	g	67	LYS
32	g	102	VAL
33	h	7	ARG
33	h	13	ASN
33	h	16	ARG
33	h	63	PRO
33	h	107	LYS
33	h	136	GLU
34	i	66	ILE
34	i	77	LYS
35	j	18	LEU
35	j	101	ALA
36	k	86	ALA
37	l	5	ALA
37	l	20	PRO

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Mol	Chain	Res	Type
37	l	28	VAL
37	l	59	THR
37	l	100	TYR
38	m	62	ILE
38	m	67	ALA
39	n	15	GLU
39	n	22	VAL
39	n	31	ALA
39	n	50	PRO
39	n	52	VAL
41	p	33	LYS
41	p	89	ILE
42	q	30	VAL
42	q	44	ILE
42	q	46	LYS
42	q	56	PRO
42	q	72	VAL
43	r	63	ASP
43	r	159	PRO
45	t	13	PRO
45	t	35	SER
46	u	11	SER
46	u	16	PRO
47	v	6	HIS
47	v	11	PRO
47	v	26	SER
47	v	31	ILE
47	v	34	GLU
47	v	44	THR
47	v	58	ARG
48	w	23	HIS
49	x	24	GLU
49	x	36	LEU
49	x	52	VAL
50	y	7	PRO
51	z	6	THR
51	z	36	LYS
51	z	55	ALA
51	z	61	LEU
53	2	7	VAL
53	2	69	PRO
53	2	77	PRO

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Mol	Chain	Res	Type
53	2	80	VAL
53	2	93	LEU
53	2	107	VAL
54	3	22	PRO
54	3	26	ALA
54	3	34	ILE
54	3	67	PHE
54	3	109	LYS
54	3	112	MET
54	3	113	PRO
2	F	24	TRP
2	F	33	TYR
2	F	77	ALA
2	F	127	ILE
2	F	169	LYS
2	F	202	PRO
3	G	16	ARG
3	G	61	ALA
3	G	74	GLY
3	G	139	GLN
3	G	181	ASN
3	G	196	LEU
4	H	24	GLU
4	H	29	PRO
4	H	32	ALA
4	H	137	SER
4	H	199	ASN
5	I	6	PHE
5	I	73	ASN
5	I	75	THR
5	I	144	THR
7	K	37	ASN
7	K	112	PRO
7	K	130	GLY
7	K	148	ASN
8	L	44	PHE
8	L	78	GLN
8	L	97	VAL
8	L	133	LEU
9	M	47	LEU
9	M	58	HIS
9	M	92	TYR

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Mol	Chain	Res	Type
9	M	127	LYS
10	N	11	PHE
10	N	36	GLY
10	N	51	ARG
10	N	54	PHE
10	N	60	ARG
11	O	52	GLY
11	O	54	ARG
12	P	6	THR
12	P	7	ILE
12	P	48	PRO
12	P	51	ALA
12	P	83	VAL
13	Q	7	VAL
13	Q	58	GLU
13	Q	63	THR
13	Q	103	THR
13	Q	109	THR
14	R	15	LYS
14	R	29	ARG
14	R	55	GLY
15	S	48	LYS
15	S	72	ARG
15	S	88	ARG
17	U	14	LYS
17	U	66	SER
18	V	21	LYS
18	V	87	ARG
19	W	47	HIS
20	X	74	LYS
21	Y	11	GLY
22	C	5	ASP
22	C	28	ARG
22	C	45	PHE
22	C	47	ASP
22	C	79	HIS
22	C	80	LEU
22	C	105	LEU
22	C	163	ALA
22	C	166	ALA
22	C	178	LEU
22	C	209	GLN

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Mol	Chain	Res	Type
22	C	217	LEU
22	C	231	TYR
22	C	232	SER
22	C	244	VAL
22	C	260	GLU
22	C	320	LEU
22	C	333	GLU
22	C	334	PRO
22	C	356	ILE
22	C	372	THR
22	C	383	LYS
22	C	405	ILE
22	C	407	GLU
22	C	444	ALA
22	C	500	VAL
22	C	501	VAL
22	C	567	VAL
22	C	588	GLY
22	C	590	VAL
25	Z	156	ILE
25	Z	159	GLY
25	Z	160	ARG
25	Z	161	ILE
25	Z	174	PRO
25	Z	206	GLY
25	Z	218	MET
26	a	10	THR
26	a	17	THR
26	a	54	ARG
26	a	59	LYS
26	a	89	SER
26	a	144	ALA
26	a	149	PRO
26	a	162	SER
26	a	170	GLY
26	a	245	PRO
26	a	260	ARG
27	b	37	ARG
27	b	57	LYS
27	b	75	VAL
27	b	83	ASP
27	b	117	MET

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Mol	Chain	Res	Type
27	b	119	ARG
27	b	145	LYS
27	b	184	VAL
28	c	58	ALA
28	c	68	LYS
28	c	89	VAL
28	c	97	TYR
28	c	126	VAL
29	d	49	ASP
29	d	115	ARG
29	d	128	ARG
30	e	57	ASP
30	e	118	PRO
30	e	152	ARG
30	e	155	SER
31	f	45	ASN
31	f	68	GLU
31	f	127	ASP
31	f	135	PRO
32	g	30	ALA
32	g	49	ARG
33	h	23	PRO
33	h	25	SER
33	h	30	THR
33	h	41	ARG
33	h	59	LEU
34	i	67	ARG
34	i	78	PRO
34	i	87	LYS
36	k	32	LEU
36	k	64	GLU
36	k	95	HIS
37	l	18	ASP
37	l	27	THR
37	l	39	ARG
38	m	54	LYS
38	m	77	SER
38	m	93	LYS
39	n	6	LYS
39	n	13	ARG
39	n	14	VAL
39	n	18	LEU

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Mol	Chain	Res	Type
39	n	57	VAL
39	n	64	HIS
39	n	68	LYS
39	n	69	LYS
39	n	90	PRO
40	o	41	LYS
41	p	44	GLU
41	p	48	LYS
41	p	53	LYS
42	q	17	SER
42	q	20	TYR
42	q	23	ARG
42	q	68	HIS
42	q	75	ILE
42	q	77	PRO
42	q	82	PRO
42	q	87	LYS
42	q	99	CYS
43	r	42	VAL
43	r	82	ARG
45	t	46	ARG
47	v	22	ILE
47	v	32	TYR
47	v	56	VAL
48	w	14	ALA
48	w	56	LYS
49	x	17	LYS
49	x	35	GLU
49	x	49	HIS
50	y	39	ARG
51	z	45	GLY
51	z	62	LEU
53	2	30	GLN
54	3	14	ALA
54	3	28	GLY
54	3	82	ALA
54	3	94	GLU
54	3	96	VAL
54	3	100	THR
54	3	134	MET
2	F	15	VAL
2	F	16	HIS

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Mol	Chain	Res	Type
2	F	78	GLN
2	F	82	ARG
2	F	204	ASN
2	F	232	PRO
3	G	137	ALA
3	G	174	PRO
4	H	4	TYR
4	H	88	VAL
4	H	131	ARG
4	H	136	PRO
5	I	12	LEU
7	K	121	ALA
8	L	22	GLU
8	L	132	GLU
9	M	23	ASN
9	M	57	GLY
9	M	88	TYR
10	N	34	VAL
11	O	111	ASP
12	P	22	SER
13	Q	28	ALA
13	Q	66	LEU
13	Q	67	GLU
14	R	32	SER
14	R	34	TYR
15	S	17	ARG
15	S	47	LYS
16	T	11	SER
17	U	99	SER
19	W	7	LYS
22	C	19	ASP
22	C	42	ARG
22	C	48	SER
22	C	84	PRO
22	C	140	LEU
22	C	170	THR
22	C	189	LYS
22	C	198	ALA
22	C	254	GLU
22	C	278	ASP
22	C	285	ARG
22	C	317	ARG

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Mol	Chain	Res	Type
22	C	328	ALA
22	C	330	LEU
22	C	335	GLU
22	C	387	GLU
22	C	399	PRO
22	C	408	PRO
22	C	418	GLU
22	C	429	GLN
22	C	496	VAL
22	C	498	GLY
22	C	503	ALA
22	C	529	PRO
25	Z	35	ALA
25	Z	37	PHE
25	Z	109	ASP
26	a	6	PHE
26	a	55	GLY
26	a	84	TYR
26	a	91	ARG
26	a	246	PRO
27	b	16	ARG
27	b	17	ASP
27	b	32	PRO
27	b	54	GLN
27	b	114	ALA
27	b	122	PHE
27	b	124	GLY
27	b	173	VAL
27	b	202	LYS
28	c	12	LEU
28	c	62	ARG
28	c	168	ARG
29	d	64	THR
29	d	132	ASN
29	d	135	LEU
29	d	177	GLY
30	e	12	PRO
30	e	21	PRO
30	e	47	GLU
30	e	48	GLY
30	e	56	SER
31	f	4	TYR

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Mol	Chain	Res	Type
31	f	48	MET
31	f	93	THR
31	f	111	PRO
32	g	4	PRO
32	g	93	PRO
33	h	36	LYS
33	h	42	SER
33	h	64	LYS
34	i	20	ALA
34	i	26	TYR
34	i	61	GLY
34	i	81	VAL
34	i	91	GLU
34	i	98	LYS
35	j	4	LEU
35	j	20	LEU
35	j	61	HIS
35	j	89	ASP
36	k	55	ALA
36	k	82	ILE
37	l	80	SER
38	m	24	TYR
38	m	64	ARG
38	m	87	GLY
39	n	66	ARG
40	o	9	TYR
40	o	15	ARG
42	q	34	LYS
42	q	94	LYS
43	r	41	LEU
43	r	146	ILE
43	r	165	VAL
43	r	170	THR
43	r	177	PRO
44	s	21	LEU
44	s	83	PRO
45	t	37	GLY
47	v	41	PRO
47	v	48	ARG
47	v	50	VAL
49	x	46	HIS
50	y	11	LYS

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Mol	Chain	Res	Type
51	z	13	ARG
51	z	38	GLY
53	2	62	ALA
54	3	10	LEU
54	3	13	PRO
54	3	24	GLY
54	3	64	SER
54	3	73	PRO
54	3	74	ALA
54	3	117	THR
54	3	126	MET
2	F	61	LEU
3	G	4	LYS
3	G	144	SER
3	G	157	ILE
4	H	40	PRO
4	H	200	GLU
9	M	117	HIS
12	P	16	GLU
13	Q	27	LYS
15	S	87	ILE
16	T	9	PHE
16	T	68	ASP
18	V	82	THR
22	C	6	LEU
22	C	35	ALA
22	C	143	ALA
22	C	145	PRO
22	C	159	PRO
22	C	164	ILE
22	C	167	SER
22	C	247	PRO
22	C	256	LEU
22	C	292	PRO
22	C	298	LYS
22	C	396	LEU
22	C	488	ASP
22	C	499	GLU
22	C	522	ASP
22	C	530	ARG
22	C	556	LYS
22	C	591	GLU

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Mol	Chain	Res	Type
25	Z	39	GLU
25	Z	72	VAL
26	a	62	TYR
26	a	118	VAL
26	a	219	PRO
26	a	271	ILE
27	b	147	PRO
28	c	54	ARG
28	c	72	ARG
29	d	65	GLY
29	d	86	MET
29	d	124	SER
29	d	151	ALA
29	d	178	PHE
30	e	41	MET
30	e	110	SER
32	g	101	PRO
33	h	18	ARG
33	h	96	THR
35	j	8	ARG
35	j	107	ASP
36	k	36	TYR
36	k	61	ASN
36	k	88	ASP
37	l	61	PHE
37	l	110	ILE
38	m	94	ASN
39	n	10	LYS
40	o	64	MET
40	o	73	ALA
40	o	89	ALA
41	p	63	LYS
42	q	40	GLU
42	q	42	VAL
42	q	74	PRO
42	q	83	THR
42	q	86	ARG
43	r	13	GLU
43	r	55	HIS
43	r	168	GLU
44	s	20	ARG
46	u	31	LEU

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Mol	Chain	Res	Type
47	v	18	CYS
47	v	27	THR
47	v	55	ARG
48	w	43	HIS
48	w	48	GLU
48	w	59	GLU
49	x	29	ASN
49	x	53	LYS
50	y	2	LYS
50	y	4	THR
50	y	15	THR
52	1	6	SER
53	2	109	SER
53	2	119	ALA
54	3	57	ILE
54	3	93	ARG
2	F	29	ALA
4	H	3	ARG
4	H	35	ARG
4	H	198	VAL
9	M	104	ARG
10	N	23	ILE
10	N	87	THR
10	N	90	LEU
12	P	61	THR
13	Q	101	GLN
17	U	68	ARG
22	C	46	LEU
22	C	64	VAL
22	C	286	PRO
22	C	505	THR
22	C	507	ILE
22	C	542	GLY
25	Z	49	ILE
25	Z	132	GLY
26	a	7	LYS
26	a	268	ARG
26	a	270	ILE
27	b	168	MET
28	c	36	VAL
28	c	69	HIS
29	d	164	GLU

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Mol	Chain	Res	Type
30	e	30	LYS
30	e	131	VAL
30	e	154	PRO
31	f	47	ALA
33	h	84	ASN
33	h	91	PHE
33	h	92	GLU
33	h	138	LEU
34	i	110	THR
36	k	102	ALA
37	l	99	LEU
39	n	41	GLY
39	n	72	VAL
40	o	63	ASP
40	o	75	TYR
42	q	6	HIS
43	r	81	ARG
43	r	123	ASP
48	w	5	PRO
49	x	28	ARG
50	y	41	ARG
51	z	4	MET
51	z	14	VAL
52	1	7	VAL
54	3	60	TYR
54	3	90	LYS
54	3	95	LYS
2	F	99	GLY
2	F	230	VAL
3	G	14	ILE
6	J	27	GLN
9	M	70	LYS
10	N	31	GLY
11	O	89	ALA
12	P	19	ARG
14	R	16	PHE
17	U	65	ILE
17	U	80	GLY
18	V	20	ALA
19	W	19	VAL
21	Y	7	ARG
22	C	33	THR

