



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:24 AM UTC

PDB ID : 6GSN / pdb_00006gsn
EMDB ID : EMD-0058
Title : Structure of a partial yeast 48S preinitiation complex in closed conformation
Authors : Llacer, J.L.; Hussain, T.; Ramakrishnan, V.
Deposited on : 2018-06-14
Resolution : 5.75 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

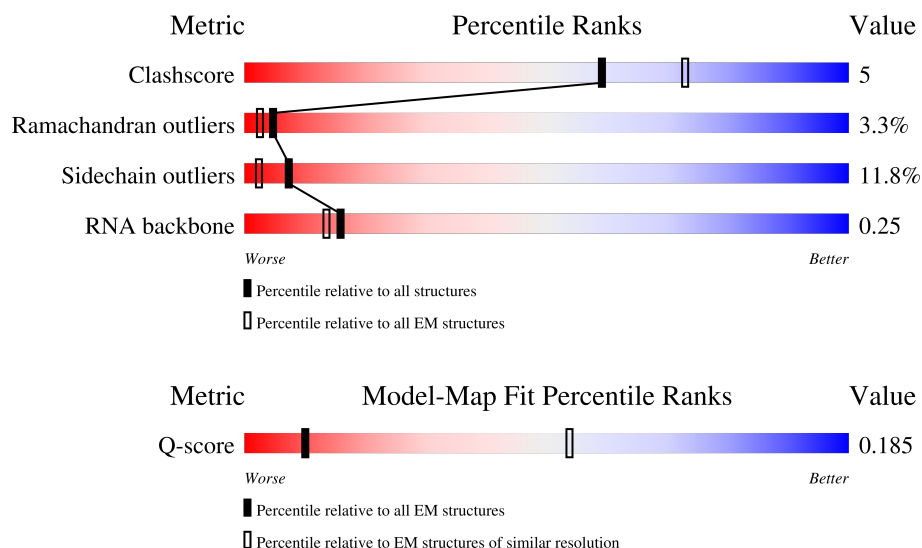
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.75 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	476 (5.25 - 6.25)

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

Mol	Chain	Length	Quality of chain
1	2	1798	
2	C	217	
3	D	223	

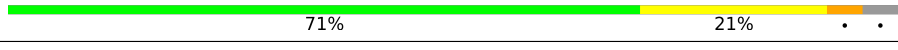
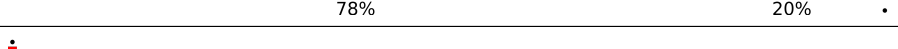
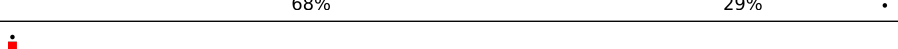
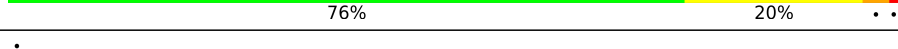
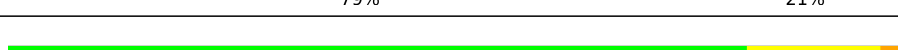
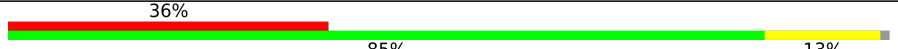
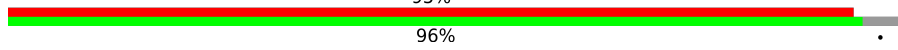
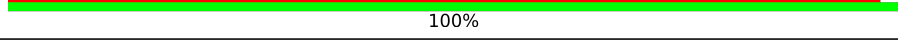
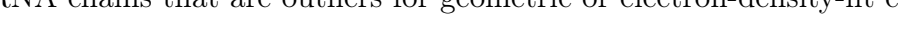
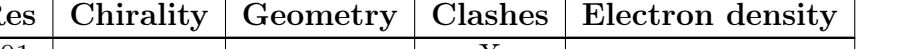
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Mol	Chain	Length	Quality of chain
4	F	206	
5	K	96	
6	M	118	
7	P	117	
8	Q	141	
9	R	130	
10	S	145	
11	T	143	
12	U	106	
13	Z	70	
14	c	62	
15	f	69	
16	g	324	
17	d	53	
18	e	58	
19	h	25	
20	3	14	
21	i	111	
22	m	90	
23	o	567	
24	q	699	
25	k	430	
26	l	144	
27	j	263	
28	1	75	

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Mol	Chain	Length	Quality of chain
29	A	219	
30	B	231	
31	E	260	
32	G	226	
33	H	184	
34	I	200	
35	J	182	
36	L	155	
37	N	150	
38	O	127	
39	V	87	
40	W	129	
41	Y	134	
42	X	144	
43	a	98	
44	b	81	
45	p	666	
46	s	342	
47	r	49	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
49	ZN	a	101	-	-	X	-

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 103798 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 18S rRNA (1798-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1798	Total	C	N	O	P	0	0
			38175	17061	6721	12595	1798		

- Molecule 2 is a protein called KLLA0F09812p.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	217	Total	C	N	O	S	0	0
			1629	1041	287	297	4		

- Molecule 3 is a protein called KLLA0D08305p.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	223	Total	C	N	O	S	0	0
			1744	1108	313	318	5		

- Molecule 4 is a protein called KLLA0D10659p.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 5 is a protein called KLLA0B08173p.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 6 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	117	Total	C	N	O	0	0
			885	553	161	171		

- Molecule 7 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	117	Total	C	N	O	S	0	0
			927	595	166	161	5		

- Molecule 8 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	141	Total	C	N	O		0	0
			1105	709	204	192			

- Molecule 9 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	130	Total	C	N	O	S	0	0
			1027	640	191	193	3		

- Molecule 10 is a protein called KLLA0B01562p.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	145	Total	C	N	O	S	0	0
			1193	741	240	210	2		

- Molecule 11 is a protein called KLLA0A07194p.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	143	Total	C	N	O		0	0
			1110	693	210	207			

- Molecule 12 is a protein called KLLA0F25542p.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 13 is a protein called KLLA0B06182p.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Z	70	Total	C	N	O	S	0	0
			558	355	104	98	1		

- Molecule 14 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	c	62	Total	C	N	O	S	0	0
			487	301	97	88	1		

- Molecule 15 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	69	Total	C	N	O	S	0	0
			546	351	101	90	4		

- Molecule 16 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	g	318	Total	C	N	O	S	0	0
			2466	1561	430	470	5		

- Molecule 17 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	d	53	Total	C	N	O	S	0	0
			446	280	89	76	1		

- Molecule 18 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	e	58	Total	C	N	O	S	0	0
			463	290	94	78	1		

- Molecule 19 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 20 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	3	14	Total	C	N	O	P	0	0
			287	129	42	102	14		

- Molecule 21 is a protein called Eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	i	111	Total	C	N	O	S	0	0
			884	542	170	167	5		

- Molecule 22 is a protein called Eukaryotic translation initiation factor eIF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	m	90	Total	C	N	O	S	0	0
			716	452	132	128	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	20	ALA	THR	conflict	UNP P32911
m	23	ALA	SER	conflict	UNP P32911

- Molecule 23 is a protein called Eukaryotic translation initiation factor 3 subunit A, eIF3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	521	Total	C	N	O	S	0	0
			3996	2554	685	750	7		

- Molecule 24 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	q	675	Total	C	N	O	S	0	0
			5179	3309	874	984	12		

- Molecule 25 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	k	414	Total	C	N	O	S	0	0
			3123	1985	560	562	16		

- Molecule 26 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	l	126	Total	C	N	O	S	0	0
			1016	646	183	180	7		

- Molecule 27 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	j	249	Total	C	N	O	S	0	0
			2006	1283	333	382	8		

- Molecule 28 is a RNA chain called tRNAi (75-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	75	Total	C	N	O	P	0	0
			1607	716	296	520	75		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	31	U	G	conflict	GB 176433
1	39	A	C	conflict	GB 176433

- Molecule 29 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A	219	Total	C	N	O	S	0	0
			1702	1085	299	316	2		

- Molecule 30 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B	222	Total	C	N	O	S	0	0
			1769	1117	324	325	3		

- Molecule 31 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 32 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	G	226	Total	C	N	O	S	0	0
			1812	1134	348	326	4		

- Molecule 33 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	H	184	Total	C	N	O	0	0
			1483	950	270	263		

- Molecule 34 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	I	188	Total	C	N	O	S	0	0
			1489	923	300	265	1		

- Molecule 35 is a protein called KLLA0E23673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 36 is a protein called KLLA0A10483p.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 37 is a protein called KLLA0F18040p.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	N	150	Total	C	N	O	S	0	0
			1187	756	223	206	2		

- Molecule 38 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	O	127	Total	C	N	O	S	0	0
			942	578	188	173	3		

- Molecule 39 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 40 is a protein called 40S ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 41 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Y	134	Total	C	N	O	S	0	0
			1061	665	207	189			

- Molecule 42 is a protein called RPS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	X	144	Total	C	N	O	S	0	0
			1119	708	218	191	2		

- Molecule 43 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	a	98	Total	C	N	O	S	0	0
			779	480	165	129	5		

- Molecule 44 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	b	81	Total	C	N	O	S	0	0
			609	379	112	113	5		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	p	658	Total	C	N	O	S	0	0
			5147	3295	889	945	18		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	330	Total	C	N	O	S	0	0
			2606	1661	429	507	9		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	r	49	Total	C	N	O	0	0
			392	240	76	76		

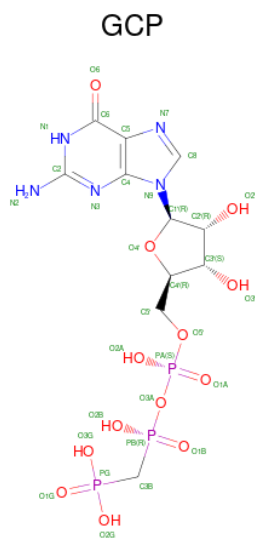
- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	2	76	Total	Mg	0
			76	76	
48	C	1	Total	Mg	0
			1	1	
48	h	1	Total	Mg	0
			1	1	
48	k	1	Total	Mg	0
			1	1	
48	B	1	Total	Mg	0
			1	1	
48	a	1	Total	Mg	0
			1	1	

- Molecule 49 is ZINC ION (CCD ID: ZN) (formula: Zn).

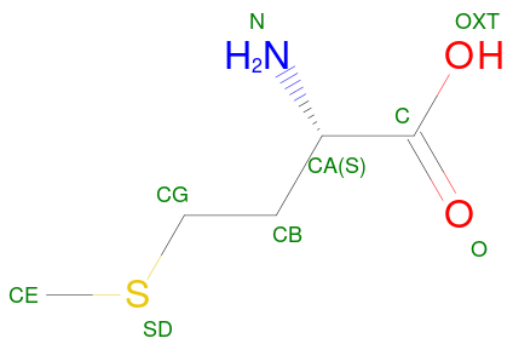
Mol	Chain	Residues	Atoms		AltConf
49	f	1	Total	Zn	0
			1	1	
49	l	1	Total	Zn	0
			1	1	
49	a	1	Total	Zn	0
			1	1	
49	b	1	Total	Zn	0
			1	1	

- Molecule 50 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
50	k	1	Total	C	N	O	P	0
			32	11	5	13	3	

- Molecule 51 is METHIONINE (CCD ID: MET) (formula: $\text{C}_5\text{H}_{11}\text{NO}_2\text{S}$).

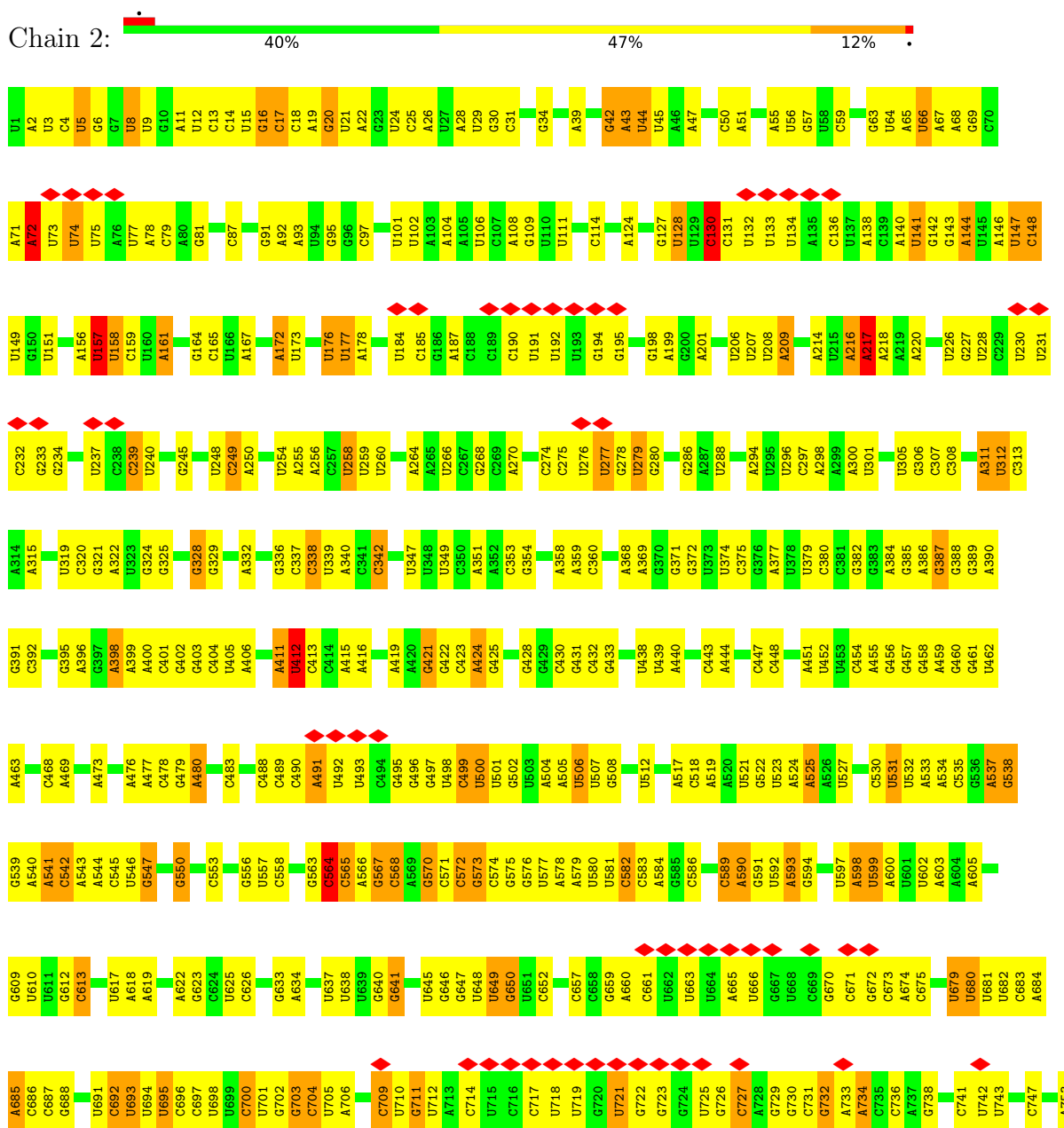


Mol	Chain	Residues	Atoms					AltConf
51	k	1	Total	C	N	O	S	0
			8	5	1	1	1	

3 Residue-property plots

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

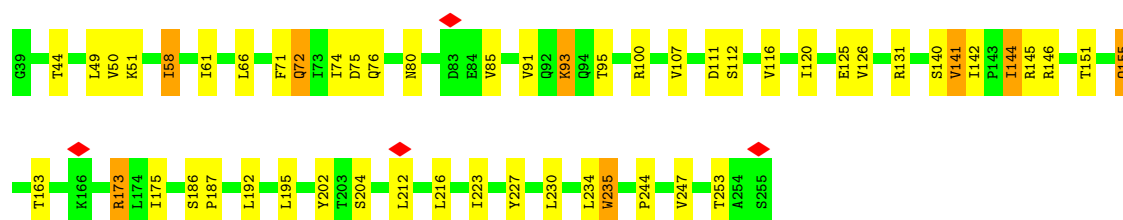
• Molecule 1: 18S rRNA (1798-MER)



G1790	G1791	G1792	U1793	G1794	A1795	U1796	U1797	A1798	G1704	A1705	G1706	G1707	U1708	G1709	A1710	G1711	G1712	G1713	G1714	G1715	A1716	A1717	A1720	G1725	A1728	A1729	A1730	G1735	A1742	G1743	A1744	G1745	A1748	A1753	G1754	G1755	U1756	G1757	G1758	U1759	A1760	A1761	G1762	A1763	A1764	G1765	G1766	U1767	U1768	U1769	A1774	G1775	G1781	G1782	G1786	G1787	A1789	A1790	A1793	A1794	G1795	G1796	U799	G800	G801	A802	A803	U804	A805	G809	A810	A811	U812	A813	G814	C817	G818	U819	U820	U821	G822	G823	U824	U825	C826																																																																																																																																																																																																																																												
U1559	U1564	U1565	C1566	A1571	G1572	G1573	G1574	A1575	U1576	U1577	C1578	U1579	U1580	A1581	G1582	U1583	A1584	A1585	G1586	G1587	G1588	G1589	A1590	U1593	C1594	A1595	U1596	C1597	G1598	A1599	C1600	U1601	U1602	G1603	C1604	G1605	U1606	U1607	G1608	U1611	A1612	C1613	G1614	U1615	C1616	C1617	C1618	U1619	G1620	U1626	G1627	U1628	A1629	C1630	G1631	C1632	A1633	G1634	C1635	G1636	C1637	C1638	G1639	G1640	A1641	C1642	G1647	U1648	C1651	G1652	A1653	U1654	U1655	G1656	G1660	G1661	C1662	U1667	G1670	G1671	C1672	A1675	G1676	U1677	G1678	A1679	U1680	U1681	U1682	G1683	C1684	U1685	U1686	G1687	G1688	A1692	G1693	G1694	G1695	G1696	G1697	U1698	A1699	A1700	C1701	U1702	C1703																																																																																																																																																																																																																						
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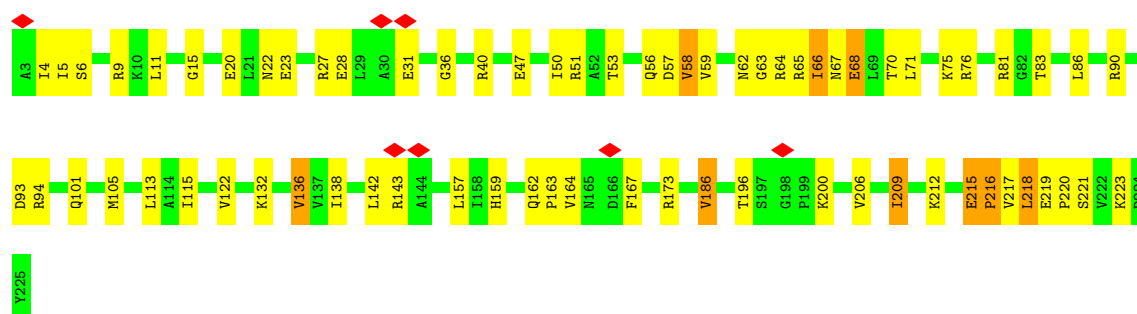
- Molecule 2: KLLA0F09812p

Chain C:  76% 21%



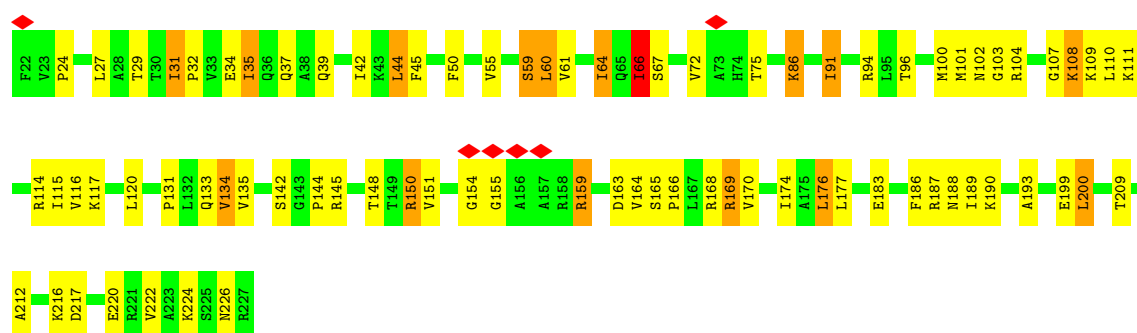
- Molecule 3: KLLA0D08305p

Chain D:  69% 27%



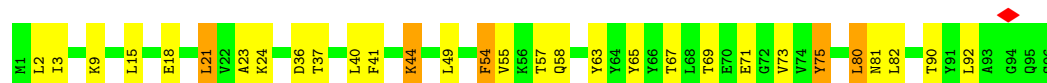
- Molecule 4: KLLA0D10659p

Chain F:  61% 32% 7%



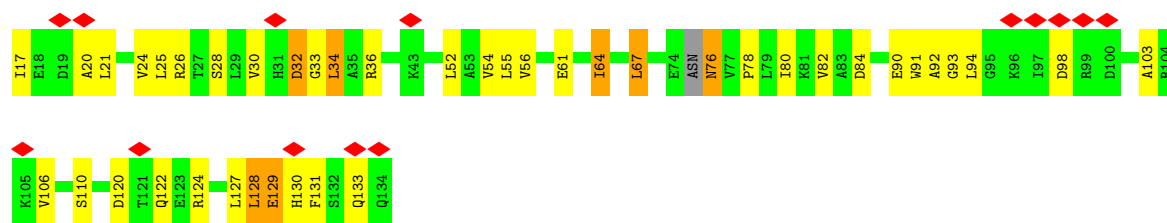
- Molecule 5: KLLA0B08173p

Chain K:  69% 26% 5%

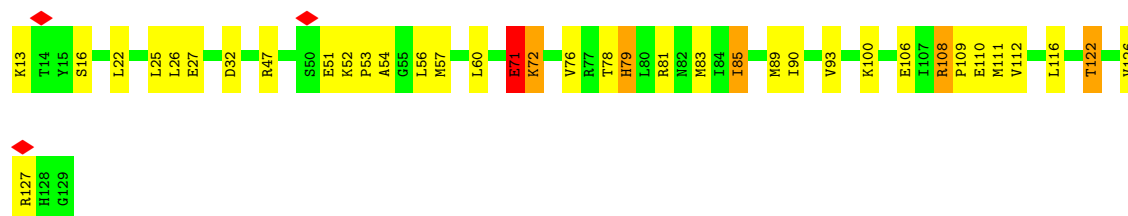


- Molecule 6: 40S ribosomal protein S12

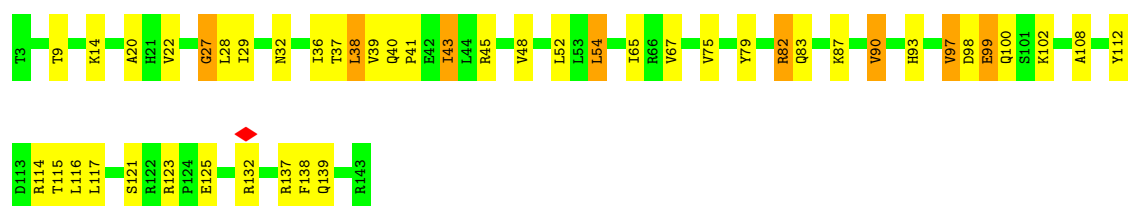
Chain M:  12% 64% 30% 6%



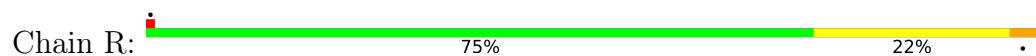
• Molecule 7: KLLA0F07843p



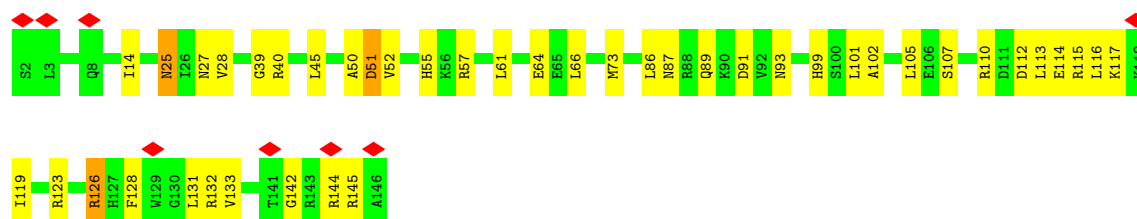
• Molecule 8: 40S ribosomal protein S16



• Molecule 9: KLLA0B01474p

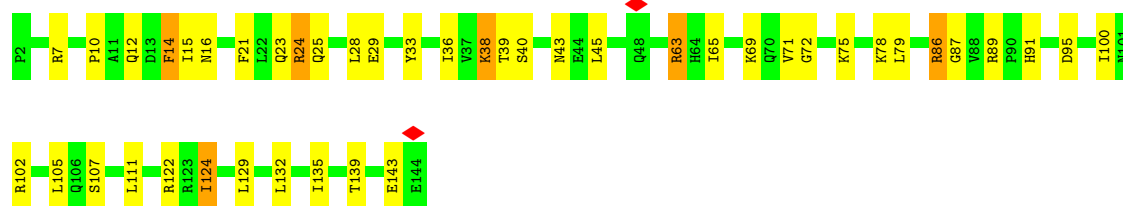


• Molecule 10: KLLA0B01562p



• Molecule 11: KLLA0A07194p

Chain T:  69% 27%



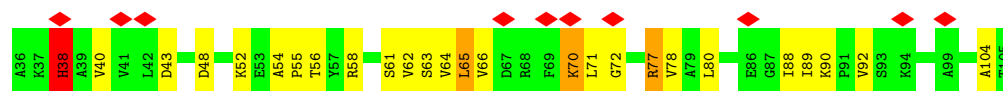
- Molecule 12: KLLA0F25542p

Chain U:  6% 69% 25% 5%



- Molecule 13: KLLA0B06182p

Chain Z:  14% 63% 31%



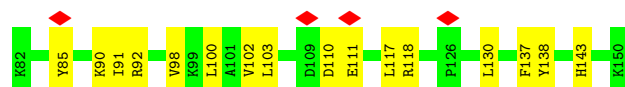
- Molecule 14: 40S ribosomal protein S28

Chain c:  6% 65% 34%



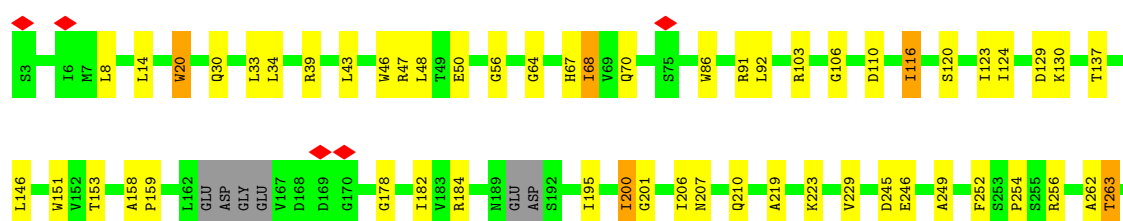
- Molecule 15: Ubiquitin-40S ribosomal protein S27a

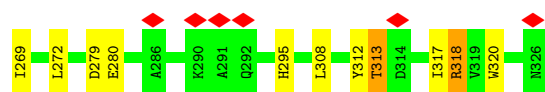
Chain f:  6% 77% 23%



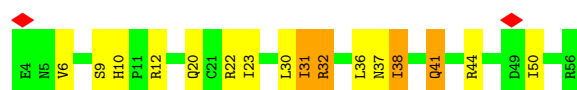
- Molecule 16: KLLA0E12277p

Chain g:  77% 19%

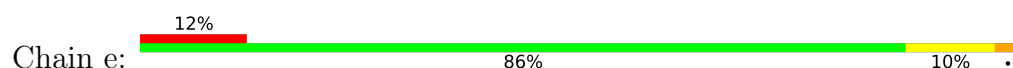




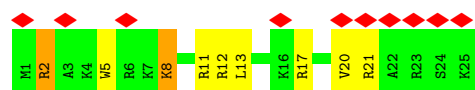
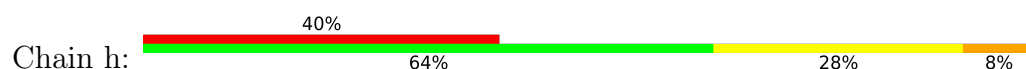
- Molecule 17: 40S ribosomal protein S29



- Molecule 18: 40S ribosomal protein S30



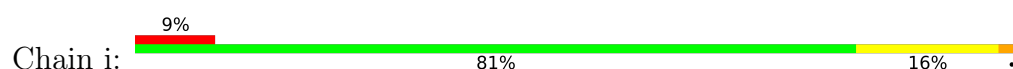
- Molecule 19: 60S ribosomal protein L41-A



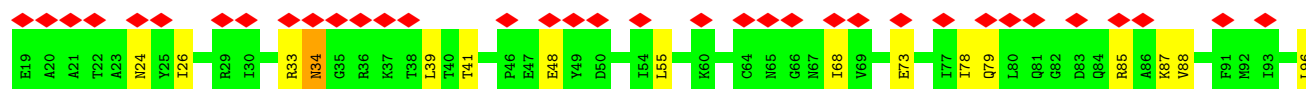
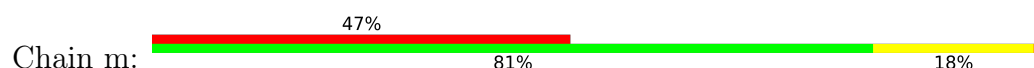
- Molecule 20: mRNA

