



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 11:06 AM UTC

PDB ID : 8HFR / pdb_00008hfr
EMDB ID : EMD-34725
Title : NPC-trapped pre-60S particle
Authors : Li, Z.Q.; Chen, S.J.; Sui, S.F.
Deposited on : 2022-11-12
Resolution : 2.64 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

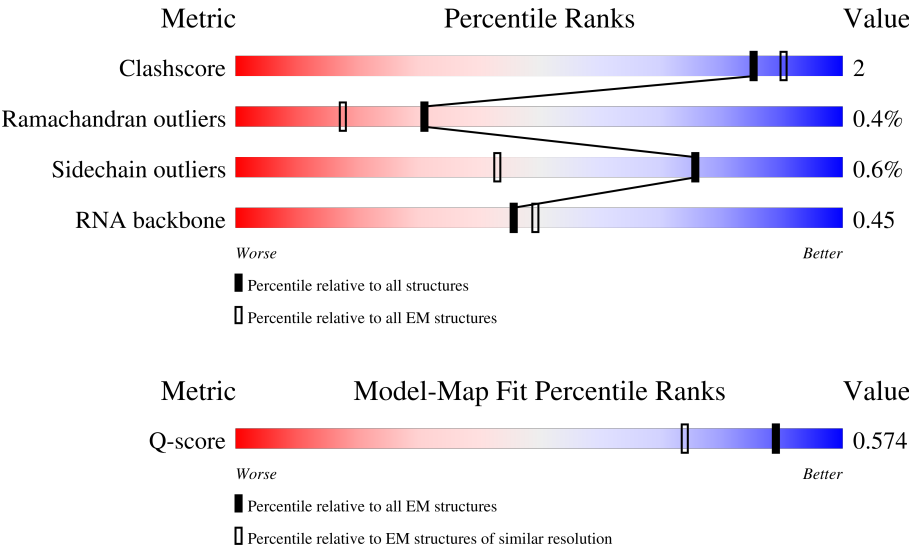
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.64 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.



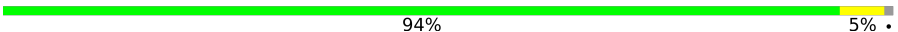
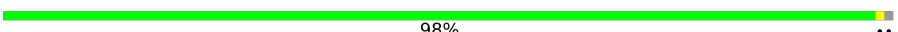
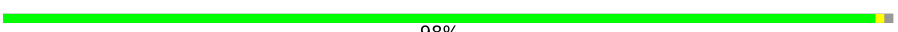
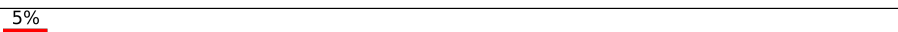
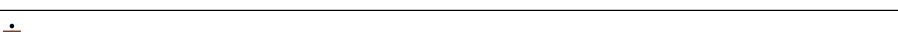
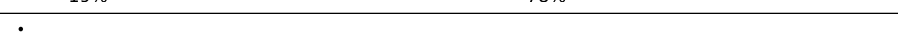
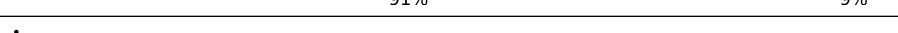
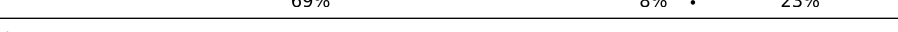
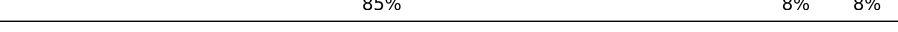
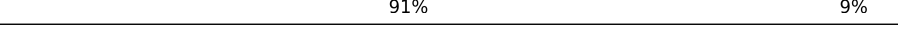
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8968 (2.14 - 3.14)

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	h1	120	92% 7% .
2	g2	121	90% . 6%
3	b3	59	88% 5% 7%

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Mol	Chain	Length	Quality of chain
4	B4	254	 94%5%.
5	V5	137	 91%9%.
6	O6	199	 98%..
7	f7	107	 98%..
8	F8	176	 5%95%..
9	v9	486	 19%..78%
10	rA	647	 91%9%
11	tB	199	 69%8%23%
12	cC	105	 85%8%8%
13	CD	387	 91%9%
14	yE	245	 89%10%.
15	UF	121	 8%89%5%5%
16	dG	113	 5%91%6%.
17	eH	130	 92%7%.
18	xI	212	 24%5%69%
19	qJ	175	 10%73%.23%
20	Bt	184	 23%85%.10%
20	DK	184	 87%82%7%10%
20	FR	184	 89%84%.10%
21	LL	199	 6%95%5%.
22	KM	165	 26%82%13%..
23	AN	599	 21%58%.38%
23	CW	599	 61%66%5%29%
23	EX	599	 58%53%..42%
24	DO	362	 96%.

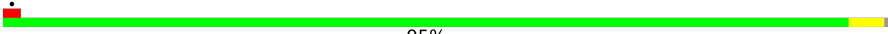
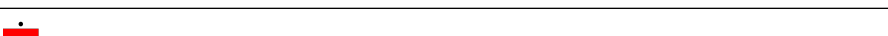
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Mol	Chain	Length	Quality of chain
25	RP	189	
26	MQ	138	
27	mS	106	
28	pT	593	
29	YU	127	
30	vV	518	
31	nY	92	
32	SZ	172	
33	ia	100	
34	Ib	191	
35	Xc	142	
36	xd	261	
37	1e	3396	
38	2f	121	
39	Wg	236	
40	jh	88	
41	li	51	
42	Hj	256	
43	Qk	186	
44	Tl	160	
45	sm	178	
46	3n	158	
47	No	204	
48	zp	106	
49	Zq	136	

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Mol	Chain	Length	Quality of chain
50	kr	78	 83% 15%
51	As	217	 15% 86% 12%
52	Gu	244	 89% 9%
53	Pv	184	 95%
54	aw	149	 97%
55	ox	166	 84% 14%
56	Jy	174	 88% 7% 5%
57	Ez	297	 92% 6%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 152374 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	h1	119	Total	C	N	O	S	0	0
			961	610	185	165	1		

- Molecule 2 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	g2	114	Total	C	N	O	S	0	0
			885	546	180	155	4		

- Molecule 3 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	b3	55	Total	C	N	O	0	0
			422	262	91	69		

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B4	251	Total	C	N	O	S	0	0
			1901	1183	386	331	1		

- Molecule 5 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V5	136	Total	C	N	O	S	0	0
			990	622	185	176	7		

- Molecule 6 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	O6	197	Total	C	N	O	S	0	0
			1548	1000	288	259	1		

- Molecule 7 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f7	106	Total	C	N	O	S	0	0
			847	537	165	144	1		

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F8	175	Total	C	N	O	S	0	0
			1241	797	231	212	1		

- Molecule 9 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	v9	106	Total	C	N	O	S	0	0
			748	475	134	138	1		

- Molecule 10 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	rA	647	Total	C	N	O	S	0	0
			5044	3164	918	938	24		

- Molecule 11 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	tB	154	Total	C	N	O	S	0	0
			1246	779	245	213	9		

- Molecule 12 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	cC	97	Total	C	N	O	S	0	0
			689	440	119	129	1		

- Molecule 13 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	CD	386	Total	C	N	O	S	0	0
			2968	1896	572	492	8		

- Molecule 14 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	yE	242	Total	C	N	O	S	0	0
			1786	1113	313	354	6		

- Molecule 15 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	UF	115	Total	C	N	O		0	0
			864	560	146	158			

- Molecule 16 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	dG	110	Total	C	N	O	S	0	0
			862	549	167	145	1		

- Molecule 17 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	eH	129	Total	C	N	O	S	0	0
			1034	655	207	171	1		

- Molecule 18 is a protein called Shuttling pre-60S factor ECM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	xI	65	Total	C	N	O	S	0	0
			524	327	97	99	1		

- Molecule 19 is a protein called Ribosome biogenesis protein ALB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	qJ	135	Total	C	N	O		0	0
			1022	640	198	184			

- Molecule 20 is a protein called mRNA transport regulator MTR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	DK	165	Total	C	N	O		0	0
			816	486	165	165			
20	FR	165	Total	C	N	O		0	0
			816	486	165	165			
20	Bt	165	Total	C	N	O		0	0
			816	486	165	165			

- Molecule 21 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	LL	198	Total	C	N	O	0	0
			1492	934	309	249		

- Molecule 22 is a protein called YEAST 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	KM	159	Total	C	N	O	0	0
			796	473	164	159		

- Molecule 23 is a protein called mRNA export factor MEX67.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	AN	371	Total	C	N	O	0	0
			1843	1101	371	371		
23	CW	427	Total	C	N	O	0	0
			2120	1266	427	427		
23	EX	347	Total	C	N	O	0	0
			1725	1031	347	347		

- Molecule 24 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	DO	361	Total	C	N	O	S	0	0
			2675	1688	516	468	3		

- Molecule 25 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	RP	188	Total	C	N	O	0	0
			1374	853	290	231		

- Molecule 26 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	MQ	136	Total	C	N	O	S	0	0
			1042	668	197	175	2		

- Molecule 27 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	mS	93	Total	C	N	O	S	0	0
			711	445	142	119	5		

- Molecule 28 is a protein called Probable metalloprotease ARX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	pT	580	Total	C	N	O	S	0	0
			4285	2690	746	834	15		

- Molecule 29 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	YU	126	Total	C	N	O	S	0	0
			989	623	192	174			

- Molecule 30 is a protein called 60S ribosomal export protein NMD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	vV	245	Total	C	N	O	S	0	0
			1875	1208	317	343	7		

- Molecule 31 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	nY	91	Total	C	N	O	S	0	0
			673	415	136	117	5		

- Molecule 32 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SZ	171	Total	C	N	O	S	0	0
			1420	916	265	236	3		

- Molecule 33 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	ia	96	Total	C	N	O	S	0	0
			718	448	143	125	2		

- Molecule 34 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ib	191	Total	C	N	O	S	0	0
			1446	926	267	250	3		

- Molecule 35 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Xc	123	Total	C	N	O	S	0	0
			963	620	170	171	2		

- Molecule 36 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	xd	72	Total	C	N	O	S	0	0
			601	373	130	97	1		

- Molecule 37 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1e	3274	Total	C	N	O	P	0	0
			69952	31234	12578	22866	3274		

- Molecule 38 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	2f	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 39 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Wg	233	Total	C	N	O		0	0
			1190	709	244	237			

- Molecule 40 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	jh	87	Total	C	N	O	S	0	0
			677	411	147	114	5		

- Molecule 41 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	li	50	Total	C	N	O	S	0	0
			433	269	97	65	2		

- Molecule 42 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Hj	230	Total	C	N	O	S	0	0
			1660	1066	298	294	2		

- Molecule 43 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Qk	185	Total	C	N	O	S	0	0
			1434	903	289	240	2		

- Molecule 44 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Tl	160	Total	C	N	O	S	0	0
			1256	790	245	217	4		

- Molecule 45 is a protein called Translation machinery-associated protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	sm	150	Total	C	N	O	S	0	0
			1036	631	213	190	2		

- Molecule 46 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3n	156	Total	C	N	O	P	0	0
			3313	1482	582	1093	156		

- Molecule 47 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	No	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 48 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	zp	88	Total	C	N	O	S	0	0
			668	412	134	121	1		

- Molecule 49 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Zq	135	Total	C	N	O		0	0
			1052	684	195	173			

- Molecule 50 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	kr	77	Total	C	N	O		0	0
			573	362	106	105			

- Molecule 51 is a protein called YEAST 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	As	217	Total	C	N	O		0	0
			1089	653	218	218			

- Molecule 52 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Gu	223	Total	C	N	O	S	0	0
			1784	1152	325	306	1		

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Pv	182	Total	C	N	O		0	0
			1383	859	277	247			

- Molecule 54 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	aw	148	Total	C	N	O	S	0	0
			1170	746	230	191	3		

- Molecule 55 is a protein called Bud site selection protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	ox	143	Total	C	N	O	S	0	0
			1147	720	210	214	3		

- Molecule 56 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Jy	166	Total	C	N	O	S	0	0
			1270	792	244	230	4		

- Molecule 57 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Ez	290	Total	C	N	O	S	0	0
			1973	1245	372	355	1		

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	g2	2	Total	Mg	0
			2	2	
58	B4	1	Total	Mg	0
			1	1	
58	CD	2	Total	Mg	0
			2	2	
58	1e	223	Total	Mg	0
			223	223	
58	2f	1	Total	Mg	0
			1	1	
58	3n	6	Total	Mg	0
			6	6	
58	No	1	Total	Mg	0
			1	1	
58	zp	1	Total	Mg	0
			1	1	

3 Residue-property plots [i](#)

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

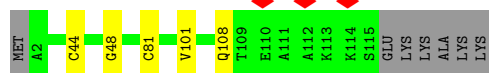
- Molecule 1: 60S ribosomal protein L35-A

Chain h1: 



- Molecule 2: 60S ribosomal protein L34-A

Chain g2: 

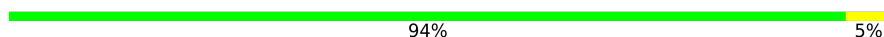


- Molecule 3: 60S ribosomal protein L29

Chain b3: 



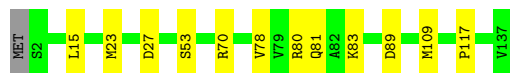
- Molecule 4: 60S ribosomal protein L2-A

Chain B4: 



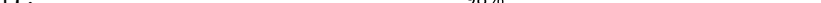
- Molecule 5: 60S ribosomal protein L23-A

Chain V5: 

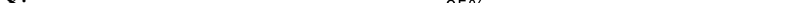


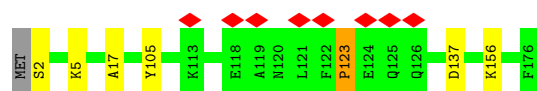
- Molecule 6: 60S ribosomal protein L16-A

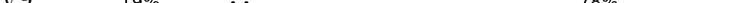
MET
SER
V3
E100
Y199

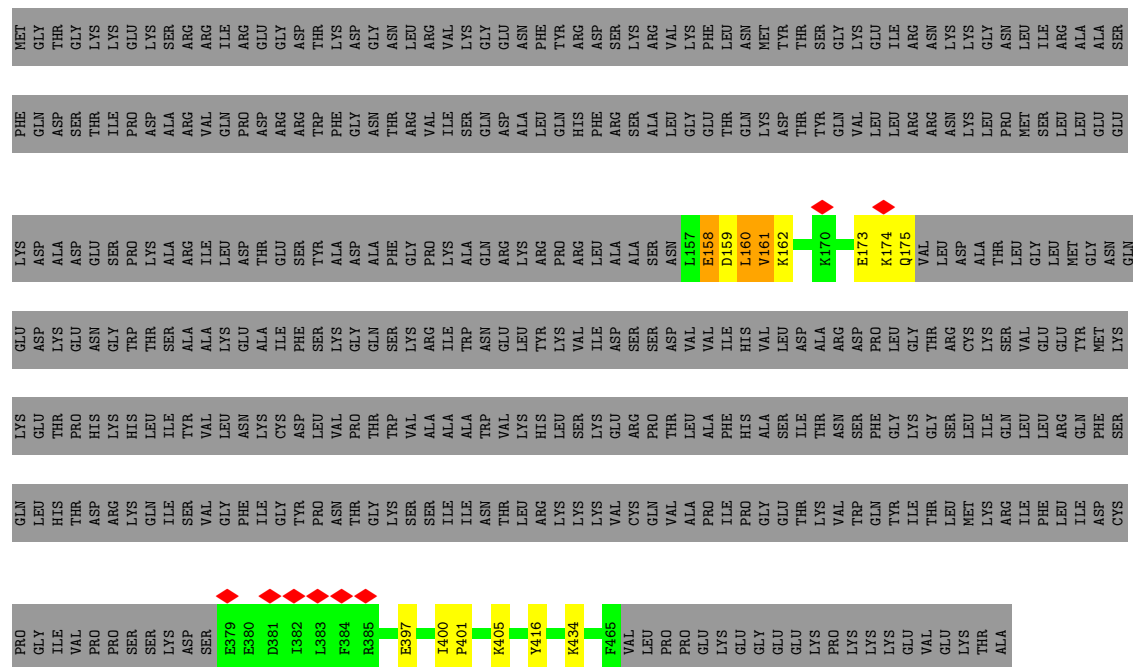
- Chain f7:  98% ..

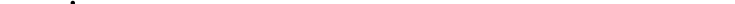


- Chain F8:  5% 95% ...

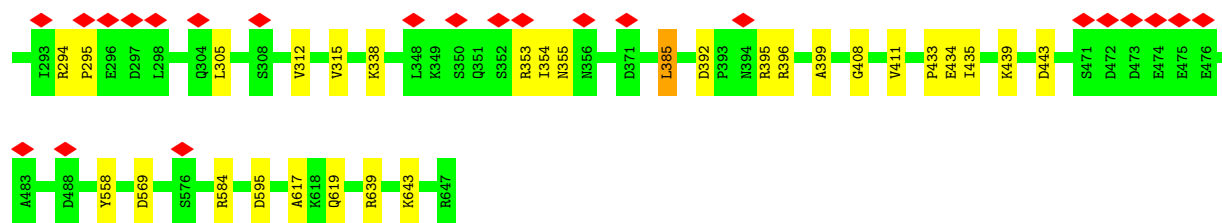


- Chain v9:  19% .. 78%

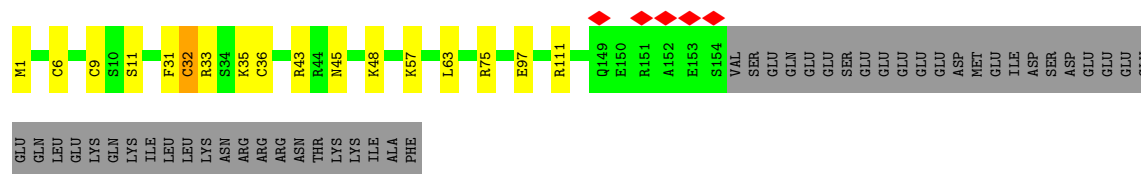


- Chain rA:  91% 9%

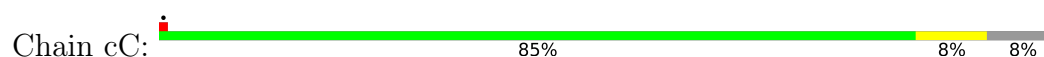




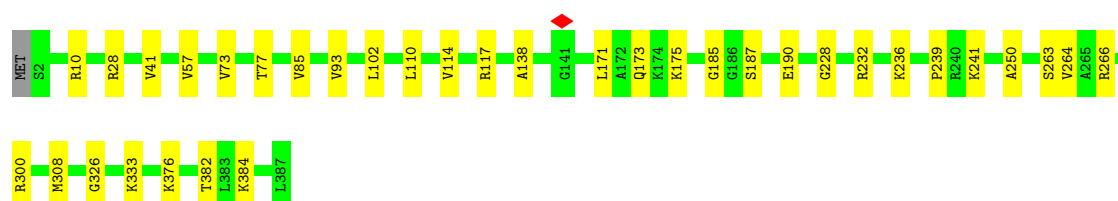
- Molecule 11: Ribosome biogenesis protein RLP24



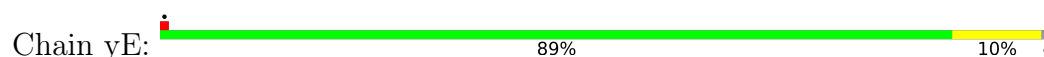
- Molecule 12: 60S ribosomal protein L30



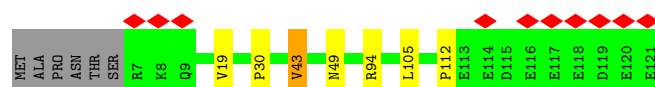
- Molecule 13: 60S ribosomal protein L3

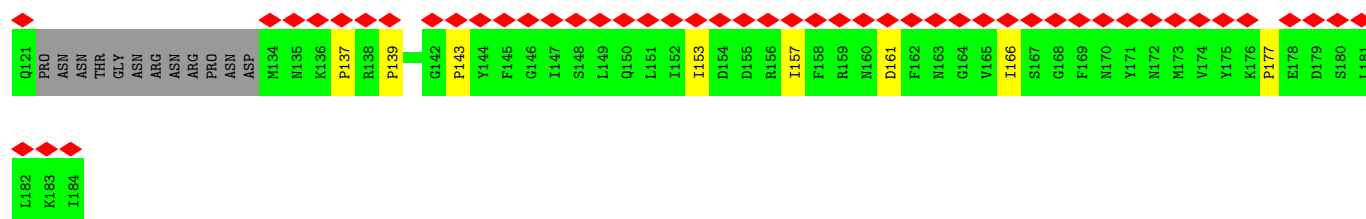


- Molecule 14: Eukaryotic translation initiation factor 6

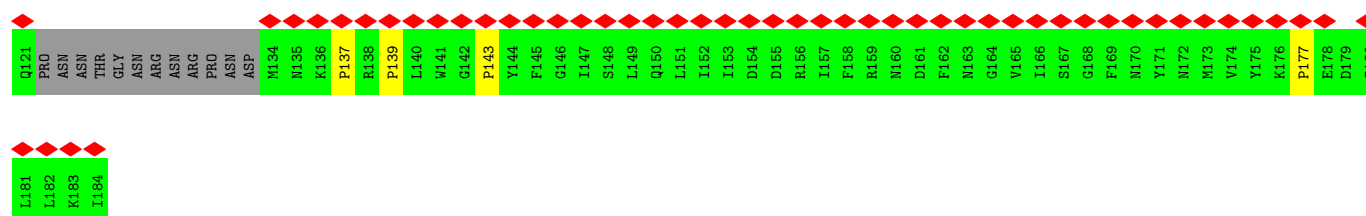
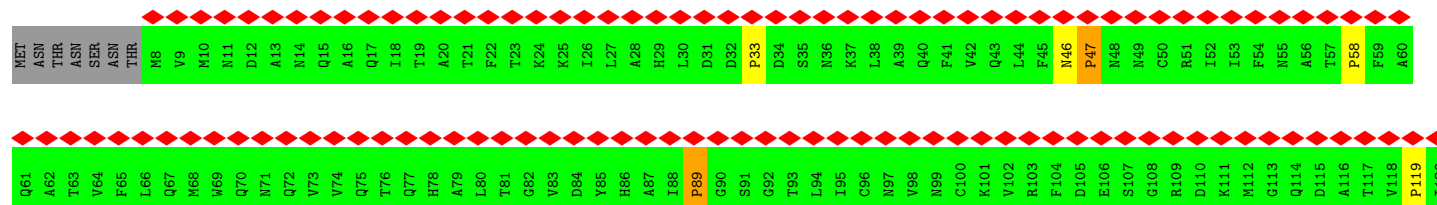
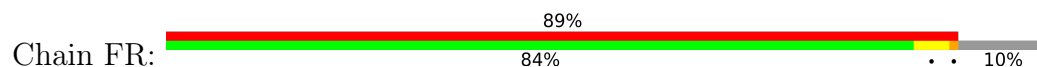