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Mol	Chain	Res	Type
22	C	44	GLN
22	C	137	LYS
22	C	353	HIS
22	C	482	ALA
25	Z	36	LYS
25	Z	158	ALA
27	b	91	VAL
28	c	16	GLY
29	d	126	ASP
30	e	125	VAL
30	e	160	LYS
30	e	168	PRO
30	e	174	GLY
32	g	78	ARG
44	s	30	VAL
49	x	27	LYS
6	J	72	VAL
15	S	29	VAL
22	C	141	PRO
22	C	152	VAL
22	C	213	PRO
22	C	536	PRO
26	a	142	VAL
27	b	126	PRO
30	e	107	VAL
35	j	73	VAL
39	n	17	GLY
42	q	15	VAL
54	3	5	VAL
54	3	52	ILE
22	C	274	VAL
22	C	486	PRO
22	C	593	PRO
32	g	119	PRO
34	i	94	VAL
43	r	147	GLY
53	2	73	GLY
54	3	135	GLY
9	M	22	GLY
22	C	133	PRO
22	C	385	GLY
22	C	527	VAL

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Mol	Chain	Res	Type
25	Z	4	GLY
26	a	28	GLU
34	i	19	GLY
43	r	39	VAL
43	r	167	PRO
3	G	138	VAL
4	H	167	GLY
8	L	75	ARG
8	L	134	ILE
10	N	40	LEU
22	C	77	VAL
22	C	225	GLY
22	C	249	GLY
22	C	390	VAL
22	C	402	ILE
22	C	454	ALA
26	a	18	VAL
27	b	116	VAL
28	c	84	VAL
30	e	126	PRO
34	i	125	LEU
45	t	12	SER
48	w	54	GLY
11	O	112	THR
13	Q	95	GLY
19	W	26	GLY
28	c	30	PRO
37	l	56	GLY
44	s	63	VAL
53	2	100	ASN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	202/220 (92%)	202 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	160/188 (85%)	160 (100%)	0	100	100
4	H	180/181 (99%)	180 (100%)	0	100	100
5	I	115/123 (94%)	115 (100%)	0	100	100
6	J	90/90 (100%)	90 (100%)	0	100	100
7	K	126/127 (99%)	126 (100%)	0	100	100
8	L	119/119 (100%)	119 (100%)	0	100	100
9	M	98/99 (99%)	98 (100%)	0	100	100
10	N	88/92 (96%)	88 (100%)	0	100	100
11	O	90/99 (91%)	90 (100%)	0	100	100
12	P	104/109 (95%)	103 (99%)	1 (1%)	73	81
13	Q	92/101 (91%)	87 (95%)	5 (5%)	18	39
14	R	49/50 (98%)	49 (100%)	0	100	100
15	S	79/80 (99%)	79 (100%)	0	100	100
16	T	72/74 (97%)	72 (100%)	0	100	100
17	U	96/97 (99%)	96 (100%)	0	100	100
18	V	64/77 (83%)	64 (100%)	0	100	100
19	W	71/80 (89%)	69 (97%)	2 (3%)	38	57
20	X	76/82 (93%)	76 (100%)	0	100	100
21	Y	19/22 (86%)	19 (100%)	0	100	100
22	C	473/505 (94%)	347 (73%)	126 (27%)	0	3
25	Z	180/181 (99%)	174 (97%)	6 (3%)	33	52
26	a	215/218 (99%)	213 (99%)	2 (1%)	75	83
27	b	166/166 (100%)	165 (99%)	1 (1%)	84	88
28	c	164/166 (99%)	164 (100%)	0	100	100
29	d	156/156 (100%)	153 (98%)	3 (2%)	52	69
30	e	143/148 (97%)	141 (99%)	2 (1%)	62	75
31	f	118/119 (99%)	118 (100%)	0	100	100
32	g	100/100 (100%)	99 (99%)	1 (1%)	73	81
33	h	111/116 (96%)	111 (100%)	0	100	100
34	i	106/111 (96%)	106 (100%)	0	100	100
35	j	100/101 (99%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	k	87/88 (99%)	87 (100%)	0	100	100
37	l	105/127 (83%)	105 (100%)	0	100	100
38	m	93/94 (99%)	93 (100%)	0	100	100
39	n	82/82 (100%)	82 (100%)	0	100	100
40	o	90/92 (98%)	90 (100%)	0	100	100
41	p	76/78 (97%)	76 (100%)	0	100	100
42	q	91/91 (100%)	91 (100%)	0	100	100
43	r	159/179 (89%)	159 (100%)	0	100	100
44	s	63/67 (94%)	63 (100%)	0	100	100
45	t	62/62 (100%)	62 (100%)	0	100	100
46	u	51/52 (98%)	51 (100%)	0	100	100
47	v	63/63 (100%)	60 (95%)	3 (5%)	21	43
48	w	50/52 (96%)	50 (100%)	0	100	100
49	x	48/52 (92%)	48 (100%)	0	100	100
50	y	42/42 (100%)	42 (100%)	0	100	100
51	z	54/55 (98%)	54 (100%)	0	100	100
52	1	34/34 (100%)	34 (100%)	0	100	100
54	3	101/111 (91%)	86 (85%)	15 (15%)	2	12
All	All	5373/5618 (96%)	5206 (97%)	167 (3%)	37	54

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	P	93	LEU
13	Q	58	GLU
13	Q	62	ASN
13	Q	66	LEU
13	Q	99	ARG
13	Q	102	ARG
19	W	5	LEU
19	W	7	LYS
22	C	3	ARG
22	C	4	MET
22	C	5	ASP
22	C	8	ARG
22	C	9	ILE

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Mol	Chain	Res	Type
22	C	10	ARG
22	C	13	SER
22	C	19	ASP
22	C	20	HIS
22	C	22	LYS
22	C	23	SER
22	C	24	THR
22	C	25	LEU
22	C	27	ASP
22	C	28	ARG
22	C	36	VAL
22	C	40	GLU
22	C	41	MET
22	C	42	ARG
22	C	43	GLU
22	C	47	ASP
22	C	49	LEU
22	C	53	ARG
22	C	55	ARG
22	C	60	LYS
22	C	74	GLU
22	C	77	VAL
22	C	78	PHE
22	C	82	ASP
22	C	95	ARG
22	C	97	LEU
22	C	104	LEU
22	C	105	LEU
22	C	120	LYS
22	C	121	PHE
22	C	125	LEU
22	C	127	HIS
22	C	136	ASN
22	C	139	ASP
22	C	140	LEU
22	C	144	ARG
22	C	150	LEU
22	C	154	GLU
22	C	165	PHE
22	C	170	THR
22	C	175	GLU
22	C	189	LYS

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Mol	Chain	Res	Type
22	C	206	ASP
22	C	208	TYR
22	C	221	ARG
22	C	223	ARG
22	C	227	ARG
22	C	229	ARG
22	C	230	ILE
22	C	232	SER
22	C	233	THR
22	C	235	LYS
22	C	246	THR
22	C	256	LEU
22	C	269	ARG
22	C	274	VAL
22	C	275	GLN
22	C	279	THR
22	C	280	ILE
22	C	287	THR
22	C	289	SER
22	C	291	TYR
22	C	294	PHE
22	C	295	ARG
22	C	315	LYS
22	C	317	ARG
22	C	321	GLU
22	C	324	LYS
22	C	325	LEU
22	C	327	ASP
22	C	330	LEU
22	C	332	PHE
22	C	337	SER
22	C	338	THR
22	C	340	LEU
22	C	342	PHE
22	C	344	PHE
22	C	349	LEU
22	C	353	HIS
22	C	369	LEU
22	C	377	VAL
22	C	381	ARG
22	C	383	LYS
22	C	392	ASN

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Mol	Chain	Res	Type
22	C	400	THR
22	C	401	ARG
22	C	403	GLU
22	C	405	ILE
22	C	406	LEU
22	C	407	GLU
22	C	418	GLU
22	C	423	SER
22	C	424	LEU
22	C	425	MET
22	C	432	ARG
22	C	446	LYS
22	C	464	HIS
22	C	467	LEU
22	C	477	MET
22	C	478	ASP
22	C	481	GLN
22	C	485	ARG
22	C	489	LEU
22	C	491	LYS
22	C	499	GLU
22	C	502	ASP
22	C	507	ILE
22	C	511	GLU
22	C	514	TYR
22	C	523	LYS
22	C	524	LEU
22	C	528	ILE
22	C	530	ARG
22	C	531	GLN
22	C	534	GLU
22	C	538	GLN
22	C	548	ARG
22	C	583	ARG
22	C	589	LYS
22	C	591	GLU
22	C	594	GLN
25	Z	161	ILE
25	Z	175	VAL
25	Z	180	PHE
25	Z	183	GLU
25	Z	184	LYS

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Mol	Chain	Res	Type
25	Z	185	LEU
26	a	25	THR
26	a	84	TYR
27	b	5	LEU
29	d	25	TYR
29	d	33	ARG
29	d	34	LEU
30	e	127	GLU
30	e	129	THR
32	g	57	VAL
47	v	28	LYS
47	v	31	ILE
47	v	32	TYR
54	3	9	LYS
54	3	11	GLN
54	3	12	LEU
54	3	63	ARG
54	3	64	SER
54	3	65	PHE
54	3	66	THR
54	3	89	HIS
54	3	93	ARG
54	3	94	GLU
54	3	105	LEU
54	3	109	LYS
54	3	111	LYS
54	3	112	MET
54	3	120	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	40	HIS
2	F	110	GLN
2	F	140	HIS
3	G	28	GLN
3	G	63	ASN
3	G	108	ASN
3	G	123	GLN
3	G	176	HIS
4	H	62	GLN
4	H	74	GLN

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Mol	Chain	Res	Type
4	H	116	GLN
4	H	129	ASN
5	I	65	ASN
5	I	78	HIS
5	I	130	ASN
6	J	64	GLN
7	K	28	ASN
7	K	68	ASN
7	K	96	GLN
7	K	109	ASN
7	K	122	HIS
8	L	15	ASN
8	L	81	HIS
8	L	82	HIS
9	M	23	ASN
9	M	34	ASN
10	N	68	HIS
11	O	22	HIS
11	O	38	ASN
11	O	116	HIS
11	O	117	ASN
12	P	76	ASN
13	Q	92	HIS
15	S	9	GLN
15	S	53	HIS
17	U	26	GLN
19	W	23	ASN
19	W	56	GLN
20	X	75	ASN
22	C	34	HIS
22	C	44	GLN
22	C	136	ASN
22	C	142	ASN
22	C	183	GLN
22	C	209	GLN
22	C	326	ASN
22	C	391	HIS
22	C	392	ASN
22	C	464	HIS
22	C	497	HIS
22	C	538	GLN
22	C	594	GLN

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Mol	Chain	Res	Type
25	Z	3	HIS
25	Z	27	HIS
25	Z	66	HIS
25	Z	71	GLN
25	Z	172	HIS
26	a	44	ASN
26	a	115	GLN
26	a	116	GLN
26	a	129	ASN
27	b	66	HIS
27	b	129	HIS
27	b	159	HIS
28	c	75	HIS
28	c	133	ASN
28	c	204	ASN
29	d	26	GLN
30	e	158	HIS
31	f	8	GLN
31	f	38	HIS
31	f	94	HIS
31	f	101	HIS
33	h	9	ASN
33	h	84	ASN
34	i	12	GLN
34	i	46	GLN
35	j	61	HIS
37	l	79	HIS
37	l	84	GLN
38	m	14	HIS
38	m	66	ASN
38	m	94	ASN
38	m	117	GLN
40	o	34	ASN
40	o	61	ASN
41	p	31	HIS
42	q	6	HIS
42	q	68	HIS
43	r	32	HIS
43	r	54	HIS
43	r	75	ASN
44	s	29	GLN
44	s	35	ASN

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Mol	Chain	Res	Type
45	t	60	ASN
46	u	19	GLN
46	u	32	GLN
46	u	46	ASN
47	v	20	ASN
47	v	47	GLN
48	w	22	HIS
48	w	23	HIS
49	x	46	HIS
50	y	36	GLN
51	z	7	HIS
52	1	34	GLN
52	1	36	GLN
54	3	29	GLN
54	3	30	HIS
54	3	42	ASN
54	3	116	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1514/1522 (99%)	640 (42%)	80 (5%)
23	D	2888/2893 (99%)	1464 (50%)	169 (5%)
24	E	122/123 (99%)	47 (38%)	4 (3%)
55	4	76/77 (98%)	30 (39%)	0
56	5	75/76 (98%)	36 (48%)	4 (5%)
All	All	4675/4691 (99%)	2217 (47%)	257 (5%)

All (2217) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	10	A
1	A	14	U
1	A	17	U
1	A	19	C
1	A	20	U
1	A	27	G
1	A	31	G

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Mol	Chain	Res	Type
1	A	32	A
1	A	34	C
1	A	37	U
1	A	38	G
1	A	39	G
1	A	47	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	52	G
1	A	53	A
1	A	54	C
1	A	56	U
1	A	57	G
1	A	58	C
1	A	59	A
1	A	61	G
1	A	64	G
1	A	66	G
1	A	80	G
1	A	87	A
1	A	89	U
1	A	90	C
1	A	91	C
1	A	93	U
1	A	96	G
1	A	101	A
1	A	106	C
1	A	108	G
1	A	110	C
1	A	112	G
1	A	116	A
1	A	119	A
1	A	120	A
1	A	121	C
1	A	122	G
1	A	123	C
1	A	125	U
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	133	U

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Mol	Chain	Res	Type
1	A	136	C
1	A	137	C
1	A	141	A
1	A	142	G
1	A	160	A
1	A	161	A
1	A	170	U
1	A	174	C
1	A	181	G
1	A	182	U
1	A	185	A
1	A	186(A)	C
1	A	188	U
1	A	189	U
1	A	190	G
1	A	191(A)	G
1	A	195	A
1	A	196	A
1	A	197	A
1	A	201	C
1	A	209	U
1	A	210	U
1	A	216	G
1	A	218	C
1	A	223	U
1	A	234	C
1	A	240	C
1	A	241	C
1	A	243	A
1	A	244	U
1	A	245	C
1	A	247	G
1	A	249	U
1	A	250	A
1	A	251	G
1	A	253	U
1	A	259	G
1	A	261	U
1	A	262	A
1	A	264	U
1	A	266	G
1	A	267	C