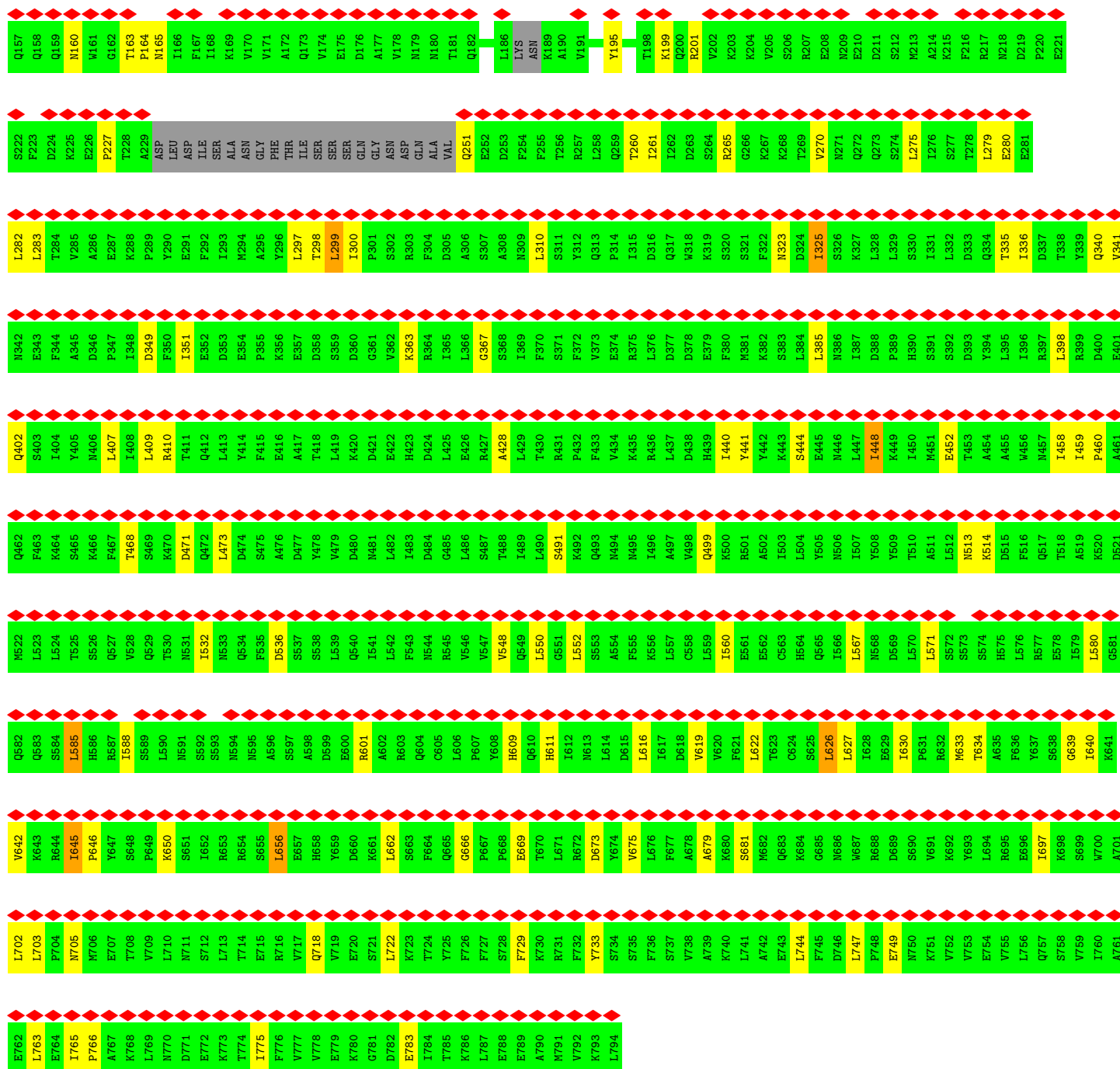


- Molecule 21: Eukaryotic translation initiation factor 1A

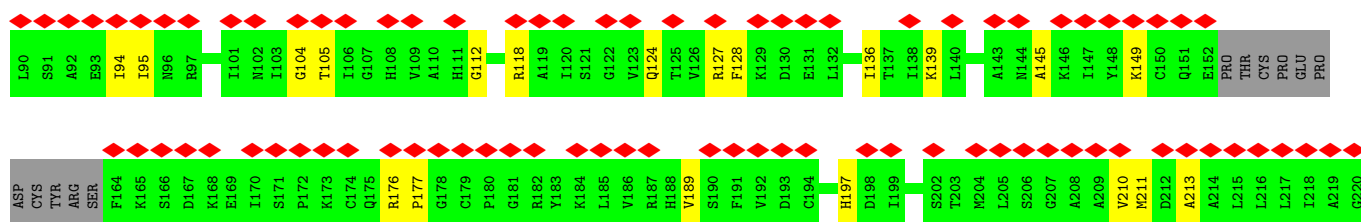
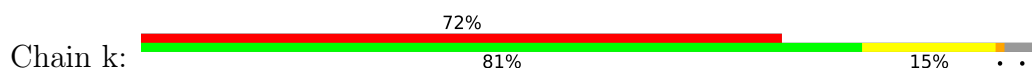


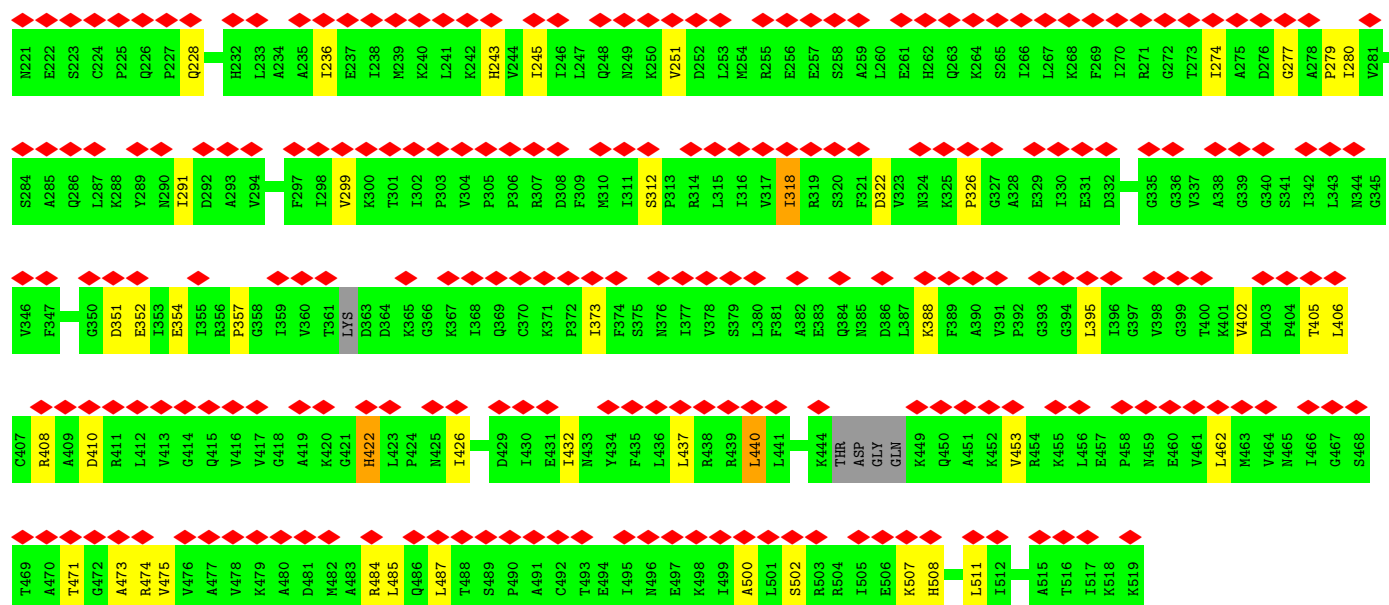
- Molecule 22: Eukaryotic translation initiation factor eIF-1



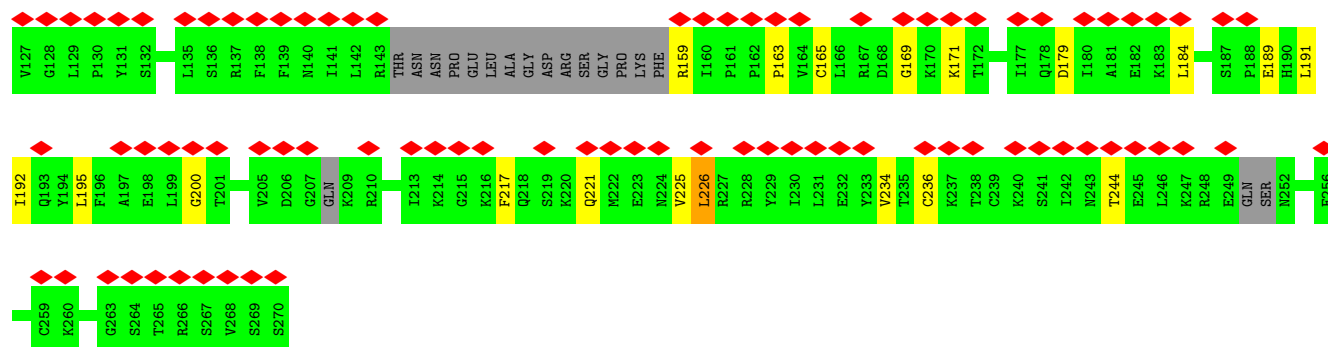
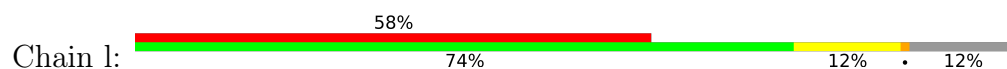


• Molecule 25: Eukaryotic translation initiation factor 2 subunit gamma

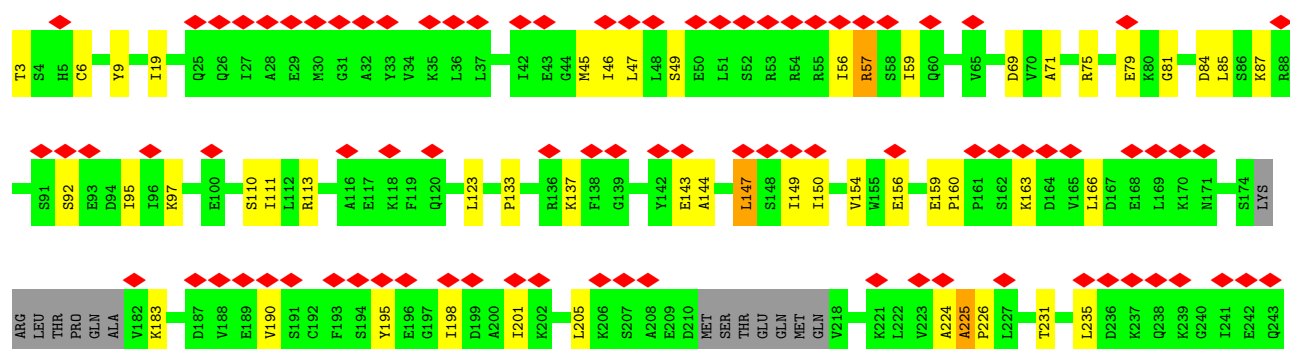
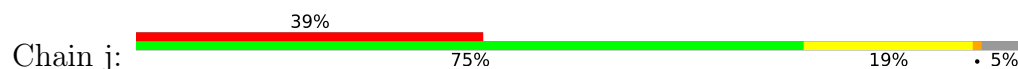




• Molecule 26: Eukaryotic translation initiation factor 2 subunit beta

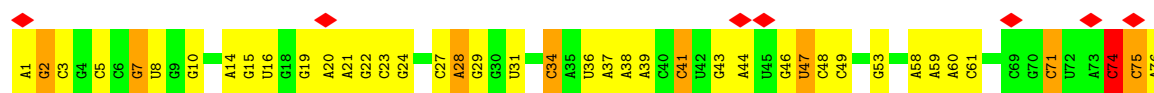
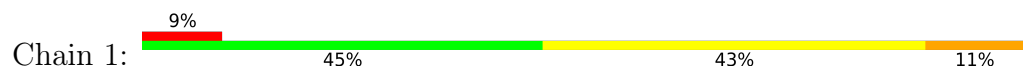


• Molecule 27: Eukaryotic translation initiation factor 2 subunit alpha

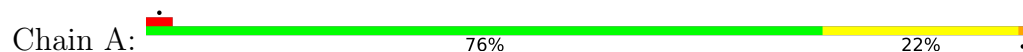




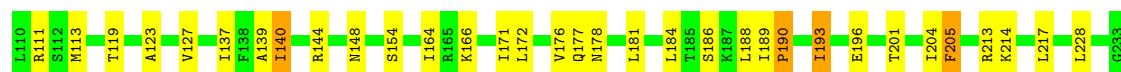
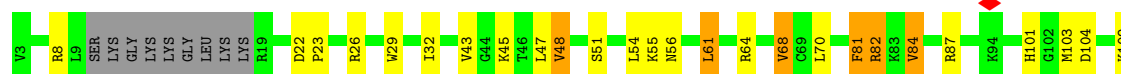
• Molecule 28: tRNAi (75-MER)



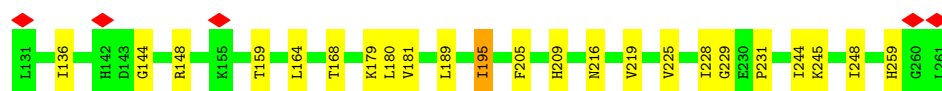
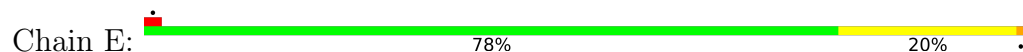
• Molecule 29: 40S ribosomal protein S0



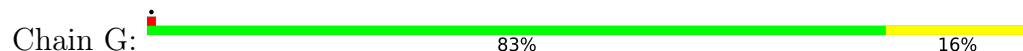
• Molecule 30: 40S ribosomal protein S1



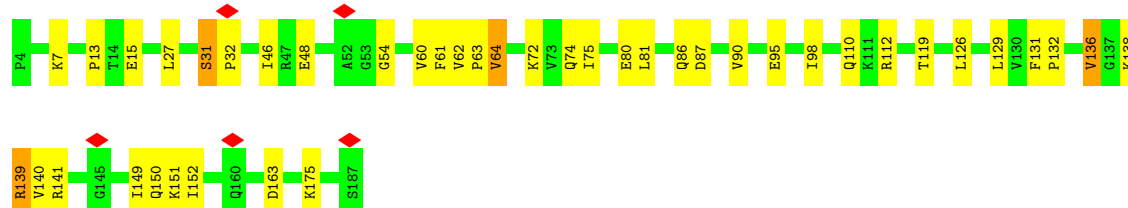
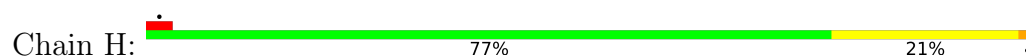
• Molecule 31: 40S ribosomal protein S4



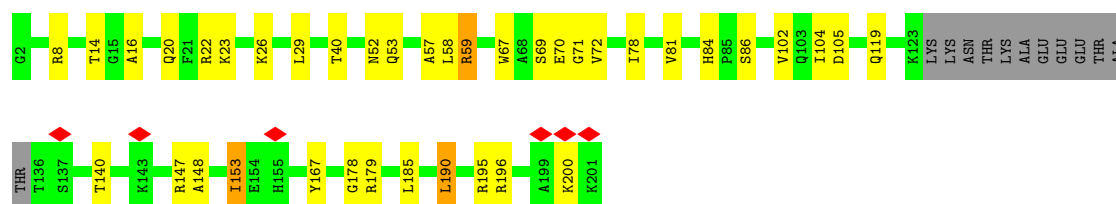
• Molecule 32: 40S ribosomal protein S6



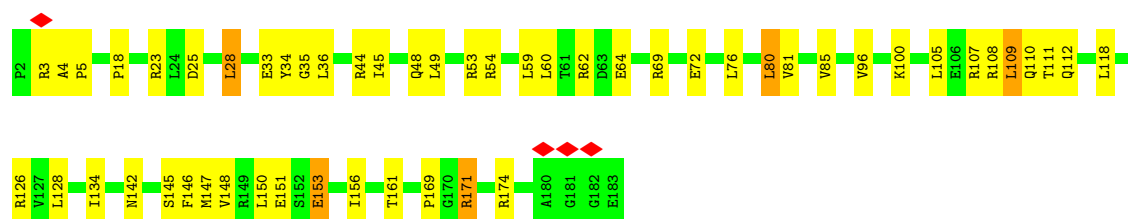
- Molecule 33: 40S ribosomal protein S7



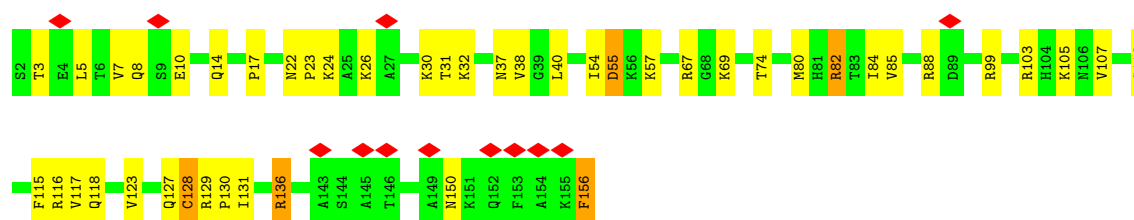
- Molecule 34: 40S ribosomal protein S8



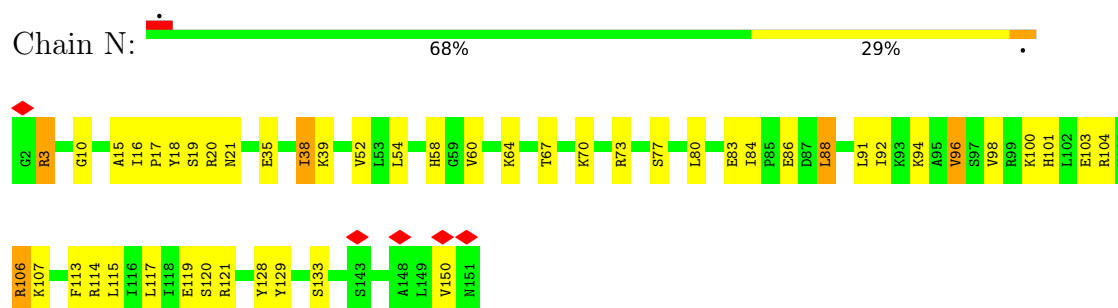
- Molecule 35: KLLA0E23673p



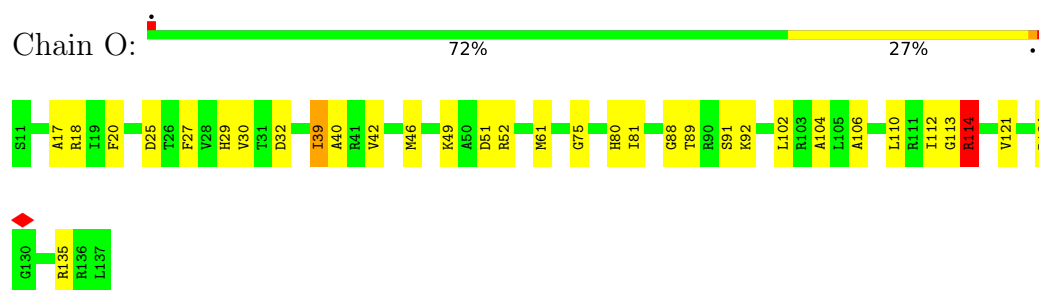
- Molecule 36: KLLA0A10483p



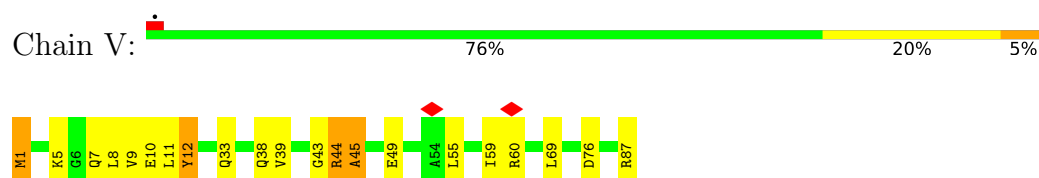
- Molecule 37: KLLA0F18040p



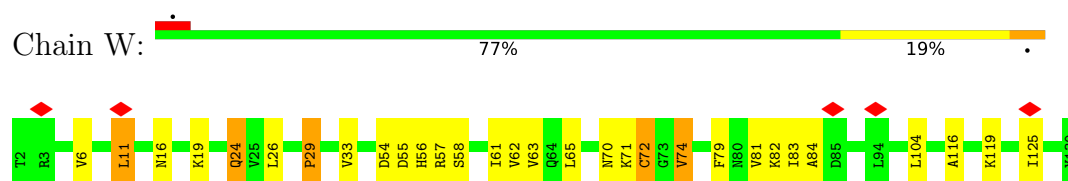
- Molecule 38: 40S ribosomal protein S14



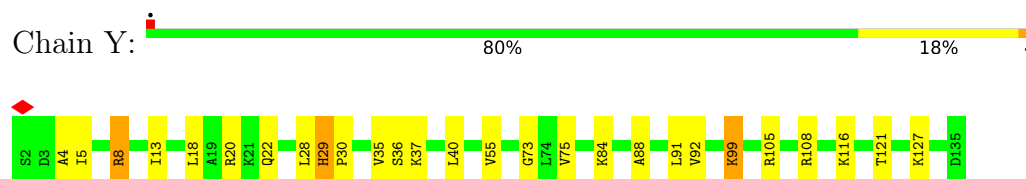
- Molecule 39: 40S ribosomal protein S21



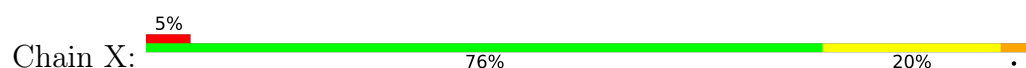
- Molecule 40: 40S ribosomal protein S22

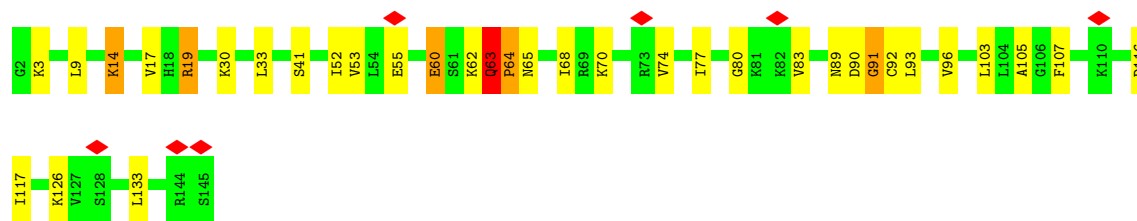


- Molecule 41: 40S ribosomal protein S24

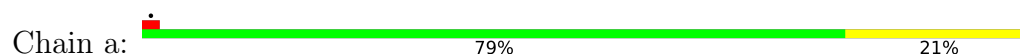


- Molecule 42: RPS23

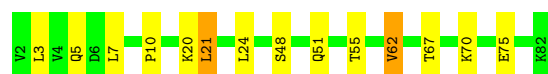
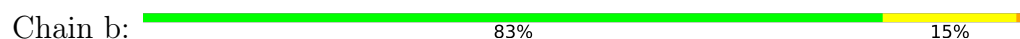




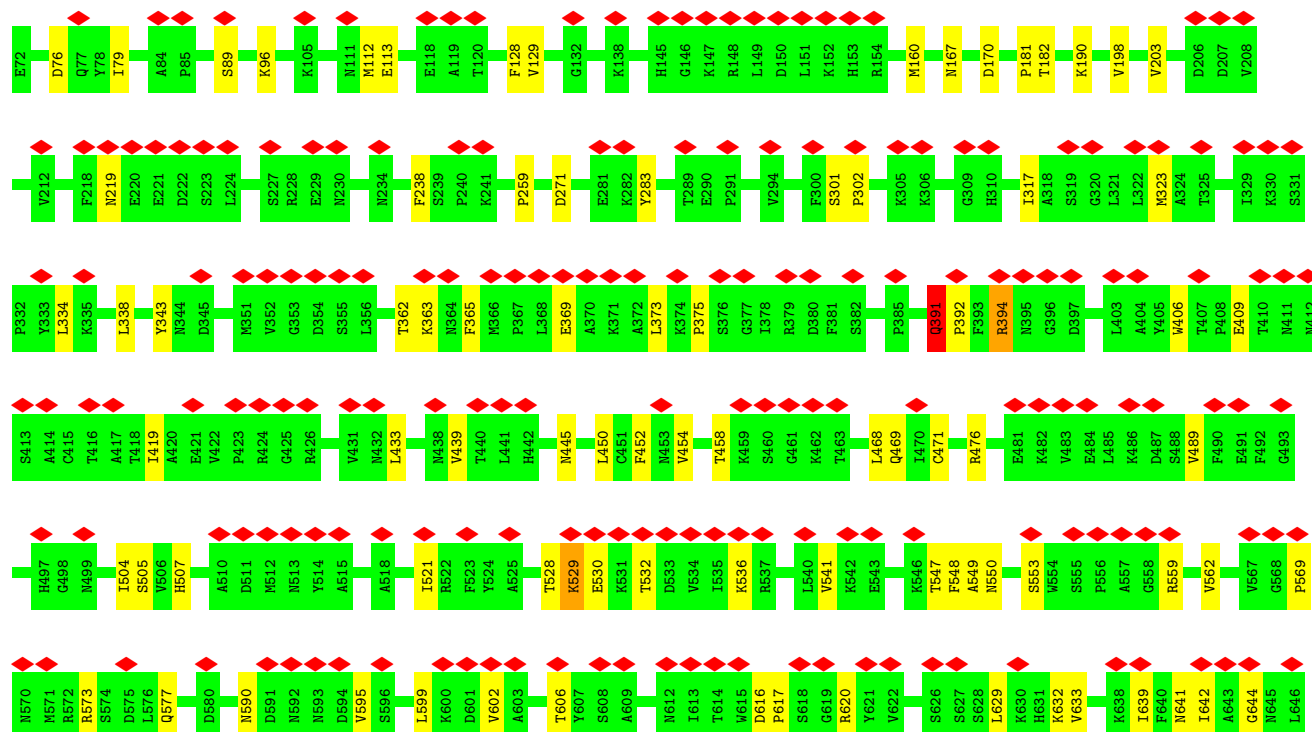
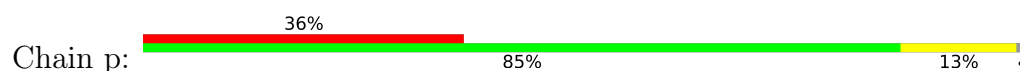
- Molecule 43: 40S ribosomal protein S26

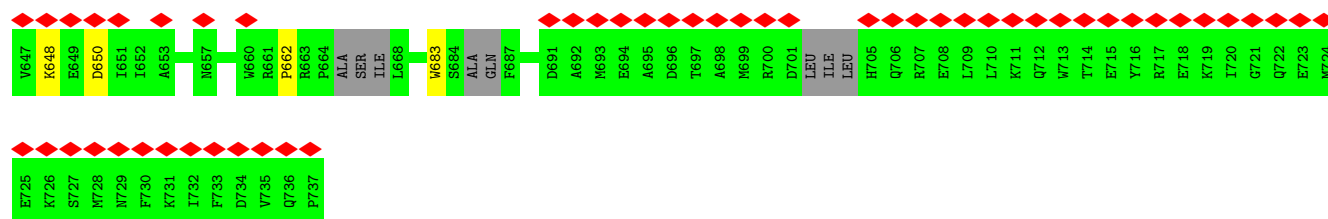


- Molecule 44: 40S ribosomal protein S27



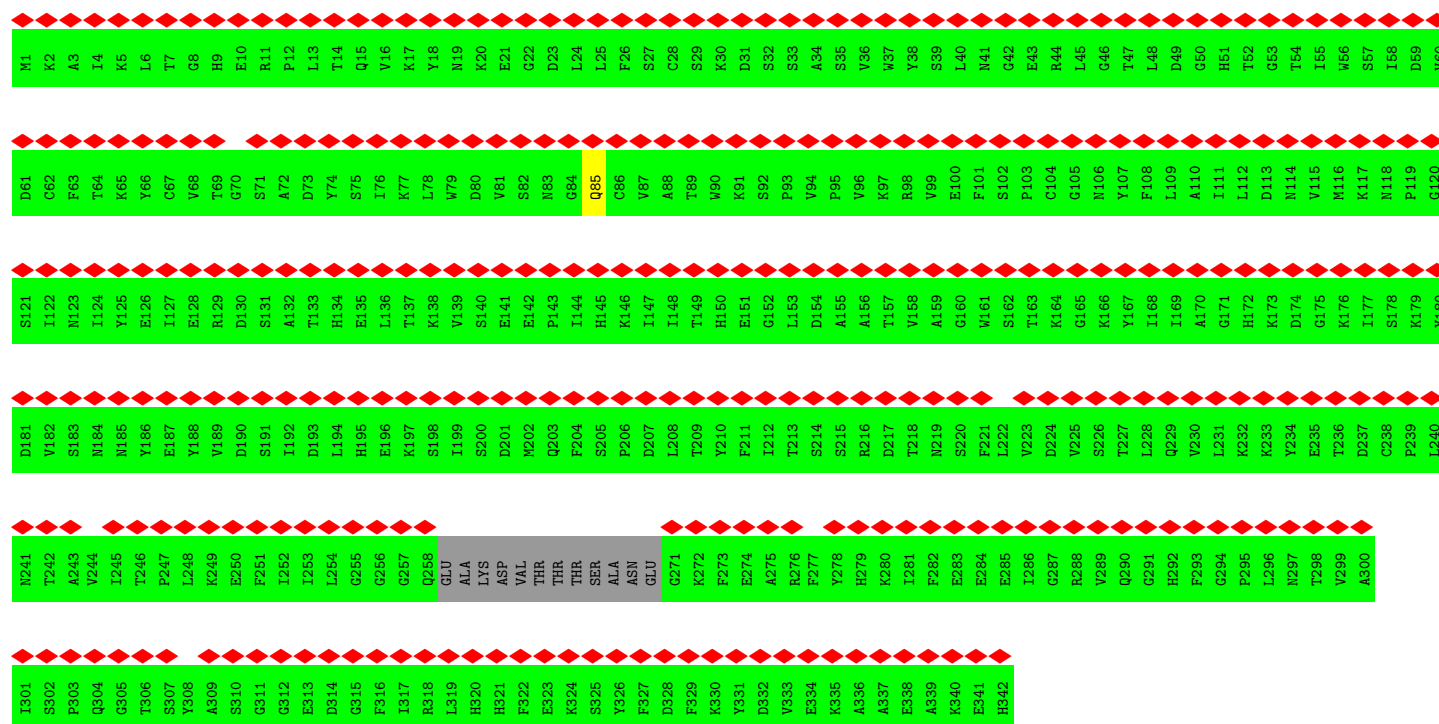
- Molecule 45: Eukaryotic translation initiation factor 3 subunit B





• Molecule 46: Eukaryotic translation initiation factor 3 subunit I

Chain s: 95%
96%



• Molecule 47: Eukaryotic translation initiation factor 3 subunit G

Chain r: 98%
100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12586	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.275	Depositor
Minimum map value	-0.119	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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, MG, ZN