- Molecule 15: 60S ribosomal protein L22-A

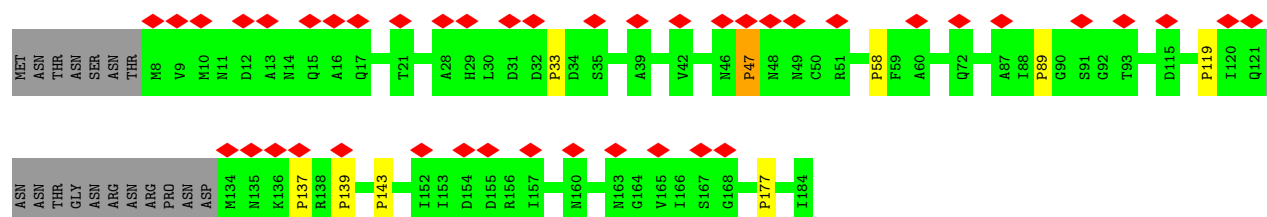
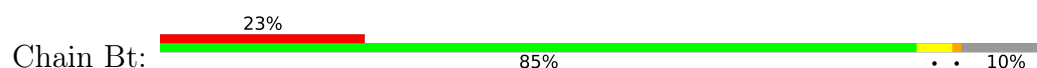




- Molecule 20: mRNA transport regulator MTR2



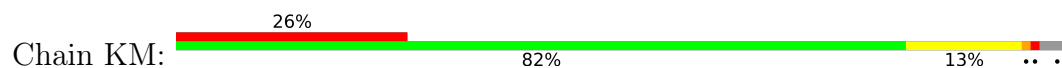
- Molecule 20: mRNA transport regulator MTR2

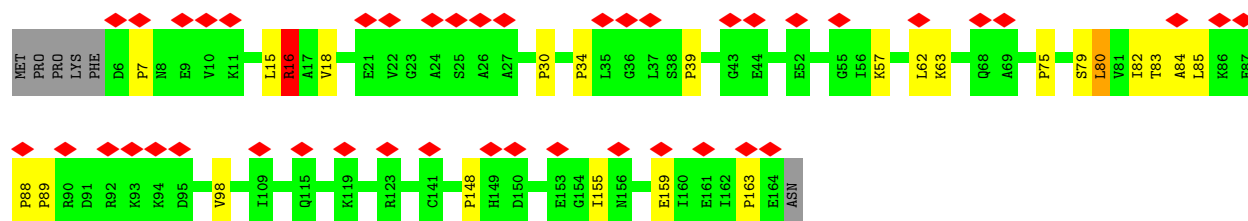


- Molecule 21: 60S ribosomal protein L13-A

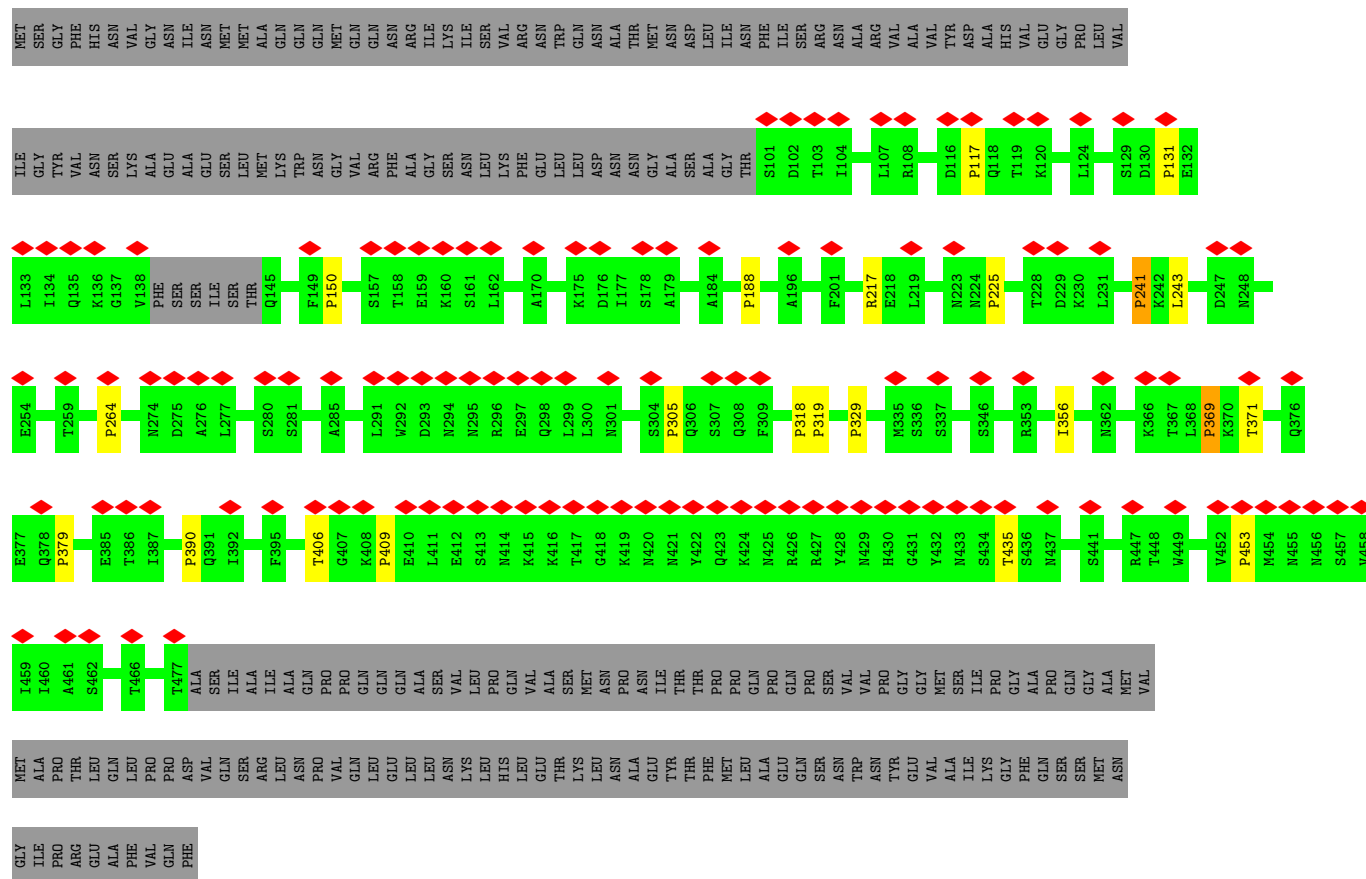


- Molecule 22: YEAST 60S ribosomal protein L12-A



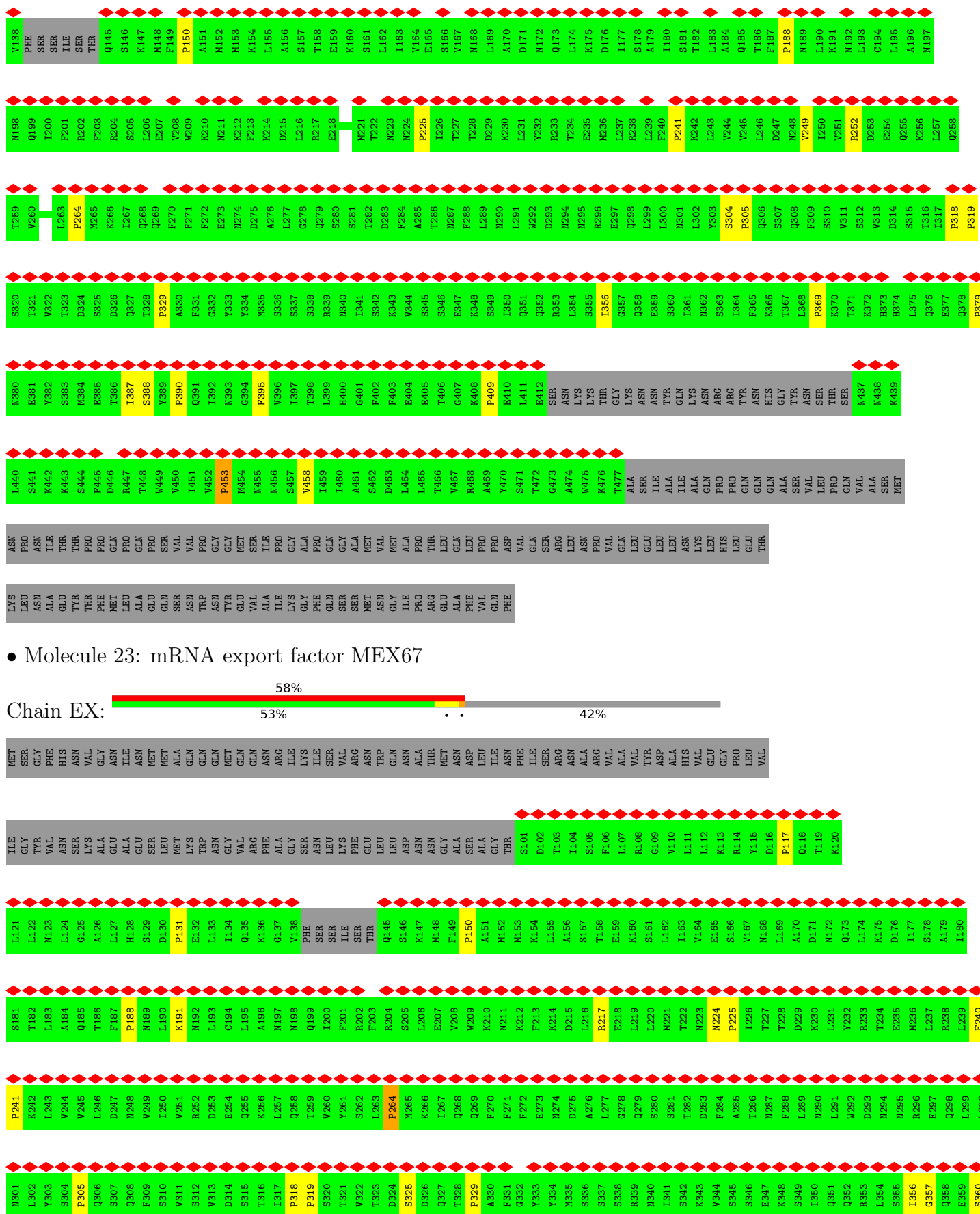


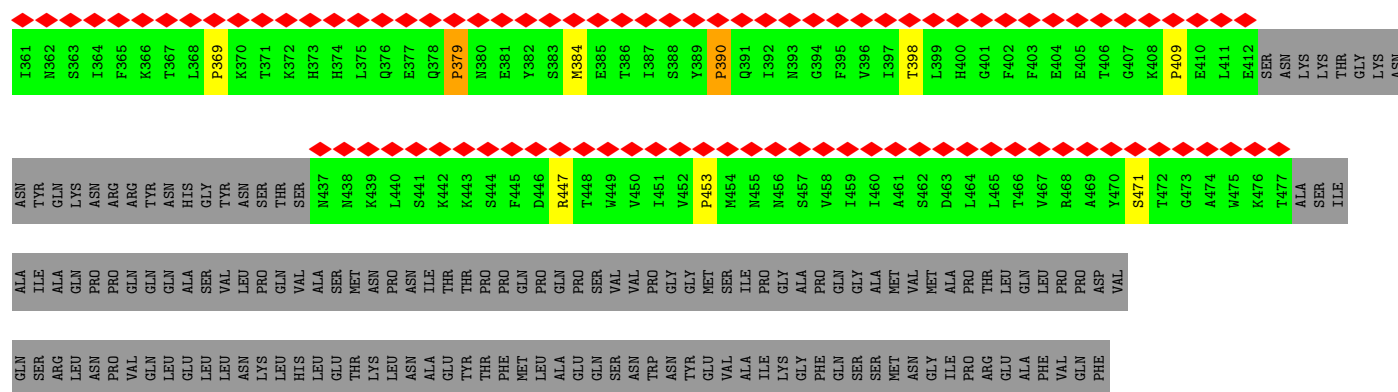
• Molecule 23: mRNA export factor MEX67



• Molecule 23: mRNA export factor MEX67







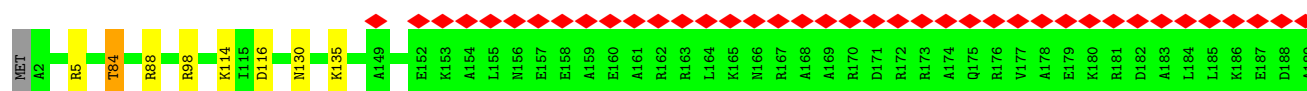
• Molecule 24: 60S ribosomal protein L4-A

Chain DO: 96%



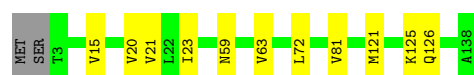
• Molecule 25: 60S ribosomal protein L19-A

Chain RP: 21% 95%



• Molecule 26: 60S ribosomal protein L14-A

Chain MQ: 91% 8%



• Molecule 27: 60S ribosomal protein L42-A

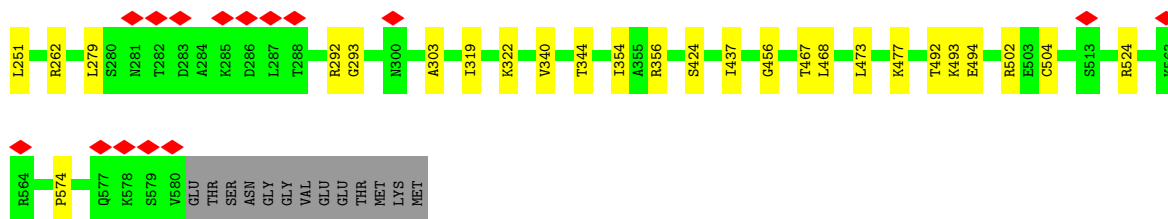
Chain mS: 80% 8% 12%



• Molecule 28: Probable metalloprotease ARX1

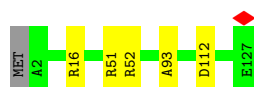
Chain pT: 6% 91% 7%





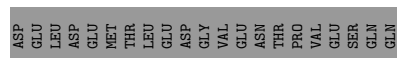
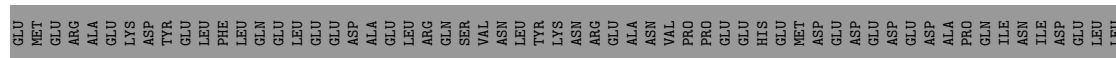
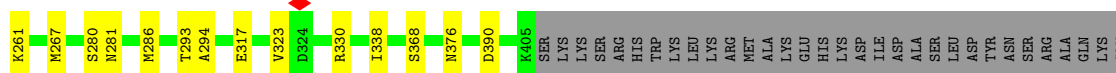
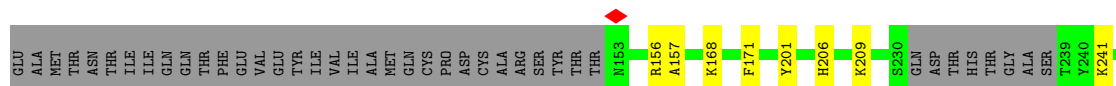
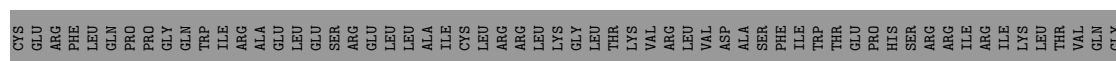
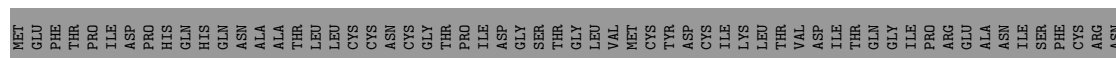
- Molecule 29: 60S ribosomal protein L26-A

Chain YU: 95%



- Molecule 30: 60S ribosomal export protein NMD3

Chain vV: 43%



- Molecule 31: 60S ribosomal protein L43-A

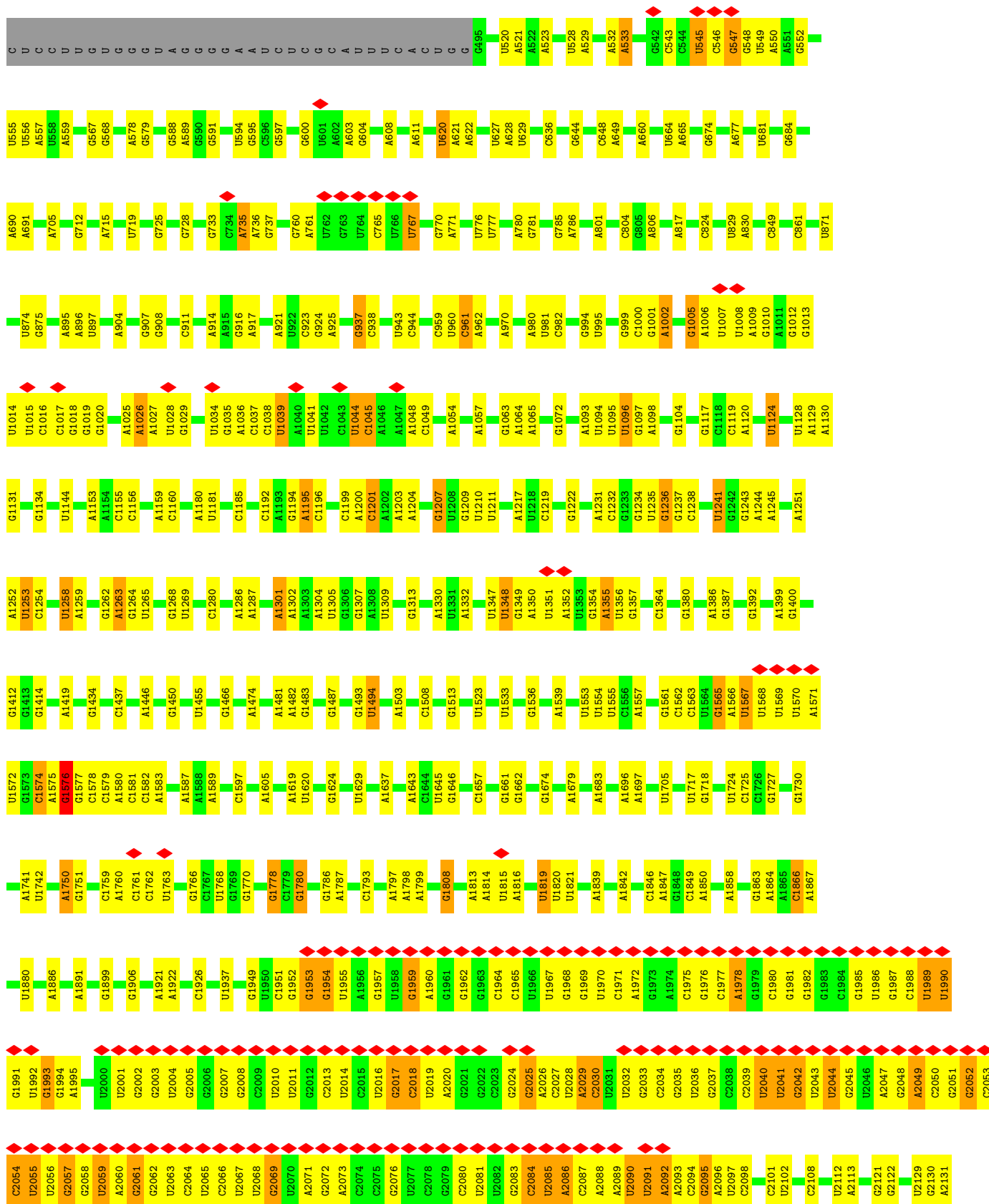
Chain nY: 91%



- Molecule 32: 60S ribosomal protein L20-A

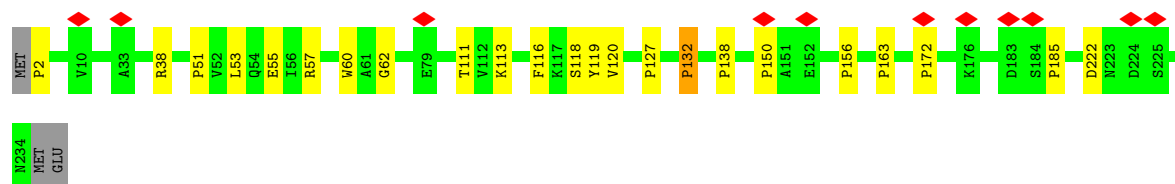
Chain SZ: 96%



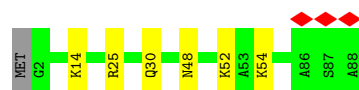
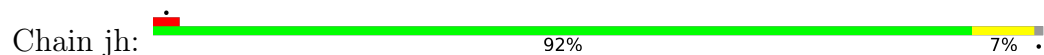




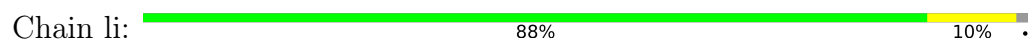
WORLDWIDE
PDB
PROTEIN DATA BANK



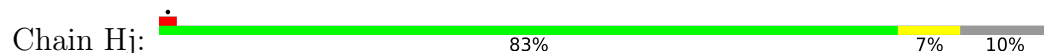
- Molecule 40: 60S ribosomal protein L37-A



- Molecule 41: 60S ribosomal protein L39



- Molecule 42: 60S ribosomal protein L8-A



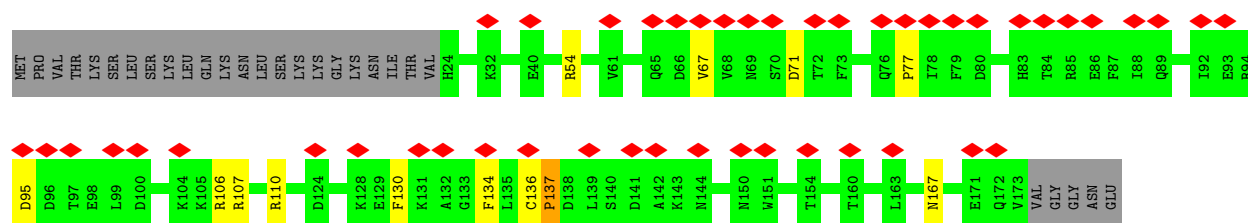
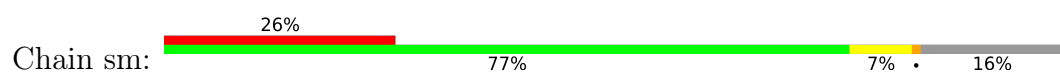
- Molecule 43: 60S ribosomal protein L18-A



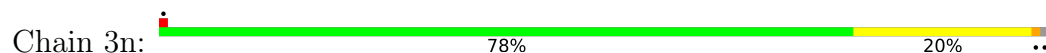
- Molecule 44: 60S ribosomal protein L21-A



- Molecule 45: Translation machinery-associated protein 16



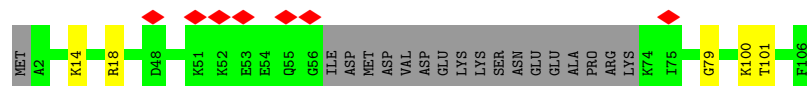
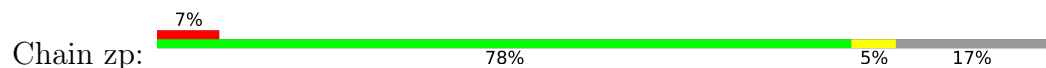
- Molecule 46: 5.8S ribosomal RNA