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Mol	Chain	Res	Type
1	A	273	A
1	A	274	A
1	A	275	G
1	A	276	G
1	A	280	C
1	A	281	G
1	A	282	A
1	A	283	C
1	A	284	G
1	A	289	G
1	A	290	C
1	A	293	G
1	A	298	A
1	A	302	G
1	A	306	G
1	A	308	C
1	A	309	G
1	A	314	C
1	A	315	A
1	A	316	G
1	A	323	U
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	334	C
1	A	336	C
1	A	345	C
1	A	346	G
1	A	347	G
1	A	348	G
1	A	349	A
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	356	A
1	A	358	U
1	A	361	G
1	A	362	G
1	A	366	C
1	A	367	U

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Mol	Chain	Res	Type
1	A	369	C
1	A	373	A
1	A	376	G
1	A	380	G
1	A	383	A
1	A	385	C
1	A	388	G
1	A	389	A
1	A	390	C
1	A	396	G
1	A	397	A
1	A	398	C
1	A	404	U
1	A	406	G
1	A	407	G
1	A	409	G
1	A	410	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	415	A
1	A	420	U
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	427	U
1	A	429	U
1	A	432	A
1	A	433	C
1	A	439	A
1	A	440	A
1	A	446	G
1	A	448	A
1	A	450	G
1	A	453	A
1	A	454	C
1	A	466	C
1	A	467	G
1	A	479	C
1	A	480	U
1	A	481	G

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Mol	Chain	Res	Type
1	A	483	C
1	A	485	G
1	A	486	U
1	A	488	C
1	A	494	U
1	A	496	A
1	A	497	U
1	A	507	C
1	A	508	C
1	A	509	A
1	A	510	A
1	A	511	C
1	A	517	G
1	A	518	C
1	A	519	C
1	A	521	G
1	A	524	G
1	A	525	C
1	A	527	G
1	A	530	G
1	A	531	U
1	A	533	A
1	A	534	U
1	A	535	A
1	A	536	C
1	A	548	G
1	A	549	C
1	A	550	G
1	A	551	U
1	A	552	U
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	567	G
1	A	570	G
1	A	571	U
1	A	572	A
1	A	573	A
1	A	574	A

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Mol	Chain	Res	Type
1	A	575	G
1	A	576	G
1	A	577	G
1	A	578	C
1	A	579	G
1	A	581	G
1	A	582	U
1	A	583	A
1	A	587	G
1	A	588	G
1	A	589	C
1	A	595	G
1	A	596	C
1	A	597	G
1	A	598	U
1	A	607	A
1	A	611	A
1	A	612	C
1	A	617	G
1	A	618	C
1	A	619	U
1	A	622	A
1	A	625	G
1	A	629	G
1	A	632	A
1	A	642	A
1	A	645	C
1	A	650	G
1	A	652	U
1	A	659	U
1	A	663	A
1	A	664	G
1	A	665	A
1	A	672	U
1	A	673	G
1	A	678	U
1	A	679	C
1	A	683	G
1	A	684	A
1	A	686	U
1	A	687	A
1	A	688	G

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Mol	Chain	Res	Type
1	A	690	G
1	A	691	G
1	A	693	G
1	A	695	A
1	A	697	U
1	A	700	G
1	A	702	A
1	A	703	G
1	A	704	A
1	A	712	A
1	A	713	G
1	A	715	A
1	A	717	C
1	A	718	G
1	A	723	U
1	A	724	G
1	A	726	C
1	A	731	G
1	A	744	C
1	A	748	C
1	A	749	C
1	A	755	G
1	A	760	G
1	A	766	A
1	A	769	G
1	A	771	G
1	A	774	G
1	A	775	G
1	A	776	G
1	A	777	A
1	A	780	A
1	A	781	A
1	A	782	A
1	A	785	G
1	A	789	U
1	A	792	A
1	A	793	U
1	A	794	A
1	A	796	C
1	A	799	G
1	A	803	G
1	A	805	C

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Mol	Chain	Res	Type
1	A	810	C
1	A	811	C
1	A	812	C
1	A	813	U
1	A	814	A
1	A	815	A
1	A	816	A
1	A	817	C
1	A	818	G
1	A	819	A
1	A	820	U
1	A	828	A
1	A	829	G
1	A	831	U
1	A	832	C
1	A	837	G
1	A	841	U
1	A	842	C
1	A	843	U
1	A	848	C
1	A	849	C
1	A	850	U
1	A	855	G
1	A	856	C
1	A	857	C
1	A	858	G
1	A	866	C
1	A	867	G
1	A	870	U
1	A	871	U
1	A	872	A
1	A	873	A
1	A	875	C
1	A	877	C
1	A	878	G
1	A	879	C
1	A	880	C
1	A	883	C
1	A	884	U
1	A	885	G
1	A	890	G
1	A	891	U

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Mol	Chain	Res	Type
1	A	898	G
1	A	900	A
1	A	901	A
1	A	902	G
1	A	907	A
1	A	913	A
1	A	914	A
1	A	917	G
1	A	919	A
1	A	922	G
1	A	926	G
1	A	927	G
1	A	932	C
1	A	934	C
1	A	936	C
1	A	938	A
1	A	939	G
1	A	945	G
1	A	947	G
1	A	950	U
1	A	954	G
1	A	955	U
1	A	958	A
1	A	960	U
1	A	961	U
1	A	965	A
1	A	966	G
1	A	969	A
1	A	971	G
1	A	972	C
1	A	973	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	979	C
1	A	980	C
1	A	981	U
1	A	984	C
1	A	985	C
1	A	986	A
1	A	991	U

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Mol	Chain	Res	Type
1	A	992	U
1	A	993	G
1	A	994	A
1	A	995	C
1	A	999	U
1	A	1001	G
1	A	1002	G
1	A	1004	A
1	A	1005	A
1	A	1009	G
1	A	1013	G
1	A	1014	A
1	A	1015	A
1	A	1024	G
1	A	1026	G
1	A	1027	C
1	A	1028(A)	C
1	A	1032(A)	G
1	A	1034	G
1	A	1035	A
1	A	1037	C
1	A	1040	U
1	A	1042	G
1	A	1045	C
1	A	1046	A
1	A	1047	G
1	A	1049	U
1	A	1050	G
1	A	1054	C
1	A	1055	A
1	A	1056	U
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1071	C
1	A	1072	G
1	A	1081	G
1	A	1084	G
1	A	1087	G
1	A	1089	G
1	A	1092	A

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Mol	Chain	Res	Type
1	A	1093	A
1	A	1095	U
1	A	1100	C
1	A	1101	A
1	A	1102	A
1	A	1104	G
1	A	1113	C
1	A	1116	C
1	A	1117	G
1	A	1118	C
1	A	1125	U
1	A	1126	U
1	A	1129	C
1	A	1131	G
1	A	1133	G
1	A	1134	G
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1142	G
1	A	1147	C
1	A	1152	A
1	A	1153	C
1	A	1154	G
1	A	1156	G
1	A	1157	A
1	A	1158	C
1	A	1159	U
1	A	1160	G
1	A	1163	C
1	A	1164	G
1	A	1174	G
1	A	1175	G
1	A	1182	G
1	A	1183	A
1	A	1184	G
1	A	1187	G
1	A	1188	A
1	A	1189	C
1	A	1191	A

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Mol	Chain	Res	Type
1	A	1192	C
1	A	1196	U
1	A	1197	G
1	A	1198	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1203	C
1	A	1205	U
1	A	1212	U
1	A	1213	A
1	A	1215	G
1	A	1218	C
1	A	1222	G
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1229	A
1	A	1232	U
1	A	1238	A
1	A	1239	A
1	A	1240	U
1	A	1241	G
1	A	1242	C
1	A	1244	C
1	A	1248	A
1	A	1249	C
1	A	1250	A
1	A	1251	A
1	A	1254	C
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1261	A
1	A	1264	C
1	A	1266	G
1	A	1267	C
1	A	1268	A
1	A	1269	A
1	A	1270	C

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Mol	Chain	Res	Type
1	A	1271	G
1	A	1275	A
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1284	C
1	A	1286	A
1	A	1287	A
1	A	1290	G
1	A	1292	U
1	A	1298	C
1	A	1299	A
1	A	1301	U
1	A	1302	U
1	A	1305	G
1	A	1306	A
1	A	1310	G
1	A	1312	G
1	A	1314	C
1	A	1318	A
1	A	1319	A
1	A	1320	C
1	A	1321	C
1	A	1322	C
1	A	1323	G
1	A	1327	C
1	A	1328	C
1	A	1329	A
1	A	1330	U
1	A	1331	G
1	A	1334	G
1	A	1335	C
1	A	1337	G
1	A	1340	A
1	A	1345	U
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1357	A

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Mol	Chain	Res	Type
1	A	1361	G
1	A	1363	A
1	A	1364	U
1	A	1365	G
1	A	1367	C
1	A	1374	A
1	A	1375	A
1	A	1377	A
1	A	1378	C
1	A	1379	G
1	A	1380	U
1	A	1381	U
1	A	1382	C
1	A	1387	G
1	A	1394	A
1	A	1395	C
1	A	1397	C
1	A	1398	A
1	A	1399	C
1	A	1400	C
1	A	1401	G
1	A	1403	C
1	A	1404	C
1	A	1410	G
1	A	1414	U
1	A	1415	G
1	A	1417	G
1	A	1419	G
1	A	1421	G
1	A	1422	G
1	A	1429	C
1	A	1433	A
1	A	1434	A
1	A	1435	G
1	A	1440	C
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1448	C
1	A	1450	U
1	A	1451	A
1	A	1452	C

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Mol	Chain	Res	Type
1	A	1453	G
1	A	1454	G
1	A	1455	G
1	A	1459	C
1	A	1465	C
1	A	1466	C
1	A	1467	G
1	A	1476	G
1	A	1483	A
1	A	1484	C
1	A	1486	G
1	A	1490	C
1	A	1492	A
1	A	1493	A
1	A	1494	G
1	A	1495	U
1	A	1497	G
1	A	1498	U
1	A	1499	A
1	A	1501	C
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1508	G
1	A	1516	G
1	A	1517	G
1	A	1520	G
1	A	1523	G
1	A	1527	C
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1532	U
1	A	1533	C
1	A	1534	A
1	A	1535	C
1	A	1537	U
1	A	1539	C
1	A	1540	U

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Mol	Chain	Res	Type
23	D	4	C
23	D	5	A
23	D	13	A
23	D	15	G
23	D	25	U
23	D	26	G
23	D	28	A
23	D	29	U
23	D	30	G
23	D	33	U
23	D	34	C
23	D	35	G
23	D	36	G
23	D	45	G
23	D	49	A
23	D	50	U
23	D	51	G
23	D	52	A
23	D	53	A
23	D	55	G
23	D	60	G
23	D	61	G
23	D	64	A
23	D	66	C
23	D	68	G
23	D	69	C
23	D	71	A
23	D	72	U
23	D	73	A
23	D	74	A
23	D	75	G
23	D	76	C
23	D	77	C
23	D	82	G
23	D	83	G
23	D	84	A
23	D	85	G
23	D	86	C
23	D	87	C
23	D	88	G
23	D	90	U
23	D	91	A

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Mol	Chain	Res	Type
23	D	92	G
23	D	94	G
23	D	95	G
23	D	96	G
23	D	98	G
23	D	101	G
23	D	102	G
23	D	103	A
23	D	105	C
23	D	109	G
23	D	110	G
23	D	111	A
23	D	112	U
23	D	113	G
23	D	115	C
23	D	119	A
23	D	120	U
23	D	121	G
23	D	122	G
23	D	125	G
23	D	127	A
23	D	128	C
23	D	130	C
23	D	131	G
23	D	136	G
23	D	137(A)	G
23	D	139	G
23	D	140	A
23	D	141(A)	C
23	D	147	U
23	D	149	A
23	D	150	C
23	D	154	G
23	D	155	C
23	D	161	U
23	D	163	U
23	D	164	U
23	D	171	G
23	D	172	C
23	D	173	G
23	D	174	C
23	D	175	G

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Mol	Chain	Res	Type
23	D	178	G
23	D	179	G
23	D	181	A
23	D	184	C
23	D	185	U
23	D	191	A
23	D	196	A
23	D	197	A
23	D	198	C
23	D	199	A
23	D	200	U
23	D	205	G
23	D	206	U
23	D	214	G
23	D	216	A
23	D	217	G
23	D	218	A
23	D	221	A
23	D	222	A
23	D	223	A
23	D	224	G
23	D	226	G
23	D	227	A
23	D	228	A
23	D	229	A
23	D	230	U
23	D	232	G
23	D	233	A
23	D	241	A
23	D	242	G
23	D	243	U
23	D	244	A
23	D	245	G
23	D	246	C
23	D	247	G
23	D	248	G
23	D	249	C
23	D	250	G
23	D	251	A
23	D	252	G
23	D	264	C
23	D	266	G

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Mol	Chain	Res	Type
23	D	268	C
23	D	270(A)	A
23	D	270(B)	A
23	D	270(C)	C
23	D	270(E)	G
23	D	270(K)	C
23	D	270(L)	U
23	D	270(M)	U
23	D	270(N)	G
23	D	270(O)	U
23	D	270(S)	G
23	D	270(Z)	U
23	D	271(A)	C
23	D	271(B)	G
23	D	271(C)	U
23	D	271	G
23	D	272	G
23	D	273(B)	C
23	D	273(E)	U
23	D	273(F)	C
23	D	274	G
23	D	275	G
23	D	276	A
23	D	277	C
23	D	279	C
23	D	280	C
23	D	281	G
23	D	282	A
23	D	283	A
23	D	284	U
23	D	287	C
23	D	289	A
23	D	290	G
23	D	293	U
23	D	294	A
23	D	296	C
23	D	298	G
23	D	299	A
23	D	301	G
23	D	302	C
23	D	305	U
23	D	307	G

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Mol	Chain	Res	Type
23	D	308	G
23	D	310	A
23	D	312	G
23	D	316	C
23	D	321	G
23	D	323	G
23	D	324	A
23	D	325	G
23	D	328	U
23	D	329	G
23	D	330	A
23	D	331	A
23	D	332	A
23	D	333	G
23	D	338	G
23	D	339	U
23	D	340	A
23	D	341	G
23	D	342	G
23	D	344	G
23	D	345	A
23	D	346	A
23	D	347	A
23	D	349	G
23	D	350	U
23	D	351	G
23	D	356	G
23	D	360	G
23	D	361	G
23	D	362	U
23	D	363(A)	A
23	D	363(F)	A
23	D	365	C
23	D	366	C
23	D	370	G
23	D	371	A
23	D	372	G
23	D	373	U
23	D	374	A
23	D	380	U
23	D	385	C
23	D	386	G