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	2	0.38	0/42691	0.74	40/66521 (0.1%)
2	C	0.56	0/1659	1.04	4/2252 (0.2%)
3	D	0.59	0/1769	1.02	0/2378
4	F	0.58	0/1628	1.11	0/2198
5	K	0.57	0/831	1.05	1/1123 (0.1%)
6	M	0.68	0/891	1.10	1/1201 (0.1%)
7	P	0.62	0/946	1.07	0/1273
8	Q	0.59	0/1125	1.05	1/1510 (0.1%)
9	R	0.62	0/1038	1.11	0/1395
10	S	0.59	0/1212	1.09	2/1629 (0.1%)
11	T	0.56	0/1129	1.08	1/1520 (0.1%)
12	U	0.60	0/857	0.99	0/1158
13	Z	0.59	0/567	0.99	0/762
14	c	0.64	0/489	0.86	0/655
15	f	0.71	0/559	1.02	0/747
16	g	0.57	0/2521	0.83	0/3431
17	d	0.52	0/457	0.86	0/607
18	e	0.58	0/471	0.94	0/628
19	h	0.53	0/234	0.83	0/300
20	3	0.38	0/317	0.81	1/489 (0.2%)
21	i	0.51	0/894	0.85	0/1188
22	m	0.61	0/723	0.88	0/965
23	o	0.73	0/3671	0.90	1/4961 (0.0%)
24	q	0.74	0/5270	0.93	3/7154 (0.0%)
25	k	0.71	0/3167	0.91	0/4278
26	l	0.69	0/1030	0.85	0/1375
27	j	0.67	0/2034	0.91	0/2737
28	1	0.39	0/1796	0.73	6/2795 (0.2%)
29	A	0.57	0/1742	1.07	0/2383
30	B	0.55	0/1793	0.97	2/2414 (0.1%)
31	E	0.56	0/2122	0.94	1/2861 (0.0%)
32	G	0.56	0/1835	0.97	0/2451

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	H	0.60	0/1507	1.03	1/2028 (0.0%)
34	I	0.53	0/1515	0.97	0/2029
35	J	0.56	0/1495	1.12	1/2001 (0.0%)
36	L	0.59	0/1276	0.95	0/1718
37	N	0.56	0/1210	1.13	1/1628 (0.1%)
38	O	0.59	0/953	0.96	0/1279
39	V	0.50	0/696	0.90	0/938
40	W	0.53	0/1039	1.03	0/1399
41	Y	0.53	0/1075	1.03	3/1433 (0.2%)
42	X	0.56	0/1137	1.02	1/1516 (0.1%)
43	a	0.57	0/791	0.98	1/1059 (0.1%)
44	b	0.56	0/619	0.92	0/837
45	p	0.64	0/5282	0.85	4/7178 (0.1%)
46	s	0.43	0/2669	0.70	0/3611
47	r	0.36	0/399	0.70	0/535
All	All	0.53	0/109131	0.87	76/156528 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
41	Y	0	1
42	X	0	1
45	p	0	1
All	All	0	3