- Molecule 47: 60S ribosomal protein L15-A



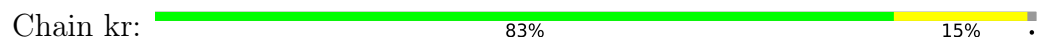
- Molecule 48: UPF0642 protein YBL028C



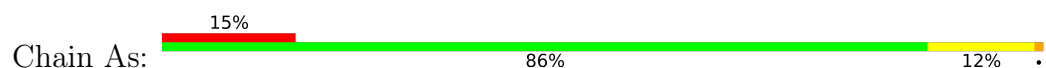
- Molecule 49: 60S ribosomal protein L27-A

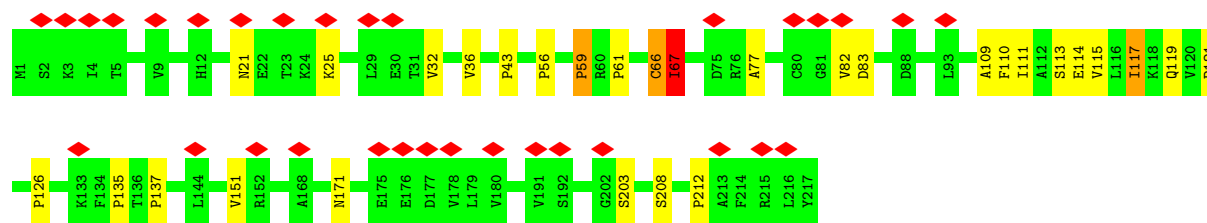


- Molecule 50: 60S ribosomal protein L38

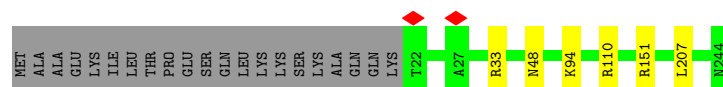
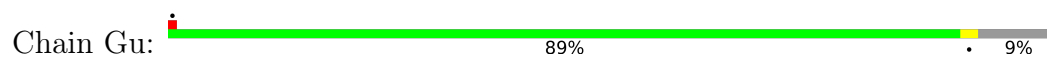


- Molecule 51: YEAST 60S ribosomal protein L1-A





- Molecule 52: 60S ribosomal protein L7-A



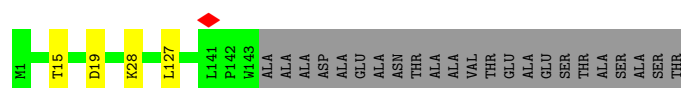
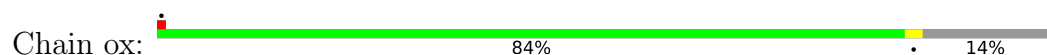
- Molecule 53: 60S ribosomal protein L17-A



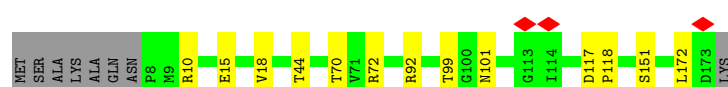
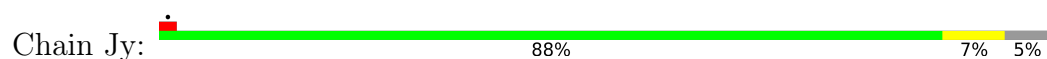
- Molecule 54: 60S ribosomal protein L28



- Molecule 55: Bud site selection protein 20



- Molecule 56: 60S ribosomal protein L11-A



- Molecule 57: 60S ribosomal protein L5





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86343	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.373	Depositor
Minimum map value	-0.495	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	534.39996, 534.39996, 534.39996	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.668, 0.668, 0.668	Depositor

5 Model quality

5.1 Standard geometry

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

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	h1	0.35	0/970	0.55	0/1292
2	g2	0.36	0/895	0.59	2/1198 (0.2%)
3	b3	0.28	0/433	0.53	0/583
4	B4	0.34	0/1935	0.61	0/2601
5	V5	0.32	0/1005	0.56	0/1353
6	O6	0.37	0/1578	0.51	0/2119
7	f7	0.38	0/865	0.53	0/1164
8	F8	0.32	0/1261	0.59	1/1715 (0.1%)
9	v9	0.50	0/761	0.75	0/1036
10	rA	0.30	0/5129	0.60	0/6913
11	tB	0.37	0/1268	0.64	3/1697 (0.2%)
12	cC	0.28	0/697	0.48	0/940
13	CD	0.39	0/3038	0.65	0/4100
14	yE	0.31	0/1808	0.58	0/2466
15	UF	0.33	0/881	0.61	0/1198
16	dG	0.33	0/876	0.55	0/1180
17	eH	0.36	0/1055	0.60	0/1413
18	xI	0.42	0/529	0.65	0/707
19	qJ	0.29	0/1033	0.55	0/1382
20	Bt	0.31	0/814	0.90	9/1131 (0.8%)
20	DK	0.29	0/814	0.95	9/1131 (0.8%)
20	FR	0.32	0/814	0.91	9/1131 (0.8%)
21	LL	0.33	0/1517	0.54	0/2049
22	KM	0.65	0/796	1.04	10/1103 (0.9%)
23	AN	0.27	0/1841	0.81	18/2567 (0.7%)
23	CW	0.27	0/2116	0.77	17/2947 (0.6%)
23	EX	0.27	0/1722	0.78	16/2400 (0.7%)
24	DO	0.34	0/2727	0.58	0/3703
25	RP	0.32	0/1391	0.48	0/1871
26	MQ	0.33	0/1057	0.61	0/1426
27	mS	0.33	0/722	0.57	0/963
28	pT	0.29	0/4360	0.57	1/5945 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
29	YU	0.32	0/1000	0.51	0/1336
30	vV	0.24	0/1913	0.55	0/2603
31	nY	0.33	0/680	0.62	0/910
32	SZ	0.32	0/1456	0.56	0/1960
33	ia	0.29	0/723	0.54	0/964
34	Ib	0.32	0/1467	0.57	0/1984
35	Xc	0.46	0/978	0.66	0/1321
36	xd	0.25	0/611	0.51	0/804
37	1e	0.38	0/78291	0.46	7/122066 (0.0%)
38	2f	0.30	0/2883	0.39	0/4491
39	Wg	0.48	0/1191	0.88	9/1651 (0.5%)
40	jh	0.40	0/692	0.65	0/919
41	li	0.39	0/440	0.60	0/584
42	Hj	0.33	0/1691	0.62	0/2308
43	Qk	0.34	0/1458	0.53	0/1956
44	Tl	0.28	0/1279	0.44	0/1718
45	sm	0.28	0/1043	0.76	2/1403 (0.1%)
46	3n	0.41	0/3702	0.43	0/5764
47	No	0.36	0/1757	0.53	0/2354
48	zp	0.32	0/675	0.60	0/898
49	Zq	0.27	0/1078	0.55	0/1453
50	kr	0.28	0/579	0.54	0/785
51	As	0.49	0/1088	0.90	9/1512 (0.6%)
52	Gu	0.35	0/1821	0.56	0/2452
53	Pv	0.34	0/1406	0.53	0/1898
54	aw	0.34	0/1201	0.53	0/1608
55	ox	0.32	0/1167	0.56	0/1574
56	Jy	0.26	0/1288	0.67	0/1728
57	Ez	0.27	0/2012	0.55	2/2750 (0.1%)
All	All	0.36	0/162278	0.54	124/237178 (0.1%)

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
5	V5	0	1
10	rA	0	4
13	CD	0	1
23	AN	0	1
24	DO	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
28	pT	0	1
36	xd	0	1
42	Hj	0	1
All	All	0	11

There are no bond length outliers.

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Bt	119	PRO	N-CA-CB	11.88	110.73	102.65
20	DK	139	PRO	N-CA-CB	11.54	110.49	102.65
20	DK	58	PRO	N-CA-CB	11.52	110.48	102.65
45	sm	77	PRO	N-CA-CB	9.95	109.48	102.81
20	FR	33	PRO	N-CA-CB	9.64	109.93	101.83
23	AN	409	PRO	N-CA-CB	9.02	110.51	103.30
20	Bt	137	PRO	N-CA-CB	8.41	110.79	103.31
23	AN	453	PRO	N-CA-CB	8.40	110.33	103.36
20	FR	89	PRO	N-CA-CB	8.33	112.00	103.25
20	FR	143	PRO	N-CA-CB	8.20	110.57	103.36
20	FR	58	PRO	N-CA-CB	7.93	110.72	103.19
20	Bt	143	PRO	N-CA-CB	7.92	110.33	103.36
23	CW	319	PRO	N-CA-CB	7.83	110.17	103.35
20	DK	143	PRO	N-CA-CB	7.81	110.59	103.33
20	Bt	177	PRO	N-CA-CB	7.79	110.21	103.36
22	KM	163	PRO	N-CA-CB	7.73	110.53	103.34
20	DK	177	PRO	N-CA-CB	7.73	110.65	103.15
23	AN	319	PRO	N-CA-CB	7.72	110.51	103.33
20	Bt	89	PRO	N-CA-CB	7.71	110.50	103.33
20	FR	137	PRO	N-CA-CB	7.67	111.03	102.67
39	Wg	172	PRO	N-CA-CB	7.61	110.06	103.36
22	KM	89	PRO	N-CA-CB	7.54	110.71	102.72
20	DK	89	PRO	N-CA-CB	7.47	111.09	103.25
22	KM	88	PRO	N-CA-CB	7.43	110.29	103.08
39	Wg	185	PRO	N-CA-CB	7.41	111.03	103.25
28	pT	574	PRO	N-CA-CB	7.39	110.20	103.33
51	As	212	PRO	N-CA-CB	7.38	110.20	103.34
23	CW	318	PRO	N-CA-CB	7.38	110.24	103.08
23	AN	369	PRO	N-CA-CB	7.30	110.91	103.25
39	Wg	156	PRO	N-CA-CB	7.28	110.10	103.33
23	AN	318	PRO	N-CA-CB	7.27	110.13	103.08
23	EX	318	PRO	N-CA-CB	7.18	110.04	103.08
51	As	137	PRO	N-CA-CB	7.18	110.11	103.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CW	329	PRO	N-CA-CB	7.15	110.76	103.25
23	EX	453	PRO	N-CA-CB	7.11	110.71	103.25
23	CW	390	PRO	N-CA-CB	7.00	109.97	103.46
23	CW	117	PRO	N-CA-CB	6.98	109.95	103.46
20	Bt	58	PRO	N-CA-CB	6.96	110.55	103.25
23	AN	117	PRO	N-CA-CB	6.93	109.90	103.46
23	CW	150	PRO	N-CA-CB	6.93	110.16	103.51
51	As	135	PRO	N-CA-CB	6.92	109.77	103.34
51	As	56	PRO	N-CA-CB	6.88	109.88	103.41
23	CW	409	PRO	N-CA-CB	6.84	110.43	103.25
51	As	59	PRO	N-CA-CB	6.83	110.42	103.25
23	EX	225	PRO	N-CA-CB	6.79	110.38	103.25
23	AN	390	PRO	N-CA-CB	6.77	110.36	103.25
23	CW	264	PRO	N-CA-CB	6.75	110.34	103.25
20	FR	177	PRO	N-CA-CB	6.73	110.32	103.25
23	EX	409	PRO	N-CA-CB	6.73	110.31	103.25
20	DK	119	PRO	N-CA-CB	6.71	110.30	103.25
39	Wg	150	PRO	N-CA-CB	6.71	111.12	102.86
20	FR	119	PRO	N-CA-CB	6.71	110.30	103.25
23	EX	329	PRO	N-CA-CB	6.70	110.29	103.25
23	AN	305	PRO	N-CA-CB	6.68	109.93	103.51
23	CW	131	PRO	N-CA-CB	6.67	109.91	103.51
22	KM	34	PRO	N-CA-CB	6.66	110.22	102.76
23	EX	319	PRO	N-CA-CB	6.64	110.22	103.25
20	DK	33	PRO	N-CA-CB	6.63	110.18	102.76
22	KM	39	PRO	N-CA-CB	6.62	110.20	103.25
8	F8	123	PRO	N-CA-CB	6.57	110.15	103.25
20	Bt	47	PRO	N-CA-CB	6.57	110.15	103.25
23	AN	329	PRO	N-CA-CB	6.57	110.27	102.85
23	EX	379	PRO	N-CA-CB	6.54	110.12	103.25
20	Bt	33	PRO	N-CA-CB	6.53	110.11	103.25
23	EX	369	PRO	N-CA-CB	6.53	110.61	103.23
20	FR	47	PRO	N-CA-CB	6.53	110.10	103.25
23	CW	369	PRO	N-CA-CB	6.51	110.09	103.25
20	DK	47	PRO	N-CA-CB	6.50	109.75	103.51
22	KM	75	PRO	N-CA-CB	6.50	109.75	102.67
23	AN	241	PRO	N-CA-CB	6.49	110.07	103.25
57	Ez	255	PRO	N-CA-CB	6.48	110.05	103.25
23	CW	225	PRO	N-CA-CB	6.48	109.94	102.88
20	DK	137	PRO	N-CA-CB	6.46	110.03	103.25
2	g2	81	CYS	CA-C-N	6.46	133.88	121.54
2	g2	81	CYS	C-N-CA	6.46	133.88	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Bt	139	PRO	N-CA-CB	6.46	110.03	103.25
23	AN	188	PRO	N-CA-CB	6.43	110.00	103.25
23	CW	58	PRO	N-CA-CB	6.43	110.00	103.25
23	EX	117	PRO	N-CA-CB	6.42	109.99	103.25
23	AN	379	PRO	N-CA-CB	6.40	109.88	102.33
23	EX	390	PRO	N-CA-CB	6.40	109.97	103.25
39	Wg	127	PRO	N-CA-CB	6.39	109.87	103.48
23	EX	264	PRO	N-CA-CB	6.39	109.96	103.25
23	AN	264	PRO	N-CA-CB	6.38	109.95	103.25
22	KM	7	PRO	N-CA-CB	6.33	109.90	103.25
23	CW	188	PRO	N-CA-CB	6.30	109.49	103.19
45	sm	137	PRO	N-CA-CB	6.26	109.82	103.25
57	Ez	251	PRO	N-CA-CB	6.23	109.79	103.25
23	AN	131	PRO	N-CA-CB	6.22	109.78	103.25
22	KM	30	PRO	N-CA-CB	6.21	109.65	102.88
37	1e	1576	G	P-O3'-C3'	6.21	129.52	120.20
23	CW	379	PRO	N-CA-CB	6.20	110.09	103.39
51	As	126	PRO	N-CA-CB	6.15	109.71	103.25
23	CW	453	PRO	N-CA-CB	6.14	110.41	102.86
39	Wg	132	PRO	N-CA-CB	6.13	109.69	103.25
23	CW	305	PRO	N-CA-CB	6.12	110.00	103.52
23	EX	188	PRO	N-CA-CB	6.01	109.89	103.52
51	As	43	PRO	N-CA-CB	6.01	110.17	103.44
39	Wg	138	PRO	N-CA-CB	5.96	110.19	102.86
23	EX	241	PRO	N-CA-CB	5.88	110.03	103.44
23	EX	305	PRO	N-CA-CB	5.88	110.03	103.44
23	EX	131	PRO	N-CA-CB	5.86	110.01	103.44
23	AN	225	PRO	N-CA-CB	5.83	109.97	103.44
20	FR	139	PRO	N-CA-CB	5.83	110.03	102.86
39	Wg	163	PRO	N-CA-CB	5.79	109.92	103.44
23	EX	150	PRO	N-CA-CB	5.76	109.89	103.44
23	CW	241	PRO	N-CA-CB	5.74	109.64	103.33
51	As	61	PRO	N-CA-CB	5.72	109.85	103.44
23	AN	150	PRO	N-CA-CB	5.67	109.79	103.44
22	KM	148	PRO	N-CA-CB	5.63	109.75	103.44
11	tB	36	CYS	CA-CB-SG	5.57	127.21	114.40
22	KM	98	VAL	CA-C-O	-5.51	117.84	122.63
37	1e	2541	U	P-O3'-C3'	5.44	128.37	120.20
51	As	121	PRO	N-CA-CB	5.42	109.29	103.33
23	AN	356	ILE	CA-C-N	5.41	129.19	121.03
23	AN	356	ILE	C-N-CA	5.41	129.19	121.03
39	Wg	51	PRO	N-CA-CB	5.40	109.49	103.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	tB	31	PHE	CA-C-N	5.36	128.86	120.82
11	tB	31	PHE	C-N-CA	5.36	128.86	120.82
37	1e	1038	C	P-O3'-C3'	5.28	128.11	120.20
37	1e	1815	U	P-O3'-C3'	5.27	128.10	120.20
37	1e	1027	A	P-O3'-C3'	5.24	128.06	120.20
37	1e	2029	A	P-O3'-C3'	5.15	127.92	120.20
37	1e	1576	G	C2'-C3'-O3'	5.11	117.17	109.50

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	AN	435	THR	Peptide
13	CD	138	ALA	Peptide
24	DO	318	LEU	Peptide
42	Hj	34	PHE	Peptide
5	V5	89	ASP	Peptide
28	pT	468	LEU	Peptide
10	rA	177	ASN	Peptide
10	rA	353	ARG	Peptide
10	rA	354	ILE	Peptide
10	rA	558	TYR	Peptide
36	xd	4	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	h1	961	0	1063	5	0
2	g2	885	0	932	11	0
3	b3	422	0	413	2	0
4	B4	1901	0	1964	10	0
5	V5	990	0	1029	7	0
6	O6	1548	0	1651	1	0
7	f7	847	0	871	1	0
8	F8	1241	0	1195	5	0
9	v9	748	0	648	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	rA	5044	0	4945	36	0
11	tB	1246	0	1236	11	0
12	cC	689	0	664	7	0
13	CD	2968	0	3006	19	0
14	yE	1786	0	1767	15	0
15	UF	864	0	844	5	0
16	dG	862	0	892	5	0
17	eH	1034	0	1101	6	0
18	xI	524	0	535	25	0
19	qJ	1022	0	1052	7	0
20	Bt	816	0	361	0	0
20	DK	816	0	361	3	0
20	FR	816	0	361	0	0
21	LL	1492	0	1490	6	0
22	KM	796	0	394	8	0
23	AN	1843	0	775	2	0
23	CW	2120	0	911	6	0
23	EX	1725	0	724	5	0
24	DO	2675	0	2740	8	0
25	RP	1374	0	1360	6	0
26	MQ	1042	0	1125	6	0
27	mS	711	0	732	4	0
28	pT	4285	0	4172	24	0
29	YU	989	0	1077	5	0
30	vV	1875	0	1845	13	0
31	nY	673	0	690	6	0
32	SZ	1420	0	1449	4	0
33	ia	718	0	778	5	0
34	Ib	1446	0	1481	7	0
35	Xc	963	0	1015	12	0
36	xd	601	0	624	8	0
37	1e	69952	0	35148	227	0
38	2f	2579	0	1304	2	0
39	Wg	1190	0	570	10	0
40	jh	677	0	674	4	0
41	li	433	0	466	5	0
42	Hj	1660	0	1634	12	0
43	Qk	1434	0	1528	6	0
44	Tl	1256	0	1287	4	0
45	sm	1036	0	881	7	0
46	3n	3313	0	1675	3	0
47	No	1720	0	1779	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	zp	668	0	643	5	0
49	Zq	1052	0	1071	4	0
50	kr	573	0	579	7	0
51	As	1089	0	502	13	0
52	Gu	1784	0	1863	5	0
53	Pv	1383	0	1374	5	0
54	aw	1170	0	1204	3	0
55	ox	1147	0	1175	4	0
56	Jy	1270	0	1271	7	0
57	Ez	1973	0	1688	9	0
58	1e	223	0	0	0	0
58	2f	1	0	0	0	0
58	3n	6	0	0	0	0
58	B4	1	0	0	0	0
58	CD	2	0	0	0	0
58	No	1	0	0	0	0
58	g2	2	0	0	0	0
58	zp	1	0	0	0	0
All	All	152374	0	108589	546	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 2.