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Mol	Chain	Res	Type
23	D	388	G
23	D	389	G
23	D	390	A
23	D	391	G
23	D	392	C
23	D	393	C
23	D	395	U
23	D	396	G
23	D	399	G
23	D	400	G
23	D	403	U
23	D	404	C
23	D	405	U
23	D	410	G
23	D	411	G
23	D	412	A
23	D	413	C
23	D	415	A
23	D	416	C
23	D	422	A
23	D	423	A
23	D	424	G
23	D	427	U
23	D	428	A
23	D	429	A
23	D	431	U
23	D	435	C
23	D	436	C
23	D	443	A
23	D	444	C
23	D	446	G
23	D	447	A
23	D	448	U
23	D	449	A
23	D	451	C
23	D	452	G
23	D	453	C
23	D	455	C
23	D	456	C
23	D	457	A
23	D	458	G
23	D	459	U

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Mol	Chain	Res	Type
23	D	464	U
23	D	467	G
23	D	470	A
23	D	471	A
23	D	473	G
23	D	475	U
23	D	476	G
23	D	477	A
23	D	478	A
23	D	480	A
23	D	481	G
23	D	482	A
23	D	483	A
23	D	492	A
23	D	493	G
23	D	503	A
23	D	504	U
23	D	505	A
23	D	506	G
23	D	507	A
23	D	508	G
23	D	509	C
23	D	510	C
23	D	511	U
23	D	512	G
23	D	517	C
23	D	519	U
23	D	520	G
23	D	521	G
23	D	522	G
23	D	523	C
23	D	527	C
23	D	528	A
23	D	530	G
23	D	531	C
23	D	532	A
23	D	533	G
23	D	541	C
23	D	547	A
23	D	549	G
23	D	551	G
23	D	554	U

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Mol	Chain	Res	Type
23	D	556	G
23	D	557	U
23	D	558	G
23	D	559	G
23	D	560	C
23	D	561	G
23	D	562	U
23	D	563	G
23	D	564	C
23	D	565	C
23	D	566	U
23	D	567	A
23	D	568	U
23	D	569	U
23	D	572	A
23	D	573	G
23	D	574	C
23	D	575	A
23	D	577	G
23	D	581	C
23	D	583	G
23	D	585	G
23	D	587	C
23	D	588	U
23	D	594	U
23	D	598	G
23	D	601	C
23	D	602	G
23	D	603	A
23	D	604	G
23	D	607	U
23	D	608	A
23	D	609	A
23	D	612	G
23	D	613	U
23	D	614	U
23	D	615	G
23	D	616	A
23	D	617	G
23	D	619	G
23	D	620	G
23	D	621	A

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Mol	Chain	Res	Type
23	D	624	C
23	D	625	G
23	D	627	A
23	D	628	G
23	D	637	A
23	D	639	U
23	D	640	C
23	D	642	G
23	D	644	A
23	D	645	C
23	D	648	G
23	D	649	G
23	D	651	G
23	D	653	A
23	D	654	A
23	D	655	A
23	D	656	G
23	D	660	G
23	D	666	G
23	D	667	U
23	D	669	G
23	D	670	A
23	D	671	C
23	D	672	C
23	D	675	A
23	D	677	A
23	D	679	C
23	D	682	G
23	D	684	G
23	D	685	A
23	D	686	G
23	D	687	C
23	D	690	G
23	D	692	C
23	D	698	C
23	D	699	A
23	D	705	A
23	D	713	G
23	D	714	U
23	D	715	G
23	D	716	A
23	D	725	G

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Mol	Chain	Res	Type
23	D	726	G
23	D	727	A
23	D	728	G
23	D	729	G
23	D	730	C
23	D	731	C
23	D	733	G
23	D	734	A
23	D	739	G
23	D	741	G
23	D	743	G
23	D	745	G
23	D	746	A
23	D	747	U
23	D	748	G
23	D	749	C
23	D	750	A
23	D	751	A
23	D	752	A
23	D	753	C
23	D	755	C
23	D	758	C
23	D	759	G
23	D	762	U
23	D	763	G
23	D	764	A
23	D	769	G
23	D	771	G
23	D	772	C
23	D	774	A
23	D	775	G
23	D	776	G
23	D	777	A
23	D	778	G
23	D	780	G
23	D	781	A
23	D	782	A
23	D	783	A
23	D	784	A
23	D	785	G
23	D	786	C
23	D	788	A

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Mol	Chain	Res	Type
23	D	789	A
23	D	790	C
23	D	791	C
23	D	792	G
23	D	793	A
23	D	794	G
23	D	796	C
23	D	797	C
23	D	799	G
23	D	800	A
23	D	801	G
23	D	802	A
23	D	803	U
23	D	804	A
23	D	805	G
23	D	806	C
23	D	811	U
23	D	812	C
23	D	819	A
23	D	820	A
23	D	822	U
23	D	823	G
23	D	824	A
23	D	827	U
23	D	828	U
23	D	830	G
23	D	831	G
23	D	832	G
23	D	833	U
23	D	834	C
23	D	842	G
23	D	846	C
23	D	847	U
23	D	848	G
23	D	850	C
23	D	855	G
23	D	857	C
23	D	858	U
23	D	859	G
23	D	860	U
23	D	861	A
23	D	863	A

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Mol	Chain	Res	Type
23	D	865	C
23	D	866	A
23	D	867	C
23	D	870	A
23	D	872	A
23	D	878	A
23	D	880	G
23	D	881	G
23	D	884	C
23	D	885	C
23	D	886	C
23	D	887	A
23	D	888	C
23	D	889	C
23	D	890	A
23	D	892	G
23	D	893	C
23	D	894	C
23	D	895	U
23	D	896	A
23	D	897	C
23	D	898	C
23	D	899	A
23	D	900	A
23	D	901	A
23	D	907	U
23	D	908	C
23	D	909	A
23	D	910	A
23	D	913	U
23	D	914	C
23	D	915	C
23	D	917	A
23	D	918	A
23	D	919	G
23	D	923	C
23	D	924	C
23	D	929	G
23	D	930	U
23	D	931	G
23	D	932	G
23	D	933	A

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Mol	Chain	Res	Type
23	D	939	G
23	D	941	A
23	D	942	G
23	D	943	U
23	D	944	G
23	D	945	A
23	D	946	G
23	D	947	G
23	D	949	C
23	D	953	A
23	D	958	U
23	D	959	A
23	D	960	A
23	D	961	C
23	D	962	G
23	D	964	C
23	D	967	C
23	D	972	G
23	D	973	A
23	D	974	G
23	D	974(A)	C
23	D	976	C
23	D	978	G
23	D	979	G
23	D	980	A
23	D	982	C
23	D	983	A
23	D	985	C
23	D	989	G
23	D	990	A
23	D	991	C
23	D	993	G
23	D	994	C
23	D	995	C
23	D	996	A
23	D	997	G
23	D	998	C
23	D	999	U
23	D	1006	C
23	D	1008	C
23	D	1011	G
23	D	1013	C

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Mol	Chain	Res	Type
23	D	1015	G
23	D	1017	G
23	D	1019	U
23	D	1020	A
23	D	1021	A
23	D	1022	G
23	D	1023	U
23	D	1024	G
23	D	1026	U
23	D	1032	A
23	D	1033	U
23	D	1034	G
23	D	1035	U
23	D	1041	C
23	D	1042	G
23	D	1043	C
23	D	1044	G
23	D	1045	A
23	D	1046	A
23	D	1047	G
23	D	1048	A
23	D	1049	C
23	D	1051	G
23	D	1052	C
23	D	1054	A
23	D	1056	G
23	D	1057	A
23	D	1058	G
23	D	1059	G
23	D	1060	U
23	D	1061	U
23	D	1062	G
23	D	1063	G
23	D	1064	C
23	D	1065	U
23	D	1066	U
23	D	1068	G
23	D	1070	A
23	D	1073	A
23	D	1074	G
23	D	1075	C
23	D	1076	C

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Mol	Chain	Res	Type
23	D	1077	A
23	D	1078	U
23	D	1079	C
23	D	1083	U
23	D	1084	A
23	D	1085	A
23	D	1086	A
23	D	1088	A
23	D	1090	U
23	D	1093	G
23	D	1094	U
23	D	1095	A
23	D	1099	G
23	D	1101	U
23	D	1102	C
23	D	1103	A
23	D	1104	C
23	D	1105	U
23	D	1106	G
23	D	1107	G
23	D	1108	U
23	D	1109	C
23	D	1110	G
23	D	1111	A
23	D	1112	G
23	D	1117	G
23	D	1126	A
23	D	1129	A
23	D	1130	U
23	D	1131	G
23	D	1134	G
23	D	1135	C
23	D	1138	G
23	D	1140	C
23	D	1141	U
23	D	1142	U
23	D	1142(A)	A
23	D	1147	C
23	D	1151	G
23	D	1155	A
23	D	1156	A
23	D	1157	G

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Mol	Chain	Res	Type
23	D	1158	C
23	D	1160	G
23	D	1161	C
23	D	1167	U
23	D	1169	G
23	D	1171	G
23	D	1173	G
23	D	1174	A
23	D	1175	U
23	D	1176	G
23	D	1177	A
23	D	1180	C
23	D	1182	A
23	D	1183	G
23	D	1184	G
23	D	1185	C
23	D	1188	U
23	D	1190	G
23	D	1195	G
23	D	1197	G
23	D	1199	U
23	D	1200	C
23	D	1203	G
23	D	1204	A
23	D	1205	U
23	D	1206	G
23	D	1208	C
23	D	1209	G
23	D	1211	U
23	D	1212	G
23	D	1213	A
23	D	1214	A
23	D	1216	G
23	D	1219	G
23	D	1220	A
23	D	1221	C
23	D	1222	C
23	D	1223	C
23	D	1224	G
23	D	1225	C
23	D	1227	A
23	D	1230	C

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Mol	Chain	Res	Type
23	D	1235	G
23	D	1236	G
23	D	1237	A
23	D	1238	G
23	D	1240	U
23	D	1241	A
23	D	1242	A
23	D	1243	G
23	D	1244	G
23	D	1248	G
23	D	1249	U
23	D	1251	C
23	D	1252	G
23	D	1253	A
23	D	1254	A
23	D	1255	U
23	D	1256	G
23	D	1264	G
23	D	1265	A
23	D	1266	G
23	D	1267	U
23	D	1268	A
23	D	1271	G
23	D	1272	A
23	D	1273	U
23	D	1274	A
23	D	1275	A
23	D	1285	G
23	D	1286	A
23	D	1287	A
23	D	1288	U
23	D	1289	C
23	D	1290	C
23	D	1294	U
23	D	1299	G
23	D	1300	U
23	D	1301	A
23	D	1303	G
23	D	1309	G
23	D	1310	G
23	D	1311	G
23	D	1312	U

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Mol	Chain	Res	Type
23	D	1318	C
23	D	1321	A
23	D	1322	A
23	D	1323	U
23	D	1324	G
23	D	1325	G
23	D	1326	U
23	D	1328	G
23	D	1329	U
23	D	1330	C
23	D	1332	G
23	D	1333	C
23	D	1335	U
23	D	1340	U
23	D	1341	U
23	D	1342	A
23	D	1343	G
23	D	1344	G
23	D	1345	C
23	D	1359	A
23	D	1360	A
23	D	1364	G
23	D	1365	A
23	D	1366	A
23	D	1368	G
23	D	1378	A
23	D	1379	A
23	D	1380	G
23	D	1381	G
23	D	1384	A
23	D	1385	G
23	D	1391	U
23	D	1392	A
23	D	1393	A
23	D	1394	U
23	D	1395	A
23	D	1397	U
23	D	1398	C
23	D	1412	A
23	D	1415	U
23	D	1416	G
23	D	1417	C

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Mol	Chain	Res	Type
23	D	1419	A
23	D	1420	U
23	D	1422	G
23	D	1425	G
23	D	1427	A
23	D	1428	C
23	D	1429	G
23	D	1430	C
23	D	1437	C
23	D	1438	U
23	D	1440	G
23	D	1444	G
23	D	1444(A)	A
23	D	1446	C
23	D	1449	A
23	D	1451	C
23	D	1453	A
23	D	1454	U
23	D	1455	G
23	D	1459	G
23	D	1460	A
23	D	1461	G
23	D	1467	C
23	D	1470	G
23	D	1471	A
23	D	1472	A
23	D	1475	G
23	D	1476	C
23	D	1477	A
23	D	1478	G
23	D	1479	G
23	D	1480	G
23	D	1482	U
23	D	1483	G
23	D	1485	G
23	D	1488	G
23	D	1489	U
23	D	1490	A
23	D	1491	G
23	D	1492	G
23	D	1493	C
23	D	1494	A

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Mol	Chain	Res	Type
23	D	1496	A
23	D	1497	U
23	D	1498	C
23	D	1499	C
23	D	1505	C
23	D	1507	A
23	D	1508	A
23	D	1509	C
23	D	1510	A
23	D	1512	G
23	D	1513	C
23	D	1514	U
23	D	1515	C
23	D	1516	U
23	D	1519	G
23	D	1520	U
23	D	1521	G
23	D	1522	G
23	D	1527	G
23	D	1528	A
23	D	1529	A
23	D	1530	G
23	D	1534	G
23	D	1537	C
23	D	1538	G
23	D	1540	G
23	D	1543	A
23	D	1544	C
23	D	1545	A
23	D	1547	C
23	D	1552	G
23	D	1553	A
23	D	1558	A
23	D	1560	G
23	D	1565	C
23	D	1566	A
23	D	1567	A
23	D	1568	G
23	D	1569	A
23	D	1570	A
23	D	1571	A
23	D	1572	A

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Mol	Chain	Res	Type
23	D	1573	G
23	D	1577	C
23	D	1578	U
23	D	1579	A
23	D	1580	A
23	D	1581	G
23	D	1583	A
23	D	1587	A
23	D	1589	C
23	D	1590	U
23	D	1591	G
23	D	1595	G
23	D	1596	A
23	D	1597	A
23	D	1600	C
23	D	1601	G
23	D	1602	U
23	D	1603	A
23	D	1604	C
23	D	1605	C
23	D	1606	G
23	D	1607	C
23	D	1608	A
23	D	1609	A
23	D	1610	A
23	D	1611	C
23	D	1612	C
23	D	1613	G
23	D	1614	A
23	D	1615	C
23	D	1617	C
23	D	1618	A
23	D	1619	G
23	D	1623	G
23	D	1624	G
23	D	1626	G
23	D	1627	G
23	D	1631	A
23	D	1633	G
23	D	1634	A
23	D	1635	G
23	D	1637	A