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1430	U	C2'-C3'-O3'	9.27	123.41	109.50
1	2	1157	C	C2'-C3'-O3'	8.06	121.59	109.50
1	2	130	C	C4'-C3'-O3'	8.04	121.46	109.40
1	2	538	G	C2'-C3'-O3'	7.89	121.33	109.50
1	2	277	U	C4'-C3'-O3'	7.88	121.23	109.40
1	2	1092	A	C4'-C3'-O3'	7.49	120.63	109.40
1	2	1206	C	C4'-C3'-O3'	7.40	120.50	109.40
1	2	1655	U	C4'-C3'-O3'	7.35	120.43	109.40
1	2	66	U	C4'-C3'-O3'	7.11	120.07	109.40
1	2	239	C	C2'-C3'-O3'	6.89	119.83	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	10	U	C4'-C3'-O3'	6.77	119.56	109.40
1	2	1765	G	C4'-C3'-O3'	6.73	119.49	109.40
1	2	810	A	C4'-C3'-O3'	6.61	119.31	109.40
28	1	7	G	C2'-C3'-O3'	6.54	119.31	109.50
42	X	90	ASP	N-CA-C	6.50	118.16	111.14
1	2	157	U	C4'-C3'-O3'	6.50	119.14	109.40
11	T	36	ILE	N-CA-C	-6.48	106.65	111.90
2	C	186	SER	CA-C-N	6.37	127.81	119.84
2	C	186	SER	C-N-CA	6.37	127.81	119.84
1	2	649	U	C2'-C3'-O3'	6.30	123.16	113.70
28	1	7	G	C4'-C3'-O3'	6.30	118.84	109.40
28	1	47	U	C4'-C3'-O3'	6.28	118.82	109.40
45	p	89	SER	N-CA-C	6.18	117.69	111.07
1	2	1571	A	C4'-C3'-O3'	6.15	118.62	109.40
1	2	695	U	C2'-C3'-O3'	6.13	118.69	109.50
28	1	74	C	C4'-C3'-O3'	6.11	118.57	109.40
41	Y	29	HIS	CA-C-N	6.03	127.38	119.84
41	Y	29	HIS	C-N-CA	6.03	127.38	119.84
24	q	642	VAL	N-CA-C	6.02	117.17	112.12
1	2	721	U	C4'-C3'-O3'	5.99	118.39	109.40
1	2	1411	U	C2'-C3'-O3'	5.98	118.47	109.50
1	2	279	U	C2'-C3'-O3'	5.91	118.37	109.50
1	2	1613	C	C4'-C3'-O3'	5.90	118.25	109.40
1	2	279	U	C4'-C3'-O3'	5.88	118.22	109.40
31	E	229	GLY	N-CA-C	5.85	117.78	110.29
1	2	1198	G	C4'-C3'-O3'	5.84	118.16	109.40
1	2	258	U	C2'-C3'-O3'	5.82	118.24	109.50
33	H	75	ILE	N-CA-C	5.82	116.28	110.23
1	2	542	C	C2'-C3'-O3'	5.79	118.19	109.50
41	Y	73	GLY	N-CA-C	5.79	119.75	110.90
1	2	828	A	C4'-C3'-O3'	5.76	118.04	109.40
1	2	564	C	C2'-C3'-O3'	5.72	118.08	109.50
45	p	445	ASN	N-CA-C	5.67	117.46	111.28
28	1	74	C	C2'-C3'-O3'	5.65	117.98	109.50
1	2	700	C	C2'-C3'-O3'	5.64	122.16	113.70
1	2	1491	A	C4'-C3'-O3'	5.63	117.85	109.40
43	a	47	ALA	N-CA-C	5.57	117.79	111.11
1	2	538	G	C4'-C3'-O3'	5.56	117.74	109.40
1	2	564	C	C4'-C3'-O3'	5.54	117.72	109.40
5	K	36	ASP	N-CA-C	5.53	117.31	111.28
1	2	74	U	C4'-C3'-O3'	5.53	117.69	109.40
30	B	205	PHE	CA-C-N	5.49	126.70	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	205	PHE	C-N-CA	5.49	126.70	119.84
1	2	1534	G	C4'-C3'-O3'	5.48	117.62	109.40
37	N	38	ILE	N-CA-CB	5.44	117.94	110.54
8	Q	90	VAL	N-CA-CB	5.44	117.93	110.54
23	o	152	THR	N-CA-C	-5.41	108.46	114.62
45	p	616	ASP	CA-C-N	5.33	125.40	119.32
45	p	616	ASP	C-N-CA	5.33	125.40	119.32
1	2	74	U	C2'-C3'-O3'	5.27	117.41	109.50
1	2	258	U	C4'-C3'-O3'	5.27	117.31	109.40
2	C	141	VAL	N-CA-C	5.26	120.28	109.34
1	2	1455	C	C4'-C3'-O3'	5.24	117.26	109.40
10	S	87	ASN	N-CA-C	5.22	116.65	111.07
1	2	412	U	C4'-C3'-O3'	-5.19	105.21	113.00
6	M	131	PHE	N-CA-C	5.16	116.59	110.97
1	2	72	A	C4'-C3'-O3'	5.15	117.13	109.40
24	q	666	GLY	N-CA-C	5.15	118.46	112.23
2	C	140	SER	N-CA-C	5.14	116.57	110.97
24	q	441	TYR	N-CA-C	5.12	119.02	112.87
10	S	86	LEU	N-CA-C	5.10	116.52	110.19
1	2	217	A	C3'-C2'-O2'	5.07	118.30	110.70
28	1	47	U	C2'-C3'-O3'	5.06	117.09	109.50
35	J	81	VAL	N-CA-CB	5.04	117.39	110.54
1	2	217	A	C2'-C3'-O3'	5.03	121.25	113.70
1	2	227	G	C4'-C3'-O3'	-5.01	105.48	113.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
42	X	63	GLN	Peptide
41	Y	29	HIS	Peptide
45	p	391	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	38175	0	19208	366	0
2	C	1629	0	1710	14	0
3	D	1744	0	1826	21	0
4	F	1609	0	1679	34	0
5	K	809	0	810	6	0
6	M	885	0	917	13	0
7	P	927	0	971	9	0
8	Q	1105	0	1170	17	0
9	R	1027	0	1071	10	0
10	S	1193	0	1217	14	0
11	T	1110	0	1124	16	0
12	U	845	0	913	10	0
13	Z	558	0	585	10	0
14	c	487	0	528	10	0
15	f	546	0	560	3	0
16	g	2466	0	2406	21	0
17	d	446	0	436	6	0
18	e	463	0	503	3	0
19	h	233	0	284	4	0
20	3	287	0	149	2	0
21	i	884	0	891	8	0
22	m	716	0	747	5	0
23	o	3996	0	3739	14	0
24	q	5179	0	4923	34	0
25	k	3123	0	3234	19	0
26	l	1016	0	1057	6	0
27	j	2006	0	2066	12	0
28	1	1607	0	816	10	0
29	A	1702	0	1695	14	0
30	B	1769	0	1829	21	0
31	E	2078	0	2157	15	0
32	G	1812	0	1911	16	0
33	H	1483	0	1579	11	0
34	I	1489	0	1504	13	0
35	J	1471	0	1554	14	0
36	L	1248	0	1311	14	0
37	N	1187	0	1251	20	0
38	O	942	0	979	13	0
39	V	687	0	682	8	0
40	W	1021	0	1056	16	0
41	Y	1061	0	1111	8	0
42	X	1119	0	1198	12	0
43	a	779	0	831	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	b	609	0	631	6	0
45	p	5147	0	4903	23	0
46	s	2606	0	2528	0	0
47	r	392	0	382	0	0
48	2	76	0	0	0	0
48	B	1	0	0	0	0
48	C	1	0	0	0	0
48	a	1	0	0	0	0
48	h	1	0	0	0	0
48	k	1	0	0	0	0
49	a	1	0	0	2	0
49	b	1	0	0	0	0
49	f	1	0	0	0	0
49	l	1	0	0	0	0
50	k	32	0	14	1	0
51	k	8	0	8	0	0
All	All	103798	0	84654	831	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (831) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1079:U:O4	1:2:1090:A:N1	1.64	1.31
1:2:813:A:N6	1:2:856:U:H3	1.28	1.28
1:2:1593:U:H3	1:2:1598:A:N6	1.35	1.24
1:2:8:U:N3	1:2:1138:A:N6	1.89	1.19
1:2:1079:U:H3	1:2:1090:A:N6	1.41	1.19
1:2:813:A:N1	1:2:856:U:O4	1.81	1.12
1:2:813:A:N6	1:2:856:U:N3	1.90	1.11
1:2:1593:U:O4	1:2:1598:A:N1	1.88	1.05
1:2:1079:U:N3	1:2:1090:A:N6	2.02	1.01
1:2:1593:U:N3	1:2:1598:A:N6	2.07	0.97
1:2:157:U:H4'	1:2:158:U:OP1	1.67	0.91
1:2:480:A:N1	1:2:506:U:C4	2.38	0.91
43:a:23:CYS:HG	49:a:101:ZN:ZN	0.74	0.88
1:2:8:U:C2	1:2:1138:A:N6	2.42	0.87
1:2:1191:C:H3'	1:2:1192:A:H5''	1.57	0.87
1:2:8:U:N3	1:2:1138:A:C6	2.42	0.86
1:2:480:A:N1	1:2:506:U:O4	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1019:A:H4'	24:q:115:ALA:HB2	1.58	0.84
1:2:71:A:H3'	1:2:72:A:H5''	1.60	0.83
1:2:8:U:C4	1:2:1138:A:N6	2.41	0.82
1:2:1079:U:C4	1:2:1090:A:N1	2.47	0.81
1:2:1240:G:H1'	7:P:79:HIS:HB2	1.64	0.80
1:2:813:A:N1	1:2:856:U:C4	2.49	0.80
1:2:1540:G:H5'	11:T:87:GLY:HA3	1.64	0.79
38:O:61:MET:HG3	38:O:104:ALA:HB2	1.65	0.78
1:2:444:A:C8	1:2:524:A:H5''	2.19	0.77
3:D:23:GLU:O	3:D:27:ARG:HG2	1.84	0.77
43:a:10:ARG:HE	43:a:12:LYS:HE2	1.49	0.77
1:2:994:A:H61	1:2:1007:G:H1	1.34	0.76
1:2:641:G:H4'	1:2:641:G:OP1	1.84	0.76
1:2:804:U:H2'	1:2:804:U:O2	1.84	0.76
1:2:1237:A:N1	1:2:1246:U:C4	2.54	0.76
1:2:444:A:H8	1:2:524:A:H5''	1.48	0.76
1:2:640:G:O6	1:2:693:U:N3	2.19	0.74
27:j:75:ARG:HB2	27:j:84:ASP:HB2	1.68	0.74
1:2:1266:G:H1	1:2:1440:U:H3	1.36	0.73
43:a:23:CYS:SG	49:a:101:ZN:ZN	1.76	0.73
1:2:29:U:H2'	1:2:29:U:O2	1.88	0.73
1:2:1774:A:H2'	1:2:1775:G:C8	2.24	0.72
1:2:1533:U:H3	4:F:189:ILE:H	1.37	0.72
1:2:459:A:H3'	1:2:460:G:H8	1.55	0.71
1:2:1174:U:H2'	1:2:1174:U:O2	1.91	0.71
1:2:1216:A:H5''	5:K:44:LYS:HG2	1.73	0.70
1:2:1079:U:O4	1:2:1090:A:C2	2.45	0.69
1:2:1108:G:H1	1:2:1135:U:H3	1.38	0.69
1:2:480:A:C6	1:2:506:U:O4	2.45	0.68
30:B:32:ILE:HB	30:B:43:VAL:HB	1.74	0.68
1:2:930:C:H3'	1:2:931:U:H5''	1.74	0.67
1:2:867:G:H1	1:2:959:U:H3	1.43	0.67
16:g:308:LEU:HB2	16:g:320:TRP:HB2	1.77	0.66
1:2:92:A:H5'	1:2:93:A:H5''	1.78	0.65
3:D:65:ARG:O	3:D:68:GLU:HG3	1.96	0.65
30:B:23:PRO:HB3	30:B:26:ARG:HH21	1.62	0.65
35:J:64:GLU:HA	35:J:69:ARG:HD3	1.79	0.65
2:C:175:ILE:HB	2:C:202:TYR:HB2	1.78	0.65
14:c:12:VAL:HG12	14:c:30:VAL:HG12	1.77	0.65
1:2:590:A:H2'	1:2:591:G:C8	2.32	0.64
37:N:88:LEU:O	37:N:92:ILE:HG13	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:15:ILE:HD11	11:T:63:ARG:HD3	1.78	0.64
23:o:210:LEU:HD22	23:o:240:ARG:HE	1.61	0.64
1:2:1285:U:H2'	1:2:1286:A:O4'	1.99	0.63
27:j:110:SER:HA	27:j:113:ARG:HD3	1.80	0.62
1:2:979:G:H1	1:2:1020:C:H42	1.46	0.62
1:2:1571:A:H4'	1:2:1572:G:O5'	1.99	0.62
1:2:1155:C:H42	1:2:1620:G:H1	1.44	0.62
1:2:1222:A:H2'	1:2:1223:A:O4'	2.00	0.62
19:h:2:ARG:HE	19:h:5:TRP:HE1	1.48	0.62
4:F:144:PRO:HD2	4:F:169:ARG:CG	2.30	0.61
1:2:216:A:H2'	1:2:217:A:C8	2.35	0.61
8:Q:29:ILE:HG12	8:Q:65:ILE:HD12	1.82	0.61
8:Q:22:VAL:HG12	8:Q:65:ILE:HG12	1.83	0.61
1:2:1258:U:H2'	1:2:1259:U:H5'	1.83	0.61
1:2:270:A:H61	32:G:185:GLN:HE22	1.48	0.61
38:O:89:THR:HB	38:O:128:LYS:HG3	1.81	0.61
1:2:411:A:H2'	1:2:412:U:H6	1.66	0.61
2:C:111:ASP:CG	2:C:112:SER:H	2.08	0.61
30:B:186:SER:O	30:B:190:PRO:HD3	2.00	0.61
1:2:1586:G:H1	1:2:1606:U:H3	1.49	0.60
4:F:27:LEU:HB2	4:F:31:ILE:HD11	1.83	0.60
1:2:828:A:H4'	1:2:829:U:O5'	2.00	0.60
1:2:1339:U:H3	8:Q:9:THR:HG22	1.67	0.60
1:2:531:U:H2'	1:2:532:U:O4'	2.02	0.60
1:2:894:G:H1	1:2:916:U:H3	1.50	0.60
4:F:135:VAL:HA	4:F:200:LEU:HD21	1.83	0.60
9:R:93:LEU:HD11	9:R:100:LEU:HB3	1.84	0.60
1:2:1756:U:H2'	1:2:1757:C:C6	2.37	0.59
1:2:1286:A:H61	1:2:1327:G:H2'	1.67	0.59
45:p:391:GLN:HB2	45:p:476:ARG:HB3	1.82	0.59
37:N:54:LEU:HA	37:N:58:HIS:HD2	1.67	0.59
1:2:843:A:H2'	1:2:844:G:C8	2.37	0.59
1:2:1593:U:C4	1:2:1598:A:N1	2.69	0.59
37:N:98:VAL:HG11	37:N:115:LEU:HB2	1.85	0.59
1:2:248:U:H3	36:L:17:PRO:HG2	1.66	0.59
16:g:20:TRP:H	16:g:20:TRP:CD1	2.21	0.59
1:2:1137:A:H2'	1:2:1138:A:C8	2.38	0.59
1:2:813:A:C6	1:2:856:U:N3	2.71	0.58
1:2:71:A:H3'	1:2:72:A:C5'	2.31	0.58
1:2:591:G:H2'	1:2:592:U:O4'	2.02	0.58
1:2:1174:U:O2	1:2:1174:U:C2'	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:25:LEU:HD22	6:M:92:ALA:HB1	1.86	0.58
2:C:230:LEU:HD12	40:W:70:ASN:HB3	1.85	0.58
4:F:148:THR:HB	4:F:159:ARG:HD2	1.85	0.58
1:2:1426:G:H5'	21:i:14:ARG:HB3	1.85	0.57
39:V:1:MET:HA	39:V:10:GLU:HB2	1.86	0.57
1:2:1775:G:H1	1:2:1782:C:H42	1.53	0.57
3:D:68:GLU:HB3	5:K:90:THR:HG23	1.86	0.57
1:2:1768:U:H2'	1:2:1769:U:C6	2.39	0.57
1:2:692:C:H2'	1:2:693:U:H4'	1.87	0.57
1:2:1670:G:H2'	1:2:1671:G:C8	2.40	0.57
1:2:1267:G:H1	1:2:1439:C:H42	1.53	0.57
14:c:20:GLY:HA2	14:c:66:LEU:HD22	1.86	0.57
12:U:98:HIS:O	12:U:102:ARG:HG3	2.03	0.56
1:2:804:U:O2	1:2:804:U:C2'	2.53	0.56
42:X:63:GLN:C	42:X:65:ASN:H	2.13	0.56
1:2:687:C:O5'	40:W:119:LYS:HG2	2.05	0.56
13:Z:66:VAL:HG22	13:Z:72:GLY:HA2	1.86	0.56
28:1:37:A:H2'	28:1:38:A:C8	2.40	0.56
1:2:824:U:H2'	1:2:825:U:C6	2.41	0.56
1:2:1052:G:H1	1:2:1065:C:H42	1.54	0.56
9:R:46:LEU:O	9:R:50:ILE:HG13	2.06	0.56
1:2:1097:U:H1'	40:W:71:LYS:HD3	1.88	0.56
1:2:1585:A:H2'	1:2:1586:G:H8	1.71	0.56
1:2:1144:U:H5'	1:2:1301:U:H5'	1.88	0.55
13:Z:61:SER:HB3	13:Z:64:VAL:HG23	1.88	0.55
24:q:552:LEU:HB3	24:q:703:LEU:HD21	1.89	0.55
1:2:12:U:H2'	1:2:13:C:C6	2.41	0.55
21:i:38:ILE:HD12	21:i:75:ASP:HB3	1.89	0.55
1:2:55:A:H3'	1:2:402:G:H1	1.71	0.55
8:Q:93:HIS:HA	8:Q:97:VAL:HB	1.87	0.55
11:T:105:LEU:HD22	11:T:122:ARG:HD3	1.89	0.55
1:2:1627:G:H2'	1:2:1628:U:O4'	2.07	0.55
16:g:245:ASP:HB2	16:g:263:THR:HG22	1.87	0.55
35:J:105:LEU:HA	35:J:108:ARG:HD3	1.88	0.55
1:2:421:G:N3	1:2:421:G:H2'	2.22	0.55
1:2:491:A:H2'	1:2:491:A:N3	2.21	0.55
1:2:582:C:H2'	1:2:583:C:C6	2.41	0.55
1:2:1186:U:O4	1:2:1199:G:N2	2.40	0.55
1:2:1564:U:H5'	10:S:39:GLY:HA3	1.89	0.55
1:2:674:A:N3	1:2:674:A:H2'	2.21	0.55
1:2:951:A:O2'	37:N:114:ARG:HD2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1540:G:C5'	11:T:87:GLY:HA3	2.36	0.55
4:F:34:GLU:HG3	4:F:35:ILE:HD12	1.89	0.54
4:F:44:LEU:HB3	4:F:50:PHE:H	1.72	0.54
5:K:3:ILE:HG12	5:K:41:PHE:HB2	1.89	0.54
27:j:160:PRO:HG2	27:j:166:LEU:HD12	1.89	0.54
34:I:57:ALA:HB2	34:I:178:GLY:HA2	1.87	0.54
11:T:86:ARG:HH11	11:T:89:ARG:HB3	1.72	0.54
7:P:85:ILE:HB	7:P:112:VAL:HA	1.88	0.54
45:p:553:SER:HB3	45:p:562:VAL:HB	1.90	0.54
1:2:1170:A:H2'	1:2:1171:G:C8	2.42	0.54
1:2:1652:G:H5'	19:h:21:ARG:HH12	1.72	0.54
11:T:14:PHE:HA	11:T:139:THR:HG21	1.90	0.54
1:2:1639:C:H2'	1:2:1640:G:C8	2.43	0.54
29:A:62:ARG:HH12	39:V:39:VAL:HB	1.73	0.54
1:2:1237:A:N1	1:2:1246:U:O4	2.40	0.54
24:q:385:LEU:HB3	24:q:585:LEU:HB2	1.89	0.54
29:A:35:PRO:HG3	39:V:87:ARG:HH21	1.72	0.54
8:Q:97:VAL:HG12	8:Q:98:ASP:N	2.22	0.54
1:2:28:A:H2'	1:2:29:U:O4'	2.08	0.54
1:2:566:A:H3'	1:2:567:G:H5''	1.88	0.54
1:2:650:G:H1	1:2:683:C:H42	1.55	0.54
1:2:1338:C:H42	1:2:1383:G:H1	1.54	0.54
36:L:130:PRO:HA	36:L:136:ARG:HG3	1.89	0.54
24:q:626:LEU:HD11	24:q:679:ALA:HB2	1.90	0.54
1:2:1356:G:H2'	1:2:1357:G:C8	2.44	0.53
1:2:1612:A:H5'	14:c:47:PRO:HG3	1.89	0.53
35:J:59:LEU:HD21	35:J:72:GLU:HB2	1.89	0.53
1:2:1176:C:H4'	1:2:1188:A:H61	1.72	0.53
1:2:1357:G:H1	1:2:1364:C:H42	1.54	0.53
1:2:1601:U:H2'	1:2:1602:U:C6	2.43	0.53
3:D:6:SER:HB3	3:D:9:ARG:HB3	1.90	0.53
42:X:63:GLN:C	42:X:65:ASN:N	2.66	0.53
1:2:1287:G:O5'	1:2:1287:G:H8	1.92	0.53
1:2:1711:G:H3'	1:2:1712:A:C8	2.42	0.53
1:2:1712:A:H2'	1:2:1713:G:C8	2.43	0.53
11:T:65:ILE:HG22	11:T:124:ILE:HG13	1.90	0.53
30:B:137:ILE:HD12	30:B:172:LEU:HD22	1.91	0.53
30:B:68:VAL:HG23	30:B:84:VAL:HG23	1.89	0.53
30:B:87:ARG:HB2	30:B:101:HIS:HB2	1.90	0.53
38:O:135:ARG:HH11	43:a:26:CYS:HA	1.74	0.53
1:2:42:G:H1	1:2:432:C:H42	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:g:68:ILE:HB	16:g:86:TRP:CD1	2.43	0.53
28:1:74:C:H4'	28:1:75:C:O5'	2.08	0.53
1:2:1171:G:H1	1:2:1465:C:H42	1.57	0.53
1:2:385:G:H2'	1:2:386:A:C8	2.44	0.53
1:2:547:G:H1	1:2:589:C:H42	1.56	0.53
1:2:16:G:H21	1:2:1137:A:H62	1.55	0.53
1:2:609:G:H21	42:X:19:ARG:HH22	1.57	0.53
10:S:25:ASN:HB3	13:Z:38:HIS:HE1	1.74	0.53
45:p:433:LEU:HD22	45:p:454:VAL:HG11	1.90	0.53
1:2:43:A:HO2'	1:2:44:U:H6	1.54	0.53
43:a:23:CYS:HB3	43:a:28:ARG:H	1.74	0.53
13:Z:62:VAL:HG11	13:Z:77:ARG:HG3	1.92	0.52
17:d:32:ARG:HA	17:d:37:ASN:H	1.74	0.52
30:B:140:ILE:HG12	30:B:213:ARG:HB2	1.89	0.52
37:N:35:GLU:O	37:N:38:ILE:HG13	2.09	0.52
4:F:66:ILE:H	4:F:91:ILE:HD11	1.74	0.52
14:c:8:THR:HB	14:c:56:LEU:HB2	1.91	0.52
23:o:233:LEU:HD13	23:o:270:SER:HA	1.91	0.52
40:W:116:ALA:HA	40:W:119:LYS:HD3	1.91	0.52
10:S:126:ARG:HD3	10:S:133:VAL:HA	1.92	0.52
24:q:645:ILE:HG13	24:q:646:PRO:HD3	1.92	0.52
1:2:1198:G:H4'	1:2:1199:G:O5'	2.08	0.52
42:X:14:LYS:O	42:X:17:VAL:HG12	2.10	0.52
1:2:1047:G:H1	1:2:1069:C:H42	1.56	0.52
1:2:1712:A:H2'	1:2:1713:G:H8	1.74	0.52
16:g:14:LEU:HB2	16:g:317:ILE:HB	1.91	0.52
32:G:14:LYS:HZ3	32:G:16:ILE:HD11	1.75	0.52
4:F:154:GLY:HA2	20:3:10:U:H3	1.74	0.52
12:U:51:VAL:HG12	12:U:94:GLU:HB3	1.91	0.52
31:E:122:LYS:HB2	31:E:164:LEU:HD12	1.90	0.52
45:p:452:PHE:HB2	45:p:469:GLN:HB2	1.92	0.52
1:2:1195:A:H4'	1:2:1196:C:H5''	1.91	0.52
31:E:31:PRO:HG3	31:E:43:PRO:HG3	1.91	0.52
35:J:169:PRO:HB2	35:J:174:ARG:HG3	1.92	0.52
1:2:1557:A:H3'	1:2:1558:U:H5'	1.92	0.52
37:N:94:LYS:O	37:N:98:VAL:HG23	2.09	0.52
44:b:55:THR:HG22	44:b:62:VAL:H	1.74	0.52
45:p:541:VAL:HG22	45:p:595:VAL:HG21	1.92	0.52
2:C:50:VAL:HG12	2:C:76:GLN:HE21	1.75	0.52
4:F:189:ILE:HD13	13:Z:66:VAL:HG21	1.91	0.52
1:2:216:A:H2'	1:2:217:A:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1:31:U:H3	28:1:39:A:H61	1.58	0.51
1:2:270:A:H61	32:G:185:GLN:NE2	2.07	0.51
1:2:817:C:H42	1:2:852:G:H1	1.57	0.51
1:2:903:G:H2'	1:2:904:A:O4'	2.11	0.51
1:2:1588:G:H1	1:2:1604:C:H42	1.56	0.51
7:P:83:MET:HB3	7:P:116:LEU:HD12	1.91	0.51
42:X:60:GLU:HG3	42:X:68:ILE:HG13	1.90	0.51
1:2:550:G:H1	1:2:572:C:H42	1.57	0.51
1:2:951:A:H2'	1:2:952:G:H8	1.76	0.51
1:2:1079:U:N3	1:2:1090:A:C6	2.76	0.51
1:2:1141:A:N6	1:2:1142:A:N6	2.58	0.51
1:2:1482:G:O2'	1:2:1483:C:H5''	2.10	0.51
1:2:15:U:H2'	1:2:16:G:O4'	2.11	0.51
1:2:1356:G:H1	1:2:1365:C:H42	1.58	0.51
1:2:17:C:H2'	1:2:18:C:C6	2.45	0.51
1:2:1096:U:O2	1:2:1096:U:O4'	2.28	0.51
1:2:176:U:H3'	1:2:177:U:H2'	1.93	0.51
1:2:867:G:H22	1:2:959:U:H3	1.57	0.51
4:F:114:ARG:HG3	8:Q:43:ILE:HG12	1.92	0.51
12:U:62:VAL:HG22	12:U:85:ARG:HB3	1.93	0.51
30:B:51:SER:HB2	30:B:56:ASN:HD22	1.76	0.51
30:B:176:VAL:HG12	30:B:177:GLN:H	1.76	0.51
32:G:2:LYS:HG3	32:G:17:GLU:HG3	1.91	0.51
27:j:144:ALA:HA	27:j:147:LEU:HB2	1.93	0.51
7:P:16:SER:HB2	10:S:93:ASN:HD22	1.76	0.51
25:k:312:SER:HB2	25:k:422:HIS:CE1	2.45	0.51
41:Y:105:ARG:HA	41:Y:108:ARG:HD3	1.93	0.51
1:2:813:A:C2	1:2:856:U:O4	2.61	0.50
1:2:1174:U:H2'	1:2:1175:G:H8	1.76	0.50
1:2:1578:C:H2'	1:2:1579:C:C6	2.47	0.50
9:R:47:ARG:HA	9:R:50:ILE:HD12	1.93	0.50
41:Y:18:LEU:HB2	41:Y:20:ARG:HG2	1.93	0.50
1:2:148:C:H42	1:2:164:G:H1	1.59	0.50
1:2:1496:G:H5''	11:T:72:GLY:HA3	1.92	0.50
2:C:93:LYS:HB3	2:C:100:ARG:HB3	1.93	0.50
13:Z:90:LYS:HB2	13:Z:104:ALA:HB2	1.93	0.50
1:2:613:C:H42	1:2:1106:G:H1	1.60	0.50
1:2:1072:G:H4'	37:N:10:GLY:HA2	1.93	0.50
1:2:1120:C:H42	1:2:1125:G:H1	1.58	0.50
1:2:1675:C:H5''	34:I:59:ARG:HH12	1.76	0.50
2:C:61:ILE:HA	2:C:66:LEU:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:136:VAL:HG22	3:D:186:VAL:HG22	1.92	0.50
1:2:6:G:H1	1:2:18:C:H42	1.58	0.50
1:2:1243:A:H2'	1:2:1243:A:N3	2.26	0.50
12:U:34:LEU:O	12:U:37:VAL:HG12	2.10	0.50
34:I:67:TRP:HB3	34:I:71:GLY:H	1.76	0.50
2:C:58:ILE:HA	2:C:61:ILE:HD12	1.93	0.50
36:L:54:ILE:HG23	36:L:55:ASP:H	1.76	0.50
1:2:78:A:H2	32:G:174:LYS:HG3	1.77	0.50
1:2:328:G:H2'	1:2:329:G:C8	2.47	0.50
1:2:1671:G:H2'	1:2:1672:C:C6	2.47	0.50
1:2:1682:U:H2'	1:2:1683:G:H8	1.76	0.50
1:2:1137:A:H2'	1:2:1138:A:H8	1.77	0.50
3:D:56:GLN:HE21	3:D:90:ARG:HH22	1.58	0.50
36:L:80:MET:HE1	36:L:85:VAL:HG23	1.94	0.50
36:L:128:CYS:SG	36:L:129:ARG:N	2.84	0.50
1:2:245:G:H1'	36:L:40:LEU:HG	1.94	0.50
24:q:616:LEU:HD11	24:q:703:LEU:HG	1.94	0.50
43:a:43:ASN:HD22	43:a:66:LYS:HE2	1.77	0.50
45:p:529:LYS:HB2	45:p:536:LYS:HD2	1.94	0.50
1:2:645:U:H2'	1:2:646:G:C8	2.47	0.50
1:2:861:A:H5'	40:W:57:ARG:HE	1.76	0.50
35:J:110:GLN:HE22	35:J:126:ARG:HD3	1.76	0.50
1:2:50:C:H42	1:2:428:G:H1	1.58	0.49
4:F:144:PRO:HD2	4:F:169:ARG:HG2	1.93	0.49
33:H:140:VAL:HG22	33:H:150:GLN:HG2	1.94	0.49
1:2:813:A:N6	1:2:856:U:C4	2.76	0.49
1:2:1210:A:H4'	7:P:100:LYS:HG3	1.93	0.49
1:2:1534:G:H2'	1:2:1534:G:N3	2.27	0.49
29:A:21:ARG:HD2	29:A:24:LEU:HD13	1.93	0.49
30:B:81:PHE:HB3	30:B:109:LYS:HG2	1.94	0.49
1:2:1137:A:C4	1:2:1138:A:N7	2.81	0.49
23:o:210:LEU:HB2	23:o:240:ARG:HH21	1.77	0.49
1:2:813:A:C6	1:2:856:U:C4	3.00	0.49
1:2:1245:C:O2	1:2:1245:C:O4'	2.30	0.49
38:O:20:PHE:HB3	38:O:27:PHE:HB2	1.93	0.49
1:2:1472:G:H2'	1:2:1473:A:C8	2.48	0.49
1:2:1558:U:O2	1:2:1558:U:O4'	2.30	0.49
1:2:1608:G:H5'	4:F:109:LYS:HD3	1.95	0.49
24:q:588:ILE:HD13	24:q:601:ARG:HB3	1.94	0.49
1:2:1316:C:H2'	1:2:1317:G:O4'	2.12	0.49
1:2:1402:C:H2'	1:2:1403:G:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:k:128:PHE:HZ	25:k:139:LYS:HB2	1.78	0.49
1:2:589:C:HO2'	1:2:590:A:H8	1.60	0.49
1:2:826:C:H2'	1:2:827:U:C6	2.47	0.49
1:2:312:U:H5'	1:2:1117:G:H21	1.77	0.49
1:2:328:G:H2'	1:2:329:G:H8	1.78	0.49
8:Q:54:LEU:HD22	8:Q:108:ALA:HB1	1.95	0.49
17:d:22:ARG:HB3	17:d:38:ILE:HG12	1.93	0.49
24:q:280:GLU:HA	24:q:283:LEU:HD12	1.95	0.49
24:q:491:SER:HA	24:q:499:GLN:HG2	1.94	0.49
26:l:184:LEU:HD22	26:l:234:VAL:HG11	1.95	0.49
9:R:4:VAL:HG12	9:R:4:VAL:O	2.12	0.49
23:o:56:LEU:HD13	23:o:96:PHE:HB2	1.94	0.49
38:O:17:ALA:HA	38:O:30:VAL:HG22	1.95	0.49
41:Y:92:VAL:HG11	41:Y:99:LYS:HE2	1.95	0.49
1:2:1585:A:H61	1:2:1607:U:H3	1.59	0.48
4:F:145:ARG:HB3	14:c:57:MET:HB2	1.95	0.48
1:2:1660:G:H2'	1:2:1661:G:H8	1.78	0.48
1:2:1774:A:H2'	1:2:1775:G:H8	1.72	0.48
32:G:68:LEU:HA	32:G:100:ALA:HB3	1.95	0.48
35:J:76:LEU:O	35:J:80:LEU:HD12	2.14	0.48
1:2:1043:U:C6	1:2:1044:C:H5	2.31	0.48
2:C:244:PRO:HA	2:C:247:VAL:HG12	1.95	0.48
16:g:116:ILE:HG22	16:g:123:ILE:HG12	1.95	0.48
38:O:80:HIS:HA	38:O:113:GLY:O	2.13	0.48
1:2:5:U:H2'	1:2:6:G:H8	1.79	0.48
1:2:1221:C:H2'	1:2:1222:A:C8	2.48	0.48
34:I:67:TRP:CD1	34:I:70:GLU:H	2.32	0.48
1:2:324:G:H1	1:2:342:C:H42	1.61	0.48
8:Q:38:LEU:HD21	11:T:10:PRO:HA	1.95	0.48
25:k:326:PRO:HG2	28:1:1:A:H2	1.78	0.48
33:H:81:LEU:HD13	33:H:90:VAL:HG11	1.96	0.48
34:I:185:LEU:HB3	34:I:190:LEU:HB2	1.95	0.48
4:F:190:LYS:HG2	13:Z:63:SER:HB3	1.95	0.48
30:B:103:MET:HE2	30:B:188:LEU:HD11	1.95	0.48
31:E:209:HIS:HA	31:E:219:VAL:HG22	1.95	0.48
45:p:79:ILE:HG13	45:p:129:VAL:HB	1.95	0.48
1:2:592:U:O3'	1:2:593:A:H4'	2.14	0.48
1:2:711:G:H22	1:2:727:C:H42	1.61	0.48
23:o:470:LEU:HD11	24:q:733:TYR:HE2	1.78	0.48
28:1:28:A:H2'	28:1:29:G:C8	2.48	0.48
1:2:249:C:H2'	1:2:250:A:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:339:U:H2'	1:2:340:A:C8	2.49	0.48
1:2:1163:G:H1	1:2:1579:C:H42	1.62	0.48
3:D:59:VAL:HG22	3:D:66:ILE:HD11	1.95	0.48
16:g:20:TRP:HB3	16:g:313:THR:HA	1.95	0.48
24:q:444:SER:HA	24:q:513:ASN:HD21	1.79	0.48
33:H:46:ILE:HG12	33:H:60:VAL:HG12	1.95	0.48
1:2:5:U:H2'	1:2:6:G:C8	2.49	0.48
14:c:25:VAL:HG22	14:c:45:LYS:HG3	1.94	0.48
14:c:31:GLU:HB3	14:c:39:THR:HG22	1.95	0.48
32:G:32:ILE:HG23	32:G:53:ALA:HA	1.95	0.48
1:2:1246:U:H5	1:2:1247:C:C4	2.32	0.48
1:2:1419:A:H5'	3:D:159:HIS:HB3	1.94	0.48
27:j:92:SER:HA	27:j:95:ILE:HD12	1.95	0.48
1:2:762:A:N3	1:2:762:A:H2'	2.29	0.47
1:2:861:A:H3'	37:N:16:ILE:HD13	1.95	0.47
1:2:1201:A:N3	1:2:1201:A:H2'	2.28	0.47
21:i:29:LYS:HE3	21:i:34:GLU:HB3	1.96	0.47
24:q:398:LEU:HD11	24:q:609:HIS:HB3	1.96	0.47
26:l:163:PRO:HB3	26:l:226:LEU:HD13	1.95	0.47
30:B:48:VAL:HG21	30:B:61:LEU:HD21	1.95	0.47
1:2:1449:C:H5'	17:d:10:HIS:HB3	1.94	0.47
1:2:1487:U:H5''	1:2:1512:U:C6	2.49	0.47
10:S:115:ARG:O	10:S:119:ILE:HG13	2.15	0.47
10:S:123:ARG:HG3	10:S:133:VAL:HG11	1.95	0.47
40:W:79:PHE:H	40:W:125:ILE:HG22	1.77	0.47
16:g:153:THR:H	16:g:178:GLY:HA2	1.79	0.47
18:e:30:PRO:HG3	18:e:38:LEU:HD13	1.95	0.47
29:A:73:VAL:HG13	29:A:120:LEU:HD12	1.97	0.47
45:p:203:VAL:HB	45:p:238:PHE:HE2	1.79	0.47
45:p:450:LEU:HD23	45:p:471:CYS:HB2	1.96	0.47
1:2:1155:C:N4	1:2:1620:G:H1	2.12	0.47
3:D:209:ILE:HG22	9:R:38:ILE:HG23	1.96	0.47
4:F:86:LYS:HG2	4:F:94:ARG:HH22	1.79	0.47
21:i:61:ILE:HG22	21:i:63:GLY:H	1.80	0.47
22:m:41:THR:HG22	22:m:79:GLN:HG2	1.96	0.47
40:W:11:LEU:HD13	40:W:72:CYS:HB3	1.96	0.47
9:R:59:LYS:O	9:R:62:GLN:HB2	2.15	0.47
14:c:18:ARG:HA	14:c:26:THR:HA	1.96	0.47
32:G:175:ILE:HB	32:G:178:LEU:HD23	1.95	0.47
36:L:69:LYS:H	36:L:127:GLN:HB3	1.77	0.47
1:2:1179:C:H42	1:2:1456:G:H1	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1402:C:H2'	1:2:1403:G:H8	1.79	0.47
8:Q:20:ALA:HA	8:Q:67:VAL:HG22	1.97	0.47
26:l:189:GLU:HA	26:l:192:ILE:HD12	1.96	0.47
1:2:92:A:H61	32:G:88:ARG:HB2	1.80	0.47
1:2:1192:A:H1'	1:2:1281:U:H4'	1.96	0.47
1:2:1485:A:H2'	1:2:1486:G:C8	2.50	0.47
3:D:218:LEU:HD11	16:g:200:ILE:HB	1.95	0.47
4:F:142:SER:O	4:F:216:LYS:HG2	2.13	0.47
8:Q:112:TYR:HB3	8:Q:114:ARG:HG2	1.97	0.47
23:o:46:SER:HB2	23:o:84:GLU:HB3	1.97	0.47
29:A:41:ARG:HG2	29:A:43:ASP:H	1.79	0.47
29:A:155:TYR:HA	39:V:60:ARG:HB3	1.97	0.47
33:H:63:PRO:O	33:H:64:VAL:HB	2.15	0.47
34:I:167:TYR:HB3	34:I:185:LEU:HD12	1.97	0.47
37:N:96:VAL:HG11	37:N:150:VAL:HG11	1.97	0.47
1:2:512:U:O2	1:2:512:U:O4'	2.32	0.47
1:2:928:A:H2	38:O:121:VAL:HG12	1.80	0.47
1:2:1289:U:H2'	1:2:1290:G:C8	2.49	0.47
4:F:27:LEU:HD22	8:Q:27:GLY:HA3	1.97	0.47
13:Z:54:ALA:HB1	13:Z:89:ILE:HD11	1.97	0.47
25:k:322:ASP:HB3	25:k:408:ARG:HA	1.97	0.47
31:E:54:TYR:HA	41:Y:22:GLN:HE22	1.80	0.47
1:2:141:U:H2'	1:2:142:G:H8	1.79	0.47
1:2:459:A:H3'	1:2:460:G:C8	2.43	0.47
1:2:1499:C:H42	1:2:1504:G:H1	1.63	0.47
25:k:118:ARG:HD2	25:k:124:GLN:HG3	1.97	0.47
38:O:17:ALA:HB3	38:O:81:ILE:HA	1.96	0.47
41:Y:88:ALA:HA	41:Y:91:LEU:HD12	1.97	0.47
1:2:29:U:O2	1:2:29:U:C2'	2.57	0.47
1:2:1556:U:O4	7:P:122:THR:OG1	2.32	0.47
16:g:219:ALA:HA	16:g:229:VAL:HA	1.97	0.47
24:q:261:ILE:HD13	24:q:279:LEU:HG	1.96	0.47
39:V:55:LEU:HB3	39:V:59:ILE:HD11	1.97	0.47
45:p:639:ILE:HD12	45:p:648:LYS:HB3	1.97	0.47
1:2:1237:A:C6	1:2:1246:U:O4	2.68	0.46
23:o:460:LEU:HD22	23:o:464:ASP:HB3	1.97	0.46
24:q:363:LYS:HE2	24:q:428:ALA:HB2	1.97	0.46
3:D:65:ARG:HA	3:D:68:GLU:HG2	1.98	0.46
24:q:279:LEU:HB2	24:q:299:LEU:HD13	1.98	0.46
42:X:91:GLY:O	42:X:93:LEU:N	2.48	0.46
1:2:21:U:H4'	35:J:18:PRO:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:67:LEU:HD13	15:f:103:LEU:HD23	1.96	0.46
24:q:718:GLN:HE21	24:q:747:LEU:HG	1.80	0.46
38:O:80:HIS:CD2	38:O:114:ARG:HB2	2.50	0.46
31:E:11:ARG:HA	31:E:28:ALA:HB2	1.96	0.46
1:2:1585:A:N6	1:2:1607:U:H3	2.14	0.46
2:C:85:VAL:HA	2:C:107:VAL:HG22	1.97	0.46
2:C:173:ARG:HB3	2:C:204:SER:HB2	1.97	0.46
1:2:297:C:H4'	31:E:30:ARG:HH12	1.80	0.46
1:2:1079:U:C4	1:2:1090:A:C6	3.03	0.46
1:2:1654:U:H3	1:2:1742:A:H61	1.63	0.46
4:F:117:LYS:HA	4:F:120:LEU:HD12	1.96	0.46
24:q:645:ILE:H	24:q:646:PRO:HD3	1.81	0.46
25:k:373:ILE:HD13	25:k:406:LEU:HD11	1.98	0.46
29:A:93:THR:HA	29:A:185:ARG:HH12	1.78	0.46
32:G:142:ARG:HA	32:G:147:LEU:HD12	1.97	0.46
33:H:31:SER:HB2	33:H:32:PRO:HD3	1.98	0.46
39:V:38:GLN:HG3	39:V:49:GLU:HG2	1.97	0.46
1:2:312:U:H5'	1:2:1117:G:N2	2.29	0.46
1:2:325:G:H4'	36:L:82:ARG:HD2	1.96	0.46
1:2:1710:A:H2'	1:2:1711:G:H4'	1.97	0.46
19:h:8:LYS:HZ2	19:h:11:ARG:HH12	1.63	0.46
27:j:71:ALA:HB1	27:j:85:LEU:HD21	1.97	0.46
33:H:61:PHE:HB3	33:H:95:GLU:HB2	1.98	0.46
36:L:57:LYS:HD3	36:L:131:ILE:HG23	1.98	0.46
1:2:97:C:O2	1:2:424:A:O2'	2.33	0.46
1:2:1651:C:H42	1:2:1745:G:H1	1.63	0.46
4:F:59:SER:C	4:F:61:VAL:H	2.23	0.46
10:S:113:LEU:HA	10:S:116:LEU:HD12	1.97	0.46
16:g:249:ALA:H	16:g:262:ALA:HB3	1.80	0.46
25:k:104:GLY:HA3	25:k:211:MET:HE3	1.97	0.46
1:2:813:A:N6	1:2:856:U:C2	2.69	0.46
1:2:1258:U:C2'	1:2:1259:U:H5'	2.46	0.46
40:W:16:ASN:HA	40:W:19:LYS:HE3	1.98	0.46
45:p:113:GLU:HB2	45:p:128:PHE:HB2	1.98	0.46
1:2:208:U:H2'	1:2:209:A:O4'	2.16	0.46
1:2:444:A:H61	1:2:460:G:N2	2.14	0.46
1:2:480:A:C2	1:2:506:U:O4	2.68	0.46
23:o:36:THR:HG22	23:o:74:GLN:HB3	1.98	0.46
32:G:138:ALA:HA	32:G:141:ILE:HD12	1.98	0.46
42:X:63:GLN:HB3	42:X:64:PRO:CD	2.46	0.46
1:2:709:C:H41	1:2:730:G:H21	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:963:U:H5'	37:N:128:TYR:HE1	1.81	0.45
1:2:1167:U:H2'	1:2:1168:G:O4'	2.16	0.45
1:2:1405:U:H2'	1:2:1406:G:C8	2.51	0.45
6:M:20:ALA:HB3	6:M:127:LEU:HD12	1.98	0.45
6:M:26:ARG:O	6:M:30:VAL:HG23	2.15	0.45
21:i:104:LYS:HE2	21:i:111:GLU:HG3	1.97	0.45
27:j:183:LYS:HG2	27:j:231:THR:HB	1.99	0.45
30:B:29:TRP:HD1	30:B:45:LYS:HB3	1.81	0.45
1:2:598:A:H4'	42:X:105:ALA:HB1	1.98	0.45
1:2:705:U:H2'	1:2:706:A:H8	1.81	0.45
1:2:1198:G:H22	17:d:31:ILE:HG23	1.80	0.45
3:D:15:GLY:HA3	17:d:50:ILE:HG23	1.97	0.45
25:k:405:THR:HG21	27:j:190:VAL:HG12	1.97	0.45
1:2:1068:A:H2'	1:2:1069:C:O4'	2.17	0.45
1:2:1172:C:H2'	1:2:1599:G:H22	1.81	0.45
1:2:1675:C:H2'	1:2:1676:A:O4'	2.16	0.45
4:F:101:MET:HB3	4:F:102:ASN:H	1.53	0.45
8:Q:48:VAL:HG12	8:Q:82:ARG:HB2	1.98	0.45
22:m:33:ARG:HG3	22:m:34:ASN:H	1.82	0.45
24:q:300:ILE:HD13	24:q:325:ILE:HG12	1.98	0.45
24:q:633:MET:HE1	24:q:656:LEU:HD22	1.99	0.45
37:N:103:GLU:HA	37:N:106:ARG:HH12	1.81	0.45
4:F:131:PRO:O	4:F:134:VAL:HG12	2.16	0.45
16:g:295:HIS:O	16:g:313:THR:OG1	2.33	0.45
24:q:341:VAL:HG21	24:q:349:ASP:HB3	1.98	0.45
26:l:217:PHE:HD1	26:l:221:GLN:HB3	1.81	0.45
1:2:398:A:H5''	34:I:26:LYS:HD3	1.98	0.45
1:2:771:A:H3'	1:2:772:G:H8	1.80	0.45
1:2:1422:A:H5'	2:C:100:ARG:HH22	1.81	0.45
1:2:1482:G:H21	1:2:1604:C:H1'	1.81	0.45
34:I:81:VAL:HA	34:I:102:VAL:HG12	1.99	0.45
1:2:747:C:H42	1:2:801:G:H1	1.64	0.45
1:2:771:A:H3'	1:2:772:G:C8	2.51	0.45
9:R:5:ARG:HB3	9:R:53:TYR:CE2	2.51	0.45
27:j:225:ALA:H	27:j:226:PRO:HD2	1.82	0.45
30:B:70:LEU:HD13	30:B:82:ARG:HG2	1.98	0.45
1:2:8:U:N3	1:2:1139:G:C6	2.85	0.45
1:2:143:G:H2'	1:2:144:A:O4'	2.17	0.45
1:2:952:G:H2'	1:2:953:G:C8	2.52	0.45
11:T:65:ILE:HA	11:T:71:VAL:HG21	1.98	0.45
13:Z:88:ILE:HG22	13:Z:89:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:p:439:VAL:HG22	45:p:454:VAL:HA	1.98	0.45
1:2:1140:G:H2'	1:2:1141:A:C8	2.52	0.45
1:2:1246:U:H5	1:2:1247:C:C2	2.35	0.45
1:2:1637:C:H42	1:2:1761:A:H61	1.65	0.45
24:q:640:ILE:HG21	24:q:763:LEU:HB3	1.97	0.45
38:O:30:VAL:HG12	38:O:39:ILE:HB	1.99	0.45
1:2:568:C:H42	1:2:573:G:H1	1.63	0.45
1:2:979:G:H1	1:2:1020:C:N4	2.14	0.45
1:2:1201:A:H61	1:2:1455:C:H5'	1.82	0.45
1:2:1471:U:H4'	4:F:111:LYS:HD3	1.98	0.45
3:D:40:ARG:HA	12:U:110:PRO:HB3	1.98	0.45
1:2:255:A:H2'	1:2:256:A:O4'	2.17	0.45
1:2:626:C:H42	1:2:971:G:H1	1.65	0.45
1:2:813:A:C6	1:2:856:U:O4	2.65	0.45
11:T:38:LYS:C	11:T:40:SER:H	2.25	0.45
38:O:106:ALA:HA	38:O:112:ILE:HD11	1.99	0.45
1:2:141:U:H3	1:2:172:A:H61	1.64	0.44
1:2:564:C:H4'	1:2:565:C:O5'	2.17	0.44
1:2:1456:G:H2'	1:2:1457:C:C6	2.52	0.44
1:2:1590:A:H61	1:2:1602:U:H3	1.64	0.44
7:P:52:LYS:HB2	7:P:53:PRO:HD3	1.99	0.44
8:Q:99:GLU:HA	8:Q:102:LYS:HE3	1.98	0.44
27:j:144:ALA:HB1	27:j:154:VAL:HG11	1.98	0.44
30:B:201:THR:HA	30:B:204:ILE:HD12	1.99	0.44
31:E:46:VAL:HG13	31:E:50:ASN:HD22	1.81	0.44
34:I:84:HIS:CE1	34:I:86:SER:HB2	2.52	0.44
42:X:80:GLY:HA3	45:p:394:ARG:HD3	1.99	0.44
45:p:96:LYS:HE2	45:p:112:MET:HB3	1.99	0.44
1:2:462:U:H2'	1:2:463:A:O4'	2.18	0.44
1:2:799:U:H2'	1:2:800:G:H8	1.81	0.44
1:2:1381:G:H2'	1:2:1382:A:C8	2.52	0.44
9:R:91:LEU:HD22	29:A:19:ALA:HB1	2.00	0.44
10:S:126:ARG:HB3	10:S:133:VAL:HG22	1.99	0.44
24:q:548:VAL:HA	24:q:567:LEU:HD21	1.99	0.44
24:q:560:ILE:HG21	24:q:627:LEU:HB2	1.98	0.44
1:2:679:U:H4'	1:2:680:U:OP2	2.17	0.44
1:2:1237:A:N6	1:2:1245:C:H42	2.14	0.44
1:2:1341:C:H5'	16:g:103:ARG:HH21	1.82	0.44
6:M:122:GLN:HB2	6:M:124:ARG:HH12	1.82	0.44
6:M:129:GLU:HA	6:M:133:GLN:HB2	1.98	0.44
1:2:347:U:H4'	34:I:14:THR:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:648:U:H3	1:2:685:A:H61	1.65	0.44
4:F:75:THR:HA	8:Q:79:TYR:OH	2.18	0.44
4:F:176:LEU:HB3	4:F:212:ALA:HB1	1.99	0.44
10:S:50:ALA:O	10:S:51:ASP:HB2	2.17	0.44
24:q:410:ARG:HD2	24:q:459:ILE:HG12	2.00	0.44
31:E:45:ILE:HA	31:E:61:VAL:HG11	1.99	0.44
35:J:109:LEU:HB2	35:J:146:PHE:HB3	1.98	0.44
1:2:108:A:H2'	1:2:109:G:C8	2.52	0.44
1:2:732:G:H1'	1:2:734:A:N6	2.32	0.44
10:S:107:SER:HA	10:S:110:ARG:HD3	1.99	0.44
21:i:81:LEU:HD12	21:i:89:CYS:HB3	2.00	0.44
41:Y:8:ARG:HH22	41:Y:28:LEU:HD13	1.82	0.44
41:Y:37:LYS:HA	41:Y:40:LEU:HD12	1.99	0.44
5:K:15:LEU:HG	5:K:21:LEU:HD23	1.99	0.44
25:k:145:ALA:HB3	25:k:189:VAL:HG23	2.00	0.44
38:O:80:HIS:HD2	38:O:114:ARG:HB2	1.83	0.44
4:F:131:PRO:O	4:F:135:VAL:HG23	2.18	0.44
42:X:103:LEU:HB3	42:X:126:LYS:HB2	2.00	0.44
1:2:387:G:H2'	1:2:388:G:C8	2.53	0.44
1:2:908:U:H2'	1:2:909:C:C6	2.53	0.44
1:2:1221:C:H2'	1:2:1222:A:H8	1.83	0.44
3:D:162:GLN:C	3:D:164:VAL:N	2.76	0.44
19:h:2:ARG:HB2	19:h:5:TRP:CD1	2.53	0.44
30:B:164:ILE:HD11	30:B:205:PHE:HB2	2.00	0.44
45:p:521:ILE:HD11	45:p:549:ALA:HB3	2.00	0.44
1:2:597:U:H2'	1:2:598:A:H8	1.82	0.44
1:2:625:U:H2'	1:2:626:C:H6	1.83	0.44
1:2:1487:U:H5''	1:2:1512:U:H6	1.82	0.44
1:2:1512:U:O2	1:2:1512:U:O4'	2.35	0.44
6:M:76:ASN:HD22	6:M:78:PRO:HD2	1.82	0.44
1:2:480:A:H61	1:2:506:U:H3	1.66	0.43
1:2:1246:U:C5	1:2:1247:C:C4	3.06	0.43
16:g:269:ILE:HD13	16:g:279:ASP:HB3	2.00	0.43
24:q:440:ILE:HG23	24:q:448:ILE:HG21	1.99	0.43
30:B:193:ILE:H	30:B:193:ILE:HG13	1.66	0.43
36:L:14:GLN:HB3	36:L:54:ILE:HG21	2.00	0.43
1:2:21:U:H2'	1:2:22:A:C8	2.52	0.43
1:2:570:G:H2'	1:2:570:G:N3	2.33	0.43
1:2:1589:C:H42	1:2:1603:G:H1	1.66	0.43
16:g:210:GLN:HE22	16:g:252:PHE:H	1.67	0.43
21:i:41:MET:HE1	21:i:71:MET:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:q:265:ARG:HH12	24:q:298:THR:HB	1.82	0.43
1:2:305:U:H2'	1:2:306:G:C8	2.53	0.43
1:2:1446:G:H2'	1:2:1446:G:N3	2.32	0.43
23:o:463:TRP:HB3	24:q:744:LEU:HD22	2.00	0.43
1:2:20:G:OP1	1:2:570:G:H8	2.01	0.43
7:P:111:MET:SD	10:S:119:ILE:HG21	2.57	0.43
1:2:524:A:H2'	1:2:525:A:C8	2.54	0.43
1:2:1038:A:O2'	1:2:1039:G:H8	2.01	0.43
1:2:1343:A:H2'	1:2:1344:A:C8	2.54	0.43
1:2:1468:C:H4'	1:2:1538:G:H21	1.83	0.43
1:2:1662:C:H42	1:2:1735:G:H1	1.66	0.43
6:M:52:LEU:HD21	6:M:80:ILE:HD12	2.01	0.43
13:Z:65:LEU:HA	13:Z:70:LYS:HE2	2.01	0.43
25:k:149:LYS:HE3	25:k:299:VAL:HG21	2.00	0.43
33:H:131:PHE:H	33:H:132:PRO:HD2	1.83	0.43
37:N:54:LEU:HB3	37:N:60:VAL:HG21	2.00	0.43
1:2:101:U:H2'	1:2:102:U:O4'	2.18	0.43
1:2:387:G:H2'	1:2:388:G:H8	1.83	0.43
29:A:139:VAL:HG23	29:A:141:ILE:HG12	2.01	0.43
32:G:50:PHE:HB3	32:G:111:LEU:HD22	2.00	0.43
35:J:4:ALA:HA	35:J:5:PRO:HD3	1.89	0.43
1:2:1231:U:H2'	1:2:1232:G:H8	1.83	0.43
15:f:130:LEU:HD22	15:f:137:PHE:HB3	2.00	0.43
16:g:34:LEU:HB3	16:g:46:TRP:HB2	2.00	0.43
1:2:151:U:H3	1:2:161:A:H61	1.67	0.43
1:2:951:A:H2'	1:2:952:G:C8	2.53	0.43
1:2:1149:G:H3'	1:2:1766:G:H21	1.84	0.43
4:F:144:PRO:HD2	4:F:169:ARG:HG3	2.01	0.43
25:k:213:ALA:HA	25:k:243:HIS:HB2	2.00	0.43
31:E:72:VAL:HG22	31:E:90:ILE:HG12	2.01	0.43
37:N:98:VAL:HB	37:N:115:LEU:HD23	2.01	0.43
45:p:283:TYR:HE1	45:p:323:MET:HG3	1.83	0.43
1:2:473:A:N6	1:2:593:A:OP1	2.52	0.43
1:2:645:U:H2'	1:2:646:G:H8	1.83	0.43
1:2:1198:G:N3	1:2:1198:G:C2'	2.81	0.43
24:q:640:ILE:HD11	24:q:765:ILE:HG12	2.01	0.43
1:2:339:U:H2'	1:2:340:A:H8	1.83	0.43
1:2:600:A:H2'	1:2:600:A:N3	2.34	0.43
1:2:623:G:H1	1:2:974:C:H42	1.66	0.43
1:2:1491:A:H4'	1:2:1492:C:OP2	2.18	0.43
1:2:1617:C:H2'	1:2:1618:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:o:485:GLU:HG2	24:q:775:ILE:HD13	2.01	0.43
27:j:149:ILE:HD12	27:j:150:ILE:HG23	2.01	0.43
37:N:101:HIS:HA	37:N:104:ARG:HD3	2.00	0.43
1:2:476:A:H2'	1:2:477:A:H8	1.83	0.42
1:2:923:A:H2'	1:2:924:G:C8	2.54	0.42
1:2:1351:U:H2'	1:2:1352:U:O4'	2.19	0.42
1:2:1429:C:OP1	1:2:1430:U:H2'	2.19	0.42
6:M:78:PRO:HB2	6:M:128:LEU:HD21	2.01	0.42
24:q:622:LEU:HB3	24:q:675:VAL:HG11	2.01	0.42
1:2:141:U:H2'	1:2:142:G:C8	2.54	0.42
1:2:882:C:H2'	1:2:883:A:O4'	2.19	0.42
1:2:883:A:H61	1:2:927:U:H3	1.67	0.42
26:l:184:LEU:HD13	26:l:234:VAL:HG21	2.01	0.42
31:E:136:ILE:HD13	31:E:148:ARG:HH12	1.84	0.42
33:H:141:ARG:HB2	33:H:149:ILE:HB	2.02	0.42
39:V:5:LYS:HB2	39:V:7:GLN:HE21	1.84	0.42
40:W:24:GLN:CD	44:b:5:GLN:H	2.27	0.42
40:W:55:ASP:C	40:W:57:ARG:H	2.26	0.42
1:2:1356:G:H2'	1:2:1357:G:H8	1.85	0.42
1:2:1458:A:H1'	26:l:169:GLY:HA2	2.00	0.42
9:R:33:ARG:HD3	16:g:86:TRP:HZ3	1.83	0.42
10:S:112:ASP:O	10:S:115:ARG:HG2	2.19	0.42
28:1:29:G:H1	28:1:41:C:H42	1.67	0.42
33:H:139:ARG:HB2	33:H:151:LYS:HB3	2.01	0.42
35:J:153:GLU:HA	35:J:156:ILE:HD12	2.00	0.42
1:2:106:U:H5'	34:I:8:ARG:HH22	1.83	0.42
1:2:147:U:H5''	1:2:148:C:H5	1.85	0.42
1:2:206:U:H2'	1:2:207:U:C6	2.54	0.42
1:2:1651:C:H2'	1:2:1652:G:O4'	2.19	0.42
4:F:150:ARG:H	4:F:150:ARG:HG3	1.69	0.42
12:U:117:ILE:HG22	12:U:118:ILE:H	1.85	0.42
35:J:108:ARG:HG2	35:J:145:SER:HA	2.01	0.42
37:N:129:TYR:O	37:N:133:SER:N	2.49	0.42
1:2:296:U:H2'	1:2:297:C:C6	2.55	0.42
1:2:599:U:O2	1:2:599:U:C2'	2.67	0.42
1:2:817:C:N4	1:2:852:G:H1	2.17	0.42
1:2:1294:G:H2'	1:2:1295:A:H5'	2.01	0.42
4:F:115:ILE:HG23	4:F:193:ALA:HB2	1.99	0.42
8:Q:87:LYS:HA	8:Q:90:VAL:HG22	2.02	0.42
12:U:28:SER:HB3	12:U:34:LEU:HD22	2.01	0.42
24:q:645:ILE:H	24:q:646:PRO:CD	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:b:48:SER:HB2	44:b:70:LYS:HE2	2.02	0.42
1:2:1160:C:H2'	1:2:1161:C:O4'	2.19	0.42
6:M:64:ILE:HG22	15:f:103:LEU:HD22	2.01	0.42
11:T:38:LYS:HE3	11:T:38:LYS:HB2	1.92	0.42
22:m:33:ARG:HB2	22:m:39:LEU:HB2	2.02	0.42
23:o:470:LEU:HD11	24:q:733:TYR:CE2	2.55	0.42
31:E:179:LYS:HA	31:E:231:PRO:HD3	2.01	0.42
33:H:62:VAL:HG12	33:H:64:VAL:H	1.84	0.42
43:a:19:LYS:HA	43:a:20:PRO:HD3	1.86	0.42
4:F:100:MET:HE3	4:F:107:GLY:HA2	2.02	0.42
5:K:80:LEU:HB3	5:K:82:LEU:HD23	2.01	0.42
11:T:21:PHE:HA	11:T:24:ARG:HH11	1.85	0.42
16:g:318:ARG:HH11	16:g:318:ARG:HB2	1.85	0.42
23:o:73:HIS:HA	23:o:168:LEU:HD13	2.01	0.42
25:k:500:ALA:HB1	25:k:511:LEU:HD11	2.01	0.42
31:E:47:PHE:HA	31:E:51:ARG:HB2	2.00	0.42
1:2:1396:U:H3'	1:2:1397:C:H5'	2.01	0.42
10:S:117:LYS:HE2	10:S:128:PHE:HB2	2.01	0.42
25:k:210:VAL:HG21	25:k:318:ILE:HD11	2.02	0.42
29:A:174:TRP:HA	29:A:177:LEU:HD12	2.02	0.42
33:H:138:LYS:HB2	40:W:54:ASP:HB3	2.02	0.42
1:2:312:U:H3	1:2:1116:U:H3	1.68	0.42
3:D:162:GLN:C	3:D:164:VAL:H	2.28	0.42
4:F:31:ILE:HA	4:F:32:PRO:HD3	1.94	0.42
25:k:312:SER:HB2	25:k:422:HIS:HE1	1.83	0.42
25:k:440:LEU:HG	25:k:453:VAL:HG22	2.02	0.42
31:E:37:LYS:HB2	31:E:40:GLU:HB2	2.01	0.42
31:E:82:PHE:HA	31:E:83:PRO:HD3	1.96	0.42
35:J:34:TYR:CD1	35:J:111:THR:HG21	2.55	0.42
37:N:17:PRO:C	37:N:19:SER:H	2.27	0.42
41:Y:55:VAL:HG13	41:Y:75:VAL:HG22	2.00	0.42
1:2:862:A:H2'	1:2:864:A:C8	2.55	0.42
28:1:27:C:H2'	28:1:28:A:C8	2.55	0.42
1:2:128:U:H5'	1:2:130:C:H41	1.84	0.41
1:2:1051:U:H3'	1:2:1052:G:C5'	2.50	0.41
1:2:1141:A:H5''	43:a:2:PRO:HB3	2.02	0.41
1:2:1381:G:H1'	12:U:57:ARG:HH21	1.85	0.41
1:2:1500:G:N7	11:T:102:ARG:NH2	2.68	0.41
1:2:1677:G:H21	1:2:1720:A:H62	1.68	0.41
16:g:30:GLN:HE22	16:g:47:ARG:HG2	1.85	0.41
30:B:123:ALA:HB3	30:B:139:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:L:22:ASN:HA	36:L:23:PRO:HD3	1.91	0.41
40:W:62:VAL:HG13	44:b:7:LEU:HD12	2.02	0.41
1:2:1198:G:N3	1:2:1198:G:H2'	2.34	0.41
1:2:1246:U:H5	1:2:1247:C:N3	2.18	0.41
1:2:1389:A:H61	1:2:1405:U:H3	1.69	0.41
3:D:58:VAL:O	3:D:65:ARG:HB3	2.20	0.41
3:D:215:GLU:HA	3:D:216:PRO:HD3	1.94	0.41
30:B:109:LYS:HG3	30:B:113:MET:HE3	2.01	0.41
1:2:537:A:H2	1:2:541:A:H62	1.69	0.41
1:2:1127:C:H2'	1:2:1128:U:O4'	2.20	0.41
1:2:1333:U:H2'	1:2:1334:U:O4'	2.20	0.41
1:2:1540:G:H22	1:2:1566:C:H2'	1.85	0.41
3:D:36:GLY:HA3	3:D:51:ARG:HH11	1.84	0.41
6:M:28:SER:HB3	6:M:34:LEU:HD12	2.03	0.41
20:3:15:G:H1	28:1:34:C:H42	1.67	0.41
29:A:126:PRO:HG2	29:A:147:THR:HG22	2.02	0.41
32:G:74:LYS:HA	32:G:96:SER:HA	2.02	0.41
45:p:632:LYS:HG3	45:p:633:VAL:H	1.85	0.41
1:2:374:U:H2'	1:2:375:C:C6	2.55	0.41
8:Q:29:ILE:HA	8:Q:65:ILE:HB	2.02	0.41
16:g:48:LEU:HA	16:g:56:GLY:HA2	2.01	0.41
18:e:10:ARG:HH21	18:e:13:LYS:HA	1.86	0.41
45:p:301:SER:HA	45:p:302:PRO:HD3	1.87	0.41
1:2:451:A:H3'	1:2:452:U:H6	1.85	0.41
1:2:1367:G:H5''	11:T:69:LYS:HB3	2.02	0.41
1:2:1660:G:H2'	1:2:1661:G:C8	2.55	0.41
18:e:39:LEU:HB3	35:J:28:LEU:HD11	2.02	0.41
22:m:68:ILE:HG12	22:m:78:ILE:HG12	2.01	0.41
27:j:133:PRO:HA	27:j:137:LYS:HB2	2.03	0.41
29:A:205:ARG:HB3	29:A:210:ILE:HG13	2.03	0.41
40:W:11:LEU:HD12	40:W:74:VAL:HG23	2.01	0.41
40:W:24:GLN:HA	40:W:63:VAL:O	2.21	0.41
1:2:602:U:H2'	1:2:603:A:H8	1.85	0.41
1:2:829:U:O2	1:2:829:U:O4'	2.38	0.41
36:L:156:PHE:CD1	37:N:77:SER:HA	2.55	0.41
37:N:15:ALA:HB2	44:b:20:LYS:HD3	2.03	0.41
1:2:897:A:H4'	38:O:46:MET:HE3	2.02	0.41
1:2:1226:A:C2	6:M:36:ARG:HD2	2.55	0.41
1:2:1626:U:H2'	1:2:1627:G:C8	2.56	0.41
6:M:122:GLN:HB2	6:M:124:ARG:NH1	2.35	0.41
25:k:473:ALA:HB2	25:k:487:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:70:LEU:HB3	30:B:82:ARG:HB3	2.02	0.41
32:G:181:PRO:HA	32:G:184:LEU:HD12	2.01	0.41
34:I:69:SER:HB3	36:L:24:LYS:HD2	2.03	0.41
36:L:112:SER:HB3	36:L:115:PHE:HD2	1.86	0.41
42:X:53:VAL:HA	42:X:74:VAL:HG22	2.02	0.41
1:2:353:C:H5''	34:I:16:ALA:HB2	2.03	0.41
4:F:168:ARG:HD3	14:c:47:PRO:HD2	2.03	0.41
7:P:71:GLU:HB3	7:P:72:LYS:H	1.64	0.41
29:A:176:LEU:O	29:A:180:GLU:HG2	2.21	0.41
40:W:6:VAL:HG13	40:W:29:PRO:HG2	2.03	0.41
40:W:82:LYS:O	40:W:84:ALA:N	2.53	0.41
42:X:62:LYS:H	42:X:116:ASP:HB2	1.85	0.41
1:2:8:U:C2	1:2:1138:A:C6	3.04	0.41
1:2:311:A:H4'	1:2:312:U:O5'	2.21	0.41
1:2:338:C:H2'	1:2:339:U:C6	2.56	0.41
1:2:430:C:H2'	1:2:431:G:O4'	2.21	0.41
1:2:703:G:H5'	1:2:704:C:OP2	2.20	0.41
1:2:1343:A:H4'	1:2:1344:A:OP1	2.20	0.41
1:2:1507:C:H2'	1:2:1508:U:O4'	2.21	0.41
2:C:72:GLN:H	2:C:72:GLN:HG2	1.73	0.41
2:C:144:ILE:HG12	2:C:223:ILE:HG23	2.02	0.41
3:D:50:ILE:HD11	3:D:86:LEU:HD22	2.02	0.41
3:D:66:ILE:H	3:D:66:ILE:HG13	1.49	0.41
3:D:115:ILE:HD13	3:D:142:LEU:HD23	2.02	0.41
4:F:60:LEU:HD23	4:F:64:ILE:HD11	2.03	0.41
4:F:165:SER:HA	4:F:166:PRO:HD3	1.94	0.41
8:Q:41:PRO:C	8:Q:43:ILE:H	2.29	0.41
9:R:93:LEU:O	9:R:98:ASP:HA	2.20	0.41
17:d:41:GLN:H	17:d:41:GLN:HE21	1.68	0.41
23:o:425:ARG:HD2	23:o:460:LEU:HD21	2.03	0.41
28:1:2:G:H1	28:1:71:C:H42	1.68	0.41
29:A:130:ALA:HA	29:A:133:ILE:HD12	2.03	0.41
30:B:176:VAL:C	30:B:178:ASN:H	2.28	0.41
31:E:32:SER:H	31:E:81:THR:HB	1.85	0.41
35:J:112:GLN:HG3	35:J:148:VAL:HG21	2.03	0.41
37:N:70:LYS:HD3	37:N:73:ARG:HH12	1.85	0.41
37:N:114:ARG:HA	37:N:117:LEU:HD12	2.03	0.41
44:b:20:LYS:O	44:b:21:LEU:HB2	2.21	0.41
45:p:489:VAL:HG22	45:p:505:SER:HB2	2.03	0.41
1:2:71:A:C3'	1:2:72:A:H5''	2.41	0.41
1:2:499:C:H2'	1:2:500:U:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1091:A:N3	1:2:1091:A:H2'	2.36	0.41
1:2:1586:G:H22	1:2:1606:U:H3	1.69	0.41
14:c:20:GLY:H	14:c:66:LEU:HD13	1.86	0.41
16:g:158:ALA:HA	16:g:159:PRO:HD3	1.93	0.41
24:q:616:LEU:HD13	24:q:702:LEU:HB2	2.03	0.41
24:q:669:GLU:H	24:q:673:ASP:HB2	1.84	0.41
45:p:617:PRO:HG3	45:p:662:PRO:HA	2.03	0.41
1:2:91:G:OP1	1:2:396:A:N6	2.53	0.40
1:2:703:G:C3'	1:2:704:C:H5'	2.52	0.40
1:2:991:A:H61	1:2:1011:U:H3	1.69	0.40
39:V:43:GLY:C	39:V:45:ALA:H	2.29	0.40
1:2:165:C:O2	32:G:132:ARG:HG3	2.21	0.40
1:2:1667:U:H3	1:2:1730:A:H61	1.69	0.40
2:C:51:LYS:HA	2:C:76:GLN:HE22	1.86	0.40
12:U:68:ARG:HH22	12:U:77:LYS:HD3	1.86	0.40
21:i:109:LEU:HA	21:i:110:PRO:HD3	1.92	0.40
23:o:430:ARG:HH22	23:o:472:ALA:HB3	1.85	0.40
25:k:176:ARG:H	25:k:177:PRO:HD2	1.86	0.40
25:k:245:ILE:HG12	25:k:279:PRO:HG2	2.03	0.40
45:p:334:LEU:HB3	45:p:338:LEU:HD21	2.04	0.40
1:2:1211:G:H1	1:2:1449:C:H42	1.69	0.40
1:2:164:G:H21	32:G:132:ARG:HD3	1.87	0.40
1:2:1079:U:C4	1:2:1090:A:N6	2.81	0.40
1:2:1744:A:H5''	45:p:363:LYS:HE2	2.03	0.40
10:S:119:ILE:HG13	10:S:119:ILE:H	1.77	0.40
22:m:34:ASN:HA	28:1:37:A:H1'	2.03	0.40
43:a:44:ILE:HD12	43:a:67:THR:HB	2.04	0.40
1:2:1157:C:N4	1:2:1162:A:H61	2.20	0.40
1:2:1300:U:H2'	1:2:1301:U:O4'	2.21	0.40
1:2:1475:G:H5'	11:T:43:ASN:HD21	1.86	0.40
1:2:1716:A:H2'	1:2:1717:A:C8	2.57	0.40
5:K:54:PHE:CE2	5:K:75:TYR:HB3	2.57	0.40
12:U:16:GLU:C	12:U:18:VAL:H	2.29	0.40
25:k:136:ILE:HG22	50:k:602:GCP:H3B1	2.04	0.40
45:p:504:ILE:HG21	45:p:550:ASN:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	215/217 (99%)	194 (90%)	14 (6%)	7 (3%)	3	21
3	D	221/223 (99%)	196 (89%)	14 (6%)	11 (5%)	1	15
4	F	204/206 (99%)	171 (84%)	22 (11%)	11 (5%)	1	14
5	K	94/96 (98%)	84 (89%)	7 (7%)	3 (3%)	3	21
6	M	113/118 (96%)	86 (76%)	17 (15%)	10 (9%)	0	8
7	P	115/117 (98%)	94 (82%)	15 (13%)	6 (5%)	1	14
8	Q	139/141 (99%)	118 (85%)	11 (8%)	10 (7%)	1	10
9	R	128/130 (98%)	107 (84%)	15 (12%)	6 (5%)	2	16
10	S	143/145 (99%)	118 (82%)	17 (12%)	8 (6%)	1	14
11	T	141/143 (99%)	132 (94%)	7 (5%)	2 (1%)	9	40
12	U	104/106 (98%)	91 (88%)	8 (8%)	5 (5%)	2	16
13	Z	68/70 (97%)	56 (82%)	9 (13%)	3 (4%)	2	16
14	c	60/62 (97%)	53 (88%)	6 (10%)	1 (2%)	7	36
15	f	67/69 (97%)	51 (76%)	7 (10%)	9 (13%)	0	3
16	g	312/324 (96%)	271 (87%)	33 (11%)	8 (3%)	4	25
17	d	51/53 (96%)	39 (76%)	11 (22%)	1 (2%)	6	30
18	e	56/58 (97%)	45 (80%)	9 (16%)	2 (4%)	2	20
19	h	23/25 (92%)	23 (100%)	0	0	100	100
21	i	109/111 (98%)	90 (83%)	18 (16%)	1 (1%)	14	50
22	m	86/90 (96%)	76 (88%)	7 (8%)	3 (4%)	3	20
23	o	435/567 (77%)	366 (84%)	62 (14%)	7 (2%)	7	37
24	q	667/699 (95%)	577 (86%)	70 (10%)	20 (3%)	3	22
25	k	404/430 (94%)	337 (83%)	60 (15%)	7 (2%)	7	36
26	l	118/144 (82%)	97 (82%)	20 (17%)	1 (1%)	16	54
27	j	243/263 (92%)	210 (86%)	27 (11%)	6 (2%)	4	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	A	217/219 (99%)	183 (84%)	24 (11%)	10 (5%)	2	16
30	B	218/231 (94%)	187 (86%)	23 (11%)	8 (4%)	2	19
31	E	258/260 (99%)	240 (93%)	13 (5%)	5 (2%)	6	31
32	G	224/226 (99%)	205 (92%)	18 (8%)	1 (0%)	30	67
33	H	182/184 (99%)	157 (86%)	15 (8%)	10 (6%)	1	14
34	I	184/200 (92%)	166 (90%)	11 (6%)	7 (4%)	2	19
35	J	180/182 (99%)	150 (83%)	25 (14%)	5 (3%)	4	24
36	L	153/155 (99%)	132 (86%)	17 (11%)	4 (3%)	4	25
37	N	148/150 (99%)	135 (91%)	12 (8%)	1 (1%)	18	56
38	O	125/127 (98%)	102 (82%)	12 (10%)	11 (9%)	0	8
39	V	85/87 (98%)	75 (88%)	7 (8%)	3 (4%)	3	20
40	W	127/129 (98%)	113 (89%)	9 (7%)	5 (4%)	2	18
41	Y	132/134 (98%)	116 (88%)	13 (10%)	3 (2%)	5	27
42	X	142/144 (99%)	119 (84%)	14 (10%)	9 (6%)	1	12
43	a	96/98 (98%)	82 (85%)	10 (10%)	4 (4%)	2	17
44	b	79/81 (98%)	70 (89%)	3 (4%)	6 (8%)	1	9
45	p	650/666 (98%)	538 (83%)	93 (14%)	19 (3%)	3	23
46	s	326/342 (95%)	318 (98%)	8 (2%)	0	100	100
47	r	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
All	All	7889/8271 (95%)	6814 (86%)	816 (10%)	259 (3%)	5	21