All (546) 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)
2:g2:101:VAL:HG23	18:xI:206:LEU:HD11	1.42	1.01
2:g2:101:VAL:CG2	18:xI:206:LEU:HD11	1.94	0.97
37:1e:1237:G:H1	37:1e:1251:A:H2	0.94	0.93
37:1e:2008:G:H1	37:1e:2014:U:H3	1.07	0.93
37:1e:1982:G:H1	37:1e:2040:U:H3	0.98	0.92
37:1e:1985:G:H1	37:1e:2036:U:H3	1.19	0.89
37:1e:1237:G:N1	37:1e:1251:A:H2	1.74	0.85
37:1e:3348:G:H1	37:1e:3357:U:H3	1.25	0.82
51:As:113:SER:C	51:As:115:VAL:H	1.92	0.77
2:g2:101:VAL:HG22	18:xI:206:LEU:CG	2.15	0.77
2:g2:101:VAL:HG22	18:xI:206:LEU:HG	1.65	0.77
37:1e:177:U:O2	37:1e:241:G:N1	2.17	0.77
37:1e:3160:U:H3	37:1e:3290:G:H1	1.33	0.74
37:1e:1237:G:N1	37:1e:1251:A:C2	2.52	0.74
2:g2:101:VAL:CG2	18:xI:206:LEU:CD1	2.67	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1e:1975:C:H42	37:1e:2048:G:H1'	1.56	0.69
37:1e:995:U:H3	37:1e:1054:A:H2	1.39	0.69
45:sm:130:PHE:HA	45:sm:134:PHE:HA	1.73	0.68
51:As:66:CYS:HA	51:As:83:ASP:O	1.94	0.67
22:KM:18:VAL:HA	22:KM:57:LYS:HA	1.75	0.67
4:B4:3:ARG:HH11	37:1e:911:C:H42	1.43	0.66
37:1e:2467:G:O2'	37:1e:2488:A:N6	2.29	0.66
37:1e:1986:U:H3	37:1e:2035:G:H1	1.43	0.65
19:qJ:20:VAL:HG21	37:1e:3171:U:H5''	1.79	0.64
9:v9:174:LYS:O	9:v9:175:GLN:C	2.41	0.64
30:vV:156:ARG:HA	30:vV:241:LYS:HG3	1.80	0.64
37:1e:177:U:O2	37:1e:241:G:C6	2.51	0.63
28:pT:292:ARG:HD3	28:pT:473:LEU:HD11	1.80	0.63
37:1e:3170:A:H1'	37:1e:3171:U:H2'	1.81	0.63
37:1e:3234:A:H61	37:1e:3253:G:H1	1.44	0.63
23:AN:371:THR:HA	23:AN:406:THR:H	1.65	0.62
18:xI:210:VAL:HG21	49:Zq:84:ARG:NH1	2.13	0.62
37:1e:173:G:O6	37:1e:246:U:O4	2.18	0.62
37:1e:937:G:N2	37:1e:961:C:OP1	2.31	0.62
17:eH:105:ARG:NH2	37:1e:1412:G:OP1	2.33	0.61
51:As:67:ILE:HD13	51:As:77:ALA:HB1	1.81	0.61
10:rA:206:VAL:O	36:xd:3:GLN:NE2	2.33	0.61
37:1e:1953:G:N2	37:1e:2091:U:OP2	2.33	0.61
1:h1:10:ARG:NH1	1:h1:60:GLU:OE2	2.33	0.61
8:F8:2:SER:N	37:1e:1387:G:HO2'	1.99	0.61
36:xd:45:TRP:NE1	37:1e:2828:G:N7	2.50	0.60
37:1e:1978:A:N7	37:1e:2044:U:O4	2.34	0.60
37:1e:2091:U:H5'	37:1e:2092:A:H5'	1.84	0.60
31:nY:49:ARG:HH21	31:nY:52:ALA:HB2	1.66	0.60
10:rA:80:ASP:OD2	10:rA:245:HIS:NE2	2.35	0.59
25:RP:5:ARG:NH2	37:1e:1513:G:OP1	2.35	0.59
10:rA:282:SER:HB3	10:rA:338:LYS:HE3	1.83	0.59
20:DK:118:VAL:H	23:CW:252:ARG:HA	1.67	0.59
36:xd:72:LYS:HG3	36:xd:73:VAL:HG23	1.83	0.59
17:eH:19:ARG:HD3	17:eH:33:ARG:HB2	1.84	0.59
51:As:113:SER:C	51:As:115:VAL:N	2.60	0.59
37:1e:2473:C:H3'	37:1e:2474:G:H4'	1.84	0.59
23:EX:398:THR:HA	23:EX:447:ARG:O	2.04	0.58
34:Ib:23:ARG:HG3	34:Ib:23:ARG:HH11	1.68	0.58
10:rA:619:GLN:O	41:li:46:ARG:NH2	2.36	0.58
4:B4:27:ALA:O	4:B4:128:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:CW:22:ARG:O	37:1e:2454:G:N2	2.37	0.58
15:UF:112:PRO:HD3	28:pT:4:ALA:HB3	1.85	0.58
10:rA:268:VAL:HG11	10:rA:305:LEU:HB2	1.85	0.57
28:pT:344:THR:HB	28:pT:354:ILE:HD13	1.86	0.57
1:h1:66:VAL:HG11	35:Xc:49:ALA:HB1	1.84	0.57
9:v9:159:ASP:O	9:v9:160:LEU:C	2.46	0.57
37:1e:1258:U:H4'	39:Wg:57:ARG:NH1	2.19	0.57
37:1e:1348:U:OP1	43:Qk:39:ARG:NH1	2.38	0.57
3:b3:35:VAL:O	3:b3:40:ARG:NH1	2.37	0.57
18:xI:207:PRO:O	49:Zq:84:ARG:HD2	2.05	0.57
37:1e:1978:A:H62	37:1e:2044:U:H3	1.51	0.57
37:1e:2452:G:O6	37:1e:2494:A:N1	2.36	0.57
17:eH:100:ILE:O	17:eH:105:ARG:NH1	2.38	0.57
36:xd:6:TYR:H	37:1e:2898:G:H22	1.53	0.57
32:SZ:113:ARG:NH1	37:1e:1211:U:O2'	2.38	0.57
19:qJ:93:ARG:NH2	37:1e:1414:G:OP1	2.38	0.56
37:1e:1566:A:N6	37:1e:1567:U:O2	2.38	0.56
9:v9:160:LEU:O	9:v9:161:VAL:C	2.48	0.56
37:1e:3351:U:O2'	37:1e:3353:G:N2	2.39	0.56
51:As:113:SER:O	51:As:115:VAL:N	2.38	0.56
17:eH:3:SER:OG	17:eH:4:LEU:N	2.38	0.56
35:Xc:24:LYS:HE3	35:Xc:26:ARG:HG2	1.87	0.56
37:1e:1982:G:N2	37:1e:2040:U:O2	2.39	0.56
2:g2:101:VAL:CG2	18:xI:206:LEU:CG	2.83	0.56
37:1e:3283:U:H2'	37:1e:3284:G:H8	1.70	0.56
10:rA:408:GLY:H	10:rA:411:VAL:HB	1.69	0.56
36:xd:30:ARG:NH1	37:1e:3120:C:OP1	2.38	0.56
29:YU:51:ARG:NH1	46:3n:71:A:OP2	2.39	0.56
37:1e:3157:U:H4'	37:1e:3158:G:H5'	1.87	0.56
14:yE:66:ASN:HD22	14:yE:112:ASP:HA	1.71	0.55
18:xI:200:THR:O	18:xI:202:ARG:HG3	2.06	0.55
37:1e:2641:U:OP2	44:Tl:10:ARG:NH2	2.40	0.55
51:As:32:VAL:HA	51:As:208:SER:HA	1.88	0.55
4:B4:128:ARG:NH1	37:1e:2177:G:OP2	2.40	0.55
10:rA:443:ASP:O	11:tB:75:ARG:NH1	2.37	0.55
37:1e:3246:G:N2	48:zp:79:GLY:O	2.40	0.55
27:mS:36:PHE:O	27:mS:41:ARG:NH1	2.40	0.55
57:Ez:198:TYR:HE1	57:Ez:203:HIS:HB3	1.72	0.55
37:1e:2008:G:N2	37:1e:2014:U:O2	2.40	0.55
37:1e:177:U:O2	37:1e:241:G:O6	2.24	0.55
30:vV:168:LYS:HB3	30:vV:171:PHE:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:Jy:10:ARG:NH2	56:Jy:151:SER:O	2.41	0.54
10:rA:584:ARG:NH2	28:pT:424:SER:O	2.39	0.54
24:DO:338:LYS:O	24:DO:340:GLY:N	2.40	0.54
37:1e:2045:G:OP2	37:1e:2047:A:N6	2.41	0.54
26:MQ:72:LEU:HD11	26:MQ:81:VAL:HG12	1.89	0.54
28:pT:262:ARG:HA	28:pT:303:ALA:HB2	1.89	0.54
10:rA:227:ARG:NH1	10:rA:231:GLU:O	2.41	0.54
14:yE:121:ILE:O	14:yE:139:ARG:NH2	2.40	0.54
24:DO:328:ASN:OD1	52:Gu:48:ASN:ND2	2.40	0.54
47:No:159:ARG:HB2	47:No:164:LEU:HB2	1.89	0.54
18:xI:204:GLY:C	18:xI:206:LEU:H	2.14	0.54
19:qJ:14:SER:OG	48:zp:100:LYS:O	2.25	0.54
37:1e:1778:G:O2'	37:1e:1780:G:OP2	2.26	0.54
37:1e:2471:U:O4	37:1e:2474:G:N2	2.41	0.54
37:1e:3100:U:OP1	48:zp:18:ARG:NH2	2.40	0.54
28:pT:110:ASP:OD1	28:pT:356:ARG:NH2	2.40	0.54
37:1e:1096:U:OP1	44:TL:116:ARG:NH2	2.40	0.54
37:1e:1986:U:O4	37:1e:2035:G:O6	2.25	0.54
5:V5:80:ARG:NH1	5:V5:117:PRO:O	2.40	0.54
34:Ib:20:ILE:HG23	34:Ib:25:VAL:HG22	1.90	0.54
1:h1:5:LYS:HB2	1:h1:8:GLU:HG3	1.89	0.53
13:CD:241:LYS:NZ	37:1e:1891:A:OP2	2.40	0.53
5:V5:81:GLN:NE2	5:V5:83:LYS:O	2.40	0.53
51:As:21:ASN:HA	51:As:25:LYS:HA	1.89	0.53
31:nY:49:ARG:NH2	37:1e:1793:C:OP2	2.40	0.53
37:1e:1969:G:H21	37:1e:2055:U:H3	1.54	0.53
37:1e:364:G:OP2	40:jh:52:LYS:NZ	2.42	0.53
24:DO:31:ARG:NH1	37:1e:674:G:OP1	2.42	0.53
43:Qk:54:LEU:O	43:Qk:59:ARG:NH1	2.41	0.53
12:cC:61:MET:HB2	18:xI:201:ASN:ND2	2.24	0.53
19:qJ:51:LYS:NZ	37:1e:436:A:OP1	2.42	0.53
34:Ib:132:VAL:HG11	34:Ib:157:ASN:HD22	1.73	0.53
42:Hj:75:ILE:HD11	47:No:18:VAL:HG23	1.90	0.53
51:As:110:PHE:O	51:As:111:ILE:HG13	2.08	0.53
6:O6:100:GLU:HG2	19:qJ:10:PRO:HA	1.90	0.53
30:vV:323:VAL:HA	30:vV:338:ILE:HG22	1.91	0.53
37:1e:1002:A:N3	57:Ez:15:ARG:NH2	2.57	0.53
39:Wg:53:LEU:C	39:Wg:55:GLU:H	2.16	0.53
37:1e:2041:U:H3'	37:1e:2042:G:H2'	1.91	0.52
18:xI:111:ASP:N	18:xI:111:ASP:OD1	2.39	0.52
11:tB:43:ARG:NH1	55:ox:15:THR:OG1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:ox:19:ASP:OD1	55:ox:19:ASP:N	2.42	0.52
37:1e:829:U:H3	37:1e:895:A:H62	1.58	0.52
35:Xc:99:LYS:HE2	35:Xc:106:VAL:H	1.75	0.52
37:1e:1156:C:OP2	52:Gu:94:LYS:NZ	2.43	0.52
10:rA:37:PHE:HE1	37:1e:2820:A:H5''	1.75	0.52
28:pT:146:HIS:HD2	28:pT:149:GLY:H	1.58	0.52
37:1e:545:U:OP2	37:1e:547:G:N2	2.43	0.52
21:LL:73:ARG:NH2	37:1e:110:G:OP2	2.41	0.52
33:ia:29:LYS:O	37:1e:266:A:N6	2.43	0.52
37:1e:1237:G:O6	37:1e:1251:A:N1	2.43	0.52
23:EX:191:LYS:O	23:EX:217:ARG:N	2.40	0.51
35:Xc:72:MET:SD	35:Xc:141:ILE:HD11	2.50	0.51
37:1e:1863:G:N1	37:1e:1866:C:OP2	2.36	0.51
41:li:43:ASN:HB3	41:li:46:ARG:HB2	1.91	0.51
10:rA:294:ARG:HE	10:rA:295:PRO:HD2	1.75	0.51
13:CD:173:GLN:HG3	37:1e:3313:U:H4'	1.92	0.51
5:V5:15:LEU:HA	5:V5:53:SER:HB3	1.92	0.51
37:1e:2356:A:H61	37:1e:2983:C:H5	1.57	0.51
23:CW:388:SER:HA	23:CW:395:PHE:HA	1.92	0.51
37:1e:2522:G:O2'	37:1e:2524:A:OP2	2.24	0.51
37:1e:1025:A:H4'	37:1e:1026:A:H5''	1.91	0.51
57:Ez:197:SER:O	57:Ez:202:GLY:N	2.42	0.51
28:pT:76:LEU:O	28:pT:87:ARG:NH1	2.44	0.51
30:vV:317:GLU:OE2	30:vV:368:SER:OG	2.29	0.51
37:1e:1253:U:H5''	37:1e:1263:A:H2	1.75	0.51
10:rA:595:ASP:OD1	10:rA:595:ASP:N	2.42	0.51
2:g2:101:VAL:HG22	18:xI:206:LEU:CD2	2.41	0.51
22:KM:79:SER:O	22:KM:80:LEU:C	2.53	0.51
27:mS:92:GLU:OE1	30:vV:376:ASN:ND2	2.44	0.51
37:1e:1013:G:N7	37:1e:1039:U:N3	2.57	0.51
37:1e:1957:G:H22	37:1e:2084:C:H1'	1.76	0.51
13:CD:77:THR:OG1	13:CD:326:GLY:O	2.29	0.51
37:1e:1236:G:N2	37:1e:1244:A:OP1	2.44	0.51
37:1e:2208:A:O2'	37:1e:2209:U:O2	2.29	0.51
25:RP:114:LYS:NZ	37:1e:1953:G:O6	2.40	0.51
18:xI:202:ARG:C	18:xI:204:GLY:H	2.19	0.50
37:1e:1241:U:O2'	37:1e:1243:G:N7	2.36	0.50
25:RP:135:LYS:NZ	37:1e:1949:G:OP2	2.45	0.50
37:1e:1959:G:H2'	37:1e:1960:A:C8	2.46	0.50
4:B4:33:ASP:OD1	4:B4:33:ASP:N	2.45	0.50
33:ia:40:VAL:HG11	47:No:5:LYS:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:UF:43:VAL:HG13	15:UF:49:ASN:HB3	1.93	0.50
15:UF:19:VAL:HG12	15:UF:105:LEU:HD23	1.94	0.50
37:1e:2584:G:O2'	42:Hj:240:ASN:OD1	2.28	0.50
10:rA:1:MET:N	10:rA:4:SER:O	2.40	0.50
11:tB:45:ASN:HB3	11:tB:48:LYS:HB2	1.94	0.50
13:CD:376:LYS:NZ	37:1e:3330:A:OP2	2.40	0.50
5:V5:23:MET:HE1	5:V5:78:VAL:HG22	1.94	0.50
30:vV:293:THR:HG23	30:vV:330:ARG:HH12	1.75	0.50
37:1e:2901:G:O2'	37:1e:3024:A:N1	2.44	0.50
10:rA:178:VAL:O	10:rA:180:LYS:N	2.45	0.50
28:pT:293:GLY:HA3	37:1e:379:C:H5''	1.93	0.50
37:1e:904:A:OP2	40:jh:30:GLN:NE2	2.45	0.50
37:1e:2570:U:OP1	37:1e:2573:G:N2	2.45	0.50
37:1e:3231:U:H2'	37:1e:3232:G:H8	1.77	0.50
15:UF:94:ARG:NH2	37:1e:1679:A:OP1	2.45	0.49
37:1e:2941:A:H5''	37:1e:2943:G:H4'	1.94	0.49
28:pT:201:ALA:HA	28:pT:218:ILE:HD13	1.92	0.49
23:CW:62:GLY:O	37:1e:2454:G:N2	2.45	0.49
37:1e:412:G:OP1	53:Pv:62:ARG:NH1	2.45	0.49
37:1e:1982:G:O6	37:1e:2040:U:O4	2.29	0.49
2:g2:101:VAL:CG2	18:xI:206:LEU:HD21	2.43	0.49
16:dG:47:ASP:OD1	16:dG:47:ASP:N	2.40	0.49
42:Hj:52:TRP:O	42:Hj:57:ARG:NH2	2.43	0.49
57:Ez:32:GLN:O	57:Ez:36:LEU:HB2	2.12	0.49
5:V5:27:ASP:OD1	5:V5:27:ASP:N	2.42	0.49
37:1e:1899:G:O2'	37:1e:2334:U:O4	2.27	0.49
28:pT:248:ARG:HB2	28:pT:251:LEU:HB2	1.93	0.49
28:pT:279:LEU:HD13	28:pT:477:LYS:HD2	1.95	0.49
37:1e:1201:C:N4	37:1e:2825:C:OP2	2.46	0.49
13:CD:171:LEU:HD21	13:CD:333:LYS:HB2	1.94	0.49
37:1e:2745:G:N2	37:1e:2748:A:OP2	2.38	0.49
10:rA:184:LEU:O	10:rA:188:THR:OG1	2.31	0.49
14:yE:90:ASP:OD1	14:yE:90:ASP:N	2.36	0.49
28:pT:319:ILE:O	28:pT:504:CYS:HA	2.12	0.49
34:Ib:23:ARG:HG3	34:Ib:23:ARG:NH1	2.27	0.49
4:B4:21:ARG:HD3	37:1e:824:C:H5''	1.95	0.49
22:KM:79:SER:O	22:KM:82:ILE:N	2.46	0.49
37:1e:1494:U:OP1	41:li:42:ARG:NH1	2.40	0.48
33:ia:26:ILE:HD11	37:1e:155:G:H1'	1.95	0.48
37:1e:1561:G:N1	37:1e:1578:C:O2	2.46	0.48
26:MQ:23:ILE:HA	26:MQ:63:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:No:183:THR:HG22	47:No:187:ARG:HB2	1.95	0.48
47:No:190:THR:HG22	47:No:193:ARG:HH12	1.79	0.48
23:EX:325:SER:HA	23:EX:471:SER:HA	1.96	0.48
13:CD:28:ARG:NH2	37:1e:3140:G:N7	2.61	0.48
26:MQ:59:ASN:ND2	37:1e:1185:C:OP1	2.47	0.48
37:1e:2017:G:H3'	37:1e:2018:C:H5'	1.95	0.48
37:1e:2452:G:O6	37:1e:2494:A:C6	2.66	0.48
10:rA:643:LYS:NZ	37:1e:2140:U:OP2	2.39	0.48
50:kr:24:THR:HG22	50:kr:76:ASN:HB3	1.96	0.48
57:Ez:30:TYR:HA	57:Ez:33:ARG:HB3	1.95	0.48
56:Jy:15:GLU:OE1	56:Jy:72:ARG:NH1	2.46	0.48
37:1e:1954:G:H4'	37:1e:1955:U:H2'	1.94	0.48
14:yE:85:ARG:NH2	14:yE:89:PRO:O	2.47	0.48
35:Xc:137:ARG:O	35:Xc:138:ILE:C	2.56	0.48
38:2f:49:G:O2'	57:Ez:58:LYS:NZ	2.46	0.48
39:Wg:60:TRP:C	39:Wg:62:GLY:H	2.21	0.48
37:1e:1565:G:O6	37:1e:1574:C:N4	2.45	0.48
53:Pv:126:ARG:HA	53:Pv:140:GLU:HG2	1.96	0.48
37:1e:1207:G:H3'	39:Wg:2:PRO:HG2	1.95	0.47
21:LL:27:ASP:HB3	46:3n:29:U:H5''	1.95	0.47
37:1e:2442:G:H2'	37:1e:2443:A:H8	1.79	0.47
37:1e:1553:U:H4'	37:1e:1554:U:H5'	1.96	0.47
37:1e:1750:A:OP1	50:kr:44:LYS:NZ	2.44	0.47
2:g2:44:CYS:HB3	2:g2:48:GLY:H	1.79	0.47
10:rA:150:LEU:HA	10:rA:153:VAL:HG22	1.96	0.47
12:cC:61:MET:HG3	18:xI:203:PHE:O	2.13	0.47
13:CD:41:VAL:HA	13:CD:185:GLY:HA3	1.96	0.47
35:Xc:130:ASP:HB3	35:Xc:133:ASP:OD2	2.14	0.47
23:AN:217:ARG:HA	23:AN:243:LEU:HA	1.95	0.47
37:1e:567:G:H2'	37:1e:568:G:C8	2.50	0.47
37:1e:1993:G:N2	37:1e:2030:C:O2'	2.47	0.47
37:1e:3310:A:OP1	53:Pv:74:LYS:NZ	2.42	0.47
51:As:67:ILE:HD11	51:As:82:VAL:CB	2.43	0.47
37:1e:2059:U:H5	37:1e:2061:G:H5'	1.80	0.47
13:CD:187:SER:O	13:CD:190:GLU:N	2.48	0.47
13:CD:384:LYS:HD2	37:1e:3368:U:H5'	1.96	0.47
37:1e:943:U:H3'	54:aw:13:GLY:HA2	1.97	0.47
47:No:36:ILE:HG12	47:No:64:VAL:HG23	1.97	0.47
18:xI:145:TRP:HZ3	31:nY:27:LYS:HD2	1.78	0.47
22:KM:15:LEU:O	22:KM:16:ARG:C	2.57	0.47
22:KM:155:ILE:HA	22:KM:159:GLU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Xc:56:LEU:HD23	35:Xc:93:GLN:HE22	1.80	0.47
37:1e:3234:A:N6	37:1e:3253:G:H1	2.13	0.47
54:aw:34:MET:HE3	54:aw:34:MET:HB3	1.75	0.47
56:Jy:99:THR:OG1	56:Jy:101:ASN:ND2	2.47	0.47
28:pT:340:VAL:HG22	28:pT:437:ILE:HB	1.97	0.47
37:1e:2433:U:H1'	47:No:125:SER:HB3	1.96	0.47
51:As:111:ILE:HD11	51:As:151:VAL:CB	2.44	0.47
10:rA:312:VAL:HG23	10:rA:315:VAL:HB	1.97	0.47
35:Xc:57:ASP:OD1	35:Xc:57:ASP:N	2.36	0.47
37:1e:2768:U:H2'	37:1e:2769:A:C8	2.50	0.47
13:CD:228:GLY:O	13:CD:232:ARG:HB2	2.15	0.46
28:pT:155:SER:HB3	28:pT:504:CYS:HB3	1.97	0.46
37:1e:1696:A:H2'	37:1e:1697:A:C8	2.50	0.46
13:CD:93:VAL:HG23	13:CD:102:LEU:HD22	1.97	0.46
22:KM:84:ALA:O	22:KM:85:LEU:C	2.59	0.46
37:1e:3160:U:O4	37:1e:3290:G:O6	2.33	0.46
32:SZ:52:LYS:H	32:SZ:55:SER:HB2	1.80	0.46
37:1e:209:A:O2'	37:1e:211:A:OP2	2.33	0.46
37:1e:2050:C:O2'	37:1e:2052:G:N2	2.49	0.46
37:1e:2068:U:H3'	37:1e:2069:G:H8	1.80	0.46
37:1e:2800:G:O6	54:aw:42:ARG:NH2	2.48	0.46
10:rA:569:ASP:O	28:pT:262:ARG:NH2	2.42	0.46
28:pT:244:VAL:HG22	28:pT:319:ILE:HG23	1.98	0.46
30:vV:157:ALA:HB3	30:vV:201:TYR:HB2	1.96	0.46
37:1e:1005:G:N2	37:1e:1044:U:OP2	2.44	0.46
37:1e:2090:U:H1'	37:1e:2095:G:H1	1.80	0.46
39:Wg:53:LEU:C	39:Wg:55:GLU:N	2.74	0.46
17:eH:89:THR:HG22	17:eH:117:ILE:HG13	1.96	0.46
28:pT:195:VAL:HG11	28:pT:524:ARG:HH11	1.81	0.46
30:vV:390:ASP:OD1	30:vV:390:ASP:N	2.45	0.46
23:EX:384:MET:HA	23:EX:398:THR:O	2.15	0.46
36:xd:54:ARG:HA	36:xd:54:ARG:HD2	1.73	0.46
13:CD:308:MET:HE2	37:1e:3329:U:H5''	1.97	0.46
37:1e:1347:U:H2'	37:1e:1355:A:H61	1.81	0.46
42:Hj:163:VAL:HA	42:Hj:166:LEU:HD23	1.98	0.46
50:kr:32:ASN:HD21	50:kr:35:GLY:H	1.63	0.46
37:1e:1124:U:O2'	37:1e:2635:A:OP1	2.33	0.46
37:1e:1637:A:H5''	49:Zq:16:GLY:HA3	1.98	0.46
37:1e:2442:G:H2'	37:1e:2443:A:C8	2.51	0.46
19:qJ:10:PRO:HD2	48:zp:101:THR:HA	1.98	0.46
37:1e:595:G:OP1	52:Gu:33:ARG:NH2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1e:3322:A:H2'	37:1e:3323:A:C8	2.51	0.46
50:kr:23:ALA:O	50:kr:75:VAL:HA	2.16	0.46
9:v9:416:TYR:O	9:v9:434:LYS:NZ	2.49	0.46
32:SZ:12:ARG:HD3	32:SZ:22:PRO:HD2	1.99	0.45