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Mol	Chain	Res	Type
23	D	1640	C
23	D	1645	G
23	D	1646	C
23	D	1647	G
23	D	1648	C
23	D	1649	G
23	D	1651	G
23	D	1652	A
23	D	1653	G
23	D	1654	A
23	D	1655	A
23	D	1656	C
23	D	1662	C
23	D	1664	A
23	D	1667	G
23	D	1668	A
23	D	1669	A
23	D	1672	C
23	D	1673	U
23	D	1674	G
23	D	1675	C
23	D	1682	G
23	D	1683	C
23	D	1695	G
23	D	1696	G
23	D	1697	G
23	D	1698	A
23	D	1699	G
23	D	1700	A
23	D	1701	A
23	D	1703	G
23	D	1707	G
23	D	1709	U
23	D	1718	G
23	D	1725	G
23	D	1727	U
23	D	1728	G
23	D	1729	A
23	D	1730	U
23	D	1731	G
23	D	1732	A
23	D	1733	G

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Mol	Chain	Res	Type
23	D	1734	C
23	D	1743	G
23	D	1746	G
23	D	1749	A
23	D	1753	G
23	D	1754	C
23	D	1756	G
23	D	1757	U
23	D	1758	G
23	D	1759	A
23	D	1761	C
23	D	1762	A
23	D	1763	G
23	D	1764	G
23	D	1767	C
23	D	1773	A
23	D	1775	U
23	D	1776	G
23	D	1779	U
23	D	1780	A
23	D	1781	C
23	D	1782	C
23	D	1783	A
23	D	1784	A
23	D	1785	A
23	D	1786	A
23	D	1787	A
23	D	1789	A
23	D	1790	C
23	D	1791	A
23	D	1799	G
23	D	1801	G
23	D	1805	U
23	D	1808	U
23	D	1809	A
23	D	1810	A
23	D	1811	G
23	D	1815	A
23	D	1816	G
23	D	1817	G
23	D	1819	A
23	D	1820	U

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Mol	Chain	Res	Type
23	D	1822	G
23	D	1825	A
23	D	1827	C
23	D	1829	A
23	D	1830	C
23	D	1834	U
23	D	1835	G
23	D	1838	C
23	D	1839	G
23	D	1840	G
23	D	1842	G
23	D	1847	A
23	D	1848	A
23	D	1852	C
23	D	1853	A
23	D	1855	G
23	D	1858	G
23	D	1861	G
23	D	1880	C
23	D	1881	C
23	D	1884	A
23	D	1885	A
23	D	1886	C
23	D	1899	G
23	D	1901	A
23	D	1906	G
23	D	1912	A
23	D	1913	A
23	D	1914	C
23	D	1915	U
23	D	1918	A
23	D	1919	A
23	D	1920	C
23	D	1921	G
23	D	1924	C
23	D	1927	A
23	D	1929	G
23	D	1931	U
23	D	1935	G
23	D	1937	A
23	D	1938	A
23	D	1939	U

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Mol	Chain	Res	Type
23	D	1940	U
23	D	1941	C
23	D	1942	C
23	D	1944	U
23	D	1945	G
23	D	1951	U
23	D	1954	G
23	D	1955	U
23	D	1956	U
23	D	1959	G
23	D	1962	C
23	D	1963	U
23	D	1964	G
23	D	1966	A
23	D	1967	C
23	D	1968	G
23	D	1970	A
23	D	1971	A
23	D	1972	A
23	D	1982	C
23	D	1984	G
23	D	1990	C
23	D	1992	G
23	D	1993	U
23	D	1996	C
23	D	1997	G
23	D	2003	G
23	D	2007	C
23	D	2009	G
23	D	2013	A
23	D	2014	A
23	D	2017	U
23	D	2018	G
23	D	2019	A
23	D	2020	A
23	D	2021	C
23	D	2022	U
23	D	2030	A
23	D	2031	A
23	D	2032	G
23	D	2033	A
23	D	2034	U

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Mol	Chain	Res	Type
23	D	2036	C
23	D	2037	G
23	D	2041	U
23	D	2043	C
23	D	2044	C
23	D	2046	G
23	D	2048	G
23	D	2049	G
23	D	2050	C
23	D	2051	A
23	D	2052	G
23	D	2055	C
23	D	2056	G
23	D	2057	A
23	D	2060	A
23	D	2061	G
23	D	2062	A
23	D	2063	C
23	D	2064	C
23	D	2065	C
23	D	2068	U
23	D	2069	G
23	D	2070	G
23	D	2075	U
23	D	2076	U
23	D	2077	A
23	D	2081	C
23	D	2083	G
23	D	2086	U
23	D	2087	G
23	D	2092	U
23	D	2093	G
23	D	2095	C
23	D	2107	C
23	D	2108	C
23	D	2109	U
23	D	2111	C
23	D	2112	G
23	D	2114	A
23	D	2116	G
23	D	2118	U
23	D	2119	A

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Mol	Chain	Res	Type
23	D	2120	G
23	D	2121	G
23	D	2123	G
23	D	2127	G
23	D	2128	C
23	D	2134	A
23	D	2135	A
23	D	2136	C
23	D	2144	U
23	D	2145	C
23	D	2147	G
23	D	2148	G
23	D	2154	G
23	D	2155	G
23	D	2156	G
23	D	2157	G
23	D	2158	A
23	D	2159	G
23	D	2171	A
23	D	2172	U
23	D	2173	A
23	D	2174	C
23	D	2175	C
23	D	2176	A
23	D	2177	C
23	D	2178	C
23	D	2179	C
23	D	2183	C
23	D	2184	G
23	D	2187	G
23	D	2189	U
23	D	2194	G
23	D	2195	C
23	D	2198	A
23	D	2208	U
23	D	2209	C
23	D	2210	G
23	D	2212	A
23	D	2213	U
23	D	2215	G
23	D	2218	G
23	D	2225	A

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Mol	Chain	Res	Type
23	D	2226	C
23	D	2228	G
23	D	2231	C
23	D	2236	C
23	D	2238	G
23	D	2240	C
23	D	2241	A
23	D	2243	U
23	D	2245	U
23	D	2247	A
23	D	2250	G
23	D	2251	G
23	D	2256	G
23	D	2258	C
23	D	2259	G
23	D	2266	A
23	D	2267	A
23	D	2270	G
23	D	2272	U
23	D	2273	A
23	D	2274	A
23	D	2276	G
23	D	2277	G
23	D	2278	A
23	D	2281	C
23	D	2282	G
23	D	2283	C
23	D	2284	C
23	D	2286	A
23	D	2287	A
23	D	2288	A
23	D	2289	G
23	D	2290	G
23	D	2296	U
23	D	2297	C
23	D	2299	G
23	D	2305	A
23	D	2307	G
23	D	2308	G
23	D	2312	U
23	D	2316	C
23	D	2318	G

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Mol	Chain	Res	Type
23	D	2319	G
23	D	2320	A
23	D	2322	A
23	D	2323	G
23	D	2325	G
23	D	2326	C
23	D	2327	A
23	D	2333	A
23	D	2335	A
23	D	2336	A
23	D	2337	G
23	D	2339	G
23	D	2345	G
23	D	2347	C
23	D	2348	U
23	D	2349	G
23	D	2350	C
23	D	2351	G
23	D	2354	G
23	D	2356	C
23	D	2357	U
23	D	2364	C
23	D	2369	A
23	D	2375	G
23	D	2377	A
23	D	2379	G
23	D	2383	G
23	D	2385	C
23	D	2386	C
23	D	2388	A
23	D	2389	G
23	D	2390	U
23	D	2392	A
23	D	2393	A
23	D	2396	G
23	D	2402	C
23	D	2405	G
23	D	2406	U
23	D	2408	U
23	D	2409	G
23	D	2416	C
23	D	2417	C

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Mol	Chain	Res	Type
23	D	2423	U
23	D	2424	C
23	D	2425	A
23	D	2426	A
23	D	2427	C
23	D	2428	G
23	D	2429	G
23	D	2430	A
23	D	2431	U
23	D	2432	A
23	D	2434	A
23	D	2437	U
23	D	2441	C
23	D	2443	C
23	D	2445	G
23	D	2446	G
23	D	2447	G
23	D	2448	A
23	D	2449	U
23	D	2453	A
23	D	2454	G
23	D	2458	G
23	D	2461	C
23	D	2462	U
23	D	2465	C
23	D	2466	C
23	D	2469	A
23	D	2470	G
23	D	2473	U
23	D	2474	C
23	D	2476	A
23	D	2477	C
23	D	2478	A
23	D	2479	G
23	D	2480	C
23	D	2481	G
23	D	2487	G
23	D	2488	A
23	D	2491	U
23	D	2492	U
23	D	2493	U
23	D	2496	C

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Mol	Chain	Res	Type
23	D	2497	A
23	D	2498	C
23	D	2499	C
23	D	2500	U
23	D	2501	C
23	D	2502	G
23	D	2503	A
23	D	2504	U
23	D	2505	G
23	D	2506	U
23	D	2508	G
23	D	2509	G
23	D	2511	U
23	D	2512	C
23	D	2517	C
23	D	2518	A
23	D	2519	U
23	D	2520	C
23	D	2524	G
23	D	2525	G
23	D	2529	G
23	D	2530	A
23	D	2531	A
23	D	2532	G
23	D	2534	A
23	D	2535	G
23	D	2540	C
23	D	2542	A
23	D	2543	G
23	D	2544	G
23	D	2551	C
23	D	2554	U
23	D	2555	U
23	D	2556	C
23	D	2560	C
23	D	2562	U
23	D	2566	A
23	D	2567	G
23	D	2571	C
23	D	2572	A
23	D	2573	C
23	D	2574	G

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Mol	Chain	Res	Type
23	D	2576	G
23	D	2577	A
23	D	2578	G
23	D	2581	G
23	D	2582	G
23	D	2584	U
23	D	2585	U
23	D	2586	C
23	D	2588	G
23	D	2592	G
23	D	2596	U
23	D	2599	G
23	D	2600	A
23	D	2601	C
23	D	2602	A
23	D	2603	G
23	D	2606	C
23	D	2607	G
23	D	2608	G
23	D	2609	U
23	D	2610	C
23	D	2611	U
23	D	2613	U
23	D	2614	A
23	D	2615	U
23	D	2616	C
23	D	2623	G
23	D	2625	G
23	D	2626	C
23	D	2628	C
23	D	2629	A
23	D	2630	G
23	D	2631	G
23	D	2632	A
23	D	2636	U
23	D	2637	U
23	D	2638	G
23	D	2640	G
23	D	2643	G
23	D	2645	G
23	D	2653	U
23	D	2655	G

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Mol	Chain	Res	Type
23	D	2656	U
23	D	2657	A
23	D	2661	G
23	D	2664	G
23	D	2665	A
23	D	2668	G
23	D	2670	A
23	D	2671	A
23	D	2678	C
23	D	2681	C
23	D	2682	U
23	D	2683	C
23	D	2684	U
23	D	2687	U
23	D	2688	U
23	D	2689	U
23	D	2690	C
23	D	2691	C
23	D	2692	C
23	D	2701	C
23	D	2702	U
23	D	2706	G
23	D	2707	G
23	D	2710	C
23	D	2711	A
23	D	2712	U
23	D	2712(A)	A
23	D	2713	A
23	D	2714	G
23	D	2715	C
23	D	2716	U
23	D	2718	G
23	D	2724	C
23	D	2725	A
23	D	2726	U
23	D	2727	G
23	D	2732	G
23	D	2733	A
23	D	2739	U
23	D	2747	G
23	D	2748	A
23	D	2749	A

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Mol	Chain	Res	Type
23	D	2750	A
23	D	2751	G
23	D	2752	C
23	D	2755	C
23	D	2756	U
23	D	2758	A
23	D	2759	G
23	D	2764	A
23	D	2765	A
23	D	2766	G
23	D	2767	C
23	D	2769	C
23	D	2772	C
23	D	2773	C
23	D	2774	C
23	D	2775	A
23	D	2778	A
23	D	2779	U
23	D	2781	A
23	D	2782	G
23	D	2784	C
23	D	2787	C
23	D	2788	C
23	D	2789	C
23	D	2790	A
23	D	2791	C
23	D	2792	G
23	D	2795	G
23	D	2798	C
23	D	2799	A
23	D	2801	A
23	D	2803	C
23	D	2804	C
23	D	2805	G
23	D	2807	G
23	D	2808	U
23	D	2809	A
23	D	2810	A
23	D	2811	G
23	D	2812	G
23	D	2815	C
23	D	2817	G

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Mol	Chain	Res	Type
23	D	2819	G
23	D	2820	A
23	D	2823	A
23	D	2824	C
23	D	2831	G
23	D	2832	U
23	D	2833	G
23	D	2834	G
23	D	2835	A
23	D	2836	U
23	D	2838	G
23	D	2840	C
23	D	2847	U
23	D	2848	G
23	D	2849	U
23	D	2850	A
23	D	2856	C
23	D	2861	G
23	D	2867	G
23	D	2868	A
23	D	2870	C
23	D	2872	G
23	D	2875	C
23	D	2879	C
23	D	2880	C
23	D	2883	A
23	D	2889	C
23	D	2891	G
23	D	2892	A
23	D	2893	G
23	D	2894	G
23	D	2895	U
23	D	2896	C
23	D	2897	U
23	D	2898	U
23	D	2899	G
24	E	0	A
24	E	1	U
24	E	3	C
24	E	5	C
24	E	7	G
24	E	8	U

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Mol	Chain	Res	Type
24	E	12	C
24	E	13	A
24	E	15	A
24	E	16	G
24	E	21	G
24	E	24	G
24	E	27	C
24	E	30	C
24	E	32	C
24	E	35	U
24	E	39	A
24	E	41	U
24	E	44	G
24	E	45	A
24	E	57	A
24	E	58	A
24	E	59	A
24	E	62	C
24	E	66	A
24	E	67	G
24	E	73	A
24	E	75	G
24	E	76	G
24	E	77	U
24	E	83	G
24	E	85	G
24	E	86	G
24	E	89	G
24	E	90	C
24	E	96	G
24	E	99	A
24	E	103	U
24	E	104	A
24	E	105	G
24	E	108	C
24	E	109	G
24	E	111	U
24	E	115	G
24	E	116	G
24	E	118	G
24	E	120	U
55	4	3	C