All (259) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	141	VAL
2	C	187	PRO
3	D	220	PRO
4	F	67	SER
6	M	82	VAL
6	M	84	ASP
8	Q	39	VAL
8	Q	40	GLN
10	S	27	ASN
10	S	28	VAL
12	U	17	VAL

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Mol	Chain	Res	Type
12	U	96	PRO
15	f	102	VAL
18	e	47	VAL
24	q	111	VAL
29	A	95	ALA
33	H	31	SER
33	H	64	VAL
34	I	147	ARG
34	I	153	ILE
41	Y	30	PRO
42	X	64	PRO
42	X	92	CYS
43	a	59	TYR
44	b	75	GLU
45	p	181	PRO
45	p	392	PRO
3	D	216	PRO
4	F	37	GLN
4	F	59	SER
4	F	60	LEU
4	F	155	GLY
5	K	54	PHE
5	K	92	LEU
7	P	54	ALA
8	Q	97	VAL
8	Q	115	THR
9	R	99	VAL
10	S	51	ASP
10	S	91	ASP
10	S	145	ARG
13	Z	55	PRO
15	f	110	ASP
15	f	143	HIS
16	g	130	LYS
17	d	23	ILE
22	m	73	GLU
23	o	294	GLY
24	q	105	GLU
24	q	160	ASN
24	q	165	ASN
26	l	200	GLY
29	A	166	GLY

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Mol	Chain	Res	Type
29	A	202	TYR
30	B	148	ASN
30	B	214	LYS
31	E	205	PHE
31	E	245	LYS
32	G	122	GLU
33	H	74	GLN
33	H	136	VAL
33	H	163	ASP
34	I	40	THR
34	I	148	ALA
35	J	150	LEU
35	J	171	ARG
36	L	30	LYS
36	L	55	ASP
36	L	105	LYS
38	O	114	ARG
39	V	45	ALA
40	W	58	SER
40	W	83	ILE
41	Y	36	SER
43	a	13	LYS
45	p	167	ASN
45	p	182	THR
45	p	365	PHE
45	p	559	ARG
2	C	155	GLN
3	D	196	THR
3	D	219	GLU
3	D	221	SER
3	D	223	LYS
4	F	24	PRO
4	F	45	PHE
4	F	66	ILE
5	K	23	ALA
6	M	98	ASP
6	M	110	SER
7	P	108	ARG
8	Q	14	LYS
8	Q	27	GLY
8	Q	32	ASN
8	Q	116	LEU

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Mol	Chain	Res	Type
8	Q	121	SER
9	R	5	ARG
9	R	116	LYS
10	S	102	ALA
11	T	29	GLU
13	Z	38	HIS
15	f	111	GLU
16	g	201	GLY
21	i	17	ASN
22	m	85	ARG
23	o	22	GLY
23	o	171	ASN
23	o	194	GLN
23	o	461	SER
24	q	468	THR
24	q	536	ASP
24	q	650	LYS
25	k	127	ARG
27	j	9	TYR
27	j	57	ARG
27	j	225	ALA
30	B	8	ARG
30	B	190	PRO
31	E	195	ILE
33	H	110	GLN
34	I	52	ASN
38	O	18	ARG
38	O	124	ASP
40	W	29	PRO
40	W	72	CYS
42	X	3	LYS
44	b	3	LEU
44	b	51	GLN
45	p	76	ASP
45	p	160	MET
45	p	170	ASP
45	p	219	ASN
45	p	271	ASP
45	p	641	ASN
45	p	644	GLY
2	C	151	THR
2	C	235	TRP

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Mol	Chain	Res	Type
2	C	253	THR
3	D	62	ASN
4	F	186	PHE
6	M	32	ASP
6	M	103	ALA
7	P	89	MET
7	P	90	ILE
7	P	109	PRO
9	R	24	LEU
9	R	88	VAL
10	S	14	ILE
10	S	142	GLY
12	U	89	ARG
14	c	35	ASP
15	f	98	VAL
15	f	100	LEU
15	f	118	ARG
16	g	106	GLY
18	e	11	ALA
22	m	24	ASN
23	o	457	PRO
24	q	113	LYS
24	q	164	PRO
24	q	460	PRO
24	q	514	LYS
24	q	645	ILE
25	k	507	LYS
27	j	49	SER
29	A	21	ARG
29	A	39	LYS
30	B	54	LEU
30	B	55	LYS
31	E	77	ARG
33	H	54	GLY
37	N	3	ARG
38	O	51	ASP
38	O	75	GLY
38	O	125	SER
39	V	12	TYR
41	Y	4	ALA
42	X	63	GLN
42	X	70	LYS

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Mol	Chain	Res	Type
44	b	21	LEU
45	p	259	PRO
45	p	529	LYS
3	D	4	ILE
3	D	217	VAL
6	M	21	LEU
6	M	120	ASP
8	Q	138	PHE
11	T	39	THR
13	Z	56	THR
15	f	90	LYS
16	g	50	GLU
16	g	120	SER
16	g	129	ASP
24	q	140	LEU
24	q	227	PRO
24	q	351	ILE
24	q	639	GLY
25	k	94	ILE
25	k	95	ILE
25	k	357	PRO
27	j	224	ALA
29	A	103	THR
30	B	154	SER
33	H	98	ILE
34	I	59	ARG
35	J	134	ILE
35	J	147	MET
36	L	5	LEU
38	O	25	ASP
38	O	40	ALA
38	O	42	VAL
38	O	91	SER
40	W	56	HIS
42	X	89	ASN
43	a	36	ILE
2	C	44	THR
3	D	163	PRO
4	F	108	LYS
7	P	71	GLU
12	U	107	THR
15	f	85	TYR

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Mol	Chain	Res	Type
25	k	112	GLY
29	A	100	GLY
29	A	158	VAL
29	A	206	ASN
31	E	144	GLY
33	H	13	PRO
33	H	87	ASP
34	I	22	ARG
38	O	88	GLY
39	V	44	ARG
43	a	61	GLU
44	b	62	VAL
45	p	198	VAL
45	p	375	PRO
4	F	103	GLY
16	g	254	PRO
29	A	25	GLY
42	X	91	GLY
45	p	391	GLN
45	p	569	PRO
24	q	163	THR
24	q	367	GLY
35	J	35	GLY
42	X	41	SER
42	X	96	VAL
6	M	33	GLY
9	R	117	LEU
12	U	117	ILE
23	o	423	PRO
24	q	336	ILE
25	k	277	GLY
27	j	81	GLY
3	D	63	GLY
6	M	93	GLY
24	q	766	PRO
44	b	10	PRO
16	g	64	GLY
30	B	22	ASP

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	C	176/176 (100%)	147 (84%)	29 (16%)	2	10
3	D	185/185 (100%)	145 (78%)	40 (22%)	1	6
4	F	174/174 (100%)	134 (77%)	40 (23%)	1	6
5	K	88/88 (100%)	67 (76%)	21 (24%)	1	5
6	M	93/94 (99%)	75 (81%)	18 (19%)	1	8
7	P	100/100 (100%)	75 (75%)	25 (25%)	0	4
8	Q	117/117 (100%)	98 (84%)	19 (16%)	2	11
9	R	115/118 (98%)	96 (84%)	19 (16%)	2	10
10	S	128/128 (100%)	109 (85%)	19 (15%)	3	13
11	T	117/117 (100%)	91 (78%)	26 (22%)	1	6
12	U	96/96 (100%)	78 (81%)	18 (19%)	1	8
13	Z	60/60 (100%)	47 (78%)	13 (22%)	1	6
14	c	54/54 (100%)	46 (85%)	8 (15%)	3	13
15	f	57/60 (95%)	53 (93%)	4 (7%)	14	35
16	g	265/270 (98%)	233 (88%)	32 (12%)	5	17
17	d	46/46 (100%)	35 (76%)	11 (24%)	1	5
18	e	51/51 (100%)	48 (94%)	3 (6%)	18	39
19	h	23/23 (100%)	17 (74%)	6 (26%)	0	3
21	i	93/93 (100%)	85 (91%)	8 (9%)	10	29
22	m	77/78 (99%)	69 (90%)	8 (10%)	7	22
23	o	398/438 (91%)	355 (89%)	43 (11%)	6	21
24	q	527/644 (82%)	484 (92%)	43 (8%)	10	30
25	k	332/364 (91%)	303 (91%)	29 (9%)	9	28
26	l	117/132 (89%)	107 (92%)	10 (8%)	10	29
27	j	224/237 (94%)	196 (88%)	28 (12%)	4	16
29	A	180/185 (97%)	159 (88%)	21 (12%)	5	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	B	198/210 (94%)	175 (88%)	23 (12%)	5	18
31	E	223/223 (100%)	198 (89%)	25 (11%)	6	19
32	G	192/192 (100%)	177 (92%)	15 (8%)	11	32
33	H	164/164 (100%)	149 (91%)	15 (9%)	9	27
34	I	147/158 (93%)	130 (88%)	17 (12%)	5	18
35	J	153/153 (100%)	126 (82%)	27 (18%)	2	9
36	L	136/136 (100%)	111 (82%)	25 (18%)	1	9
37	N	127/127 (100%)	105 (83%)	22 (17%)	2	9
38	O	96/96 (100%)	86 (90%)	10 (10%)	7	22
39	V	73/73 (100%)	64 (88%)	9 (12%)	4	17
40	W	110/110 (100%)	101 (92%)	9 (8%)	10	30
41	Y	108/108 (100%)	99 (92%)	9 (8%)	10	30
42	X	119/119 (100%)	106 (89%)	13 (11%)	6	20
43	a	83/83 (100%)	79 (95%)	4 (5%)	23	44
44	b	71/71 (100%)	69 (97%)	2 (3%)	38	59
45	p	537/597 (90%)	508 (95%)	29 (5%)	20	41
46	s	287/297 (97%)	286 (100%)	1 (0%)	86	85
47	r	40/40 (100%)	40 (100%)	0	100	100
All	All	6757/7085 (95%)	5961 (88%)	796 (12%)	7	18

All (796) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	49	LEU
2	C	58	ILE
2	C	71	PHE
2	C	72	GLN
2	C	74	ILE
2	C	75	ASP
2	C	80	ASN
2	C	91	VAL
2	C	93	LYS
2	C	95	THR
2	C	116	VAL
2	C	120	ILE
2	C	125	GLU