37:1e:767:U:O2'	37:1e:2772:C:N4	2.48	0.45
37:1e:1661:G:H2'	37:1e:1662:G:C8	2.51	0.45
47:No:84:PRO:HA	47:No:87:GLN:HG3	1.98	0.45
8:F8:17:ALA:O	37:1e:591:G:O2'	2.34	0.45
16:dG:24:SER:HB2	16:dG:27:LYS:HD2	1.98	0.45
10:rA:184:LEU:HD22	10:rA:220:ASP:HB2	1.98	0.45
27:mS:72:LEU:O	27:mS:80:ARG:HA	2.16	0.45
37:1e:2039:C:H2'	37:1e:2040:U:C6	2.51	0.45
38:2f:39:C:H4'	56:Jy:44:THR:HG23	1.98	0.45
2:g2:101:VAL:HG22	18:xI:206:LEU:HD21	1.98	0.45
37:1e:3100:U:OP2	48:zp:14:LYS:NZ	2.47	0.45
45:sm:134:PHE:N	45:sm:167:ASN:O	2.48	0.45
56:Jy:92:ARG:HG3	56:Jy:172:LEU:HD12	1.98	0.45
11:tB:6:CYS:SG	11:tB:9:CYS:N	2.88	0.45
11:tB:33:ARG:HG3	11:tB:35:LYS:H	1.80	0.45
37:1e:120:G:N2	42:Hj:126:SER:O	2.45	0.45
37:1e:2048:G:H5''	37:1e:2049:A:H5'	1.98	0.45
44:Tl:102:ARG:HA	44:Tl:102:ARG:HD2	1.78	0.45
47:No:17:ASP:N	47:No:17:ASP:OD1	2.49	0.45
50:kr:66:ILE:HD13	50:kr:77:ARG:HH12	1.82	0.45
14:yE:14:GLY:O	14:yE:61:ARG:NH1	2.49	0.45
25:RP:116:ASP:OD1	25:RP:116:ASP:N	2.49	0.45
37:1e:1717:U:H2'	37:1e:1718:G:C8	2.52	0.45
14:yE:142:ILE:HG23	14:yE:145:ASN:HB2	1.99	0.45
16:dG:87:ASN:OD1	16:dG:87:ASN:N	2.49	0.45
37:1e:2538:U:OP1	37:1e:2539:C:N4	2.50	0.45
37:1e:3302:U:H3	37:1e:3312:U:H3	1.64	0.45
10:rA:392:ASP:O	10:rA:395:ARG:NE	2.48	0.45
42:Hj:227:ASP:OD1	42:Hj:227:ASP:N	2.50	0.45
51:As:36:VAL:HA	51:As:203:SER:O	2.16	0.45
36:xd:44:GLY:HA2	37:1e:1301:A:H1'	1.99	0.45
37:1e:664:U:H2'	37:1e:665:A:C8	2.52	0.45
37:1e:2864:A:N7	37:1e:2865:U:N3	2.64	0.45
42:Hj:144:GLU:HA	42:Hj:173:MET:HE2	1.99	0.45
10:rA:170:LEU:O	10:rA:218:ALA:HA	2.17	0.44
13:CD:266:ARG:NH2	37:1e:2392:C:O2'	2.49	0.44
42:Hj:95:ASN:HD21	42:Hj:98:ARG:HH21	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:CD:236:LYS:HD3	37:1e:2880:U:H5''	1.98	0.44
24:DO:181:VAL:HG11	24:DO:224:GLY:HA3	1.98	0.44
35:Xc:32:ARG:NH1	37:1e:1579:C:O2	2.50	0.44
37:1e:1991:G:H2'	37:1e:1992:U:C2	2.52	0.44
37:1e:2495:C:H2'	37:1e:2496:C:H2'	1.99	0.44
30:vV:280:SER:OG	30:vV:281:ASN:N	2.51	0.44
32:SZ:47:LYS:HB2	32:SZ:47:LYS:HE3	1.86	0.44
37:1e:2357:A:H2'	37:1e:2358:A:C8	2.51	0.44
8:F8:5:LYS:HA	8:F8:5:LYS:HD2	1.78	0.44
8:F8:105:TYR:OH	8:F8:137:ASP:OD2	2.31	0.44
10:rA:242:ALA:O	10:rA:246:LEU:HB2	2.18	0.44
25:RP:84:THR:O	25:RP:88:ARG:HB2	2.18	0.44
27:mS:12:CYS:SG	27:mS:21:THR:OG1	2.69	0.44
35:Xc:26:ARG:HD2	42:Hj:50:VAL:HG21	1.99	0.44
37:1e:3160:U:H5''	37:1e:3396:U:H2'	1.99	0.44
37:1e:1364:C:OP1	52:Gu:110:ARG:NH2	2.50	0.44
42:Hj:156:ASP:OD1	42:Hj:156:ASP:N	2.50	0.44
57:Ez:129:TYR:OH	57:Ez:175:HIS:O	2.28	0.44
10:rA:433:PRO:HB3	13:CD:300:ARG:HG3	1.98	0.44
14:yE:9:ASN:ND2	37:1e:3018:C:OP1	2.51	0.44
29:YU:112:ASP:OD1	29:YU:112:ASP:N	2.50	0.44
30:vV:286:MET:HE3	30:vV:286:MET:HB3	1.80	0.44
37:1e:1119:C:H2'	37:1e:1120:A:H8	1.83	0.44
37:1e:1194:G:H2'	37:1e:1195:A:C8	2.53	0.44
37:1e:2836:C:H3'	37:1e:2837:A:C8	2.53	0.44
29:YU:16:ARG:NH1	37:1e:216:G:OP1	2.51	0.44
39:Wg:111:THR:C	39:Wg:113:LYS:H	2.26	0.44
40:jh:14:LYS:HZ2	40:jh:25:ARG:HH21	1.65	0.44
4:B4:33:ASP:O	4:B4:37:ARG:HB2	2.17	0.44
10:rA:26:GLN:HE22	37:1e:1301:A:H62	1.66	0.44
12:cC:69:TYR:HE2	18:xI:200:THR:HG1	1.63	0.44
24:DO:308:LYS:NZ	37:1e:594:U:O2'	2.51	0.44
37:1e:3348:G:O6	37:1e:3357:U:O4	2.34	0.44
37:1e:3375:A:O2'	37:1e:3378:C:OP2	2.33	0.44
2:g2:108:GLN:HE22	18:xI:205:VAL:CG2	2.30	0.43
4:B4:97:ASN:OD1	31:nY:87:ARG:NH1	2.51	0.43
9:v9:158:GLU:O	9:v9:159:ASP:C	2.60	0.43
12:cC:27:TYR:OH	12:cC:55:GLU:OE1	2.32	0.43
15:UF:19:VAL:HG21	15:UF:30:PRO:HB3	2.00	0.43
44:Tl:14:MET:HE3	44:Tl:14:MET:HB2	1.80	0.43
4:B4:117:GLU:OE2	4:B4:163:ARG:NH2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:yE:158:GLY:HA2	14:yE:179:VAL:HB	2.00	0.43
26:MQ:121:MET:HE2	26:MQ:125:LYS:HD2	2.00	0.43
37:1e:1786:G:H2'	37:1e:1787:A:C8	2.53	0.43
37:1e:358:G:N2	37:1e:361:A:OP2	2.41	0.43
1:h1:77:PRO:HD2	1:h1:80:LEU:HD12	2.00	0.43
10:rA:434:GLU:OE2	14:yE:79:GLN:NE2	2.52	0.43
30:vV:267:MET:HG2	30:vV:294:ALA:HB1	2.01	0.43
45:sm:67:VAL:O	45:sm:71:ASP:CB	2.67	0.43
9:v9:173:GLU:O	9:v9:174:LYS:C	2.61	0.43
10:rA:639:ARG:HB2	37:1e:2400:G:C5	2.53	0.43
11:tB:6:CYS:HB3	11:tB:11:SER:H	1.83	0.43
24:DO:98:ARG:NH2	37:1e:804:C:OP1	2.46	0.43
37:1e:158:G:H2'	37:1e:159:A:H8	1.84	0.43
37:1e:549:U:H2'	37:1e:550:A:H8	1.84	0.43
37:1e:2768:U:H2'	37:1e:2769:A:H8	1.82	0.43
1:h1:79:ASP:OD1	1:h1:79:ASP:N	2.45	0.43
26:MQ:126:GLN:NE2	37:1e:3261:C:OP1	2.47	0.43
37:1e:1624:G:O6	37:1e:1819:U:O4	2.37	0.43
13:CD:250:ALA:HB1	37:1e:2947:G:C2	2.53	0.43
22:KM:62:LEU:O	22:KM:63:LYS:C	2.61	0.43
28:pT:100:ILE:O	28:pT:140:LYS:NZ	2.50	0.43
33:ia:47:ILE:HD12	33:ia:47:ILE:HA	1.92	0.43
37:1e:1970:U:HO2'	37:1e:2054:C:H42	1.66	0.43
11:tB:111:ARG:NH1	37:1e:3367:C:OP1	2.52	0.43
21:LL:27:ASP:OD1	21:LL:27:ASP:N	2.45	0.43
19:qJ:41:SER:HB3	37:1e:620:U:H5'	2.01	0.42
28:pT:79:TYR:O	28:pT:87:ARG:NH1	2.52	0.42
37:1e:994:G:N2	37:1e:995:U:O4	2.43	0.42
12:cC:64:LYS:HB2	12:cC:64:LYS:HE2	1.72	0.42
18:xI:201:ASN:C	18:xI:203:PHE:H	2.25	0.42
28:pT:492:THR:HG22	28:pT:494:GLU:H	1.84	0.42
37:1e:2129:U:H2'	37:1e:2130:G:C8	2.54	0.42
37:1e:2213:A:H2'	37:1e:2214:A:C8	2.53	0.42
11:tB:57:LYS:NZ	11:tB:63:LEU:O	2.45	0.42
51:As:32:VAL:H	51:As:171:ASN:HA	1.84	0.42
16:dG:11:GLU:OE2	16:dG:74:ARG:NE	2.51	0.42
37:1e:94:G:H2'	37:1e:95:A:C8	2.54	0.42
37:1e:549:U:H2'	37:1e:550:A:C8	2.54	0.42
37:1e:1493:G:O6	41:li:2:ALA:N	2.52	0.42
37:1e:2452:G:C6	37:1e:2494:A:N1	2.88	0.42
41:li:27:ILE:HD13	46:3n:52:A:H62	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:sm:95:ASP:OD1	45:sm:95:ASP:N	2.52	0.42
57:Ez:40:HIS:HB3	57:Ez:43:LYS:HD2	2.01	0.42
9:v9:160:LEU:O	9:v9:162:LYS:N	2.52	0.42
18:xI:204:GLY:C	18:xI:206:LEU:N	2.78	0.42
29:YU:51:ARG:HG2	29:YU:52:ARG:H	1.84	0.42
37:1e:644:G:N2	37:1e:2372:A:O4'	2.52	0.42
42:Hj:144:GLU:OE2	47:No:6:TYR:OH	2.28	0.42
5:V5:109:MET:HE2	5:V5:109:MET:HB3	1.77	0.42
35:Xc:66:ILE:HD12	35:Xc:120:LYS:HG3	2.02	0.42
37:1e:1565:G:O2'	37:1e:1576:G:OP1	2.37	0.42
37:1e:2057:G:H1	37:1e:2072:G:H5''	1.85	0.42
4:B4:28:LYS:HE2	4:B4:28:LYS:HB3	1.87	0.42
13:CD:57:VAL:HG22	13:CD:73:VAL:HG22	2.02	0.42
13:CD:117:ARG:HA	13:CD:175:LYS:HE3	2.00	0.42
18:xI:208:ASP:O	18:xI:209:ASP:C	2.62	0.42
47:No:103:GLU:OE2	47:No:118:SER:OG	2.32	0.42
51:As:117:ILE:C	51:As:119:GLN:H	2.27	0.42
53:Pv:16:SER:HB3	53:Pv:149:VAL:HG22	2.00	0.42
14:yE:229:PRO:HD2	14:yE:232:ILE:HB	2.02	0.42
25:RP:98:ARG:NH2	25:RP:130:ASN:OD1	2.41	0.42
37:1e:1646:G:O2'	37:1e:1808:G:N2	2.40	0.42
39:Wg:116:PHE:C	39:Wg:118:SER:H	2.27	0.42
50:kr:27:ILE:HG13	50:kr:41:THR:HG22	2.01	0.42
37:1e:339:C:OP1	37:1e:1380:G:O2'	2.37	0.42
10:rA:214:LEU:HD21	14:yE:239:THR:HA	2.02	0.42
13:CD:10:ARG:HH12	13:CD:263:SER:HB2	1.85	0.42
14:yE:68:ARG:NH1	14:yE:112:ASP:O	2.49	0.42
23:EX:357:GLY:O	23:EX:360:SER:N	2.53	0.42
37:1e:528:U:H2'	37:1e:529:A:C8	2.54	0.42
37:1e:2048:G:H4'	37:1e:2049:A:H8	1.85	0.42
3:b3:19:ASN:ND2	37:1e:970:A:OP2	2.51	0.41
10:rA:48:ARG:NH1	37:1e:2938:G:OP1	2.41	0.41
10:rA:385:LEU:HD23	10:rA:396:ARG:HH12	1.85	0.41
20:DK:157:ILE:HA	20:DK:161:ASP:H	1.84	0.41
26:MQ:121:MET:HG3	37:1e:3214:U:C4	2.55	0.41
37:1e:532:A:H2'	37:1e:533:A:C8	2.54	0.41
37:1e:2660:G:OP1	37:1e:2750:U:O2'	2.38	0.41
42:Hj:161:GLU:HA	42:Hj:164:VAL:HG22	2.02	0.41
43:Qk:178:ARG:HE	43:Qk:178:ARG:HB3	1.71	0.41
12:cC:24:THR:HG22	12:cC:91:SER:HB3	2.01	0.41
24:DO:206:LEU:HD23	24:DO:248:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1e:1989:U:H2'	37:1e:1990:U:C5	2.55	0.41
37:1e:2063:U:H2'	37:1e:2064:C:C6	2.55	0.41
37:1e:2711:C:O2'	37:1e:2744:U:OP1	2.35	0.41
28:pT:322:LYS:HG2	28:pT:502:ARG:HG3	2.03	0.41
37:1e:1970:U:O2'	37:1e:2054:C:N4	2.45	0.41
37:1e:3283:U:H2'	37:1e:3284:G:C8	2.53	0.41
45:sm:106:ARG:NH1	45:sm:107:ARG:O	2.52	0.41
7:f7:99:ARG:NH1	37:1e:3275:U:O2'	2.53	0.41
12:cC:30:THR:HG23	12:cC:91:SER:HB2	2.02	0.41
21:LL:176:GLU:OE2	21:LL:183:ARG:NH1	2.53	0.41
33:ia:32:ALA:HA	37:1e:298:U:H5'	2.01	0.41
37:1e:1000:C:O2'	37:1e:1045:C:N4	2.53	0.41
37:1e:1597:C:H5'	37:1e:1696:A:H1'	2.01	0.41
5:V5:70:ARG:NH2	9:v9:397:GLU:OE1	2.40	0.41
14:yE:11:ASN:HB3	14:yE:207:GLY:HA3	2.02	0.41
31:nY:36:ARG:HG3	31:nY:48:LYS:HD3	2.02	0.41
37:1e:396:A:O2'	37:1e:399:A:OP1	2.33	0.41
55:ox:127:LEU:HD23	55:ox:127:LEU:HA	1.92	0.41
57:Ez:116:ASP:OD1	57:Ez:116:ASP:N	2.49	0.41
14:yE:117:VAL:HB	14:yE:121:ILE:HD12	2.02	0.41
17:eH:126:LEU:HD23	17:eH:126:LEU:HA	1.85	0.41
22:KM:82:ILE:O	22:KM:83:THR:C	2.63	0.41
23:CW:453:PRO:HA	23:CW:458:VAL:HA	2.01	0.41
40:jh:48:ASN:OD1	40:jh:54:LYS:NZ	2.50	0.41
43:Qk:123:THR:OG1	43:Qk:125:ASP:OD1	2.36	0.41
56:Jy:117:ASP:HA	56:Jy:118:PRO:HD3	1.93	0.41
10:rA:617:ALA:HB2	53:Pv:125:GLN:HE21	1.86	0.41
21:LL:195:ALA:O	21:LL:199:LYS:CB	2.68	0.41
37:1e:728:G:H5''	43:Qk:43:PRO:HB2	2.01	0.41
37:1e:1231:A:H5''	37:1e:1232:C:H5'	2.03	0.41
39:Wg:116:PHE:C	39:Wg:118:SER:N	2.79	0.41
4:B4:136:ILE:HD13	4:B4:148:VAL:HG12	2.03	0.41
10:rA:439:LYS:NZ	11:tB:97:GLU:OE1	2.54	0.41
34:Ib:85:GLY:HA3	34:Ib:187:ILE:HD12	2.02	0.41
36:xd:63:LYS:HE2	36:xd:63:LYS:HB2	1.91	0.41
39:Wg:38:ARG:O	39:Wg:222:ASP:HA	2.21	0.41
50:kr:32:ASN:OD1	50:kr:36:LYS:N	2.52	0.41
11:tB:6:CYS:HB2	11:tB:32:CYS:HB3	1.78	0.41
14:yE:163:PRO:HA	14:yE:183:ALA:HB1	2.03	0.41
18:xI:210:VAL:HG21	49:Zq:84:ARG:HH12	1.83	0.41
24:DO:113:VAL:HB	24:DO:118:LYS:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Ib:21:LYS:HA	34:Ib:21:LYS:HD3	1.99	0.41
37:1e:627:U:H2'	37:1e:628:A:C8	2.56	0.41
37:1e:735:A:H2'	37:1e:736:A:C8	2.56	0.41
39:Wg:118:SER:O	39:Wg:119:TYR:C	2.64	0.41
43:Qk:147:ARG:HG3	43:Qk:150:VAL:HG23	2.03	0.41
56:Jy:18:VAL:HG13	56:Jy:70:THR:HG22	2.03	0.41
28:pT:456:GLY:H	29:YU:93:ALA:HB2	1.85	0.41
30:vV:206:HIS:HA	30:vV:209:LYS:HG2	2.02	0.41
45:sm:54:ARG:HA	45:sm:54:ARG:HD2	1.90	0.40
10:rA:435:ILE:HD12	11:tB:1:MET:HE3	2.04	0.40
28:pT:493:LYS:HA	28:pT:493:LYS:HD3	1.93	0.40
30:vV:261:LYS:HB2	30:vV:261:LYS:HE2	1.90	0.40
37:1e:159:A:H2'	37:1e:160:G:H8	1.86	0.40
37:1e:1957:G:N2	37:1e:2084:C:O2'	2.54	0.40
37:1e:2108:C:H1'	37:1e:3344:A:C8	2.57	0.40
52:Gu:151:ARG:HD2	52:Gu:207:LEU:HD23	2.02	0.40
55:ox:28:LYS:HA	55:ox:28:LYS:HD2	1.95	0.40
18:xI:122:ARG:NH1	37:1e:2156:C:OP2	2.40	0.40
31:nY:44:LYS:NZ	37:1e:1727:G:OP1	2.54	0.40
34:Ib:128:VAL:HA	34:Ib:157:ASN:HD21	1.85	0.40
37:1e:1798:A:H2'	37:1e:1799:A:C8	2.57	0.40
37:1e:2140:U:H1'	37:1e:2978:U:H5'	2.03	0.40
9:v9:400:ILE:HD13	9:v9:400:ILE:HA	1.90	0.40
10:rA:33:ILE:HD12	10:rA:33:ILE:HA	1.90	0.40
10:rA:175:TYR:HD1	10:rA:175:TYR:HA	1.77	0.40
16:dG:57:GLN:OE1	37:1e:1474:A:O2'	2.36	0.40
20:DK:153:ILE:HA	20:DK:166:ILE:HA	2.03	0.40
23:CW:34:THR:O	23:CW:38:LEU:CB	2.69	0.40
35:Xc:132:LEU:HA	35:Xc:132:LEU:HD23	1.72	0.40
37:1e:307:A:H2'	37:1e:308:A:C8	2.56	0.40
37:1e:733:G:N1	37:1e:736:A:OP2	2.39	0.40
37:1e:1921:A:H2'	37:1e:1922:A:C8	2.57	0.40
37:1e:2024:G:H1'	37:1e:2025:G:C8	2.56	0.40
8:F8:156:LYS:HE3	8:F8:156:LYS:HB3	1.94	0.40
9:v9:401:PRO:O	9:v9:405:LYS:HG2	2.21	0.40
10:rA:95:LEU:HD22	37:1e:2863:G:C2	2.55	0.40
21:LL:171:ARG:HA	21:LL:171:ARG:HD2	1.83	0.40
37:1e:1219:C:N3	45:sm:110:ARG:NH1	2.70	0.40
37:1e:2085:U:O2'	37:1e:2086:A:O5'	2.38	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	h1	117/120 (98%)	114 (97%)	3 (3%)	0	100	100
2	g2	112/121 (93%)	109 (97%)	3 (3%)	0	100	100
3	b3	53/59 (90%)	49 (92%)	4 (8%)	0	100	100
4	B4	249/254 (98%)	226 (91%)	23 (9%)	0	100	100
5	V5	134/137 (98%)	131 (98%)	3 (2%)	0	100	100
6	O6	195/199 (98%)	194 (100%)	1 (0%)	0	100	100
7	f7	104/107 (97%)	98 (94%)	6 (6%)	0	100	100
8	F8	173/176 (98%)	157 (91%)	15 (9%)	1 (1%)	21	31
9	v9	102/486 (21%)	89 (87%)	10 (10%)	3 (3%)	3	4
10	rA	645/647 (100%)	581 (90%)	57 (9%)	7 (1%)	11	16
11	tB	152/199 (76%)	143 (94%)	9 (6%)	0	100	100
12	cC	95/105 (90%)	93 (98%)	2 (2%)	0	100	100
13	CD	384/387 (99%)	358 (93%)	25 (6%)	1 (0%)	36	50
14	yE	240/245 (98%)	227 (95%)	13 (5%)	0	100	100
15	UF	113/121 (93%)	103 (91%)	10 (9%)	0	100	100
16	dG	108/113 (96%)	100 (93%)	8 (7%)	0	100	100
17	eH	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
18	xI	61/212 (29%)	55 (90%)	5 (8%)	1 (2%)	7	10
19	qJ	127/175 (73%)	117 (92%)	10 (8%)	0	100	100
20	Bt	161/184 (88%)	143 (89%)	17 (11%)	1 (1%)	21	31
20	DK	161/184 (88%)	142 (88%)	18 (11%)	1 (1%)	21	31
20	FR	161/184 (88%)	140 (87%)	18 (11%)	3 (2%)	6	8
21	LL	196/199 (98%)	190 (97%)	6 (3%)	0	100	100
22	KM	157/165 (95%)	127 (81%)	29 (18%)	1 (1%)	21	31
23	AN	367/599 (61%)	329 (90%)	36 (10%)	2 (0%)	24	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	CW	419/599 (70%)	363 (87%)	51 (12%)	5 (1%)	10	15
23	EX	341/599 (57%)	287 (84%)	48 (14%)	6 (2%)	6	9
24	DO	359/362 (99%)	333 (93%)	25 (7%)	1 (0%)	36	50
25	RP	186/189 (98%)	182 (98%)	4 (2%)	0	100	100
26	MQ	134/138 (97%)	124 (92%)	10 (8%)	0	100	100
27	mS	91/106 (86%)	82 (90%)	9 (10%)	0	100	100
28	pT	578/593 (98%)	529 (92%)	49 (8%)	0	100	100
29	YU	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
30	vV	241/518 (46%)	219 (91%)	22 (9%)	0	100	100
31	nY	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
32	SZ	169/172 (98%)	157 (93%)	12 (7%)	0	100	100
33	ia	94/100 (94%)	84 (89%)	10 (11%)	0	100	100
34	Ib	189/191 (99%)	176 (93%)	13 (7%)	0	100	100
35	Xc	121/142 (85%)	111 (92%)	9 (7%)	1 (1%)	16	24
36	xd	70/261 (27%)	66 (94%)	4 (6%)	0	100	100
39	Wg	231/236 (98%)	196 (85%)	33 (14%)	2 (1%)	14	21
40	jh	85/88 (97%)	79 (93%)	6 (7%)	0	100	100
41	li	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
42	Hj	228/256 (89%)	214 (94%)	13 (6%)	1 (0%)	30	42
43	Qk	183/186 (98%)	174 (95%)	9 (5%)	0	100	100
44	Tl	158/160 (99%)	154 (98%)	4 (2%)	0	100	100
45	sm	148/178 (83%)	121 (82%)	25 (17%)	2 (1%)	9	12
47	No	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
48	zp	84/106 (79%)	72 (86%)	12 (14%)	0	100	100
49	Zq	133/136 (98%)	123 (92%)	10 (8%)	0	100	100
50	kr	75/78 (96%)	68 (91%)	7 (9%)	0	100	100
51	As	215/217 (99%)	176 (82%)	34 (16%)	5 (2%)	5	6
52	Gu	221/244 (91%)	208 (94%)	13 (6%)	0	100	100
53	Pv	180/184 (98%)	174 (97%)	6 (3%)	0	100	100
54	aw	146/149 (98%)	134 (92%)	12 (8%)	0	100	100
55	ox	141/166 (85%)	132 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	Jy	164/174 (94%)	144 (88%)	20 (12%)	0	100	100
57	Ez	288/297 (97%)	274 (95%)	14 (5%)	0	100	100
All	All	10628/12807 (83%)	9740 (92%)	844 (8%)	44 (0%)	31	42