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Mol	Chain	Res	Type
55	4	5	G
55	4	8	U
55	4	13	C
55	4	17	C
55	4	18	G
55	4	19	G
55	4	20	U
55	4	21	A
55	4	28	C
55	4	32	C
55	4	33	U
55	4	34	C
55	4	35	A
55	4	38	A
55	4	41	C
55	4	47	U
55	4	48	C
55	4	49	G
55	4	52	G
55	4	53	G
55	4	56	C
55	4	57	A
55	4	58	A
55	4	64	G
55	4	72	A
55	4	73	A
55	4	74	C
55	4	75	C
55	4	76	A
56	5	3	C
56	5	4	C
56	5	8	U
56	5	9	A
56	5	14	A
56	5	15	G
56	5	16	U
56	5	17	C
56	5	18	G
56	5	19	G
56	5	20	U
56	5	21	A
56	5	22	G

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Mol	Chain	Res	Type
56	5	23	A
56	5	24	G
56	5	27	G
56	5	34	G
56	5	37	A
56	5	39	U
56	5	40	C
56	5	41	C
56	5	42	C
56	5	47	U
56	5	48	C
56	5	50	U
56	5	52	G
56	5	53	G
56	5	57	G
56	5	59	U
56	5	62	C
56	5	65	G
56	5	71	G
56	5	72	C
56	5	74	C
56	5	75	C
56	5	76	A

All (257) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	13	U
1	A	30	U
1	A	51	A
1	A	60	A
1	A	121	C
1	A	129(A)	G
1	A	195	A
1	A	196	A
1	A	209	U
1	A	210	U
1	A	243	A
1	A	244	U
1	A	246	A
1	A	250	A

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Mol	Chain	Res	Type
1	A	279	A
1	A	281	G
1	A	308	C
1	A	328	C
1	A	372	C
1	A	413	G
1	A	428	G
1	A	447	G
1	A	484	G
1	A	485	G
1	A	518	C
1	A	534	U
1	A	547	A
1	A	559	A
1	A	566	G
1	A	571	U
1	A	575	G
1	A	686	U
1	A	696	A
1	A	703	G
1	A	723	U
1	A	776	G
1	A	812	C
1	A	841	U
1	A	843	U
1	A	870	U
1	A	872	A
1	A	882	C
1	A	890	G
1	A	913	A
1	A	918	A
1	A	975	A
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1004	A
1	A	1036	G
1	A	1101	A
1	A	1103	C
1	A	1125	U
1	A	1139	G
1	A	1182	G

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Mol	Chain	Res	Type
1	A	1196	U
1	A	1214	C
1	A	1224	G
1	A	1226	C
1	A	1240	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1304	G
1	A	1346	A
1	A	1347	G
1	A	1356	G
1	A	1363	A
1	A	1373	G
1	A	1380	U
1	A	1394	A
1	A	1397	C
1	A	1399	C
1	A	1400	C
1	A	1432	G
1	A	1443	G
1	A	1449	C
1	A	1483	A
23	D	12	U
23	D	27	G
23	D	49	A
23	D	67	U
23	D	72	U
23	D	74	A
23	D	90	U
23	D	119	A
23	D	120	U
23	D	148	C
23	D	177	G
23	D	205	G
23	D	215	G
23	D	221	A
23	D	227	A
23	D	246	C
23	D	267	C
23	D	270(B)	A
23	D	270(L)	U

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Mol	Chain	Res	Type
23	D	281	G
23	D	311	A
23	D	323	G
23	D	350	U
23	D	371	A
23	D	389	G
23	D	421	U
23	D	434	U
23	D	442	G
23	D	446	G
23	D	455	C
23	D	470	A
23	D	481	G
23	D	503	A
23	D	506	G
23	D	529	A
23	D	559	G
23	D	574	C
23	D	587	C
23	D	606	U
23	D	616	A
23	D	643	A
23	D	644	A
23	D	686	G
23	D	747	U
23	D	752	A
23	D	757	U
23	D	776	G
23	D	785	G
23	D	788	A
23	D	793	A
23	D	822	U
23	D	831	G
23	D	859	G
23	D	860	U
23	D	865	C
23	D	884	C
23	D	886	C
23	D	930	U
23	D	943	U
23	D	944	G
23	D	945	A

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Mol	Chain	Res	Type
23	D	958	U
23	D	960	A
23	D	973	A
23	D	1062	G
23	D	1077	A
23	D	1103	A
23	D	1105	U
23	D	1183	G
23	D	1187	G
23	D	1204	A
23	D	1210	A
23	D	1221	C
23	D	1236	G
23	D	1237	A
23	D	1240	U
23	D	1241	A
23	D	1242	A
23	D	1265	A
23	D	1266	G
23	D	1289	C
23	D	1310	G
23	D	1340	U
23	D	1426	G
23	D	1427	A
23	D	1458	C
23	D	1489	U
23	D	1492	G
23	D	1498	C
23	D	1515	C
23	D	1521	G
23	D	1568	G
23	D	1586	A
23	D	1614	A
23	D	1618	A
23	D	1626	G
23	D	1634	A
23	D	1650	G
23	D	1672	C
23	D	1673	U
23	D	1681	G
23	D	1758	G
23	D	1778	U

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Mol	Chain	Res	Type
23	D	1819	A
23	D	1828	G
23	D	1854	A
23	D	1880	C
23	D	1900	A
23	D	1905	C
23	D	1918	A
23	D	1920	C
23	D	1930	G
23	D	1937	A
23	D	1938	A
23	D	1943	U
23	D	1966	A
23	D	1969	A
23	D	1991	U
23	D	1996	C
23	D	2006	C
23	D	2020	A
23	D	2030	A
23	D	2033	A
23	D	2047	U
23	D	2049	G
23	D	2056	G
23	D	2111	C
23	D	2126	A
23	D	2157	G
23	D	2158	A
23	D	2194	G
23	D	2225	A
23	D	2227	A
23	D	2242	G
23	D	2275	C
23	D	2276	G
23	D	2281	C
23	D	2283	C
23	D	2311	A
23	D	2319	G
23	D	2322	A
23	D	2350	C
23	D	2382	G
23	D	2423	U
23	D	2425	A

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Mol	Chain	Res	Type
23	D	2427	C
23	D	2436	G
23	D	2468	G
23	D	2500	U
23	D	2519	U
23	D	2572	A
23	D	2576	G
23	D	2581	G
23	D	2585	U
23	D	2602	A
23	D	2610	C
23	D	2612	C
23	D	2660	A
23	D	2664	G
23	D	2670	A
23	D	2681	C
23	D	2705	A
23	D	2712(A)	A
23	D	2725	A
23	D	2749	A
23	D	2754	U
23	D	2773	C
23	D	2777	G
23	D	2882	A
24	E	7	G
24	E	56	G
24	E	66	A
24	E	84	C
56	5	15	G
56	5	38	A
56	5	58	A
56	5	74	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

1 ligand is 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
57	GCP	C	701	-	27,34,34	3.19	8 (29%)	34,54,54	2.76	9 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	GCP	C	701	-	-	9/15/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	C	701	GCP	C3'-C4'	-9.42	1.28	1.53
57	C	701	GCP	O4'-C4'	7.70	1.62	1.45
57	C	701	GCP	O4'-C1'	-6.76	1.31	1.41
57	C	701	GCP	C2-N2	6.08	1.46	1.33
57	C	701	GCP	O2'-C2'	-3.10	1.35	1.43
57	C	701	GCP	O3'-C3'	2.57	1.49	1.43
57	C	701	GCP	C5-C4	-2.40	1.34	1.40
57	C	701	GCP	PB-O2B	-2.13	1.51	1.56

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	C	701	GCP	N2-C2-N3	8.57	131.76	117.79
57	C	701	GCP	N2-C2-N1	-6.11	107.75	117.25
57	C	701	GCP	C1'-N9-C4	-6.03	116.05	126.64
57	C	701	GCP	N3-C2-N1	-5.05	120.48	127.22
57	C	701	GCP	PB-O3A-PA	-4.93	116.91	132.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	C	701	GCP	C2-N3-C4	3.80	119.70	115.36
57	C	701	GCP	C3'-C2'-C1'	3.66	106.49	100.98
57	C	701	GCP	C2-N1-C6	2.28	119.55	115.93
57	C	701	GCP	C5-C6-N1	-2.13	120.52	123.43

There are no chirality outliers.

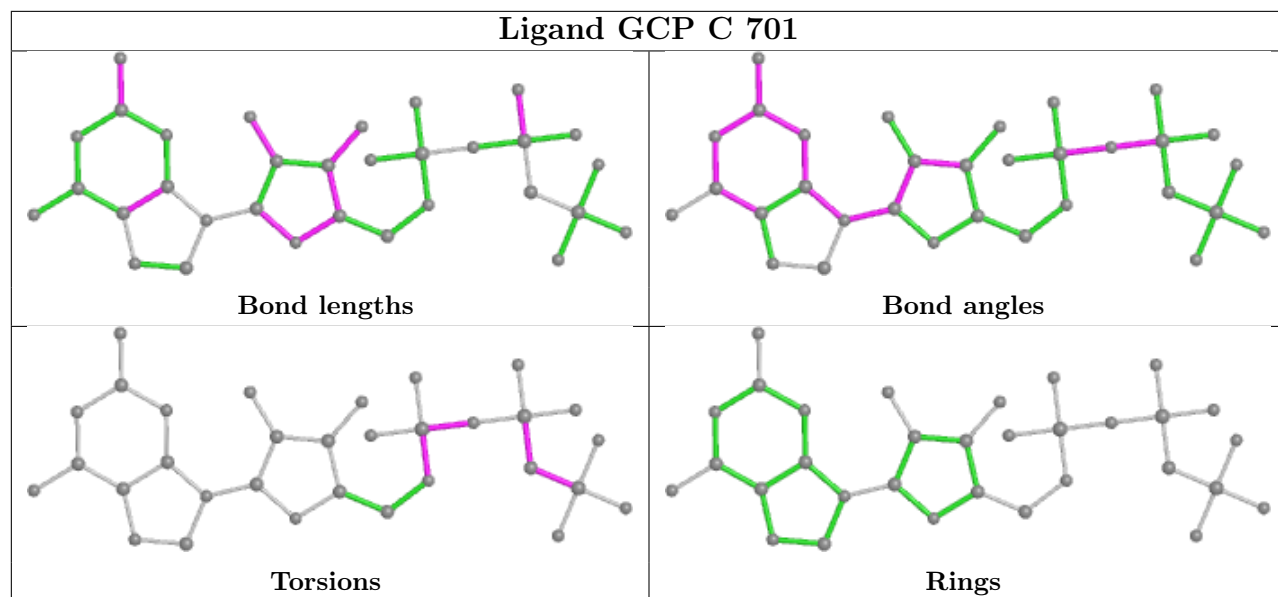
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	C	701	GCP	PG-C3B-PB-O1B
57	C	701	GCP	PG-C3B-PB-O2B
57	C	701	GCP	PG-C3B-PB-O3A
57	C	701	GCP	C5'-O5'-PA-O3A
57	C	701	GCP	C5'-O5'-PA-O1A
57	C	701	GCP	C5'-O5'-PA-O2A
57	C	701	GCP	PB-O3A-PA-O1A
57	C	701	GCP	PB-C3B-PG-O1G
57	C	701	GCP	PB-O3A-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



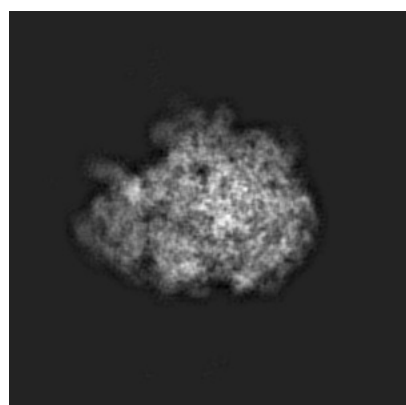
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6585. These allow visual inspection of the internal detail of the map and identification of artifacts.

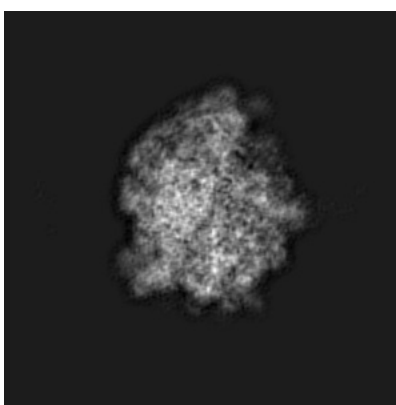
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

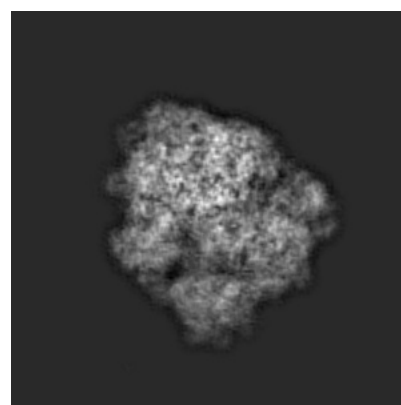
#### 6.1.1 Primary map



X



Y

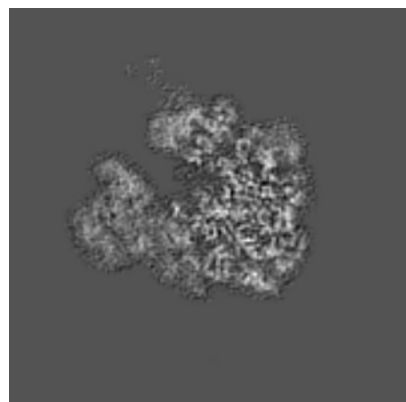


Z

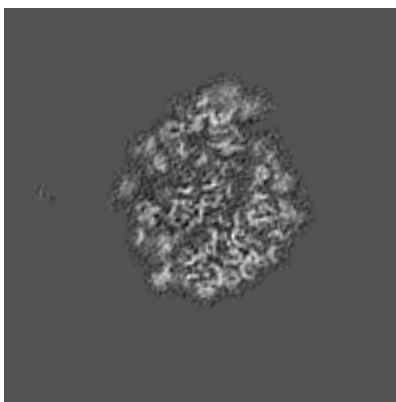
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

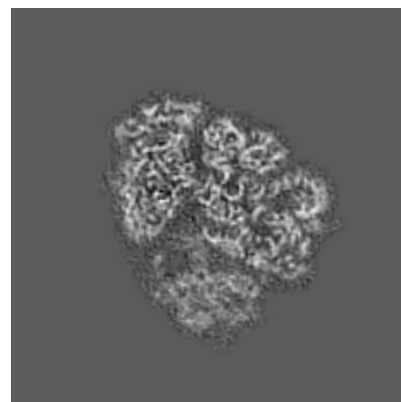
#### 6.2.1 Primary map



X Index: 162



Y Index: 162

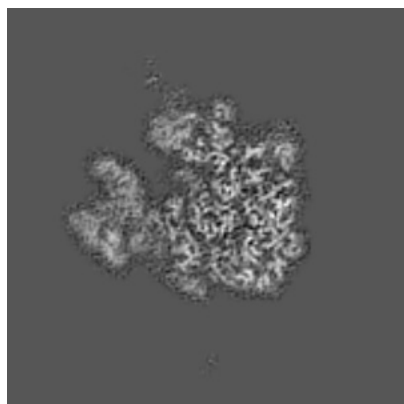


Z Index: 162

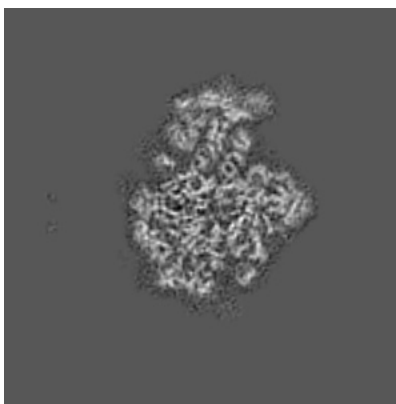
The images above show central slices of the map in three orthogonal directions.