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Mol	Chain	Res	Type
2	C	126	VAL
2	C	131	ARG
2	C	142	ILE
2	C	144	ILE
2	C	145	ARG
2	C	146	ARG
2	C	155	GLN
2	C	163	THR
2	C	173	ARG
2	C	192	LEU
2	C	195	LEU
2	C	212	LEU
2	C	216	LEU
2	C	227	TYR
2	C	234	LEU
2	C	235	TRP
3	D	5	ILE
3	D	11	LEU
3	D	20	GLU
3	D	22	ASN
3	D	28	GLU
3	D	31	GLU
3	D	47	GLU
3	D	53	THR
3	D	57	ASP
3	D	58	VAL
3	D	64	ARG
3	D	66	ILE
3	D	67	ASN
3	D	68	GLU
3	D	70	THR
3	D	71	LEU
3	D	75	LYS
3	D	76	ARG
3	D	81	ARG
3	D	83	THR
3	D	93	ASP
3	D	94	ARG
3	D	101	GLN
3	D	105	MET
3	D	113	LEU
3	D	122	VAL

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Mol	Chain	Res	Type
3	D	132	LYS
3	D	136	VAL
3	D	138	ILE
3	D	143	ARG
3	D	157	LEU
3	D	167	PHE
3	D	173	ARG
3	D	186	VAL
3	D	200	LYS
3	D	206	VAL
3	D	209	ILE
3	D	212	LYS
3	D	215	GLU
3	D	218	LEU
4	F	29	THR
4	F	31	ILE
4	F	35	ILE
4	F	39	GLN
4	F	42	ILE
4	F	44	LEU
4	F	55	VAL
4	F	64	ILE
4	F	66	ILE
4	F	72	VAL
4	F	86	LYS
4	F	91	ILE
4	F	96	THR
4	F	104	ARG
4	F	108	LYS
4	F	110	LEU
4	F	116	VAL
4	F	133	GLN
4	F	134	VAL
4	F	150	ARG
4	F	151	VAL
4	F	159	ARG
4	F	163	ASP
4	F	164	VAL
4	F	169	ARG
4	F	170	VAL
4	F	174	ILE
4	F	176	LEU

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Mol	Chain	Res	Type
4	F	177	LEU
4	F	183	GLU
4	F	187	ARG
4	F	188	ASN
4	F	199	GLU
4	F	200	LEU
4	F	209	THR
4	F	217	ASP
4	F	220	GLU
4	F	222	VAL
4	F	224	LYS
4	F	226	ASN
5	K	2	LEU
5	K	9	LYS
5	K	18	GLU
5	K	21	LEU
5	K	24	LYS
5	K	37	THR
5	K	40	LEU
5	K	44	LYS
5	K	49	LEU
5	K	55	VAL
5	K	57	THR
5	K	58	GLN
5	K	63	TYR
5	K	65	TYR
5	K	67	THR
5	K	69	THR
5	K	71	GLU
5	K	73	VAL
5	K	75	TYR
5	K	80	LEU
5	K	81	ASN
6	M	17	ILE
6	M	24	VAL
6	M	32	ASP
6	M	34	LEU
6	M	54	VAL
6	M	55	LEU
6	M	56	VAL
6	M	61	GLU
6	M	64	ILE

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Mol	Chain	Res	Type
6	M	67	LEU
6	M	76	ASN
6	M	90	GLU
6	M	91	TRP
6	M	94	LEU
6	M	106	VAL
6	M	128	LEU
6	M	129	GLU
6	M	130	HIS
7	P	13	LYS
7	P	22	LEU
7	P	25	LEU
7	P	26	LEU
7	P	27	GLU
7	P	32	ASP
7	P	47	ARG
7	P	51	GLU
7	P	56	LEU
7	P	57	MET
7	P	60	LEU
7	P	71	GLU
7	P	72	LYS
7	P	76	VAL
7	P	78	THR
7	P	79	HIS
7	P	81	ARG
7	P	85	ILE
7	P	93	VAL
7	P	106	GLU
7	P	108	ARG
7	P	110	GLU
7	P	122	THR
7	P	126	VAL
7	P	127	ARG
8	Q	28	LEU
8	Q	36	ILE
8	Q	37	THR
8	Q	38	LEU
8	Q	43	ILE
8	Q	45	ARG
8	Q	52	LEU
8	Q	54	LEU

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Mol	Chain	Res	Type
8	Q	75	VAL
8	Q	82	ARG
8	Q	83	GLN
8	Q	99	GLU
8	Q	100	GLN
8	Q	117	LEU
8	Q	123	ARG
8	Q	125	GLU
8	Q	132	ARG
8	Q	137	ARG
8	Q	139	GLN
9	R	3	ARG
9	R	5	ARG
9	R	6	THR
9	R	14	LYS
9	R	16	LEU
9	R	25	THR
9	R	26	MET
9	R	33	ARG
9	R	36	ASP
9	R	37	GLU
9	R	45	ARG
9	R	46	LEU
9	R	47	ARG
9	R	48	ASN
9	R	58	MET
9	R	78	ARG
9	R	99	VAL
9	R	106	THR
9	R	128	ARG
10	S	25	ASN
10	S	40	ARG
10	S	45	LEU
10	S	52	VAL
10	S	55	HIS
10	S	57	ARG
10	S	61	LEU
10	S	64	GLU
10	S	66	LEU
10	S	73	MET
10	S	89	GLN
10	S	99	HIS

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Mol	Chain	Res	Type
10	S	101	LEU
10	S	105	LEU
10	S	114	GLU
10	S	126	ARG
10	S	131	LEU
10	S	132	ARG
10	S	144	ARG
11	T	7	ARG
11	T	12	GLN
11	T	14	PHE
11	T	16	ASN
11	T	23	GLN
11	T	24	ARG
11	T	25	GLN
11	T	28	LEU
11	T	33	TYR
11	T	38	LYS
11	T	45	LEU
11	T	63	ARG
11	T	75	LYS
11	T	78	LYS
11	T	79	LEU
11	T	86	ARG
11	T	91	HIS
11	T	95	ASP
11	T	100	ILE
11	T	107	SER
11	T	111	LEU
11	T	124	ILE
11	T	129	LEU
11	T	132	LEU
11	T	135	ILE
11	T	143	GLU
12	U	17	VAL
12	U	27	THR
12	U	31	VAL
12	U	33	GLN
12	U	35	GLU
12	U	37	VAL
12	U	40	ASN
12	U	51	VAL
12	U	56	VAL

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Mol	Chain	Res	Type
12	U	62	VAL
12	U	82	TYR
12	U	83	GLU
12	U	89	ARG
12	U	90	TYR
12	U	91	ILE
12	U	93	LEU
12	U	109	GLU
12	U	117	ILE
13	Z	38	HIS
13	Z	40	VAL
13	Z	43	ASP
13	Z	48	ASP
13	Z	52	LYS
13	Z	58	ARG
13	Z	65	LEU
13	Z	70	LYS
13	Z	71	LEU
13	Z	77	ARG
13	Z	78	VAL
13	Z	80	LEU
13	Z	92	VAL
14	c	8	THR
14	c	13	ILE
14	c	16	LEU
14	c	19	THR
14	c	38	ARG
14	c	43	ASN
14	c	54	LEU
14	c	58	GLU
15	f	91	ILE
15	f	92	ARG
15	f	117	LEU
15	f	138	TYR
16	g	8	LEU
16	g	20	TRP
16	g	33	LEU
16	g	39	ARG
16	g	43	LEU
16	g	67	HIS
16	g	68	ILE
16	g	70	GLN

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Mol	Chain	Res	Type
16	g	91	ARG
16	g	92	LEU
16	g	110	ASP
16	g	116	ILE
16	g	124	ILE
16	g	137	THR
16	g	145	LEU
16	g	146	LEU
16	g	151	TRP
16	g	182	ILE
16	g	184	ARG
16	g	195	ILE
16	g	200	ILE
16	g	206	ILE
16	g	207	ASN
16	g	223	LYS
16	g	246	GLU
16	g	256	ARG
16	g	263	THR
16	g	272	LEU
16	g	280	GLU
16	g	312	TYR
16	g	313	THR
16	g	318	ARG
17	d	6	VAL
17	d	9	SER
17	d	12	ARG
17	d	20	GLN
17	d	30	LEU
17	d	31	ILE
17	d	32	ARG
17	d	36	LEU
17	d	38	ILE
17	d	41	GLN
17	d	44	ARG
18	e	38	LEU
18	e	39	LEU
18	e	54	ARG
19	h	2	ARG
19	h	8	LYS
19	h	12	ARG
19	h	13	LEU

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Mol	Chain	Res	Type
19	h	17	ARG
19	h	20	VAL
21	i	30	GLU
21	i	34	GLU
21	i	41	MET
21	i	42	LEU
21	i	58	MET
21	i	62	ARG
21	i	91	VAL
21	i	111	GLU
22	m	26	ILE
22	m	34	ASN
22	m	48	GLU
22	m	55	LEU
22	m	87	LYS
22	m	88	VAL
22	m	96	LEU
22	m	104	LYS
23	o	18	LEU
23	o	19	ILE
23	o	28	LEU
23	o	56	LEU
23	o	60	VAL
23	o	61	GLU
23	o	62	LEU
23	o	67	LEU
23	o	70	ASP
23	o	73	HIS
23	o	89	VAL
23	o	94	ARG
23	o	98	ASP
23	o	100	VAL
23	o	108	GLN
23	o	110	ARG
23	o	172	ASN
23	o	183	VAL
23	o	202	LEU
23	o	204	GLU
23	o	210	LEU
23	o	211	ASP
23	o	229	ASP
23	o	246	VAL

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Mol	Chain	Res	Type
23	o	254	HIS
23	o	264	PHE
23	o	278	THR
23	o	321	PHE
23	o	328	ILE
23	o	333	ILE
23	o	337	LEU
23	o	351	MET
23	o	357	LEU
23	o	374	GLU
23	o	376	ILE
23	o	397	VAL
23	o	404	LEU
23	o	406	ASN
23	o	408	LEU
23	o	428	ILE
23	o	438	GLN
23	o	465	ILE
23	o	470	LEU
24	q	149	ILE
24	q	195	TYR
24	q	199	LYS
24	q	201	ARG
24	q	251	GLN
24	q	260	THR
24	q	270	VAL
24	q	275	LEU
24	q	282	LEU
24	q	297	LEU
24	q	299	LEU
24	q	310	LEU
24	q	323	ASN
24	q	325	ILE
24	q	335	THR
24	q	340	GLN
24	q	402	GLN
24	q	407	LEU
24	q	409	LEU
24	q	448	ILE
24	q	452	GLU
24	q	458	ILE
24	q	471	ASP

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Mol	Chain	Res	Type
24	q	473	LEU
24	q	532	ILE
24	q	550	LEU
24	q	571	LEU
24	q	580	LEU
24	q	585	LEU
24	q	611	HIS
24	q	619	VAL
24	q	626	LEU
24	q	630	ILE
24	q	634	THR
24	q	656	LEU
24	q	662	LEU
24	q	681	SER
24	q	697	ILE
24	q	705	ASN
24	q	722	LEU
24	q	729	PHE
24	q	749	GLU
24	q	783	GLU
25	k	105	THR
25	k	197	HIS
25	k	228	GLN
25	k	236	ILE
25	k	251	VAL
25	k	274	ILE
25	k	280	ILE
25	k	291	ILE
25	k	318	ILE
25	k	351	ASP
25	k	352	GLU
25	k	354	GLU
25	k	388	LYS
25	k	395	LEU
25	k	402	VAL
25	k	410	ASP
25	k	422	HIS
25	k	426	ILE
25	k	432	ILE
25	k	437	LEU
25	k	440	LEU
25	k	462	LEU

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Mol	Chain	Res	Type
25	k	471	THR
25	k	474	ARG
25	k	475	VAL
25	k	484	ARG
25	k	485	LEU
25	k	502	SER
25	k	508	HIS
26	l	159	ARG
26	l	165	CYS
26	l	171	LYS
26	l	179	ASP
26	l	191	LEU
26	l	195	LEU
26	l	225	VAL
26	l	226	LEU
26	l	236	CYS
26	l	244	THR
27	j	3	THR
27	j	6	CYS
27	j	19	ILE
27	j	45	MET
27	j	46	ILE
27	j	47	LEU
27	j	56	ILE
27	j	57	ARG
27	j	59	ILE
27	j	69	ASP
27	j	79	GLU
27	j	87	LYS
27	j	97	LYS
27	j	111	ILE
27	j	123	LEU
27	j	143	GLU
27	j	147	LEU
27	j	156	GLU
27	j	159	GLU
27	j	163	LYS
27	j	195	TYR
27	j	198	ILE
27	j	201	ILE
27	j	205	LEU
27	j	235	LEU

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Mol	Chain	Res	Type
27	j	244	LEU
27	j	251	ILE
27	j	255	ILE
29	A	3	LEU
29	A	33	GLN
29	A	48	ILE
29	A	58	VAL
29	A	59	LEU
29	A	80	THR
29	A	88	LYS
29	A	93	THR
29	A	101	ARG
29	A	108	THR
29	A	112	THR
29	A	117	GLU
29	A	120	LEU
29	A	122	ILE
29	A	143	VAL
29	A	165	ARG
29	A	170	ILE
29	A	172	LEU
29	A	173	ILE
29	A	193	GLN
29	A	201	LEU
30	B	47	LEU
30	B	48	VAL
30	B	61	LEU
30	B	64	ARG
30	B	68	VAL
30	B	81	PHE
30	B	82	ARG
30	B	84	VAL
30	B	104	ASP
30	B	111	ARG
30	B	119	THR
30	B	127	VAL
30	B	140	ILE
30	B	144	ARG
30	B	166	LYS
30	B	171	ILE
30	B	181	LEU
30	B	184	LEU

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Mol	Chain	Res	Type
30	B	189	ILE
30	B	193	ILE
30	B	196	GLU
30	B	217	LEU
30	B	228	LEU
31	E	7	LYS
31	E	19	MET
31	E	22	LYS
31	E	42	LEU
31	E	51	ARG
31	E	60	GLU
31	E	65	LEU
31	E	69	HIS
31	E	75	LYS
31	E	77	ARG
31	E	102	VAL
31	E	113	ARG
31	E	123	LEU
31	E	159	THR
31	E	168	THR
31	E	180	LEU
31	E	181	VAL
31	E	189	LEU
31	E	195	ILE
31	E	216	ASN
31	E	225	VAL
31	E	228	ILE
31	E	244	ILE
31	E	248	ILE
31	E	259	HIS
32	G	5	ILE
32	G	12	THR
32	G	52	ILE
32	G	69	LEU
32	G	76	LEU
32	G	88	ARG
32	G	121	ILE
32	G	164	LYS
32	G	177	ARG
32	G	178	LEU
32	G	193	LEU
32	G	195	ILE

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Mol	Chain	Res	Type
32	G	211	LEU
32	G	214	LYS
32	G	215	ARG
33	H	7	LYS
33	H	15	GLU
33	H	27	LEU
33	H	48	GLU
33	H	72	LYS
33	H	80	GLU
33	H	86	GLN
33	H	112	ARG
33	H	119	THR
33	H	126	LEU
33	H	129	LEU
33	H	136	VAL
33	H	139	ARG
33	H	152	ILE
33	H	175	LYS
34	I	20	GLN
34	I	23	LYS
34	I	29	LEU
34	I	53	GLN
34	I	58	LEU
34	I	72	VAL
34	I	78	ILE
34	I	104	ILE
34	I	105	ASP
34	I	119	GLN
34	I	140	THR
34	I	153	ILE
34	I	179	ARG
34	I	190	LEU
34	I	195	ARG
34	I	196	ARG
34	I	200	LYS
35	J	3	ARG
35	J	23	ARG
35	J	25	ASP
35	J	28	LEU
35	J	33	GLU
35	J	36	LEU
35	J	44	ARG

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Mol	Chain	Res	Type
35	J	45	ILE
35	J	48	GLN
35	J	49	LEU
35	J	53	ARG
35	J	54	ARG
35	J	60	LEU
35	J	62	ARG
35	J	80	LEU
35	J	85	VAL
35	J	96	VAL
35	J	100	LYS
35	J	107	ARG
35	J	109	LEU
35	J	118	LEU
35	J	128	LEU
35	J	142	ASN
35	J	151	GLU
35	J	153	GLU
35	J	161	THR
35	J	171	ARG
36	L	3	THR
36	L	7	VAL
36	L	8	GLN
36	L	10	GLU
36	L	26	LYS
36	L	31	THR
36	L	32	LYS
36	L	37	ASN
36	L	38	VAL
36	L	67	ARG
36	L	74	THR
36	L	82	ARG
36	L	84	ILE
36	L	88	ARG
36	L	99	ARG
36	L	103	ARG
36	L	107	VAL
36	L	116	ARG
36	L	117	VAL
36	L	118	GLN
36	L	123	VAL
36	L	128	CYS

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Mol	Chain	Res	Type
36	L	136	ARG
36	L	150	ASN
36	L	156	PHE
37	N	3	ARG
37	N	18	TYR
37	N	20	ARG
37	N	21	ASN
37	N	39	LYS
37	N	52	VAL
37	N	64	LYS
37	N	67	THR
37	N	80	LEU
37	N	83	GLU
37	N	84	ILE
37	N	86	GLU
37	N	88	LEU
37	N	91	LEU
37	N	96	VAL
37	N	100	LYS
37	N	106	ARG
37	N	107	LYS
37	N	113	PHE
37	N	119	GLU
37	N	120	SER
37	N	121	ARG
38	O	29	HIS
38	O	32	ASP
38	O	39	ILE
38	O	49	LYS
38	O	52	ARG
38	O	92	LYS
38	O	102	LEU
38	O	110	LEU
38	O	114	ARG
38	O	129	LYS
39	V	1	MET
39	V	8	LEU
39	V	9	VAL
39	V	11	LEU
39	V	12	TYR
39	V	33	GLN
39	V	44	ARG

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Mol	Chain	Res	Type
39	V	69	LEU
39	V	76	ASP
40	W	11	LEU
40	W	24	GLN
40	W	26	LEU
40	W	33	VAL
40	W	61	ILE
40	W	65	LEU
40	W	74	VAL
40	W	81	VAL
40	W	104	LEU
41	Y	5	ILE
41	Y	8	ARG
41	Y	13	ILE
41	Y	35	VAL
41	Y	84	LYS
41	Y	99	LYS
41	Y	116	LYS
41	Y	121	THR
41	Y	127	LYS
42	X	9	LEU
42	X	14	LYS
42	X	19	ARG
42	X	30	LYS
42	X	33	LEU
42	X	52	ILE
42	X	55	GLU
42	X	60	GLU
42	X	77	ILE
42	X	83	VAL
42	X	107	PHE
42	X	117	ILE
42	X	133	LEU
43	a	34	LYS
43	a	38	ARG
43	a	50	ILE
43	a	69	ASN
44	b	24	LEU
44	b	67	THR
45	p	190	LYS
45	p	317	ILE
45	p	343	TYR

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Mol	Chain	Res	Type
45	p	362	THR
45	p	369	GLU
45	p	373	LEU
45	p	394	ARG
45	p	406	TRP
45	p	409	GLU
45	p	419	ILE
45	p	458	THR
45	p	468	LEU
45	p	507	HIS
45	p	528	THR
45	p	530	GLU
45	p	532	THR
45	p	547	THR
45	p	548	PHE
45	p	573	ARG
45	p	577	GLN
45	p	590	ASN
45	p	599	LEU
45	p	602	VAL
45	p	606	THR
45	p	620	ARG
45	p	629	LEU
45	p	642	ILE
45	p	650	ASP
45	p	683	TRP
46	s	85	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (159) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	76	GLN
2	C	94	GLN
2	C	113	ASN
2	C	115	HIS
2	C	155	GLN
3	D	56	GLN
3	D	165	ASN
3	D	179	GLN
4	F	102	ASN
4	F	105	ASN
4	F	106	ASN

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Mol	Chain	Res	Type
4	F	124	ASN
4	F	129	GLN
4	F	141	ASN
4	F	160	GLN
4	F	171	ASN
4	F	188	ASN
5	K	85	HIS
6	M	31	HIS
6	M	76	ASN
6	M	116	ASN
6	M	122	GLN
6	M	133	GLN
7	P	82	ASN
8	Q	83	GLN
8	Q	93	HIS
8	Q	94	GLN
10	S	12	GLN
10	S	13	HIS
10	S	71	GLN
10	S	75	ASN
10	S	78	HIS
10	S	93	ASN
11	T	17	ASN
11	T	43	ASN
11	T	48	GLN
11	T	77	ASN
12	U	36	ASN
12	U	72	ASN
12	U	98	HIS
12	U	105	GLN
13	Z	38	HIS
13	Z	98	GLN
14	c	27	GLN
16	g	30	GLN
16	g	94	ASN
16	g	189	ASN
16	g	203	ASN
16	g	210	GLN
16	g	292	GLN
17	d	10	HIS
17	d	41	GLN
18	e	29	GLN

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Mol	Chain	Res	Type
18	e	46	ASN
21	i	37	GLN
21	i	44	ASN
21	i	60	HIS
21	i	73	GLN
22	m	24	ASN
22	m	81	GLN
23	o	209	HIS
23	o	222	ASN
23	o	223	ASN
23	o	281	ASN
23	o	348	HIS
23	o	356	ASN
24	q	323	ASN
24	q	342	ASN
24	q	386	ASN
24	q	457	ASN
24	q	462	GLN
24	q	506	ASN
24	q	513	ASN
24	q	564	HIS
24	q	591	ASN
24	q	604	GLN
24	q	658	HIS
24	q	665	GLN
24	q	686	ASN
24	q	718	GLN
25	k	98	GLN
25	k	228	GLN
25	k	324	ASN
25	k	422	HIS
25	k	496	ASN
26	l	218	GLN
27	j	11	ASN
27	j	23	ASN
27	j	68	ASN
27	j	103	GLN
27	j	140	HIS
27	j	233	GLN
29	A	33	GLN
29	A	83	GLN
29	A	131	GLN

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Mol	Chain	Res	Type
29	A	193	GLN
29	A	213	GLN
30	B	56	ASN
30	B	124	ASN
30	B	160	HIS
30	B	177	GLN
30	B	183	GLN
30	B	209	ASN
30	B	211	HIS
31	E	16	HIS
31	E	50	ASN
31	E	57	ASN
31	E	69	HIS
31	E	98	ASN
31	E	130	GLN
31	E	142	HIS
32	G	4	ASN
32	G	10	ASN
32	G	13	GLN
32	G	65	GLN
32	G	185	GLN
32	G	189	GLN
33	H	5	GLN
33	H	110	GLN
33	H	174	ASN
33	H	180	GLN
34	I	64	ASN
34	I	84	HIS
34	I	116	HIS
35	J	38	ASN
35	J	123	HIS
36	L	16	GLN
36	L	22	ASN
36	L	98	ASN
36	L	110	HIS
36	L	138	ASN
36	L	150	ASN
37	N	49	GLN
37	N	58	HIS
37	N	78	ASN
38	O	29	HIS
38	O	65	GLN

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Mol	Chain	Res	Type
39	V	3	ASN
39	V	7	GLN
40	W	42	GLN
40	W	92	ASN
40	W	98	GLN
41	Y	22	GLN
41	Y	106	GLN
42	X	21	ASN
42	X	22	ASN
42	X	48	HIS
42	X	89	ASN
42	X	94	ASN
44	b	42	ASN
45	p	205	GLN
45	p	311	GLN
45	p	364	ASN
45	p	438	ASN
45	p	457	HIS
45	p	464	GLN
45	p	469	GLN
45	p	588	ASN
45	p	645	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1797/1798 (99%)	833 (46%)	69 (3%)
20	3	13/14 (92%)	8 (61%)	2 (15%)
28	1	73/75 (97%)	33 (45%)	6 (8%)
All	All	1883/1887 (99%)	874 (46%)	77 (4%)

All (874) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	U
1	2	4	C
1	2	5	U
1	2	8	U
1	2	9	U
1	2	11	A

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Mol	Chain	Res	Type
1	2	14	C
1	2	16	G
1	2	17	C
1	2	19	A
1	2	20	G
1	2	24	U
1	2	25	C
1	2	26	A
1	2	30	G
1	2	31	C
1	2	34	G
1	2	39	A
1	2	42	G
1	2	43	A
1	2	44	U
1	2	45	U
1	2	47	A
1	2	51	A
1	2	56	U
1	2	57	G
1	2	59	C
1	2	63	G
1	2	64	U
1	2	65	A
1	2	66	U
1	2	67	A
1	2	68	A
1	2	69	G
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	77	U
1	2	79	C
1	2	81	G
1	2	87	C
1	2	95	G
1	2	104	A
1	2	111	U
1	2	114	C
1	2	124	A
1	2	127	G

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Mol	Chain	Res	Type
1	2	128	U
1	2	130	C
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	136	C
1	2	138	A
1	2	140	A
1	2	141	U
1	2	144	A
1	2	146	A
1	2	147	U
1	2	148	C
1	2	149	U
1	2	156	A
1	2	157	U
1	2	158	U
1	2	159	C
1	2	161	A
1	2	167	A
1	2	172	A
1	2	173	U
1	2	176	U
1	2	177	U
1	2	178	A
1	2	184	U
1	2	185	C
1	2	187	A
1	2	190	C
1	2	191	U
1	2	192	U
1	2	194	G
1	2	195	G
1	2	198	G
1	2	199	A
1	2	201	A
1	2	209	A
1	2	214	A
1	2	217	A
1	2	218	A
1	2	220	A

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Mol	Chain	Res	Type
1	2	226	U
1	2	228	U
1	2	230	U
1	2	231	U
1	2	232	C
1	2	233	G
1	2	234	G
1	2	237	U
1	2	239	C
1	2	240	U
1	2	249	C
1	2	254	U
1	2	258	U
1	2	259	U
1	2	260	U
1	2	264	A
1	2	266	U
1	2	268	G
1	2	274	C
1	2	275	C
1	2	276	U
1	2	277	U
1	2	278	G
1	2	279	U
1	2	280	G
1	2	286	G
1	2	288	U
1	2	294	A
1	2	298	A
1	2	300	A
1	2	301	U
1	2	307	C
1	2	308	C
1	2	311	A
1	2	312	U
1	2	313	C
1	2	315	A
1	2	319	U
1	2	320	C
1	2	321	G
1	2	322	A
1	2	328	G

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Mol	Chain	Res	Type
1	2	332	A
1	2	336	G
1	2	337	C
1	2	338	C
1	2	342	C
1	2	349	U
1	2	351	A
1	2	354	G
1	2	358	A
1	2	359	A
1	2	360	C
1	2	368	A
1	2	369	A
1	2	371	G
1	2	372	G
1	2	377	A
1	2	379	U
1	2	380	C
1	2	382	G
1	2	384	A
1	2	387	G
1	2	389	G
1	2	390	A
1	2	391	G
1	2	392	C
1	2	395	G
1	2	398	A
1	2	399	A
1	2	400	A
1	2	401	C
1	2	403	G
1	2	404	C
1	2	405	U
1	2	406	A
1	2	411	A
1	2	412	U
1	2	413	C
1	2	415	A
1	2	416	A
1	2	419	A
1	2	421	G
1	2	422	G

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Mol	Chain	Res	Type
1	2	423	C
1	2	424	A
1	2	425	G
1	2	433	G
1	2	438	U
1	2	439	U
1	2	440	A
1	2	443	C
1	2	447	C
1	2	448	C
1	2	454	C
1	2	455	A
1	2	456	G
1	2	457	G
1	2	458	G
1	2	461	G
1	2	468	C
1	2	469	A
1	2	478	C
1	2	479	G
1	2	480	A
1	2	483	C
1	2	488	C
1	2	489	C
1	2	490	C
1	2	491	A
1	2	492	U
1	2	493	U
1	2	495	G
1	2	496	G
1	2	497	G
1	2	498	U
1	2	499	C
1	2	500	U
1	2	501	U
1	2	502	G
1	2	504	A
1	2	505	A
1	2	506	U
1	2	507	U
1	2	508	G
1	2	517	A

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Mol	Chain	Res	Type
1	2	518	C
1	2	519	A
1	2	521	U
1	2	522	G
1	2	523	U
1	2	525	A
1	2	527	U
1	2	530	C
1	2	531	U
1	2	533	A
1	2	534	A
1	2	535	C
1	2	537	A
1	2	538	G
1	2	539	G
1	2	540	A
1	2	541	A
1	2	542	C
1	2	543	A
1	2	544	A
1	2	545	C
1	2	546	U
1	2	547	G
1	2	550	G
1	2	553	C
1	2	556	G
1	2	557	U
1	2	558	C
1	2	563	G
1	2	564	C
1	2	565	C
1	2	567	G
1	2	568	C
1	2	570	G
1	2	571	C
1	2	572	C
1	2	573	G
1	2	574	C
1	2	575	G
1	2	576	G
1	2	577	U
1	2	578	A

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Mol	Chain	Res	Type
1	2	579	A
1	2	580	U
1	2	581	U
1	2	582	C
1	2	584	A
1	2	586	C
1	2	589	C
1	2	590	A
1	2	593	A
1	2	594	G
1	2	598	A
1	2	599	U
1	2	605	A
1	2	610	U
1	2	612	G
1	2	613	C
1	2	617	U
1	2	618	A
1	2	619	A
1	2	622	A
1	2	633	G
1	2	634	A
1	2	637	U
1	2	638	U
1	2	641	G
1	2	647	G
1	2	650	G
1	2	652	C
1	2	657	C
1	2	659	G
1	2	660	A
1	2	661	C
1	2	663	U
1	2	665	A
1	2	666	U
1	2	671	C
1	2	672	G
1	2	673	C
1	2	675	C
1	2	679	U
1	2	680	U
1	2	681	U

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Mol	Chain	Res	Type
1	2	682	U
1	2	684	A
1	2	685	A
1	2	686	C
1	2	688	G
1	2	691	U
1	2	692	C
1	2	693	U
1	2	694	U
1	2	695	U
1	2	696	C
1	2	697	C
1	2	698	U
1	2	700	C
1	2	701	U
1	2	702	G
1	2	703	G
1	2	704	C
1	2	709	C
1	2	710	U
1	2	711	G
1	2	712	U
1	2	714	C
1	2	717	C
1	2	718	U
1	2	719	U
1	2	721	U
1	2	722	G
1	2	723	G
1	2	725	U
1	2	726	G
1	2	727	C
1	2	729	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	736	C
1	2	738	G
1	2	741	C
1	2	742	U
1	2	743	U