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	F8	123	PRO
9	v9	158	GLU
24	DO	339	LEU
20	FR	89	PRO
23	EX	379	PRO
39	Wg	132	PRO
51	As	59	PRO
20	Bt	47	PRO
9	v9	160	LEU
9	v9	161	VAL
22	KM	16	ARG
23	CW	387	ILE
35	Xc	21	LYS
39	Wg	120	VAL
51	As	114	GLU
10	rA	228	PRO
10	rA	355	ASN
10	rA	399	ALA
20	DK	89	PRO
45	sm	137	PRO
51	As	66	CYS
51	As	109	ALA
10	rA	178	VAL
10	rA	225	LEU
13	CD	239	PRO
23	AN	241	PRO
20	FR	46	ASN
20	FR	47	PRO
23	CW	249	VAL
10	rA	9	PRO
10	rA	179	GLY
23	CW	356	ILE
23	EX	264	PRO
23	EX	390	PRO

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Mol	Chain	Res	Type
42	Hj	204	ARG
23	AN	369	PRO
23	EX	356	ILE
18	xI	205	VAL
23	EX	224	ASN
23	CW	23	ILE
23	CW	304	SER
23	EX	240	PHE
45	sm	136	CYS
51	As	67	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	h1	102/105 (97%)	102 (100%)	0	100	100
2	g2	94/103 (91%)	94 (100%)	0	100	100
3	b3	39/47 (83%)	39 (100%)	0	100	100
4	B4	191/196 (97%)	190 (100%)	1 (0%)	81	89
5	V5	101/105 (96%)	101 (100%)	0	100	100
6	O6	158/162 (98%)	158 (100%)	0	100	100
7	f7	89/91 (98%)	89 (100%)	0	100	100
8	F8	108/153 (71%)	108 (100%)	0	100	100
9	v9	62/428 (14%)	62 (100%)	0	100	100
10	rA	521/573 (91%)	520 (100%)	1 (0%)	87	94
11	tB	125/180 (69%)	124 (99%)	1 (1%)	73	84
12	cC	62/88 (70%)	62 (100%)	0	100	100
13	CD	292/323 (90%)	287 (98%)	5 (2%)	53	72
14	yE	196/211 (93%)	195 (100%)	1 (0%)	81	89
15	UF	86/107 (80%)	85 (99%)	1 (1%)	63	78
16	dG	87/97 (90%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	eH	110/111 (99%)	110 (100%)	0	100	100
18	xI	57/184 (31%)	55 (96%)	2 (4%)	32	51
19	qJ	107/153 (70%)	106 (99%)	1 (1%)	70	82
21	LL	133/159 (84%)	131 (98%)	2 (2%)	57	74
22	KM	3/136 (2%)	1 (33%)	2 (67%)	0	0
24	DO	267/289 (92%)	266 (100%)	1 (0%)	84	91
25	RP	117/154 (76%)	116 (99%)	1 (1%)	70	82
26	MQ	104/109 (95%)	101 (97%)	3 (3%)	37	57
27	mS	72/91 (79%)	71 (99%)	1 (1%)	59	75
28	pT	453/520 (87%)	451 (100%)	2 (0%)	84	91
29	YU	108/110 (98%)	108 (100%)	0	100	100
30	vV	201/467 (43%)	201 (100%)	0	100	100
31	nY	65/72 (90%)	65 (100%)	0	100	100
32	SZ	150/156 (96%)	150 (100%)	0	100	100
33	ia	73/82 (89%)	72 (99%)	1 (1%)	59	75
34	Ib	150/171 (88%)	144 (96%)	6 (4%)	28	45
35	Xc	101/118 (86%)	97 (96%)	4 (4%)	28	45
36	xd	59/229 (26%)	59 (100%)	0	100	100
39	Wg	9/213 (4%)	9 (100%)	0	100	100
40	jh	69/71 (97%)	69 (100%)	0	100	100
41	li	44/46 (96%)	44 (100%)	0	100	100
42	Hj	153/208 (74%)	153 (100%)	0	100	100
43	Qk	148/151 (98%)	148 (100%)	0	100	100
44	Tl	130/137 (95%)	130 (100%)	0	100	100
45	sm	75/162 (46%)	75 (100%)	0	100	100
47	No	175/176 (99%)	175 (100%)	0	100	100
48	zp	63/95 (66%)	63 (100%)	0	100	100
49	Zq	105/116 (90%)	104 (99%)	1 (1%)	68	80
50	kr	58/69 (84%)	58 (100%)	0	100	100
51	As	4/198 (2%)	2 (50%)	2 (50%)	0	0
52	Gu	185/205 (90%)	185 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	Pv	131/146 (90%)	131 (100%)	0	100	100
54	aw	117/119 (98%)	117 (100%)	0	100	100
55	ox	126/141 (89%)	126 (100%)	0	100	100
56	Jy	130/150 (87%)	130 (100%)	0	100	100
57	Ez	143/245 (58%)	143 (100%)	0	100	100
All	All	6508/8928 (73%)	6469 (99%)	39 (1%)	76	87

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B4	45	VAL
10	rA	385	LEU
11	tB	32	CYS
13	CD	85	VAL
13	CD	110	LEU
13	CD	114	VAL
13	CD	264	VAL
13	CD	382	THR
14	yE	92	VAL
15	UF	43	VAL
18	xI	200	THR
18	xI	202	ARG
19	qJ	89	LEU
21	LL	58	VAL
21	LL	159	VAL
22	KM	16	ARG
22	KM	80	LEU
24	DO	230	VAL
25	RP	84	THR
26	MQ	15	VAL
26	MQ	20	VAL
26	MQ	21	VAL
27	mS	59	HIS
28	pT	218	ILE
28	pT	467	THR
33	ia	93	ILE
34	Ib	20	ILE
34	Ib	21	LYS
34	Ib	22	SER
34	Ib	65	VAL

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Mol	Chain	Res	Type
34	Ib	101	VAL
34	Ib	134	ILE
35	Xc	24	LYS
35	Xc	25	VAL
35	Xc	132	LEU
35	Xc	141	ILE
49	Zq	23	VAL
51	As	67	ILE
51	As	117	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	h1	99	GLN
1	h1	104	GLN
2	g2	33	GLN
2	g2	108	GLN
3	b3	17	HIS
4	B4	86	GLN
4	B4	205	ASN
6	O6	50	ASN
6	O6	193	GLN
7	f7	5	HIS
7	f7	24	ASN
7	f7	26	ASN
10	rA	78	HIS
10	rA	195	GLN
10	rA	384	ASN
10	rA	406	ASN
10	rA	546	GLN
10	rA	626	ASN
11	tB	5	GLN
13	CD	121	ASN
13	CD	165	GLN
13	CD	198	HIS
13	CD	224	HIS
14	yE	50	HIS
16	dG	21	HIS
19	qJ	17	HIS
19	qJ	21	HIS
19	qJ	24	ASN
19	qJ	64	ASN

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Mol	Chain	Res	Type
21	LL	6	ASN
21	LL	105	ASN
24	DO	5	GLN
24	DO	328	ASN
25	RP	3	ASN
26	MQ	41	GLN
28	pT	26	ASN
28	pT	82	ASN
28	pT	146	HIS
28	pT	398	ASN
30	vV	163	GLN
30	vV	351	GLN
32	SZ	138	GLN
33	ia	91	ASN
34	Ib	9	GLN
34	Ib	125	ASN
34	Ib	157	ASN
34	Ib	183	HIS
36	xd	14	HIS
36	xd	40	GLN
36	xd	49	GLN
39	Wg	54	GLN
40	jh	13	ASN
40	jh	69	HIS
41	li	33	ASN
42	Hj	38	GLN
42	Hj	95	ASN
43	Qk	45	ASN
43	Qk	136	ASN
44	Tl	66	ASN
44	Tl	134	GLN
45	sm	120	GLN
47	No	86	ASN
49	Zq	127	ASN
52	Gu	48	ASN
52	Gu	61	ASN
52	Gu	93	ASN
52	Gu	197	GLN
52	Gu	200	ASN
52	Gu	244	ASN
53	Pv	34	GLN
53	Pv	72	GLN

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Mol	Chain	Res	Type
53	Pv	125	GLN
54	aw	39	HIS
55	ox	32	GLN
56	Jy	101	ASN
57	Ez	57	ASN
57	Ez	151	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
37	1e	3270/3396 (96%)	763 (23%)	0
38	2f	120/121 (99%)	15 (12%)	0
46	3n	155/158 (98%)	31 (20%)	0
All	All	3545/3675 (96%)	809 (22%)	0

All (809) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
37	1e	6	A
37	1e	26	A
37	1e	40	A
37	1e	43	A
37	1e	49	A
37	1e	59	G
37	1e	60	A
37	1e	65	A
37	1e	66	A
37	1e	72	C
37	1e	92	G
37	1e	99	A
37	1e	109	A
37	1e	110	G
37	1e	111	C
37	1e	117	U
37	1e	118	U
37	1e	119	U
37	1e	120	G
37	1e	122	A
37	1e	130	A
37	1e	134	U
37	1e	135	C

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Mol	Chain	Res	Type
37	1e	136	G
37	1e	155	G
37	1e	156	G
37	1e	157	A
37	1e	164	A
37	1e	165	A
37	1e	169	U
37	1e	170	G
37	1e	171	G
37	1e	172	G
37	1e	173	G
37	1e	177	U
37	1e	187	A
37	1e	190	U
37	1e	191	U
37	1e	192	C
37	1e	200	C
37	1e	206	G
37	1e	210	U
37	1e	211	A
37	1e	213	A
37	1e	218	G
37	1e	219	A
37	1e	220	G
37	1e	240	U
37	1e	241	G
37	1e	242	C
37	1e	243	G
37	1e	245	U
37	1e	247	C
37	1e	248	U
37	1e	249	U
37	1e	251	G
37	1e	253	A
37	1e	259	C
37	1e	269	G
37	1e	270	U
37	1e	286	U
37	1e	295	A
37	1e	297	G
37	1e	298	U
37	1e	305	U

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Mol	Chain	Res	Type
37	1e	323	A
37	1e	329	U
37	1e	337	G
37	1e	338	A
37	1e	339	C
37	1e	376	G
37	1e	398	A
37	1e	399	A
37	1e	401	U
37	1e	402	A
37	1e	403	C
37	1e	420	G
37	1e	421	G
37	1e	422	A
37	1e	439	C
37	1e	520	U
37	1e	521	A
37	1e	523	A
37	1e	533	A
37	1e	543	C
37	1e	545	U
37	1e	546	C
37	1e	547	G
37	1e	548	G
37	1e	552	G
37	1e	555	U
37	1e	556	U
37	1e	557	A
37	1e	559	A
37	1e	578	A
37	1e	579	G
37	1e	588	G
37	1e	589	A
37	1e	597	G
37	1e	600	G
37	1e	603	A
37	1e	604	G
37	1e	608	A
37	1e	611	A
37	1e	620	U
37	1e	621	A
37	1e	622	A

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Mol	Chain	Res	Type
37	1e	629	U
37	1e	636	C
37	1e	648	C
37	1e	649	A
37	1e	660	A
37	1e	677	A
37	1e	681	U
37	1e	684	G
37	1e	690	A
37	1e	691	A
37	1e	705	A
37	1e	712	G
37	1e	715	A
37	1e	719	U
37	1e	725	G
37	1e	735	A
37	1e	737	G
37	1e	760	G
37	1e	761	A
37	1e	765	C
37	1e	767	U
37	1e	770	G
37	1e	771	A
37	1e	776	U
37	1e	777	U
37	1e	780	A
37	1e	781	G
37	1e	785	G
37	1e	786	A
37	1e	801	A
37	1e	806	A
37	1e	817	A
37	1e	830	A
37	1e	849	C
37	1e	861	C
37	1e	871	U
37	1e	874	U
37	1e	875	G
37	1e	896	A
37	1e	897	U
37	1e	907	G
37	1e	908	G

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Mol	Chain	Res	Type
37	1e	914	A
37	1e	916	G
37	1e	917	A
37	1e	921	A
37	1e	923	C
37	1e	924	G
37	1e	925	A
37	1e	937	G
37	1e	938	C
37	1e	944	C
37	1e	959	C
37	1e	960	U
37	1e	961	C
37	1e	962	A
37	1e	980	A
37	1e	981	U
37	1e	982	C
37	1e	999	G
37	1e	1001	G
37	1e	1002	A
37	1e	1005	G
37	1e	1006	A
37	1e	1007	U
37	1e	1008	U
37	1e	1009	A
37	1e	1010	G
37	1e	1012	G
37	1e	1014	U
37	1e	1015	U
37	1e	1016	C
37	1e	1017	C
37	1e	1018	G
37	1e	1019	G
37	1e	1020	G
37	1e	1026	A
37	1e	1028	U
37	1e	1029	G
37	1e	1034	U
37	1e	1035	G
37	1e	1036	A
37	1e	1037	C
37	1e	1039	U

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Mol	Chain	Res	Type
37	1e	1041	U
37	1e	1044	U
37	1e	1045	C
37	1e	1048	A
37	1e	1049	C
37	1e	1057	A
37	1e	1063	G
37	1e	1064	A
37	1e	1065	A
37	1e	1072	G
37	1e	1093	A
37	1e	1094	U
37	1e	1095	U
37	1e	1096	U
37	1e	1097	G
37	1e	1098	A
37	1e	1104	G
37	1e	1117	G
37	1e	1124	U
37	1e	1128	U
37	1e	1129	A
37	1e	1130	A
37	1e	1131	G
37	1e	1134	G
37	1e	1144	U
37	1e	1153	A
37	1e	1155	C
37	1e	1159	A
37	1e	1160	C
37	1e	1180	A
37	1e	1181	U
37	1e	1192	C
37	1e	1195	A
37	1e	1196	C
37	1e	1199	C
37	1e	1200	A
37	1e	1201	C
37	1e	1203	A
37	1e	1204	A
37	1e	1207	G
37	1e	1209	G
37	1e	1210	U

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Mol	Chain	Res	Type
37	1e	1217	A
37	1e	1222	G
37	1e	1234	G
37	1e	1235	U
37	1e	1236	G
37	1e	1238	C
37	1e	1241	U
37	1e	1245	A
37	1e	1252	A
37	1e	1253	U
37	1e	1254	C
37	1e	1258	U
37	1e	1259	A
37	1e	1262	G
37	1e	1263	A
37	1e	1264	G
37	1e	1265	U
37	1e	1268	G
37	1e	1269	U
37	1e	1280	C
37	1e	1286	A
37	1e	1287	A
37	1e	1301	A
37	1e	1302	A
37	1e	1304	A
37	1e	1305	U
37	1e	1307	G
37	1e	1309	U
37	1e	1313	G
37	1e	1330	A
37	1e	1332	A
37	1e	1348	U
37	1e	1349	G
37	1e	1350	A
37	1e	1351	U
37	1e	1352	A
37	1e	1354	G
37	1e	1355	A
37	1e	1356	U
37	1e	1357	G
37	1e	1386	A
37	1e	1392	G

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Mol	Chain	Res	Type
37	1e	1399	A
37	1e	1400	G
37	1e	1419	A
37	1e	1434	G
37	1e	1437	C
37	1e	1446	A
37	1e	1450	G
37	1e	1455	U
37	1e	1466	G
37	1e	1481	A
37	1e	1482	A
37	1e	1483	G
37	1e	1487	G
37	1e	1494	U
37	1e	1503	A
37	1e	1508	C
37	1e	1523	U
37	1e	1533	U
37	1e	1536	G
37	1e	1539	A
37	1e	1555	U
37	1e	1557	A
37	1e	1562	C
37	1e	1563	C
37	1e	1565	G
37	1e	1567	U
37	1e	1568	U
37	1e	1569	U
37	1e	1570	U
37	1e	1571	A
37	1e	1572	U
37	1e	1574	C
37	1e	1575	A
37	1e	1576	G
37	1e	1577	G
37	1e	1580	A
37	1e	1581	C
37	1e	1582	C
37	1e	1583	A
37	1e	1587	A
37	1e	1589	A
37	1e	1605	A

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Mol	Chain	Res	Type
37	1e	1619	A
37	1e	1620	U
37	1e	1629	U
37	1e	1643	A
37	1e	1645	U
37	1e	1657	C
37	1e	1674	G
37	1e	1683	A
37	1e	1705	U
37	1e	1724	U
37	1e	1725	C
37	1e	1730	G
37	1e	1741	A
37	1e	1742	U
37	1e	1750	A
37	1e	1751	G
37	1e	1759	C
37	1e	1760	A
37	1e	1761	C
37	1e	1762	C
37	1e	1763	U
37	1e	1766	G
37	1e	1768	U
37	1e	1770	G
37	1e	1778	G
37	1e	1780	G
37	1e	1797	A
37	1e	1808	G
37	1e	1813	A
37	1e	1814	A
37	1e	1816	A
37	1e	1819	U
37	1e	1820	U
37	1e	1821	U
37	1e	1839	A
37	1e	1842	A
37	1e	1846	C
37	1e	1847	A
37	1e	1849	C
37	1e	1850	A
37	1e	1858	A
37	1e	1864	A

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Mol	Chain	Res	Type
37	1e	1866	C
37	1e	1867	A
37	1e	1880	U
37	1e	1886	A
37	1e	1906	G
37	1e	1926	C
37	1e	1937	U
37	1e	1951	C
37	1e	1952	G
37	1e	1953	G
37	1e	1954	G
37	1e	1959	G
37	1e	1962	G
37	1e	1964	C
37	1e	1965	C
37	1e	1967	U
37	1e	1968	G
37	1e	1971	C
37	1e	1972	A
37	1e	1976	G
37	1e	1977	C
37	1e	1978	A
37	1e	1980	C
37	1e	1981	G
37	1e	1987	G
37	1e	1988	C
37	1e	1989	U
37	1e	1990	U
37	1e	1993	G
37	1e	1994	G
37	1e	1995	A
37	1e	2001	U
37	1e	2002	G
37	1e	2003	G
37	1e	2004	U
37	1e	2005	G
37	1e	2007	G
37	1e	2010	U
37	1e	2011	U
37	1e	2013	C
37	1e	2016	U
37	1e	2017	G

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Mol	Chain	Res	Type
37	1e	2018	C
37	1e	2019	U
37	1e	2020	A
37	1e	2025	G
37	1e	2026	A
37	1e	2027	C
37	1e	2028	U
37	1e	2029	A
37	1e	2030	C
37	1e	2032	U
37	1e	2033	G
37	1e	2034	C
37	1e	2037	G
37	1e	2040	U
37	1e	2041	U
37	1e	2042	G
37	1e	2043	U
37	1e	2044	U
37	1e	2049	A
37	1e	2051	G
37	1e	2052	G
37	1e	2053	C
37	1e	2054	C
37	1e	2055	U
37	1e	2056	U
37	1e	2057	G
37	1e	2058	G
37	1e	2059	U
37	1e	2060	A
37	1e	2061	G
37	1e	2062	G
37	1e	2065	U
37	1e	2066	C
37	1e	2067	U
37	1e	2069	G
37	1e	2071	A
37	1e	2073	A
37	1e	2076	G
37	1e	2080	C
37	1e	2081	U
37	1e	2083	G
37	1e	2084	C

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Mol	Chain	Res	Type
37	1e	2085	U
37	1e	2086	A
37	1e	2087	C
37	1e	2088	A
37	1e	2089	A
37	1e	2090	U
37	1e	2091	U
37	1e	2092	A
37	1e	2093	A
37	1e	2094	C
37	1e	2095	G
37	1e	2096	A
37	1e	2097	U
37	1e	2098	C
37	1e	2101	C
37	1e	2102	U
37	1e	2112	U
37	1e	2113	A
37	1e	2121	G
37	1e	2122	G
37	1e	2131	A
37	1e	2140	U
37	1e	2142	A
37	1e	2158	A
37	1e	2160	G
37	1e	2169	G
37	1e	2176	U
37	1e	2188	A
37	1e	2205	U
37	1e	2206	G
37	1e	2209	U
37	1e	2210	G
37	1e	2214	A
37	1e	2244	A
37	1e	2319	U
37	1e	2334	U
37	1e	2335	G
37	1e	2336	U
37	1e	2373	A
37	1e	2375	G
37	1e	2385	G
37	1e	2388	U