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

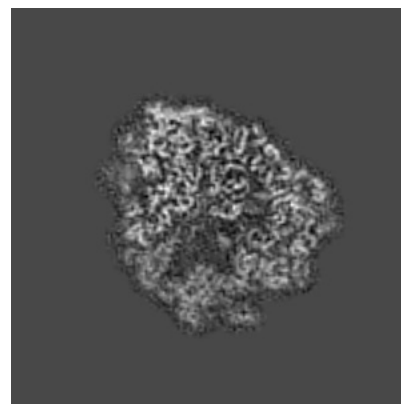
### 6.3.1 Primary map



X Index: 167



Y Index: 170

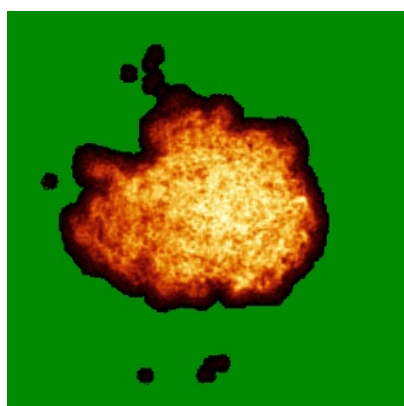


Z Index: 170

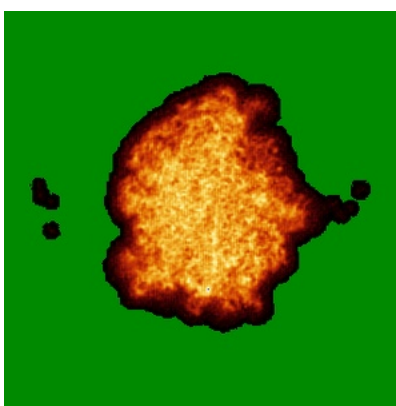
The images above show the largest variance slices of the map in three orthogonal directions.

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

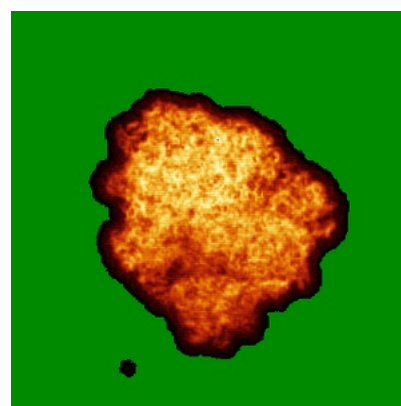
### 6.4.1 Primary map



X



Y

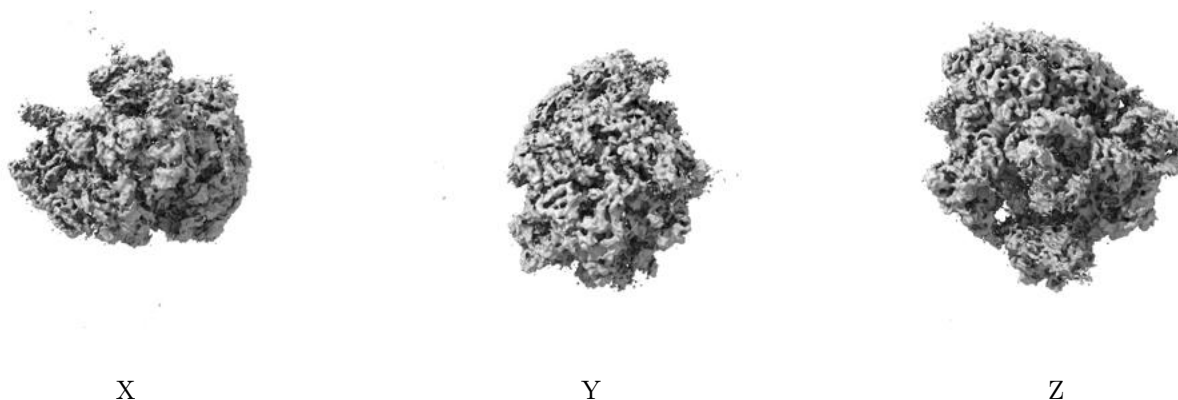


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.161. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

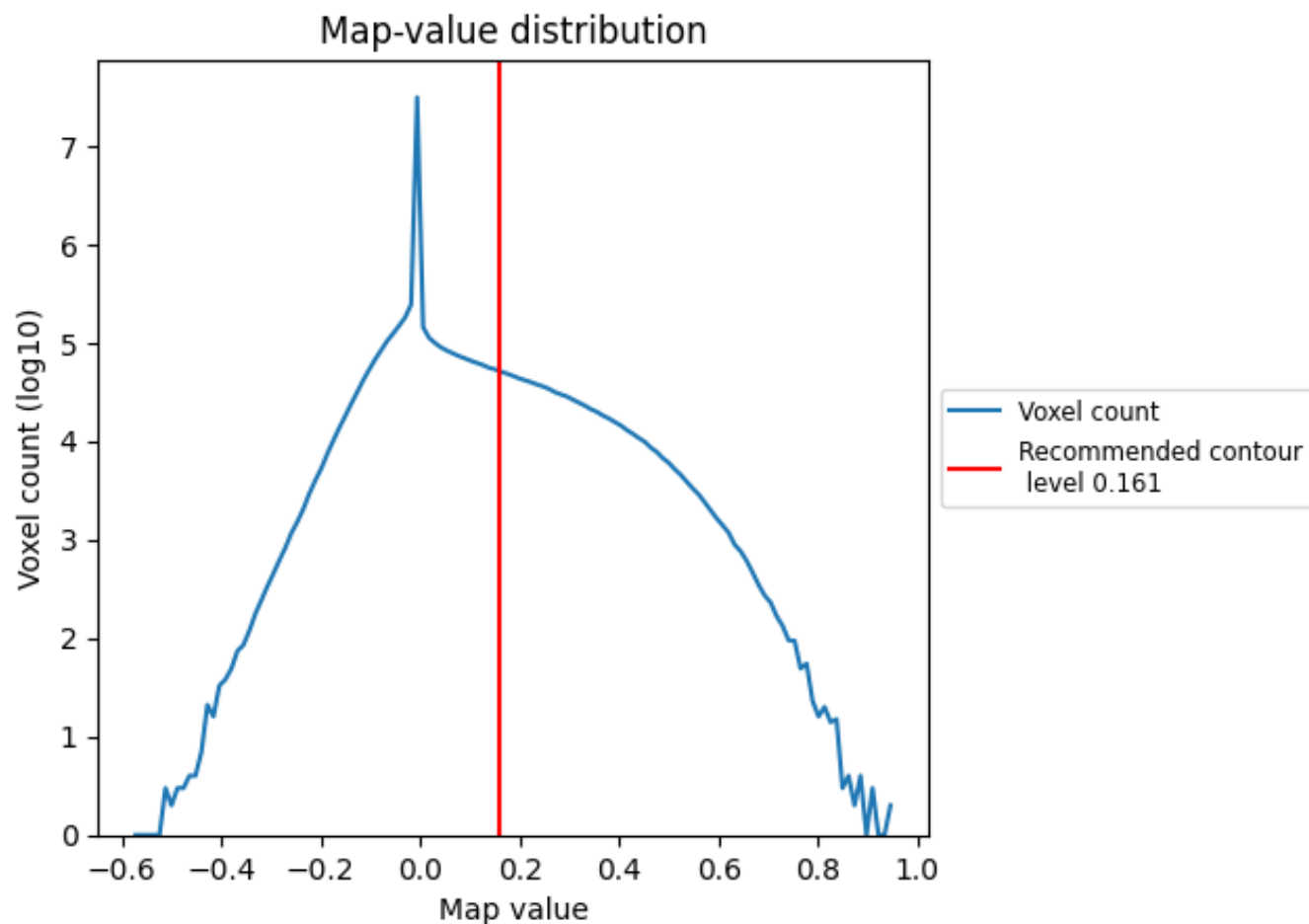
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

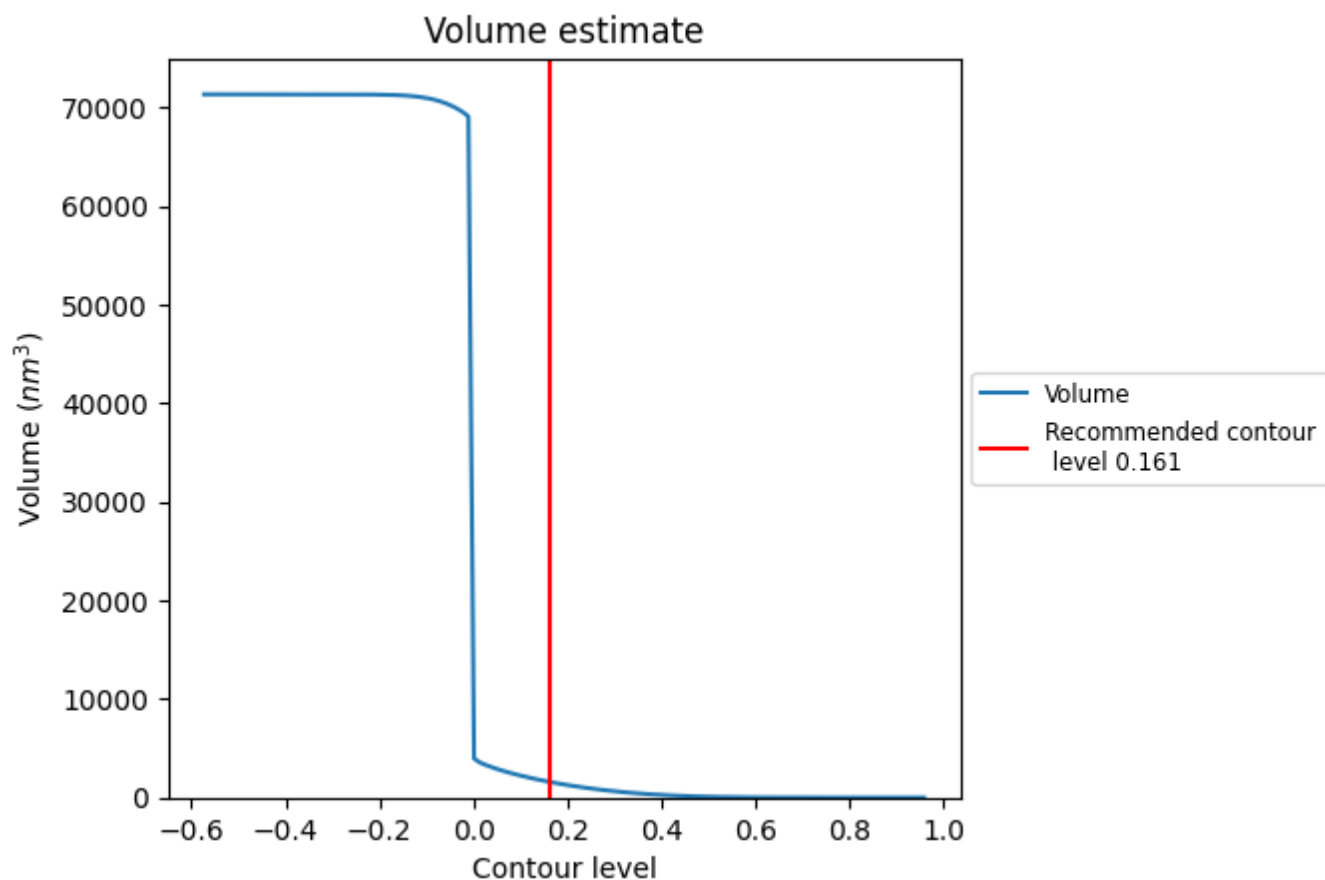
This section contains the results of statistical analysis of the map.