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Mol	Chain	Res	Type
1	2	753	A
1	2	755	A
1	2	762	A
1	2	763	G
1	2	765	G
1	2	766	U
1	2	767	U
1	2	768	C
1	2	771	A
1	2	774	A
1	2	778	G
1	2	779	A
1	2	780	A
1	2	781	A
1	2	782	G
1	2	784	U
1	2	785	C
1	2	786	G
1	2	788	A
1	2	790	A
1	2	793	U
1	2	794	U
1	2	795	A
1	2	796	G
1	2	802	A
1	2	805	A
1	2	809	G
1	2	811	A
1	2	812	U
1	2	813	A
1	2	814	G
1	2	817	C
1	2	819	U
1	2	820	U
1	2	822	G
1	2	823	G
1	2	826	C
1	2	827	U
1	2	828	A
1	2	829	U
1	2	837	G
1	2	839	U

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Mol	Chain	Res	Type
1	2	840	U
1	2	845	G
1	2	847	C
1	2	855	A
1	2	856	U
1	2	860	U
1	2	861	A
1	2	862	A
1	2	863	U
1	2	864	A
1	2	871	G
1	2	872	U
1	2	875	G
1	2	885	U
1	2	886	A
1	2	891	A
1	2	895	U
1	2	897	A
1	2	898	G
1	2	903	G
1	2	904	A
1	2	905	A
1	2	907	U
1	2	908	U
1	2	910	U
1	2	911	U
1	2	912	G
1	2	913	G
1	2	914	A
1	2	915	U
1	2	916	U
1	2	918	A
1	2	919	U
1	2	920	U
1	2	925	A
1	2	927	U
1	2	930	C
1	2	931	U
1	2	932	A
1	2	934	U
1	2	936	C
1	2	939	A

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Mol	Chain	Res	Type
1	2	941	G
1	2	944	U
1	2	946	U
1	2	947	G
1	2	950	A
1	2	956	G
1	2	958	U
1	2	959	U
1	2	962	A
1	2	963	U
1	2	965	A
1	2	970	A
1	2	974	C
1	2	978	A
1	2	981	U
1	2	982	A
1	2	983	G
1	2	987	A
1	2	990	G
1	2	991	A
1	2	993	G
1	2	994	A
1	2	996	G
1	2	999	C
1	2	1002	A
1	2	1003	U
1	2	1004	A
1	2	1008	U
1	2	1009	C
1	2	1011	U
1	2	1015	C
1	2	1018	A
1	2	1022	A
1	2	1024	A
1	2	1025	A
1	2	1026	A
1	2	1027	C
1	2	1028	U
1	2	1030	U
1	2	1031	G
1	2	1034	G
1	2	1038	A

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Mol	Chain	Res	Type
1	2	1039	G
1	2	1041	G
1	2	1042	A
1	2	1044	C
1	2	1048	U
1	2	1049	G
1	2	1050	G
1	2	1051	U
1	2	1052	G
1	2	1054	U
1	2	1055	U
1	2	1056	U
1	2	1057	U
1	2	1058	C
1	2	1059	U
1	2	1062	U
1	2	1065	C
1	2	1070	U
1	2	1071	C
1	2	1075	A
1	2	1077	C
1	2	1081	C
1	2	1082	G
1	2	1084	G
1	2	1085	A
1	2	1086	A
1	2	1089	C
1	2	1092	A
1	2	1093	G
1	2	1095	C
1	2	1096	U
1	2	1097	U
1	2	1098	U
1	2	1099	G
1	2	1100	G
1	2	1101	G
1	2	1102	U
1	2	1103	U
1	2	1105	U
1	2	1107	G
1	2	1108	G
1	2	1110	G

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Mol	Chain	Res	Type
1	2	1111	G
1	2	1112	A
1	2	1113	G
1	2	1116	U
1	2	1117	G
1	2	1118	G
1	2	1125	G
1	2	1128	U
1	2	1132	A
1	2	1133	C
1	2	1135	U
1	2	1136	A
1	2	1137	A
1	2	1138	A
1	2	1142	A
1	2	1145	G
1	2	1146	A
1	2	1149	G
1	2	1150	A
1	2	1154	G
1	2	1155	C
1	2	1157	C
1	2	1158	C
1	2	1160	C
1	2	1161	C
1	2	1162	A
1	2	1163	G
1	2	1164	G
1	2	1166	G
1	2	1168	G
1	2	1169	G
1	2	1172	C
1	2	1173	C
1	2	1174	U
1	2	1176	C
1	2	1184	U
1	2	1188	A
1	2	1189	C
1	2	1190	U
1	2	1191	C
1	2	1192	A
1	2	1193	A

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Mol	Chain	Res	Type
1	2	1195	A
1	2	1196	C
1	2	1197	G
1	2	1198	G
1	2	1199	G
1	2	1201	A
1	2	1202	A
1	2	1206	C
1	2	1207	A
1	2	1208	C
1	2	1211	G
1	2	1216	A
1	2	1217	G
1	2	1218	A
1	2	1224	U
1	2	1225	A
1	2	1226	A
1	2	1227	G
1	2	1228	G
1	2	1229	A
1	2	1236	G
1	2	1237	A
1	2	1240	G
1	2	1243	A
1	2	1244	G
1	2	1245	C
1	2	1250	U
1	2	1254	G
1	2	1255	A
1	2	1256	U
1	2	1258	U
1	2	1259	U
1	2	1260	G
1	2	1268	U
1	2	1269	G
1	2	1272	G
1	2	1273	C
1	2	1275	U
1	2	1282	U
1	2	1283	C
1	2	1284	U
1	2	1286	A

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Mol	Chain	Res	Type
1	2	1287	G
1	2	1292	U
1	2	1294	G
1	2	1295	A
1	2	1296	G
1	2	1300	U
1	2	1305	C
1	2	1306	U
1	2	1307	G
1	2	1309	U
1	2	1312	A
1	2	1313	U
1	2	1314	U
1	2	1315	G
1	2	1317	G
1	2	1319	U
1	2	1320	A
1	2	1321	A
1	2	1324	A
1	2	1332	C
1	2	1336	A
1	2	1337	C
1	2	1338	C
1	2	1339	U
1	2	1340	A
1	2	1343	A
1	2	1344	A
1	2	1345	A
1	2	1347	A
1	2	1349	G
1	2	1353	G
1	2	1355	U
1	2	1358	C
1	2	1359	A
1	2	1361	U
1	2	1362	U
1	2	1363	G
1	2	1364	C
1	2	1366	G
1	2	1369	U
1	2	1370	G
1	2	1371	A

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Mol	Chain	Res	Type
1	2	1376	U
1	2	1379	U
1	2	1380	A
1	2	1381	G
1	2	1382	A
1	2	1386	A
1	2	1387	C
1	2	1388	U
1	2	1391	C
1	2	1393	G
1	2	1396	U
1	2	1397	C
1	2	1398	A
1	2	1400	G
1	2	1408	A
1	2	1409	A
1	2	1411	U
1	2	1412	U
1	2	1413	U
1	2	1414	G
1	2	1416	G
1	2	1418	C
1	2	1419	A
1	2	1420	A
1	2	1422	A
1	2	1423	A
1	2	1424	C
1	2	1425	A
1	2	1426	G
1	2	1428	U
1	2	1429	C
1	2	1430	U
1	2	1431	G
1	2	1433	G
1	2	1434	A
1	2	1442	A
1	2	1443	G
1	2	1444	A
1	2	1450	U
1	2	1455	C
1	2	1456	G
1	2	1457	C

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Mol	Chain	Res	Type
1	2	1458	A
1	2	1461	C
1	2	1463	C
1	2	1465	C
1	2	1466	U
1	2	1467	A
1	2	1469	A
1	2	1470	C
1	2	1471	U
1	2	1476	G
1	2	1479	C
1	2	1480	C
1	2	1481	A
1	2	1482	G
1	2	1484	G
1	2	1488	A
1	2	1489	C
1	2	1490	A
1	2	1491	A
1	2	1492	C
1	2	1494	U
1	2	1497	G
1	2	1498	C
1	2	1505	G
1	2	1509	G
1	2	1512	U
1	2	1513	A
1	2	1514	A
1	2	1515	U
1	2	1516	C
1	2	1519	G
1	2	1521	G
1	2	1522	A
1	2	1523	A
1	2	1528	C
1	2	1529	G
1	2	1533	U
1	2	1534	G
1	2	1535	C
1	2	1538	G
1	2	1540	G
1	2	1544	G

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Mol	Chain	Res	Type
1	2	1546	G
1	2	1548	A
1	2	1551	G
1	2	1554	A
1	2	1555	U
1	2	1557	A
1	2	1558	U
1	2	1559	U
1	2	1564	U
1	2	1566	C
1	2	1571	A
1	2	1572	G
1	2	1573	G
1	2	1574	A
1	2	1575	A
1	2	1577	U
1	2	1578	C
1	2	1579	C
1	2	1580	U
1	2	1581	A
1	2	1582	G
1	2	1583	U
1	2	1584	A
1	2	1588	G
1	2	1590	A
1	2	1593	U
1	2	1594	C
1	2	1595	A
1	2	1597	C
1	2	1599	G
1	2	1600	C
1	2	1603	G
1	2	1604	C
1	2	1608	G
1	2	1611	U
1	2	1612	A
1	2	1613	C
1	2	1614	G
1	2	1616	C
1	2	1617	C
1	2	1628	U
1	2	1629	A

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Mol	Chain	Res	Type
1	2	1631	A
1	2	1632	C
1	2	1633	A
1	2	1634	C
1	2	1635	C
1	2	1637	C
1	2	1642	C
1	2	1647	G
1	2	1648	U
1	2	1652	G
1	2	1655	U
1	2	1656	G
1	2	1660	G
1	2	1662	C
1	2	1676	A
1	2	1678	G
1	2	1679	A
1	2	1680	U
1	2	1682	U
1	2	1685	U
1	2	1686	U
1	2	1687	A
1	2	1688	G
1	2	1692	A
1	2	1693	G
1	2	1694	G
1	2	1695	G
1	2	1696	G
1	2	1697	G
1	2	1698	C
1	2	1699	A
1	2	1700	A
1	2	1701	C
1	2	1702	U
1	2	1703	C
1	2	1705	A
1	2	1706	U
1	2	1708	U
1	2	1709	C
1	2	1710	A
1	2	1711	G
1	2	1712	A

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Mol	Chain	Res	Type
1	2	1715	G
1	2	1725	G
1	2	1728	A
1	2	1730	A
1	2	1742	A
1	2	1745	G
1	2	1748	A
1	2	1753	A
1	2	1755	G
1	2	1758	G
1	2	1760	A
1	2	1763	A
1	2	1766	G
1	2	1767	U
1	2	1768	U
1	2	1781	C
1	2	1786	G
1	2	1787	G
1	2	1789	A
1	2	1790	G
1	2	1791	G
1	2	1792	A
1	2	1793	U
1	2	1794	C
1	2	1795	A
1	2	1796	U
1	2	1797	U
1	2	1798	A
20	3	4	U
20	3	6	U
20	3	7	C
20	3	8	U
20	3	10	U
20	3	11	C
20	3	12	U
20	3	16	C
28	1	2	G
28	1	3	C
28	1	5	C
28	1	7	G
28	1	8	U
28	1	10	G

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Mol	Chain	Res	Type
28	1	14	A
28	1	15	G
28	1	16	U
28	1	19	G
28	1	20	A
28	1	21	A
28	1	22	G
28	1	23	C
28	1	24	G
28	1	28	A
28	1	34	C
28	1	36	U
28	1	41	C
28	1	43	G
28	1	44	A
28	1	46	G
28	1	47	U
28	1	48	C
28	1	49	C
28	1	53	G
28	1	59	A
28	1	60	A
28	1	61	C
28	1	71	C
28	1	74	C
28	1	75	C
28	1	76	A

All (77) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	66	U
1	2	68	A
1	2	72	A
1	2	74	U
1	2	130	C
1	2	131	C
1	2	157	U
1	2	177	U
1	2	190	C
1	2	216	A
1	2	217	A

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Mol	Chain	Res	Type
1	2	239	C
1	2	258	U
1	2	275	C
1	2	277	U
1	2	279	U
1	2	321	G
1	2	412	U
1	2	439	U
1	2	497	G
1	2	538	G
1	2	542	C
1	2	563	G
1	2	564	C
1	2	593	A
1	2	649	U
1	2	670	G
1	2	673	C
1	2	685	A
1	2	693	U
1	2	695	U
1	2	700	C
1	2	721	U
1	2	736	C
1	2	793	U
1	2	810	A
1	2	812	U
1	2	826	C
1	2	828	A
1	2	860	U
1	2	896	C
1	2	907	U
1	2	938	A
1	2	1092	A
1	2	1107	G
1	2	1110	G
1	2	1132	A
1	2	1157	C
1	2	1194	C
1	2	1195	A
1	2	1198	G
1	2	1199	G
1	2	1206	C

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Mol	Chain	Res	Type
1	2	1226	A
1	2	1283	C
1	2	1343	A
1	2	1389	A
1	2	1411	U
1	2	1430	U
1	2	1455	C
1	2	1465	C
1	2	1491	A
1	2	1534	G
1	2	1571	A
1	2	1599	G
1	2	1613	C
1	2	1655	U
1	2	1678	G
1	2	1765	G
20	3	10	U
20	3	11	C
28	1	7	G
28	1	20	A
28	1	47	U
28	1	58	A
28	1	59	A
28	1	74	C

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 87 ligands modelled in this entry, 85 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
51	MET	k	603	-	6,7,8	0.48	0	2,7,9	0.11	0
50	GCP	k	602	-	32,34,34	2.02	10 (31%)	49,54,54	1.82	9 (18%)

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
51	MET	k	603	-	-	3/5/6/8	-
50	GCP	k	602	-	-	4/19/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	k	602	GCP	PG-O1G	5.60	1.61	1.50
50	k	602	GCP	PB-O1B	4.25	1.61	1.51
50	k	602	GCP	C5-C4	3.43	1.48	1.38
50	k	602	GCP	PB-O3A	3.34	1.62	1.58
50	k	602	GCP	PB-O2B	-3.27	1.48	1.56
50	k	602	GCP	PG-O2G	2.95	1.61	1.55
50	k	602	GCP	PG-O3G	-2.88	1.48	1.55
50	k	602	GCP	PA-O3A	2.43	1.62	1.59
50	k	602	GCP	C6-N1	-2.07	1.35	1.38
50	k	602	GCP	C5-N7	-2.01	1.35	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	k	602	GCP	C5-C4-N3	-6.46	118.11	128.39
50	k	602	GCP	C2-N3-C4	5.44	121.67	112.30
50	k	602	GCP	N9-C4-N3	4.79	135.52	125.95
50	k	602	GCP	C6-C5-N7	3.31	136.31	130.29
50	k	602	GCP	PB-O3A-PA	-2.78	123.30	132.37
50	k	602	GCP	C4-C5-N7	-2.56	106.62	110.67
50	k	602	GCP	C3'-C2'-C1'	2.32	105.85	101.46
50	k	602	GCP	O6-C6-C5	-2.13	120.90	126.53
50	k	602	GCP	C5-C6-N1	2.05	118.46	113.25

There are no chirality outliers.

All (7) torsion outliers are listed below:

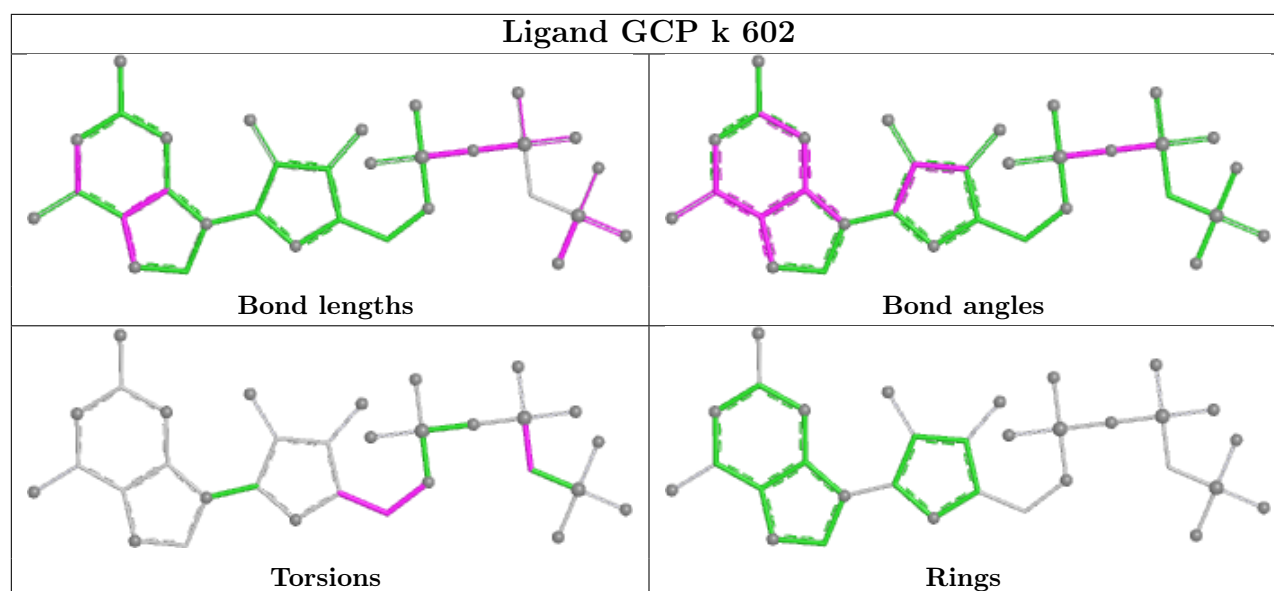
Mol	Chain	Res	Type	Atoms
51	k	603	MET	O-C-CA-CB
50	k	602	GCP	O4'-C4'-C5'-O5'
51	k	603	MET	CA-CB-CG-SD
51	k	603	MET	N-CA-CB-CG
50	k	602	GCP	C4'-C5'-O5'-PA
50	k	602	GCP	PG-C3B-PB-O1B
50	k	602	GCP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	k	602	GCP	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	o	2
28	1	1
22	m	1
25	k	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	o	492:ALA	C	693:UNK	N	230.47
1	1	16:U	O3'	18:G	P	5.21
1	m	75:GLY	C	76:GLU	N	4.38
1	k	372:PRO	C	373:ILE	N	3.76
1	o	5:PRO	C	6:PHE	N	3.57

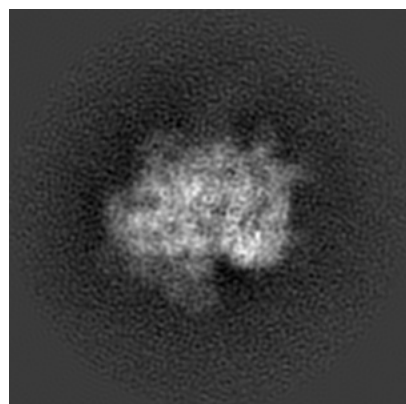
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0058. These allow visual inspection of the internal detail of the map and identification of artifacts.

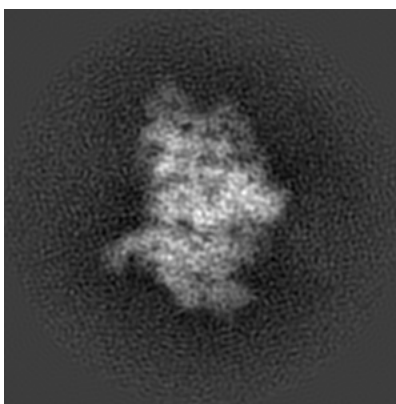
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

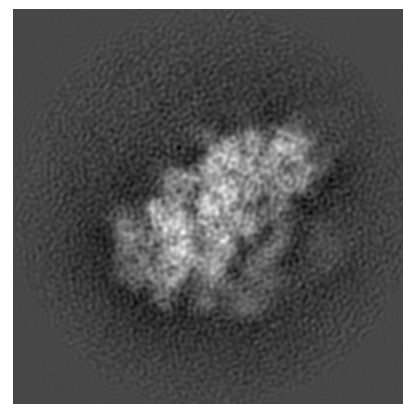
6.1.1 Primary map



X

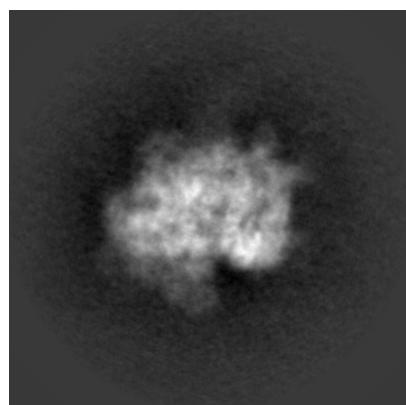


Y

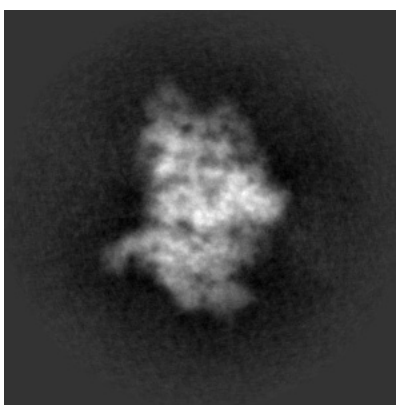


Z

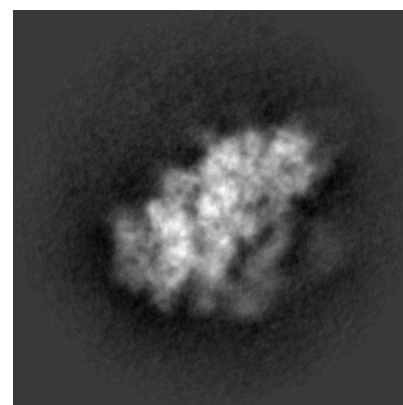
6.1.2 Raw map



X



Y

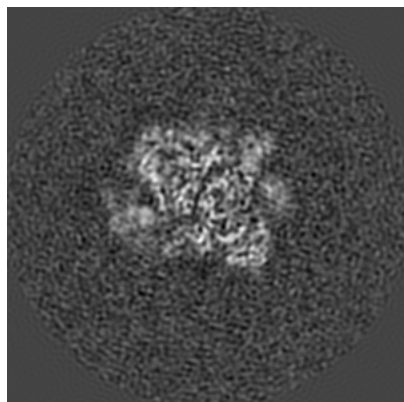


Z

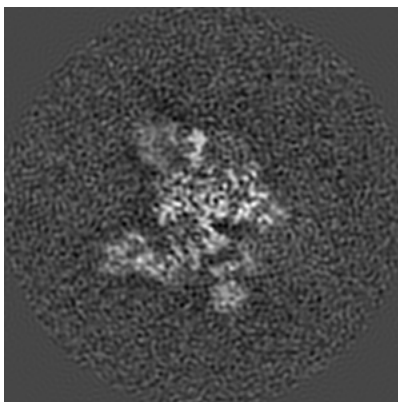
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

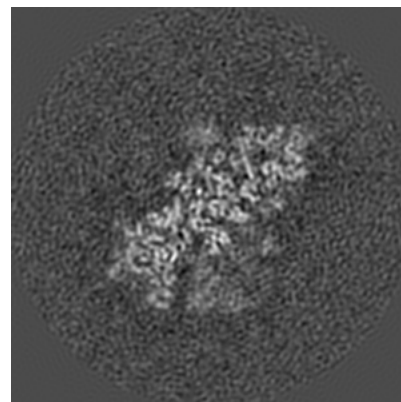
6.2.1 Primary map



X Index: 150

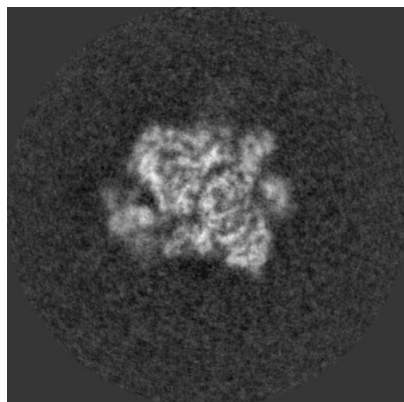


Y Index: 150

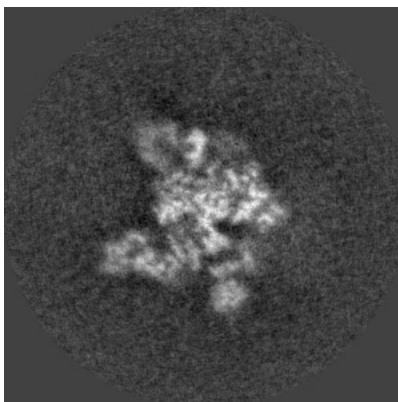


Z Index: 150

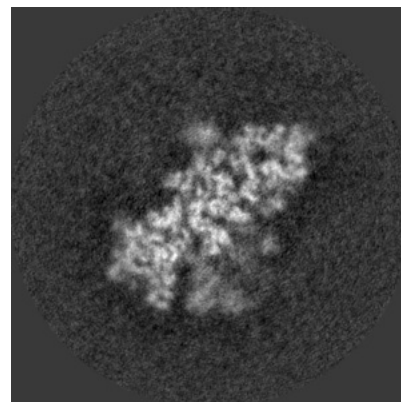
6.2.2 Raw map



X Index: 150



Y Index: 150

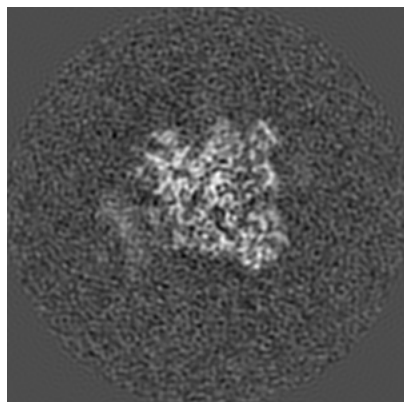


Z Index: 150

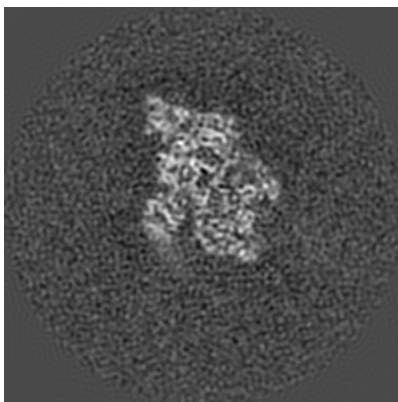
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

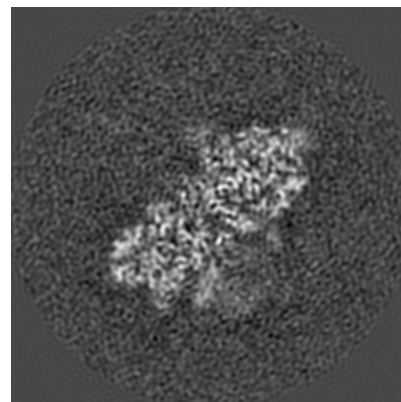
6.3.1 Primary map



X Index: 160

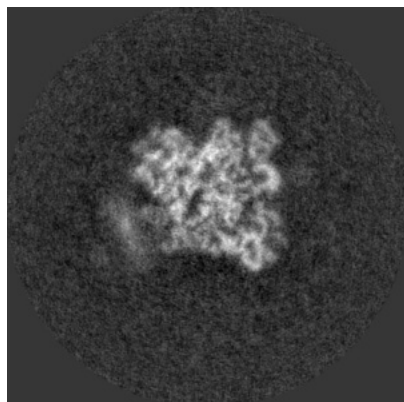


Y Index: 172

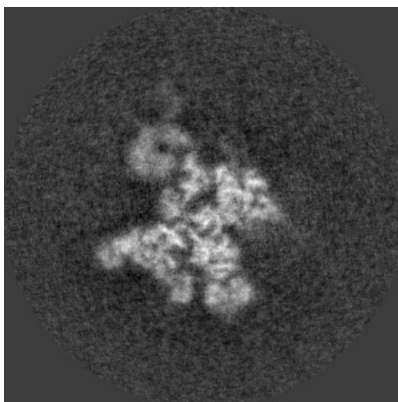


Z Index: 143

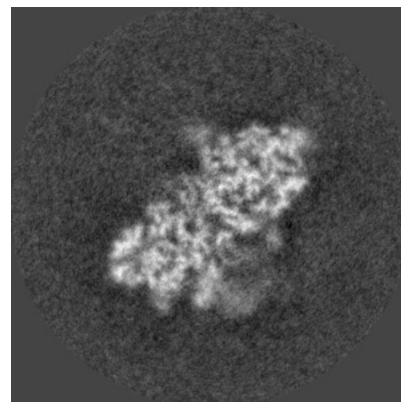
6.3.2 Raw map



X Index: 158



Y Index: 139

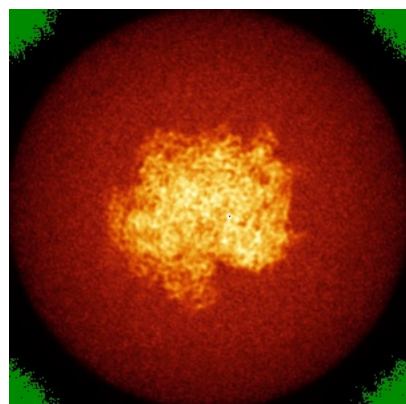


Z Index: 143

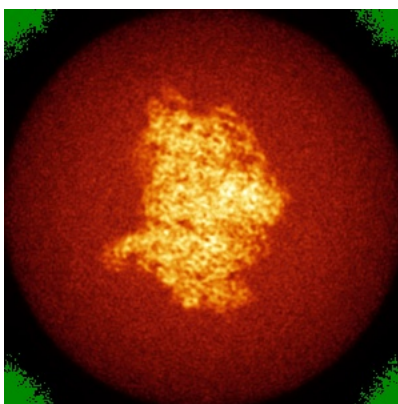
The images above show the largest variance slices of the map in three orthogonal directions.