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Mol	Chain	Res	Type
37	1e	2393	G
37	1e	2400	G
37	1e	2401	A
37	1e	2411	U
37	1e	2419	A
37	1e	2422	C
37	1e	2443	A
37	1e	2444	C
37	1e	2446	U
37	1e	2449	A
37	1e	2451	G
37	1e	2452	G
37	1e	2453	U
37	1e	2454	G
37	1e	2455	U
37	1e	2456	A
37	1e	2458	A
37	1e	2459	A
37	1e	2460	U
37	1e	2461	A
37	1e	2462	A
37	1e	2463	G
37	1e	2464	U
37	1e	2465	G
37	1e	2467	G
37	1e	2468	A
37	1e	2470	C
37	1e	2472	U
37	1e	2473	C
37	1e	2474	G
37	1e	2475	G
37	1e	2477	G
37	1e	2480	A
37	1e	2481	G
37	1e	2483	G
37	1e	2484	A
37	1e	2485	A
37	1e	2488	A
37	1e	2489	C
37	1e	2490	C
37	1e	2491	A
37	1e	2492	C

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Mol	Chain	Res	Type
37	1e	2494	A
37	1e	2495	C
37	1e	2496	C
37	1e	2497	U
37	1e	2498	U
37	1e	2502	A
37	1e	2505	U
37	1e	2506	U
37	1e	2507	C
37	1e	2511	A
37	1e	2514	U
37	1e	2515	A
37	1e	2522	G
37	1e	2530	G
37	1e	2531	C
37	1e	2532	U
37	1e	2537	U
37	1e	2538	U
37	1e	2539	C
37	1e	2540	A
37	1e	2541	U
37	1e	2542	U
37	1e	2544	U
37	1e	2546	C
37	1e	2549	G
37	1e	2550	U
37	1e	2552	C
37	1e	2555	G
37	1e	2561	A
37	1e	2566	C
37	1e	2569	A
37	1e	2570	U
37	1e	2571	U
37	1e	2572	C
37	1e	2573	G
37	1e	2576	G
37	1e	2581	U
37	1e	2585	G
37	1e	2593	A
37	1e	2606	G
37	1e	2607	G
37	1e	2614	G

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Mol	Chain	Res	Type
37	1e	2626	A
37	1e	2628	A
37	1e	2635	A
37	1e	2648	G
37	1e	2651	G
37	1e	2652	U
37	1e	2656	A
37	1e	2672	G
37	1e	2674	A
37	1e	2677	G
37	1e	2679	A
37	1e	2689	A
37	1e	2690	G
37	1e	2691	A
37	1e	2694	A
37	1e	2696	A
37	1e	2705	A
37	1e	2714	G
37	1e	2719	U
37	1e	2727	A
37	1e	2728	G
37	1e	2729	U
37	1e	2753	G
37	1e	2755	C
37	1e	2762	A
37	1e	2771	U
37	1e	2772	C
37	1e	2777	G
37	1e	2778	G
37	1e	2792	A
37	1e	2794	G
37	1e	2796	G
37	1e	2800	G
37	1e	2801	A
37	1e	2802	A
37	1e	2803	A
37	1e	2804	A
37	1e	2810	C
37	1e	2817	A
37	1e	2818	U
37	1e	2819	A
37	1e	2820	A

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Mol	Chain	Res	Type
37	1e	2821	C
37	1e	2822	U
37	1e	2823	G
37	1e	2825	C
37	1e	2826	U
37	1e	2836	C
37	1e	2837	A
37	1e	2838	A
37	1e	2840	C
37	1e	2841	G
37	1e	2842	U
37	1e	2843	U
37	1e	2845	A
37	1e	2846	U
37	1e	2847	A
37	1e	2848	G
37	1e	2855	U
37	1e	2856	G
37	1e	2857	C
37	1e	2858	U
37	1e	2859	U
37	1e	2860	U
37	1e	2861	U
37	1e	2862	U
37	1e	2864	A
37	1e	2865	U
37	1e	2866	U
37	1e	2867	C
37	1e	2868	U
37	1e	2869	U
37	1e	2870	C
37	1e	2871	G
37	1e	2874	G
37	1e	2876	C
37	1e	2887	A
37	1e	2898	G
37	1e	2899	C
37	1e	2900	A
37	1e	2914	G
37	1e	2921	U
37	1e	2935	U
37	1e	2936	A

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Mol	Chain	Res	Type
37	1e	2941	A
37	1e	2942	C
37	1e	2943	G
37	1e	2945	G
37	1e	2946	A
37	1e	2947	G
37	1e	2950	G
37	1e	2971	A
37	1e	2978	U
37	1e	2979	U
37	1e	2980	U
37	1e	2981	U
37	1e	2983	C
37	1e	2997	G
37	1e	3011	A
37	1e	3012	A
37	1e	3014	U
37	1e	3027	A
37	1e	3040	A
37	1e	3056	U
37	1e	3058	U
37	1e	3059	G
37	1e	3078	U
37	1e	3079	U
37	1e	3080	G
37	1e	3086	A
37	1e	3092	C
37	1e	3093	C
37	1e	3099	C
37	1e	3104	U
37	1e	3109	G
37	1e	3113	A
37	1e	3119	U
37	1e	3127	A
37	1e	3129	A
37	1e	3130	A
37	1e	3131	U
37	1e	3142	A
37	1e	3143	C
37	1e	3153	U
37	1e	3154	C
37	1e	3155	U

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Mol	Chain	Res	Type
37	1e	3156	U
37	1e	3157	U
37	1e	3158	G
37	1e	3165	A
37	1e	3167	A
37	1e	3168	A
37	1e	3169	U
37	1e	3170	A
37	1e	3171	U
37	1e	3172	A
37	1e	3173	G
37	1e	3174	A
37	1e	3175	U
37	1e	3176	G
37	1e	3179	U
37	1e	3181	C
37	1e	3187	A
37	1e	3195	U
37	1e	3196	U
37	1e	3206	C
37	1e	3207	U
37	1e	3210	A
37	1e	3216	G
37	1e	3217	C
37	1e	3218	A
37	1e	3219	G
37	1e	3228	C
37	1e	3229	G
37	1e	3234	A
37	1e	3243	A
37	1e	3245	A
37	1e	3246	G
37	1e	3247	G
37	1e	3252	G
37	1e	3254	G
37	1e	3259	U
37	1e	3270	U
37	1e	3275	U
37	1e	3276	G
37	1e	3280	U
37	1e	3281	U
37	1e	3286	G

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Mol	Chain	Res	Type
37	1e	3288	G
37	1e	3289	G
37	1e	3295	A
37	1e	3304	U
37	1e	3316	A
37	1e	3317	U
37	1e	3318	G
37	1e	3319	U
37	1e	3320	A
37	1e	3330	A
37	1e	3341	U
37	1e	3342	A
37	1e	3345	G
37	1e	3349	C
37	1e	3350	C
37	1e	3352	U
37	1e	3354	U
37	1e	3355	U
37	1e	3356	G
37	1e	3359	A
37	1e	3369	G
37	1e	3378	C
37	1e	3382	U
37	1e	3386	G
37	1e	3389	U
37	1e	3391	A
38	2f	10	C
38	2f	22	A
38	2f	31	U
38	2f	32	U
38	2f	33	U
38	2f	53	U
38	2f	54	U
38	2f	55	A
38	2f	65	G
38	2f	73	C
38	2f	74	C
38	2f	90	U
38	2f	99	G
38	2f	102	A
38	2f	112	G
46	3n	2	A

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Mol	Chain	Res	Type
46	3n	21	C
46	3n	23	U
46	3n	34	U
46	3n	35	C
46	3n	38	U
46	3n	52	A
46	3n	53	A
46	3n	59	A
46	3n	62	C
46	3n	63	G
46	3n	79	A
46	3n	80	A
46	3n	82	U
46	3n	84	C
46	3n	85	G
46	3n	86	U
46	3n	88	A
46	3n	90	U
46	3n	95	G
46	3n	105	A
46	3n	106	C
46	3n	111	A
46	3n	113	U
46	3n	124	G
46	3n	125	U
46	3n	126	A
46	3n	138	A
46	3n	148	G
46	3n	152	G
46	3n	156	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 237 ligands modelled in this entry, 237 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

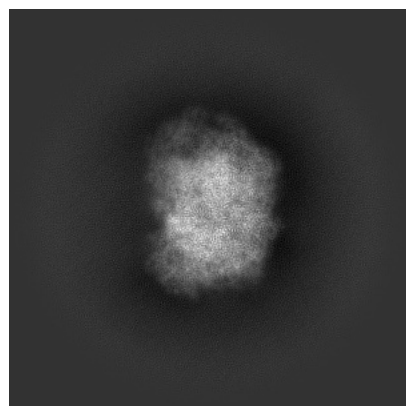
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34725. These allow visual inspection of the internal detail of the map and identification of artifacts.

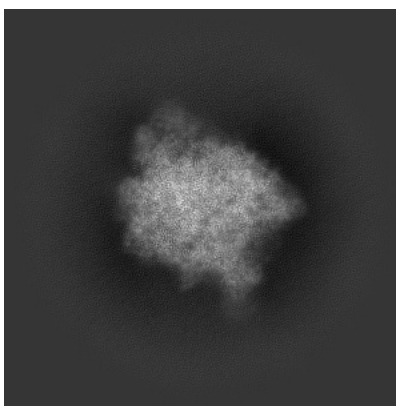
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

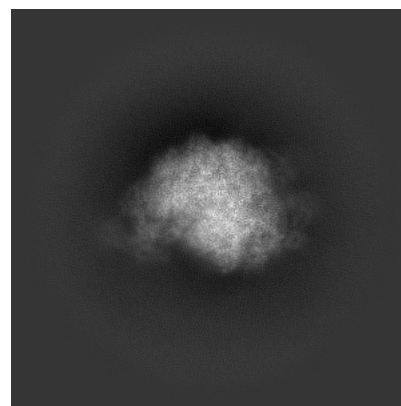
6.1.1 Primary map



X

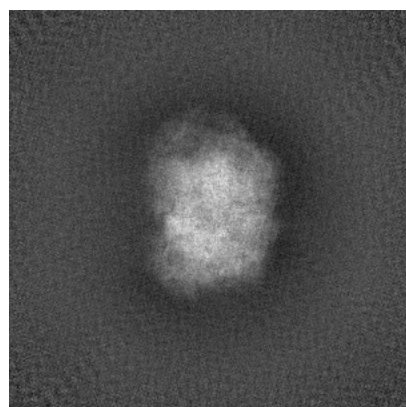


Y

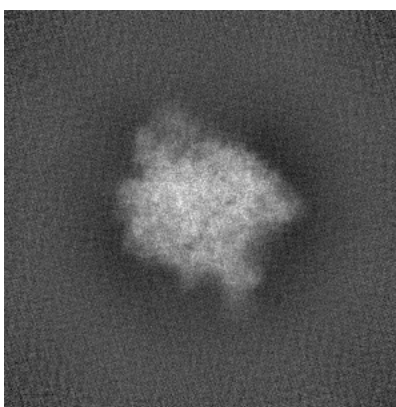


Z

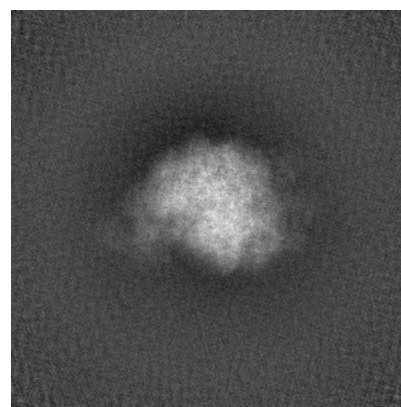
6.1.2 Raw map



X



Y

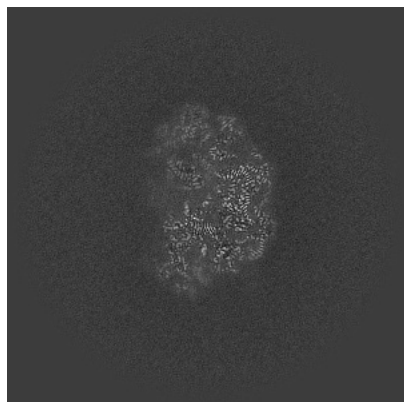


Z

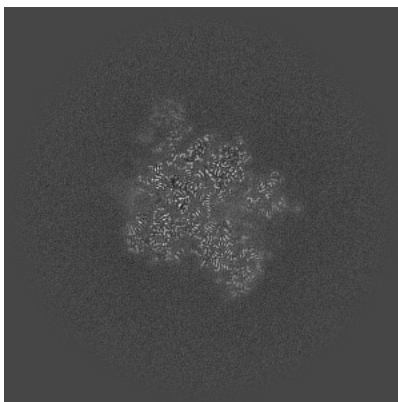
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

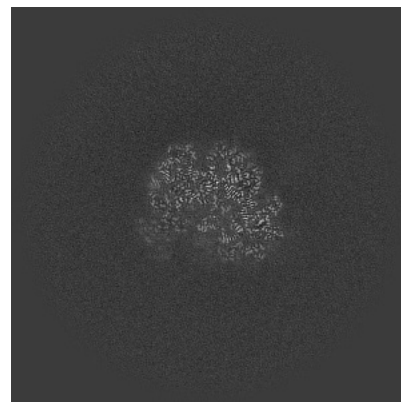
6.2.1 Primary map



X Index: 400

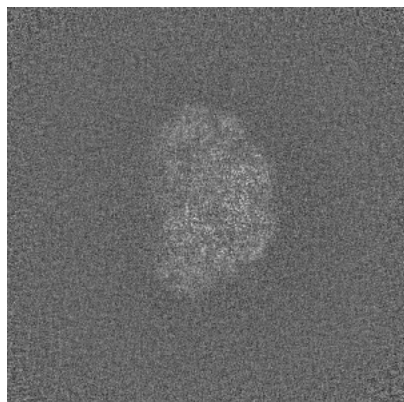


Y Index: 400

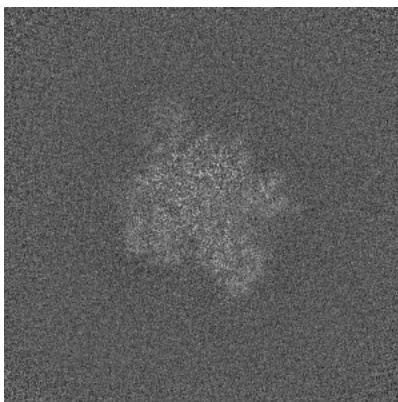


Z Index: 400

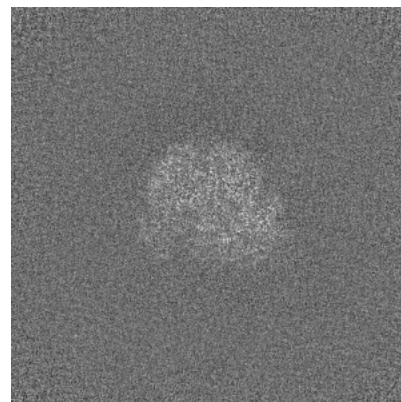
6.2.2 Raw map



X Index: 400



Y Index: 400

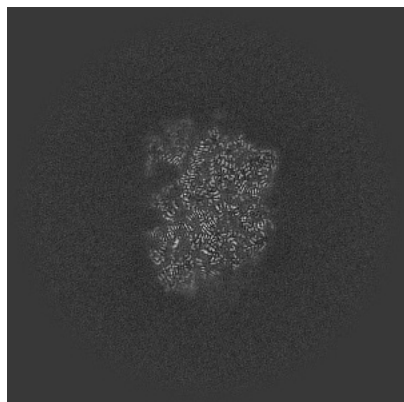


Z Index: 400

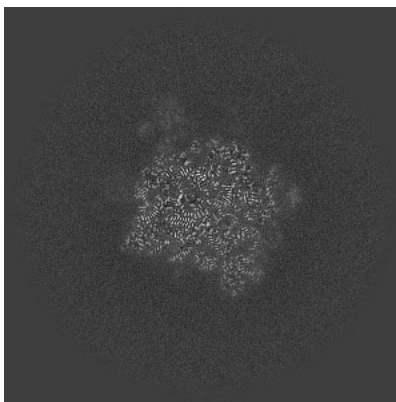
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

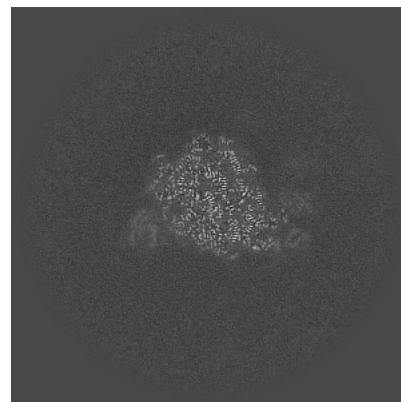
6.3.1 Primary map



X Index: 443

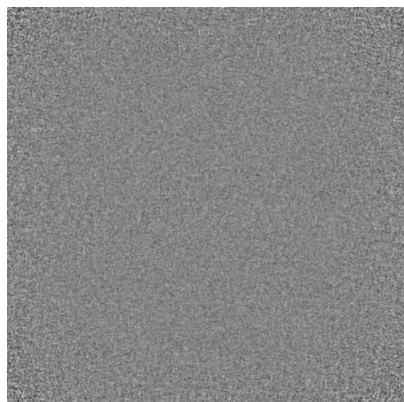


Y Index: 424

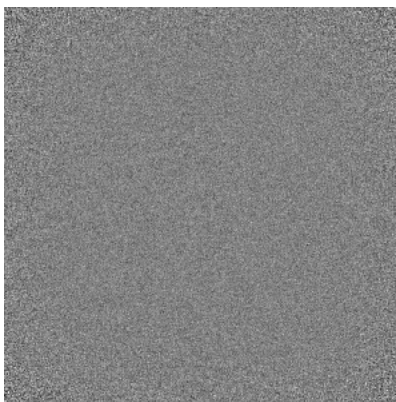


Z Index: 357

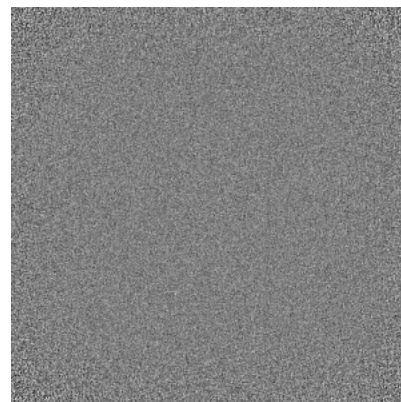
6.3.2 Raw map



X Index: 0



Y Index: 0

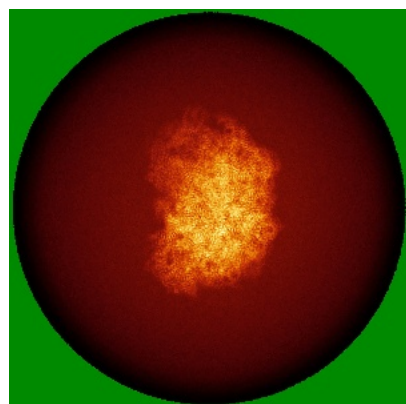


Z Index: 0

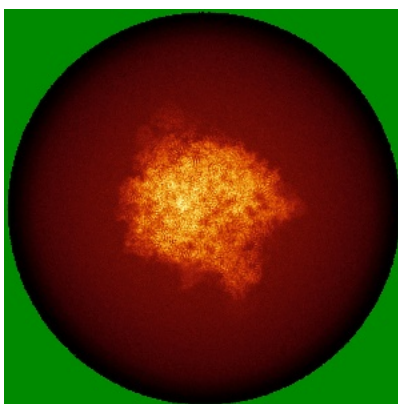
The images above show the largest variance slices of the map in three orthogonal directions.

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

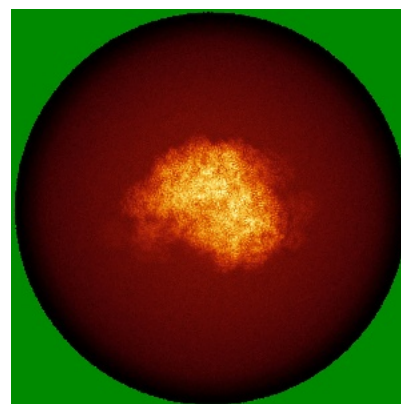
6.4.1 Primary map



X

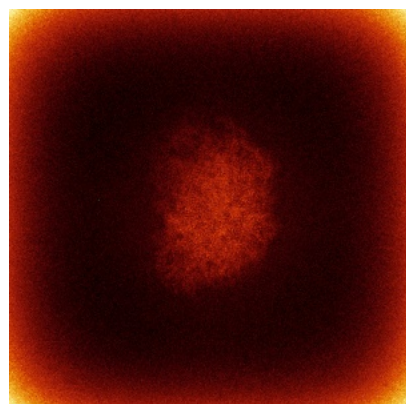


Y

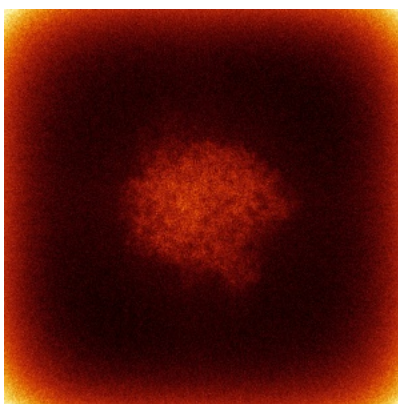


Z

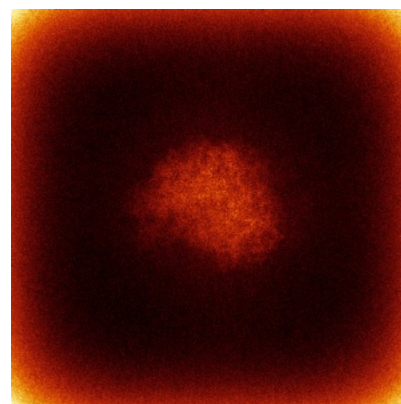
6.4.2 Raw map



X



Y

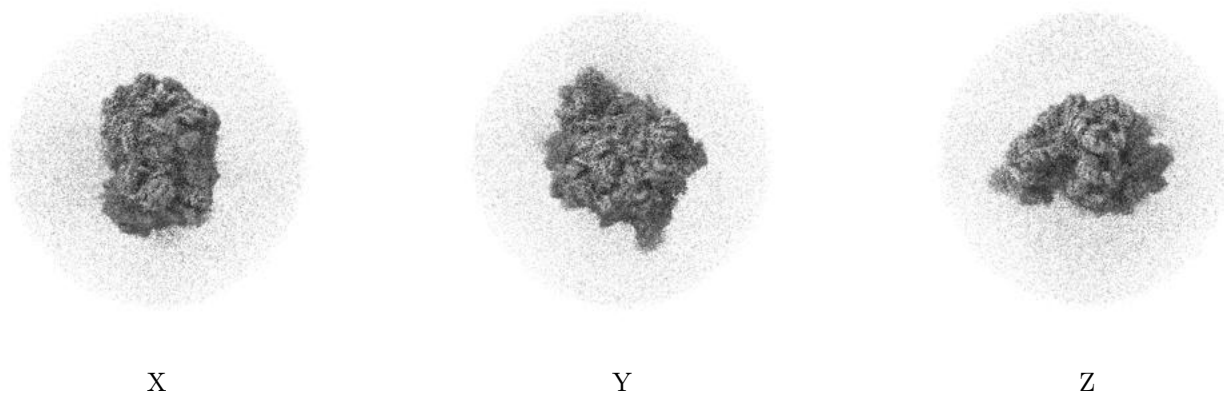


Z

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.