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



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

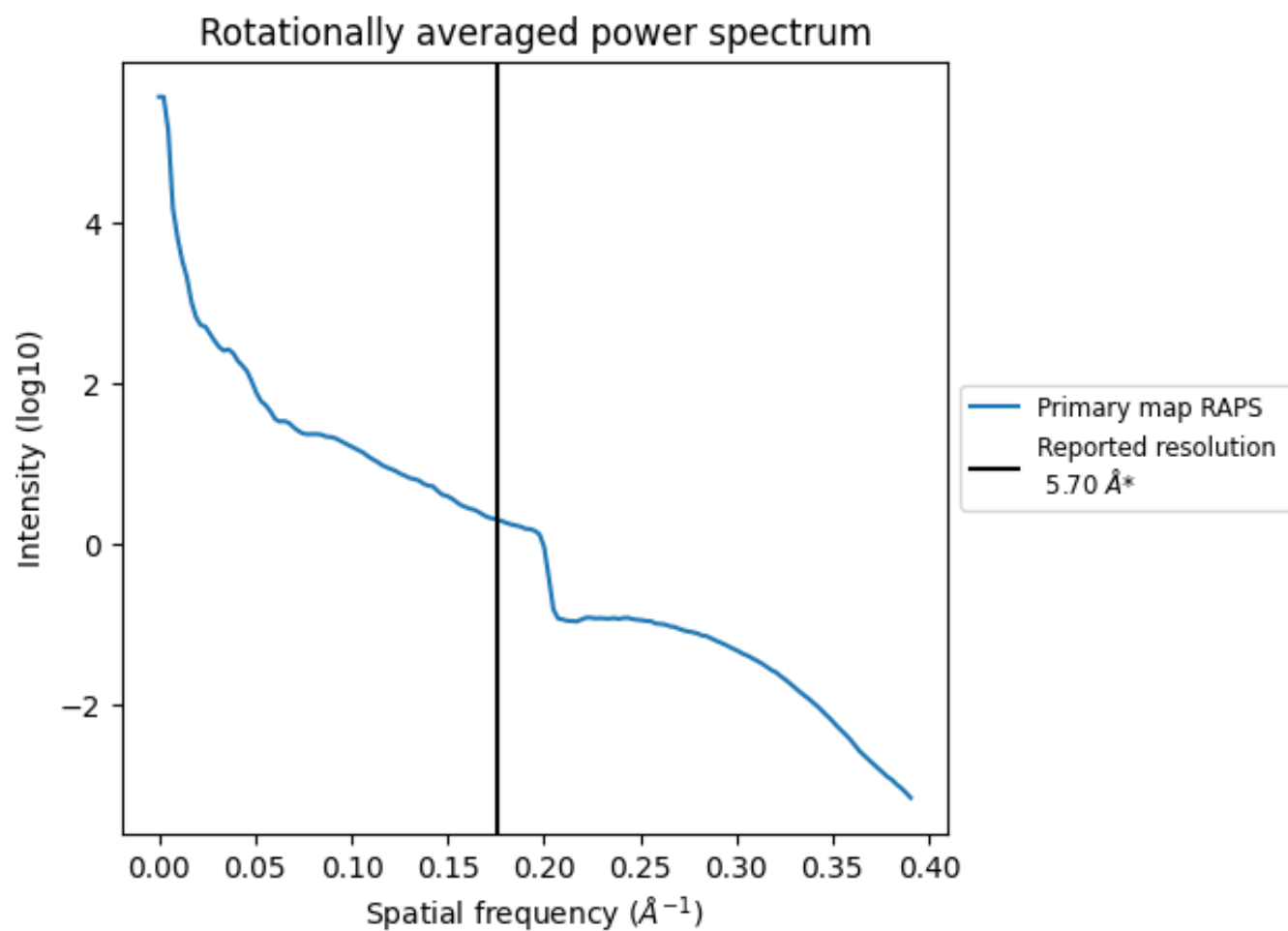
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1597 nm<sup>3</sup>; this corresponds to an approximate mass of 1443 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.175 Å<sup>-1</sup>

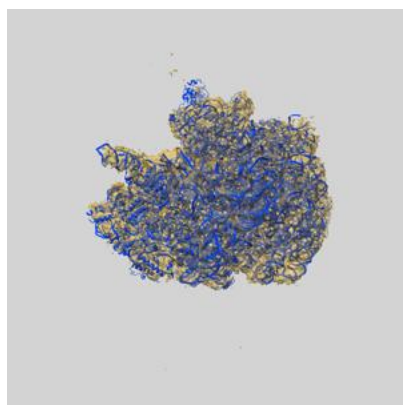
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

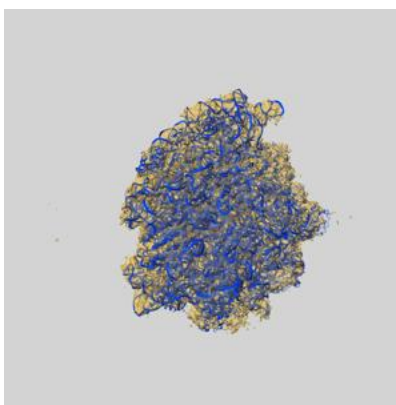
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6585 and PDB model 5IMR. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

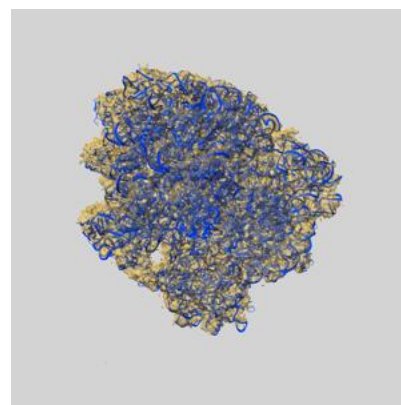
### 9.1 Map-model overlay [i](#)



X



Y

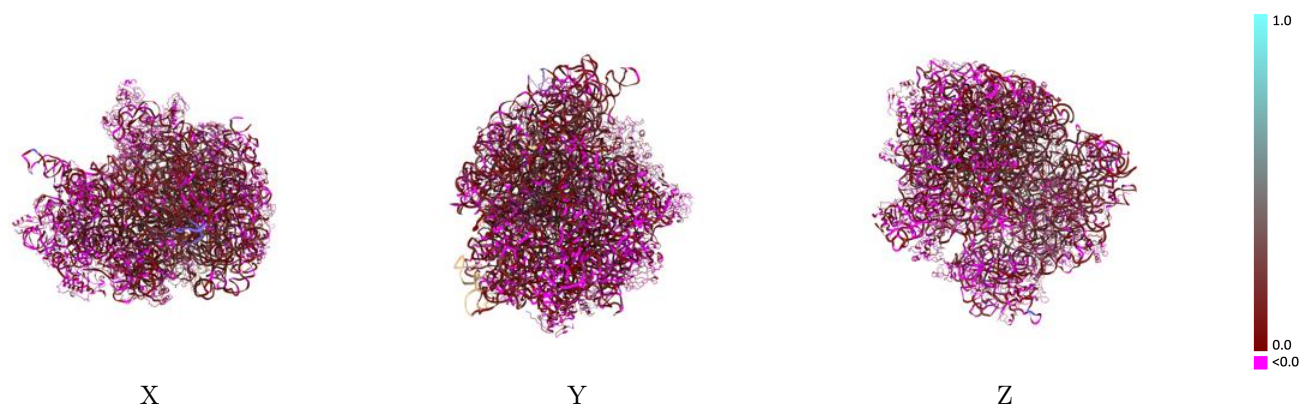


Z

The images above show the 3D surface view of the map at the recommended contour level 0.161 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.

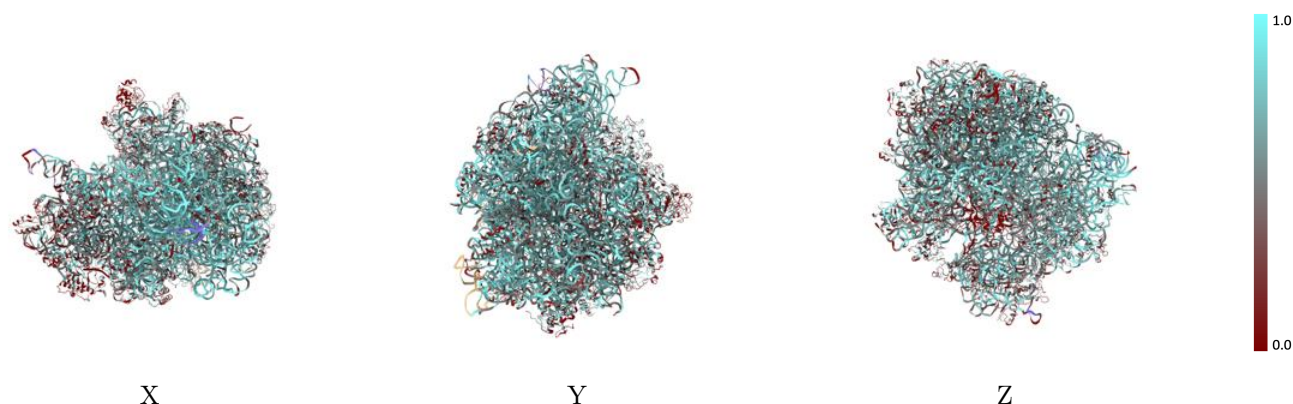


## 9.2 Q-score mapped to coordinate model [i](#)



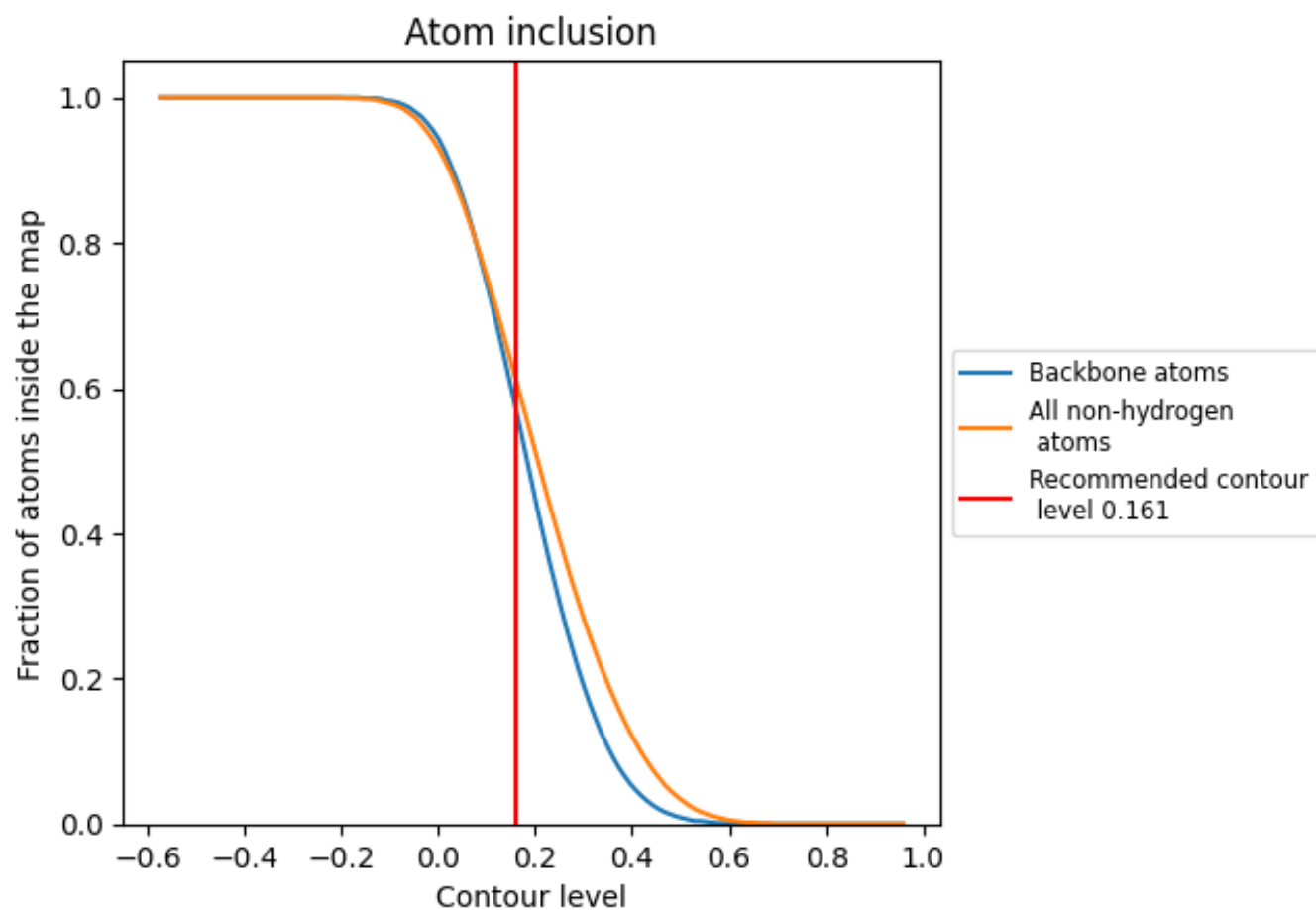
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.161).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 61% 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 (0.161) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6110	 0.1000
1	 0.5100	 0.0940
2	 0.0370	 0.0020
3	 0.3710	 0.0270
4	 0.3630	 0.1310
5	 0.5870	 0.1030
A	 0.7040	 0.1120
C	 0.4590	 0.0940
D	 0.7180	 0.1300
E	 0.6380	 0.0400
F	 0.3260	 0.0200
G	 0.3200	 0.0180
H	 0.4550	 0.0590
I	 0.4890	 0.0960
J	 0.4270	 0.0670
K	 0.3150	 0.0270
L	 0.4960	 0.0610
M	 0.3700	 0.0290
N	 0.3080	 0.0180
O	 0.5250	 0.1180
P	 0.5060	 0.1290
Q	 0.4460	 0.0260
R	 0.3230	 0.0250
S	 0.4630	 0.0880
T	 0.5340	 0.0280
U	 0.5290	 0.0990
V	 0.4290	 0.0820
W	 0.4520	 -0.0270
X	 0.4670	 0.0570
Y	 0.3510	 -0.0210
Z	 0.1620	 0.0120
a	 0.5880	 0.1510
b	 0.4920	 0.0860
c	 0.4520	 0.0640
d	 0.3990	 0.0230



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Chain	Atom inclusion	Q-score
e	 0.4790	 0.0370
f	 0.4250	 0.0370
g	 0.5090	 0.1400
h	 0.4840	 0.0750
i	 0.4460	 0.0850
j	 0.4480	 0.0250
k	 0.4960	 0.0110
l	 0.5070	 0.1240
m	 0.4160	 0.0340
n	 0.4080	 0.0160
o	 0.4270	 0.0540
p	 0.4680	 0.0670
q	 0.4280	 0.0270
r	 0.3180	 0.0200
s	 0.4340	 0.0550
t	 0.4460	 0.0290
u	 0.4250	 0.0400
v	 0.4860	 0.1120
w	 0.3880	 0.0100
x	 0.5160	 0.0970
y	 0.4650	 0.1110
z	 0.3740	 0.0400