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

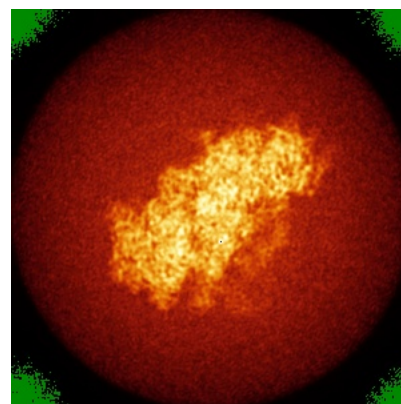
6.4.1 Primary map



X

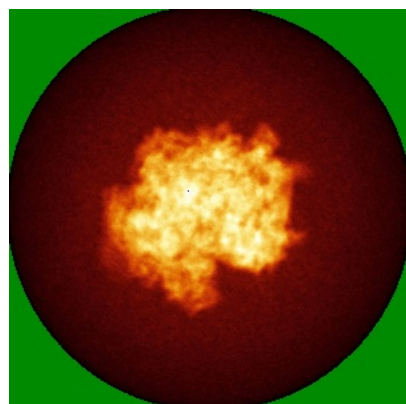


Y

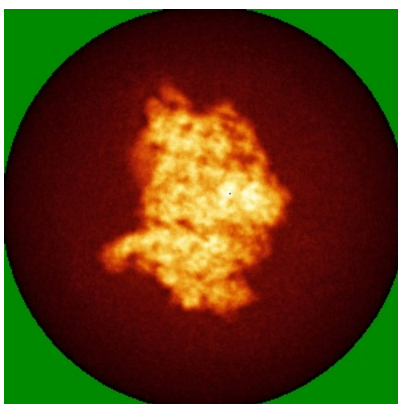


Z

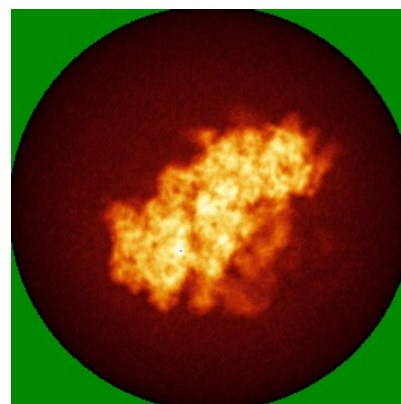
6.4.2 Raw map



X



Y

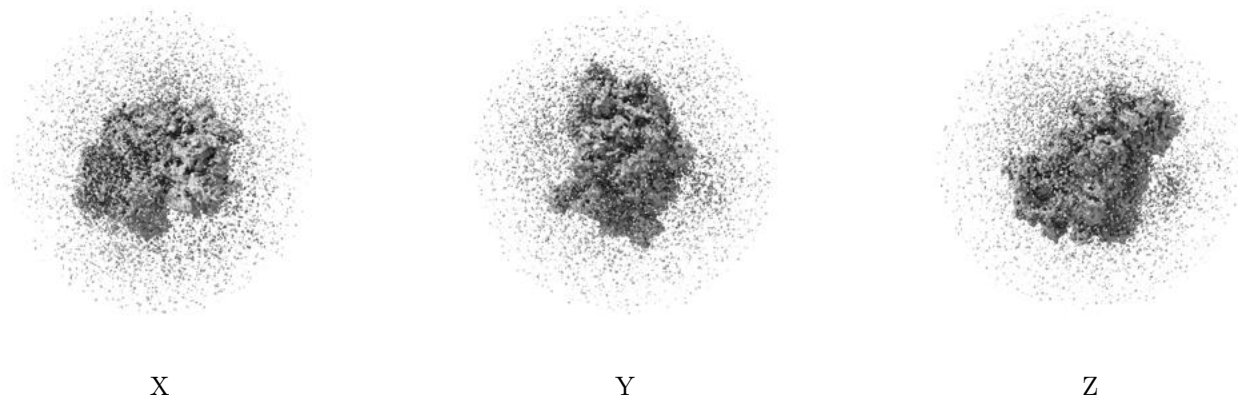


Z

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

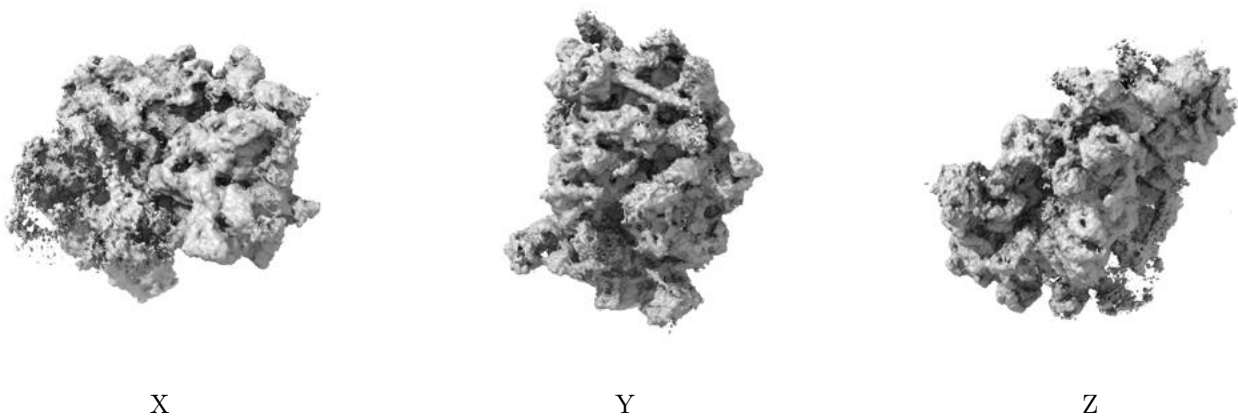
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

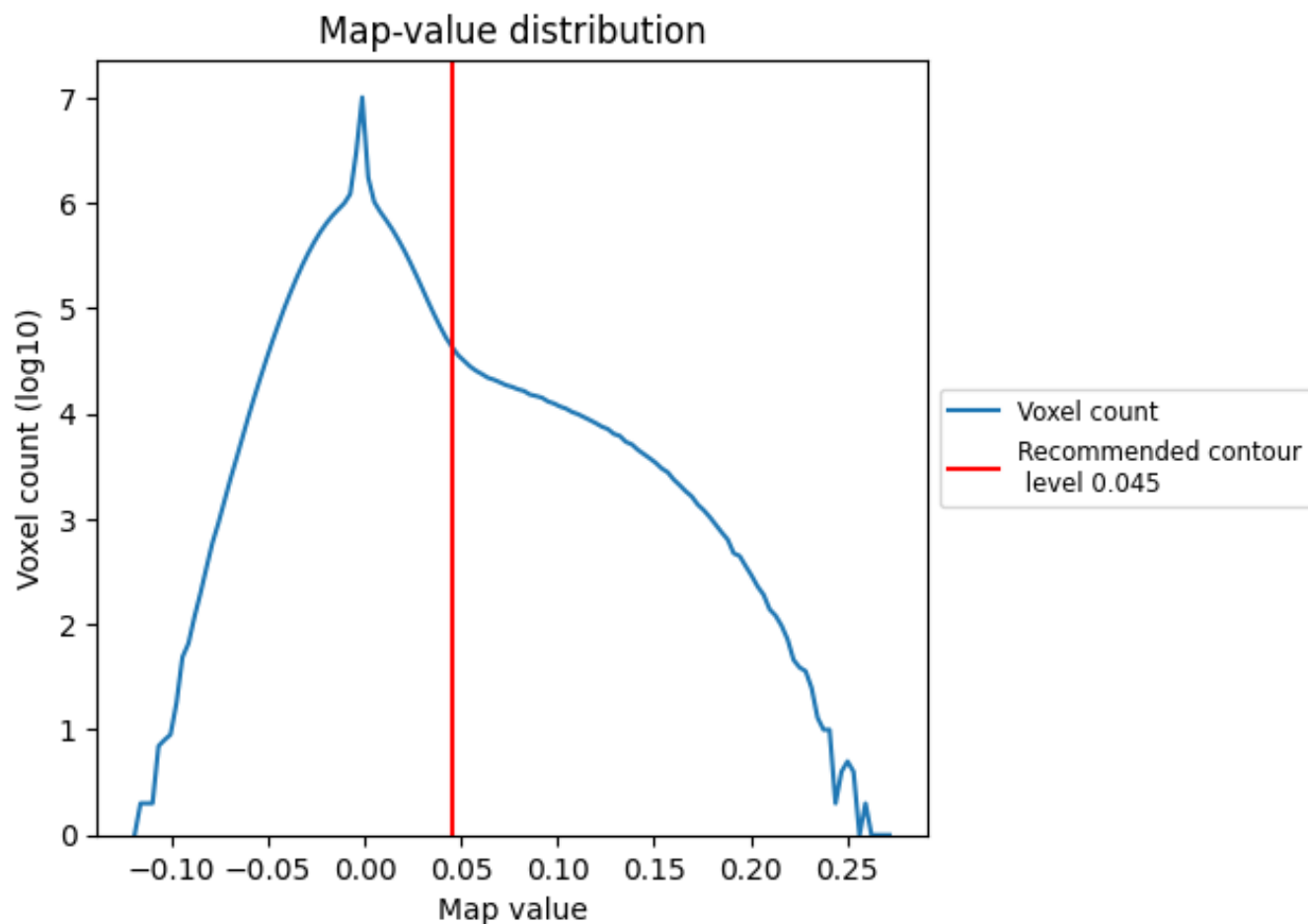
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

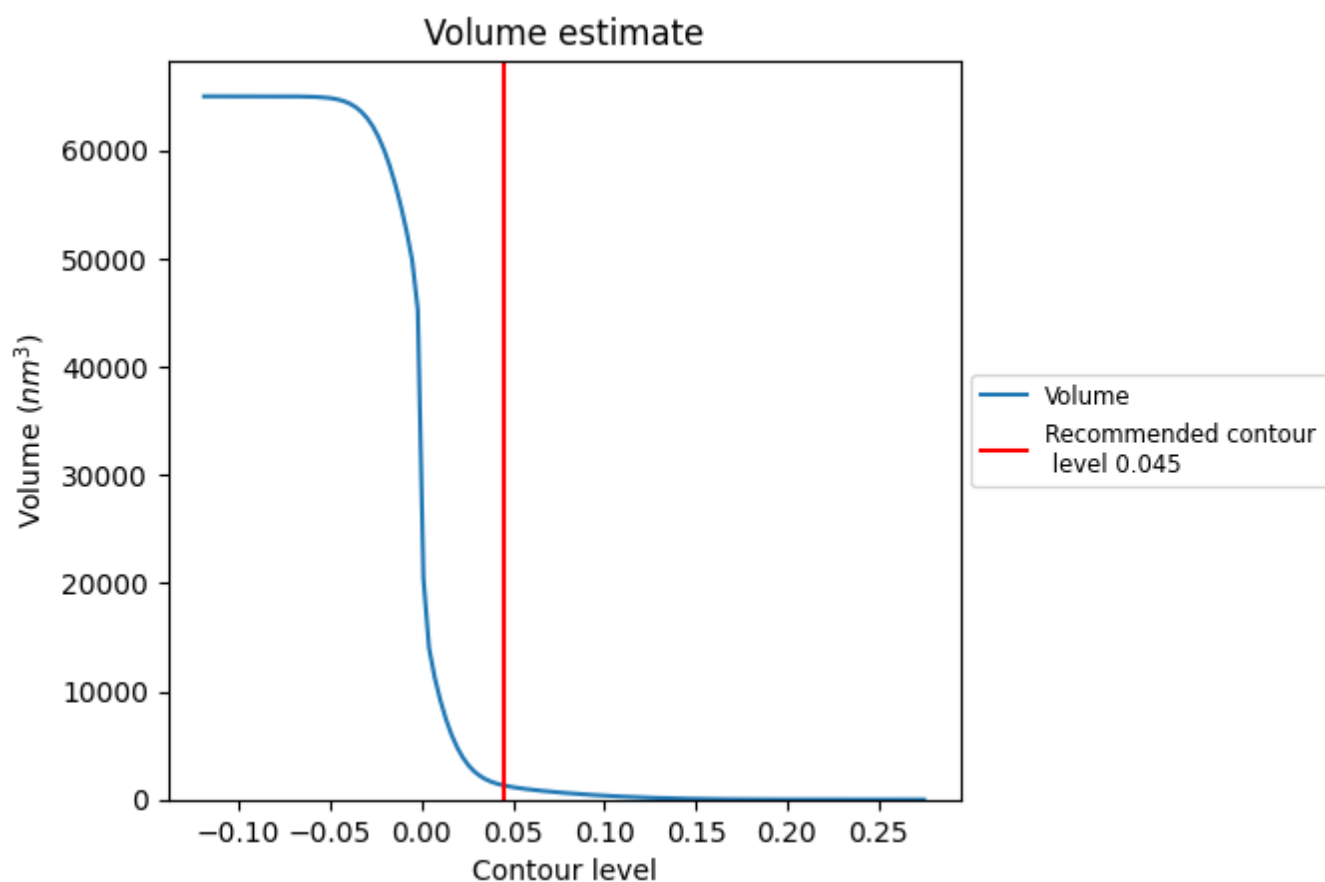
This section contains the results of statistical analysis of the map.

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.

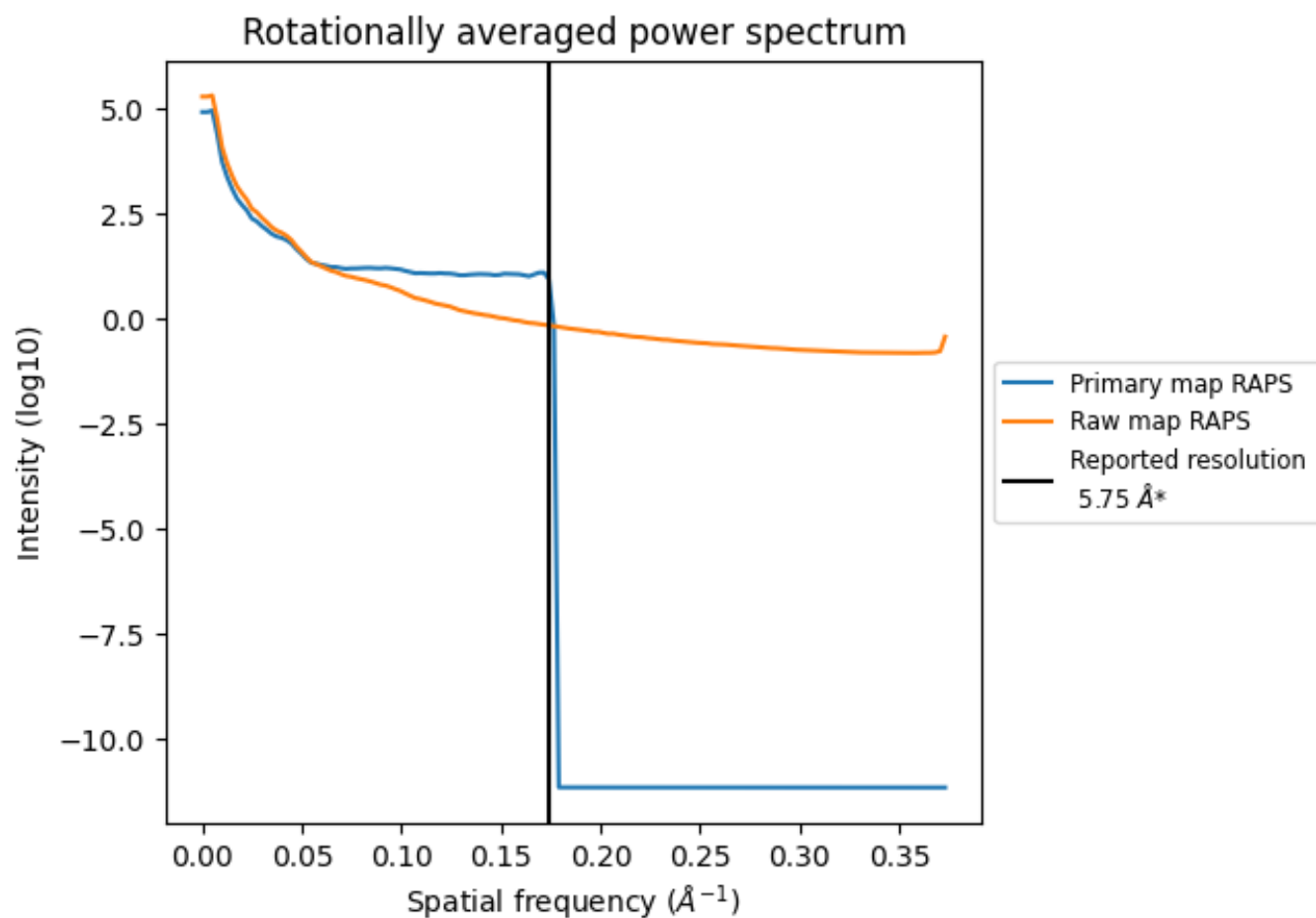
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1308 nm^3 ; this corresponds to an approximate mass of 1181 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 ⓘ

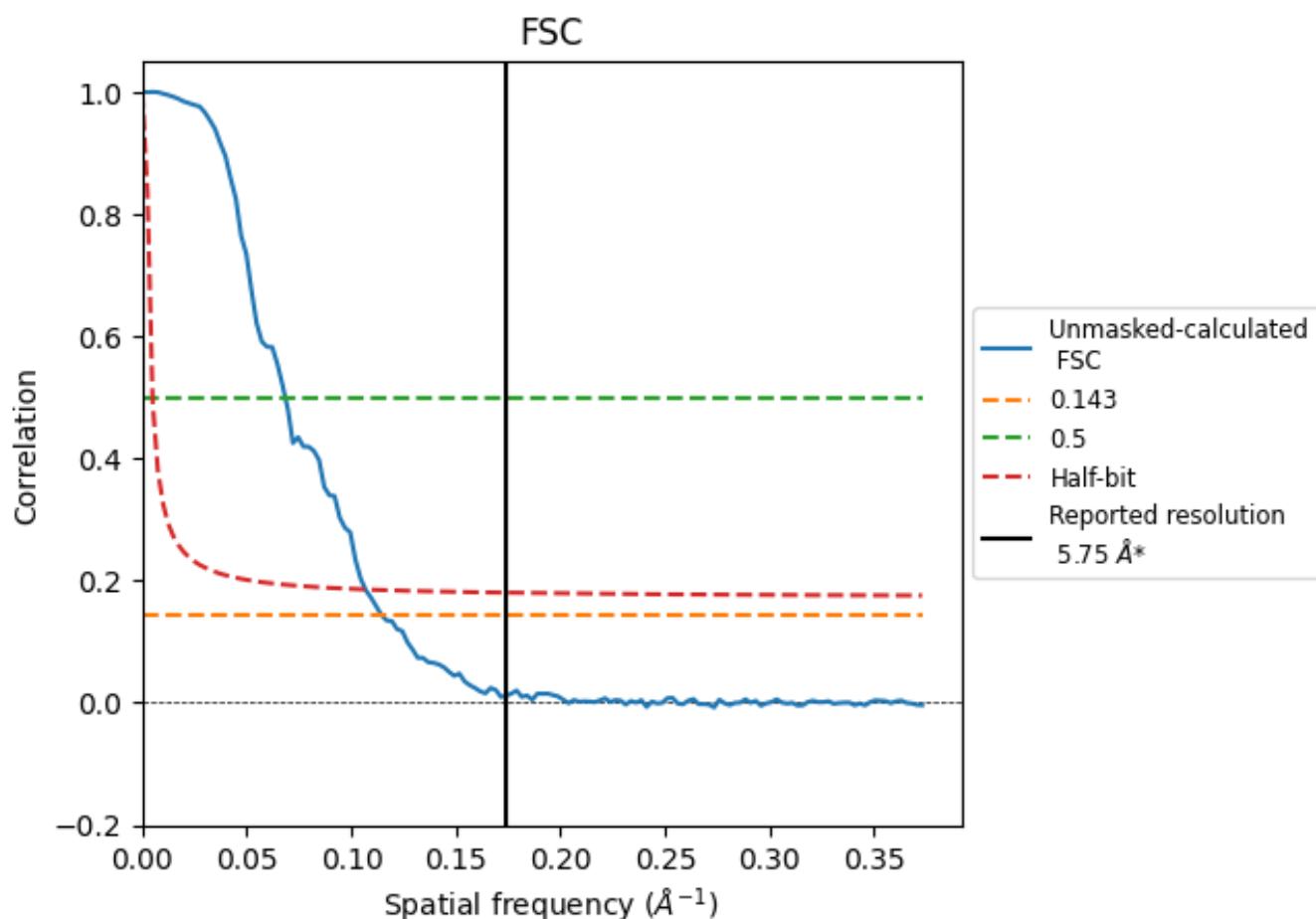


*Reported resolution corresponds to spatial frequency of 0.174 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.174 Å⁻¹

8.2 Resolution estimates [i](#)

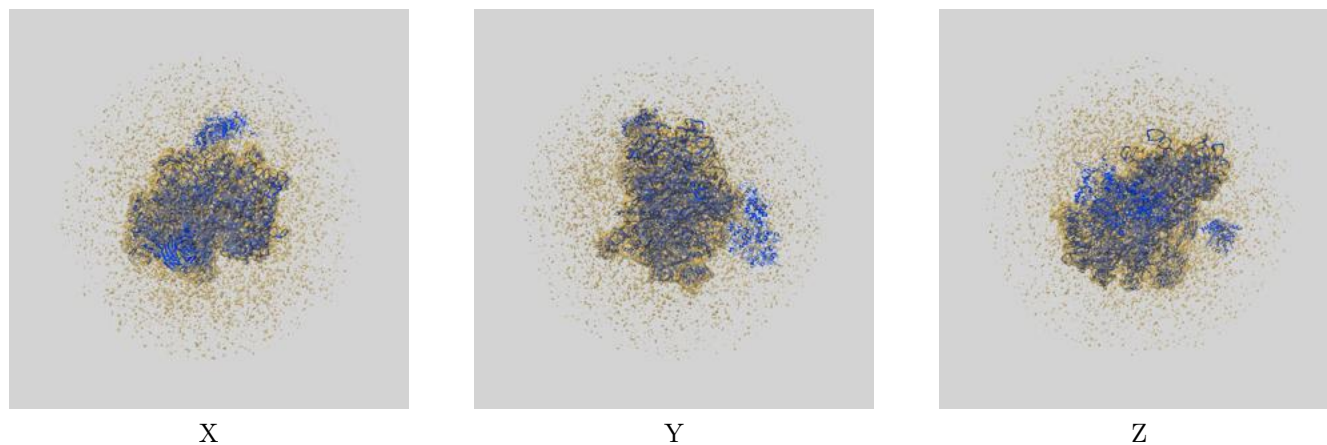
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.75	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.73	14.62	9.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.73 differs from the reported value 5.75 by more than 10 %

9 Map-model fit [i](#)

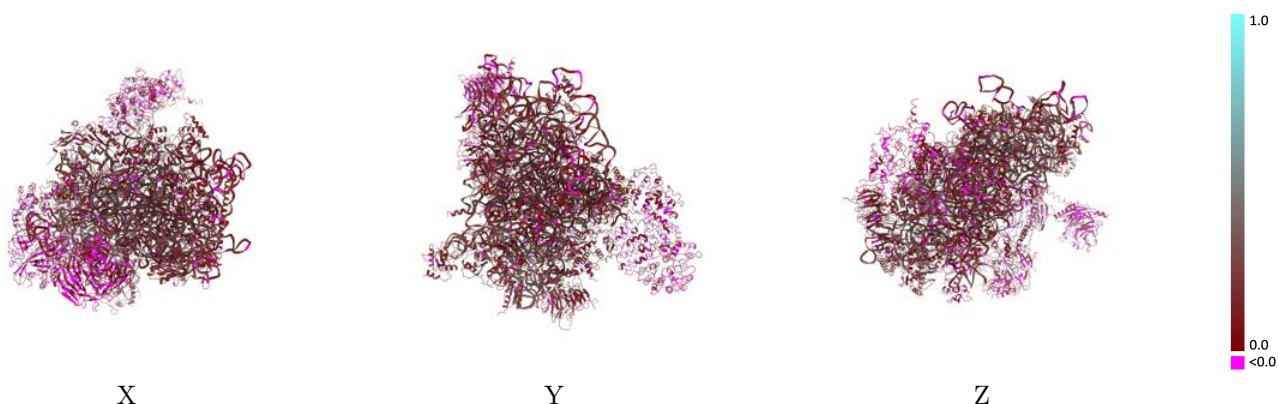
This section contains information regarding the fit between EMDB map EMD-0058 and PDB model 6GSN. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



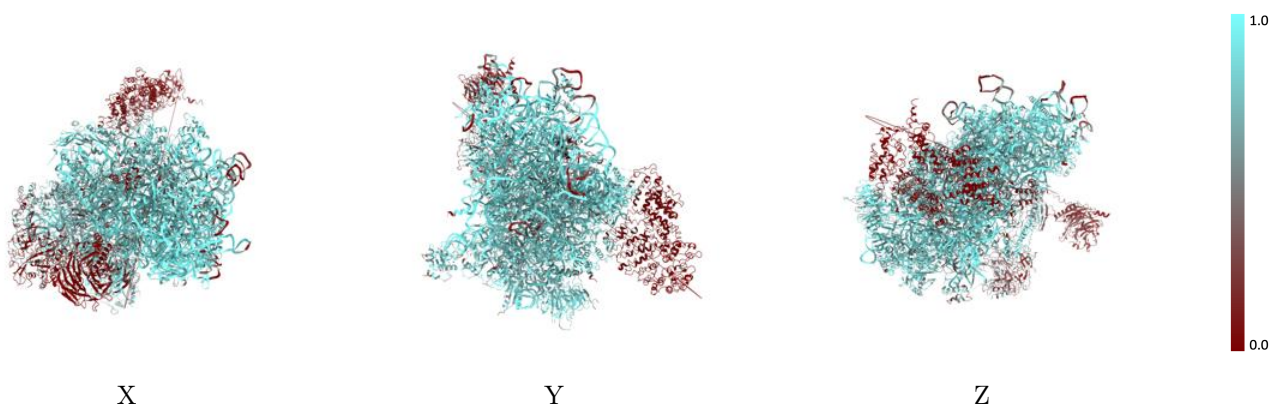
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



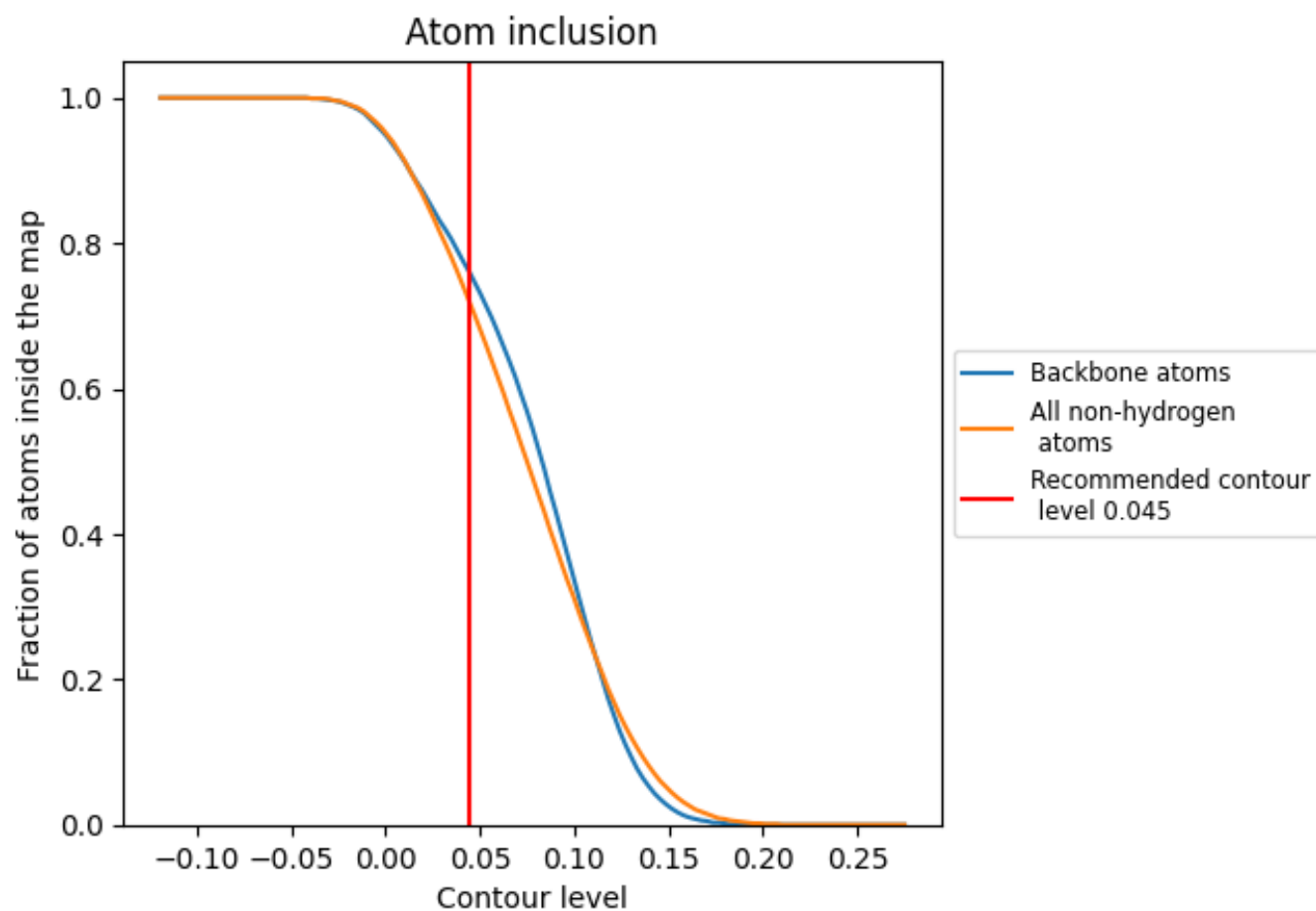
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7170	 0.1850
1	 0.8130	 0.1580
2	 0.9260	 0.2360
3	 0.7350	 0.1800
A	 0.8200	 0.2010
B	 0.8440	 0.1950
C	 0.7730	 0.2070
D	 0.7760	 0.2120
E	 0.7920	 0.1980
F	 0.7870	 0.1950
G	 0.8350	 0.1770
H	 0.8230	 0.1830
I	 0.8020	 0.1920
J	 0.7920	 0.2000
K	 0.8250	 0.1880
L	 0.7670	 0.2080
M	 0.6960	 0.1600
N	 0.8170	 0.1930
O	 0.8550	 0.2030
P	 0.8400	 0.1940
Q	 0.8150	 0.1760
R	 0.7820	 0.1940
S	 0.7940	 0.1800
T	 0.8270	 0.1810
U	 0.7510	 0.1810
V	 0.8430	 0.2120
W	 0.7920	 0.1980
X	 0.7260	 0.2060
Y	 0.8330	 0.2070
Z	 0.7350	 0.1580
a	 0.8330	 0.2220
b	 0.8410	 0.2140
c	 0.7940	 0.2100
d	 0.7840	 0.1930
e	 0.6930	 0.2070



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Chain	Atom inclusion	Q-score
f	 0.7900	 0.1870
g	 0.8280	 0.1720
h	 0.5400	 0.1350
i	 0.7160	 0.2200
j	 0.4780	 0.1290
k	 0.2490	 0.0930
l	 0.3020	 0.1060
m	 0.4460	 0.1650
o	 0.0950	 0.0710
p	 0.5480	 0.1290
q	 0.0460	 0.0870
r	 0.0210	 0.0550
s	 0.0230	 0.0020