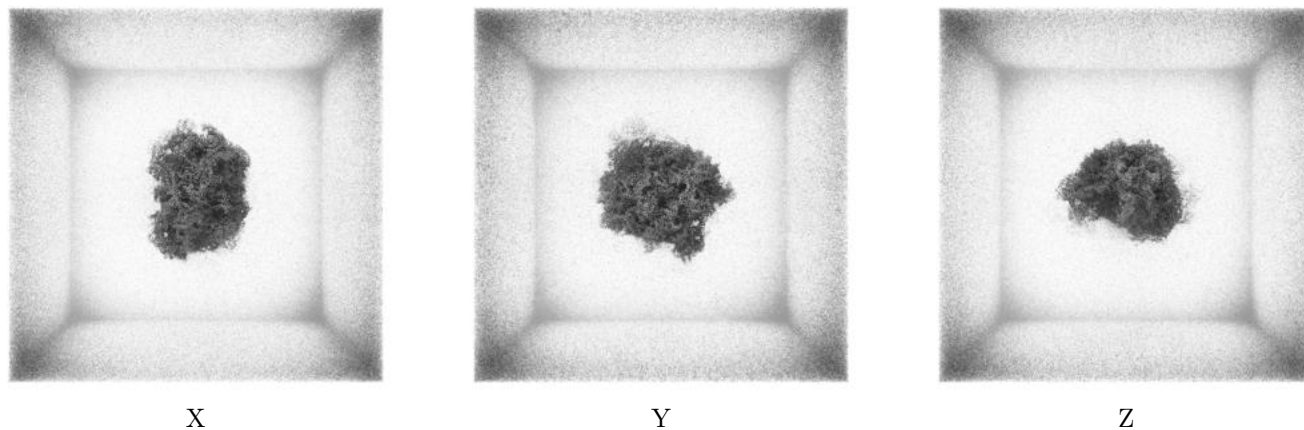
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

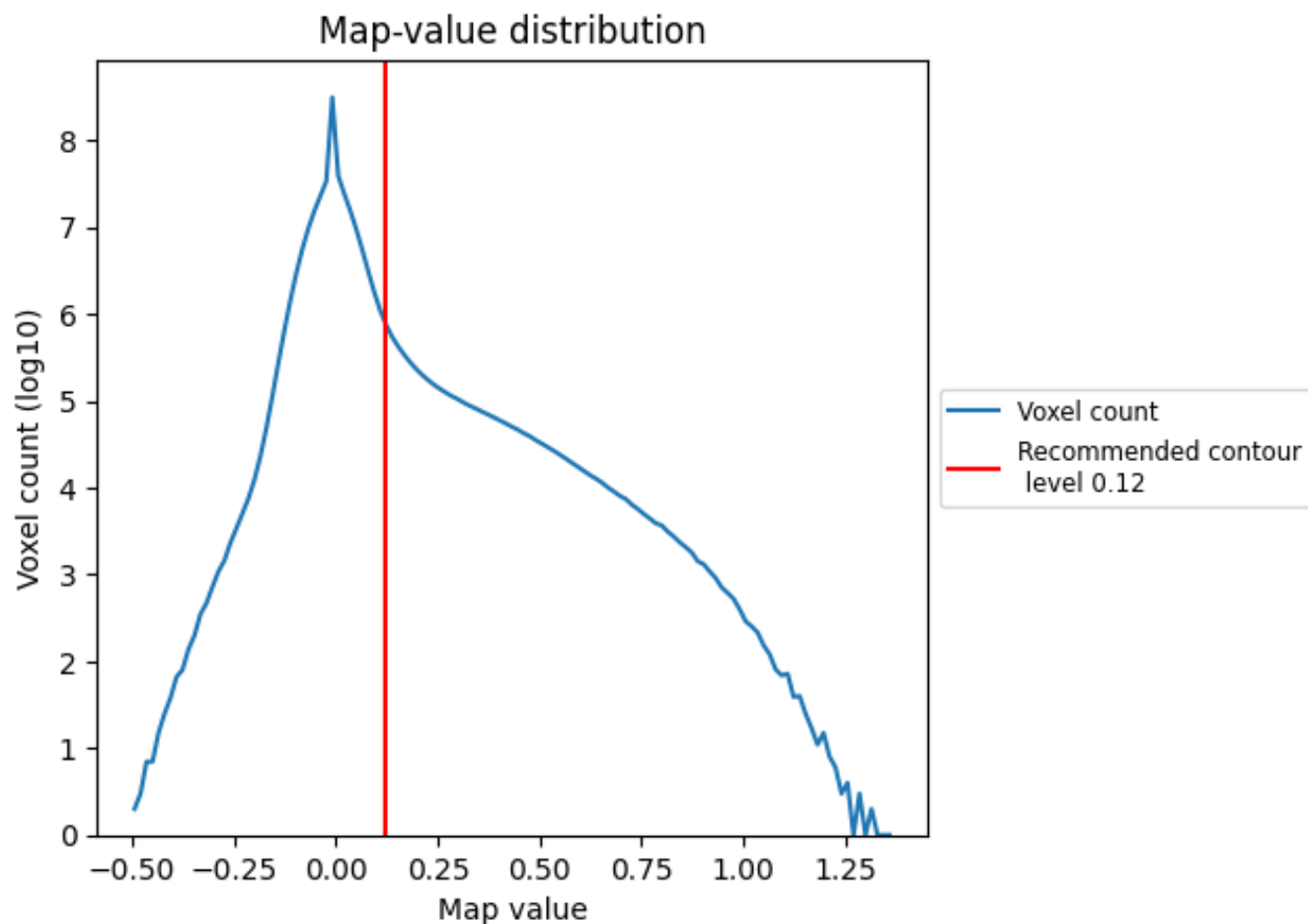
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

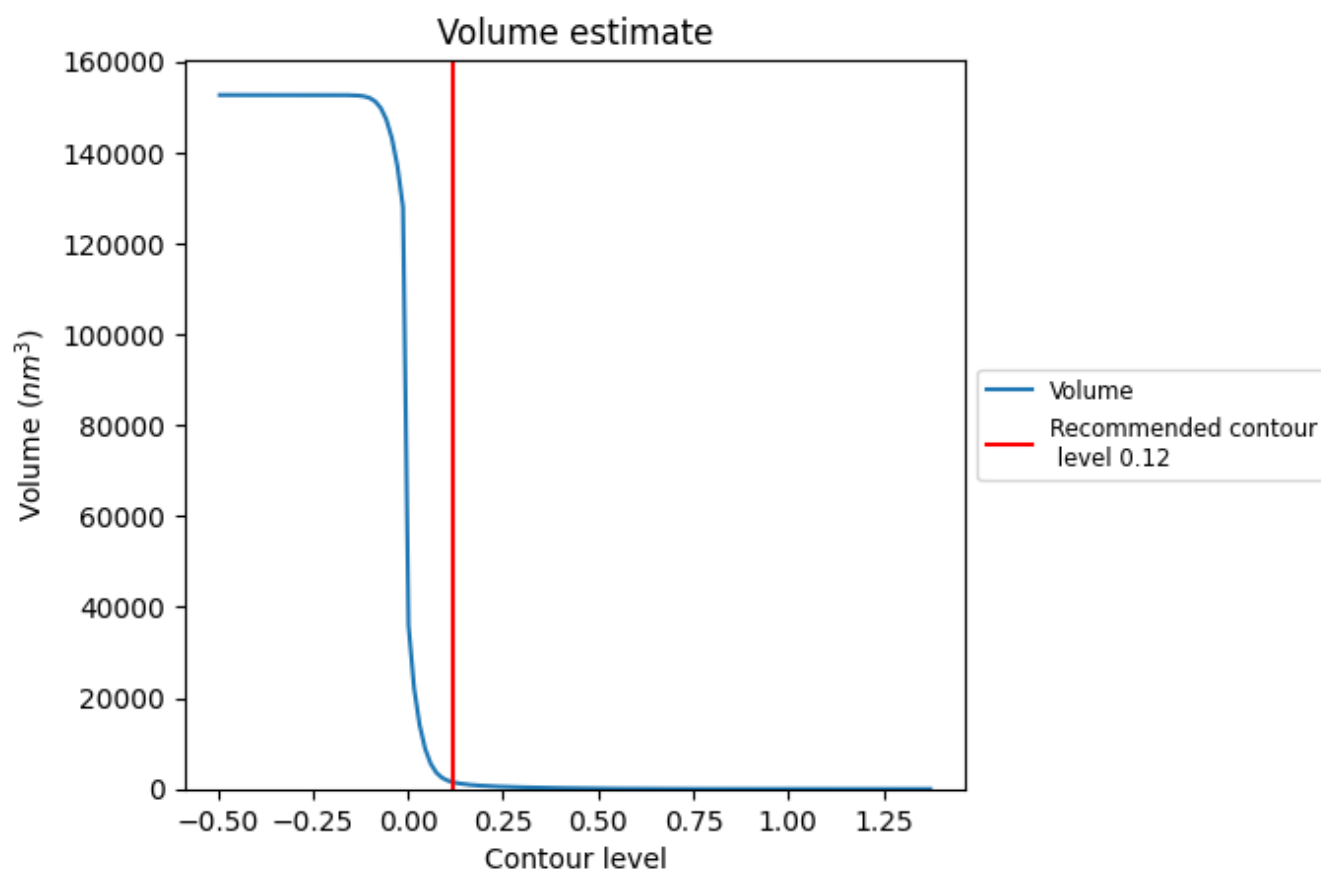
This section contains the results of statistical analysis of the map.

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.

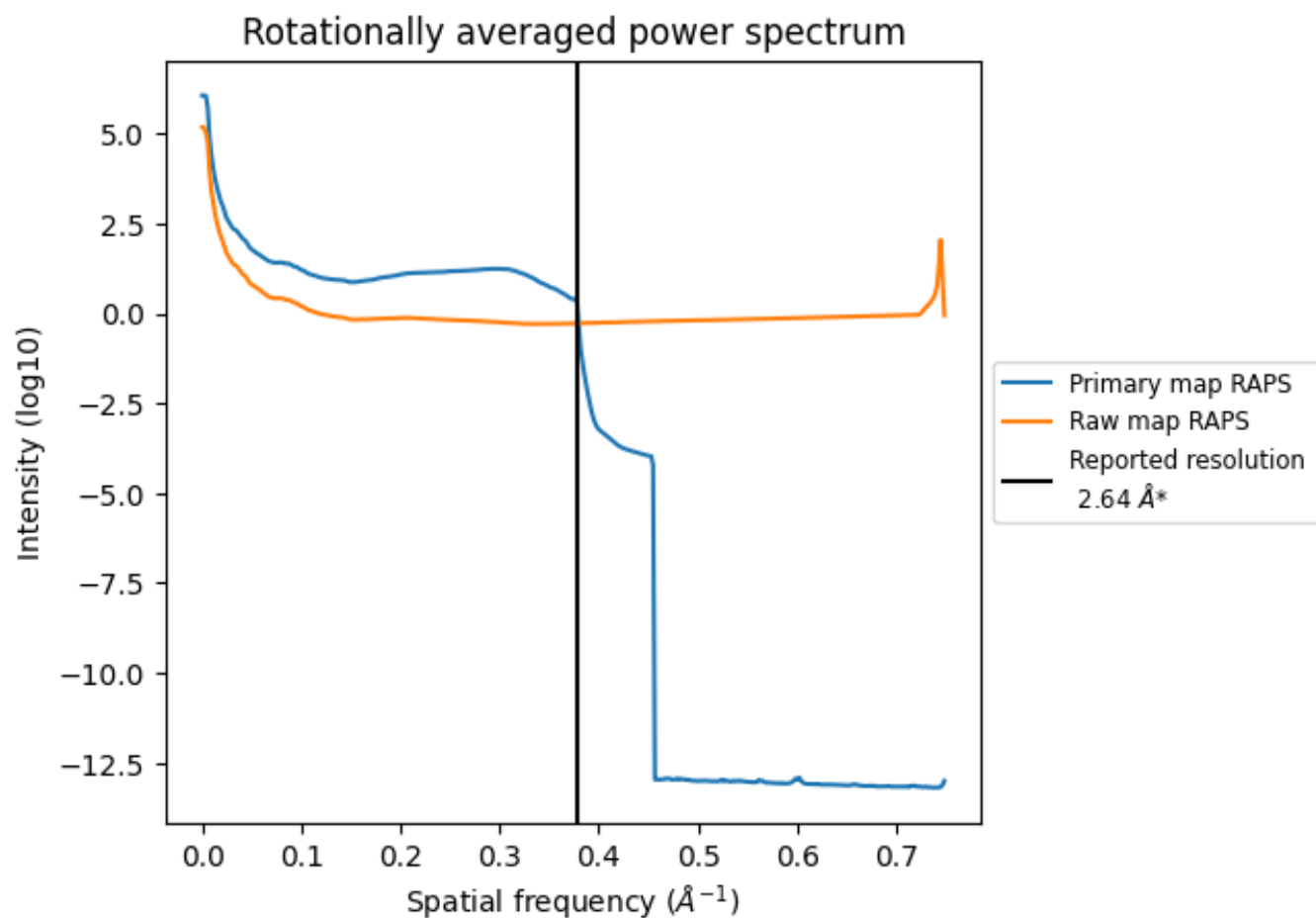
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1460 nm^3 ; this corresponds to an approximate mass of 1319 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 ⓘ

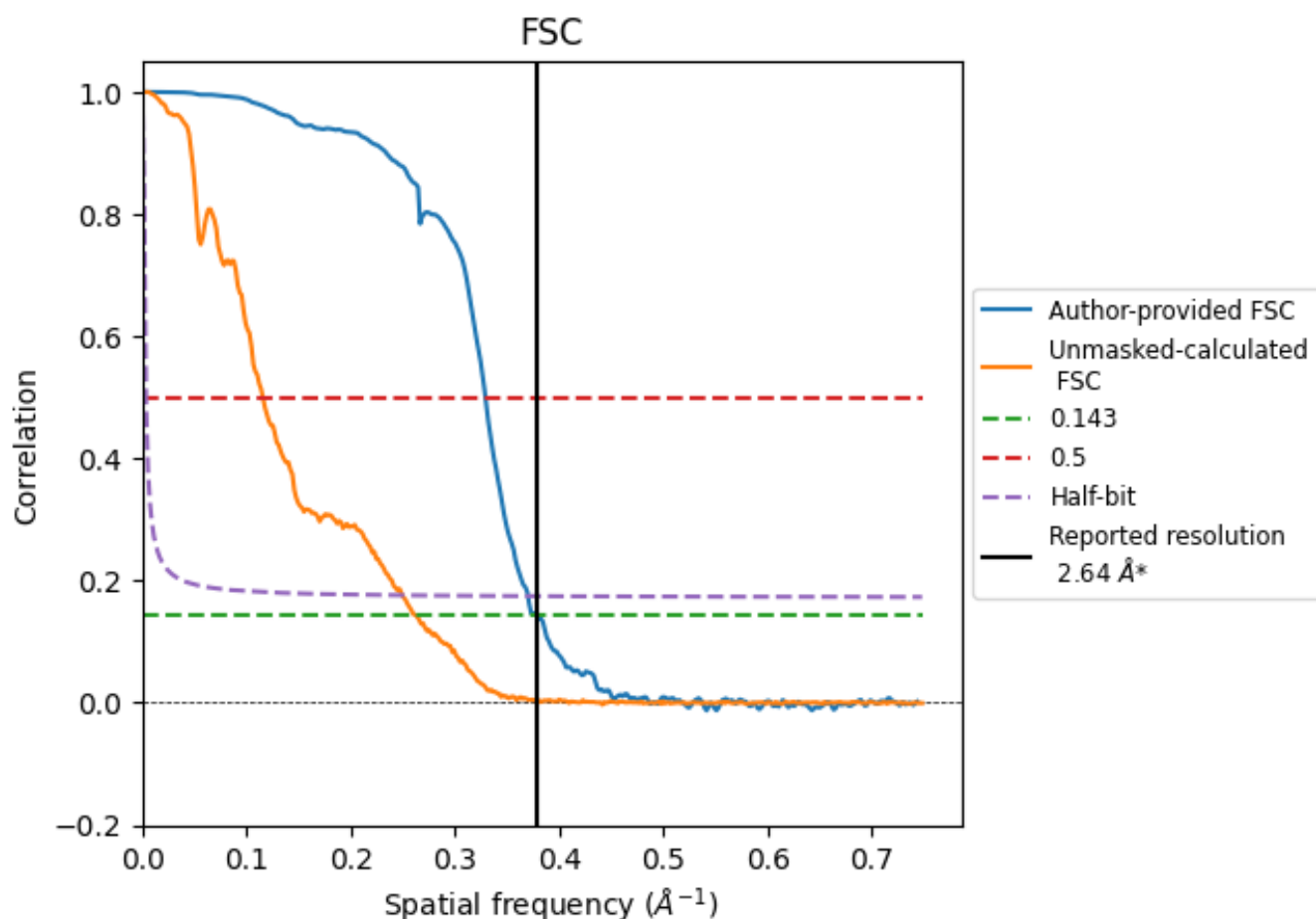


*Reported resolution corresponds to spatial frequency of 0.379 Å⁻¹

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 0.379 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

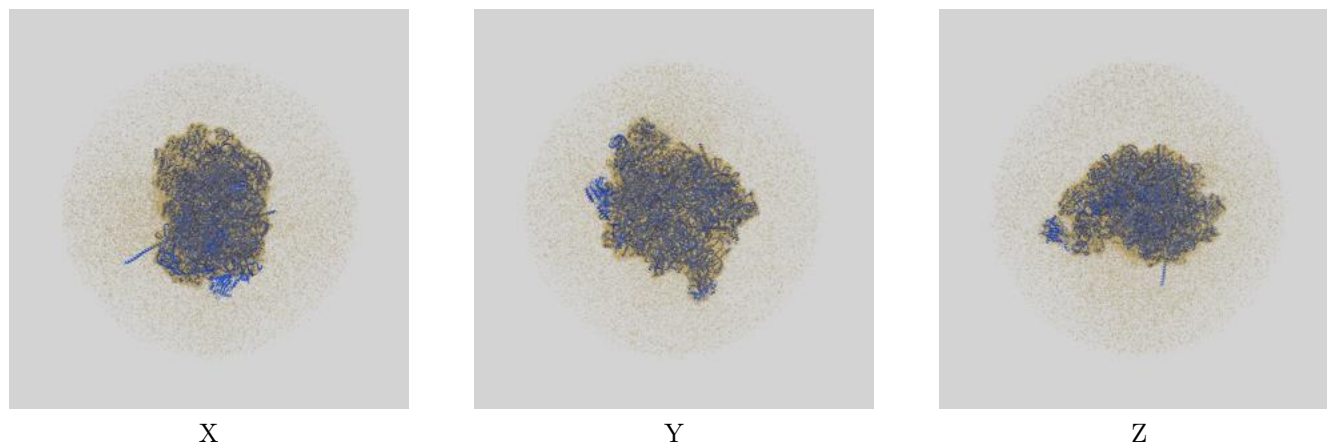
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.64	-	-
Author-provided FSC curve	2.64	3.04	2.70
Unmasked-calculated*	3.81	8.63	4.00

*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 3.81 differs from the reported value 2.64 by more than 10 %

9 Map-model fit [i](#)

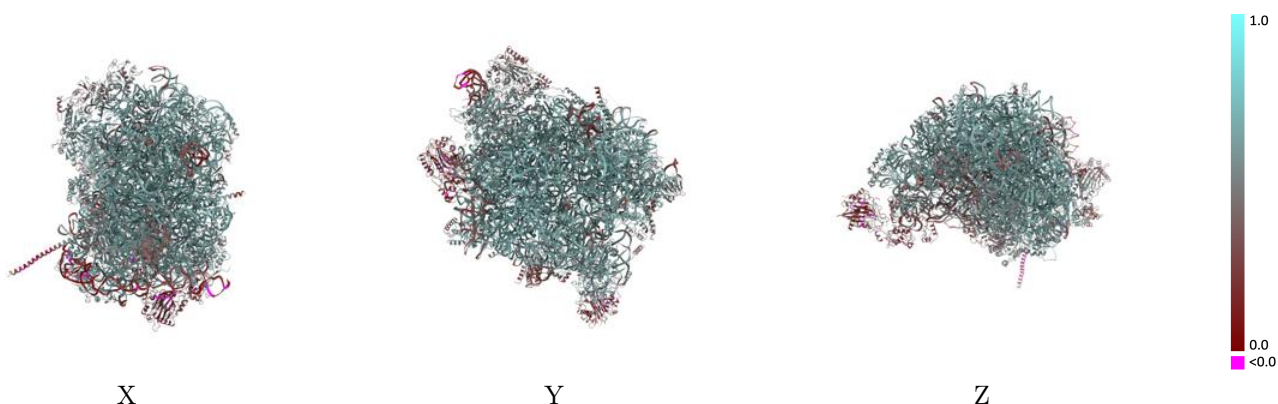
This section contains information regarding the fit between EMDB map EMD-34725 and PDB model 8HFR. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



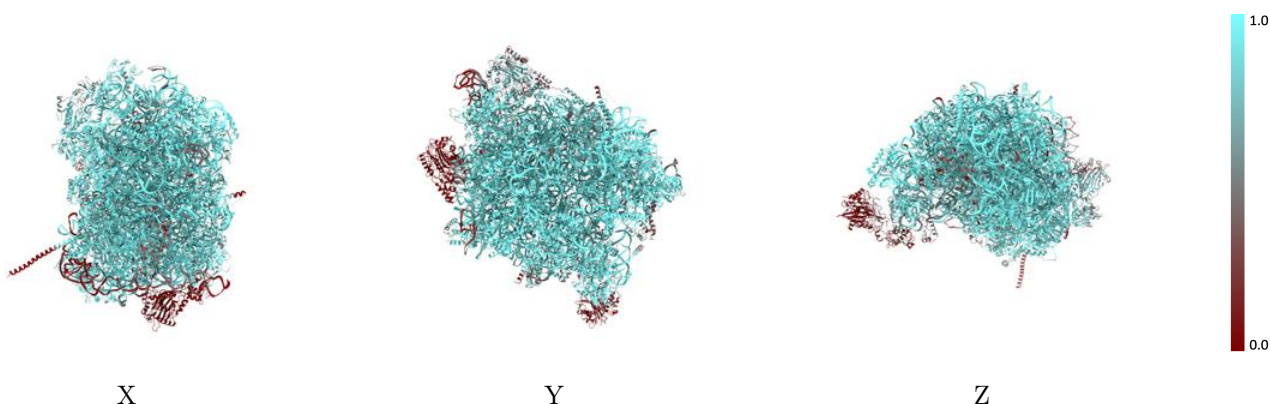
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



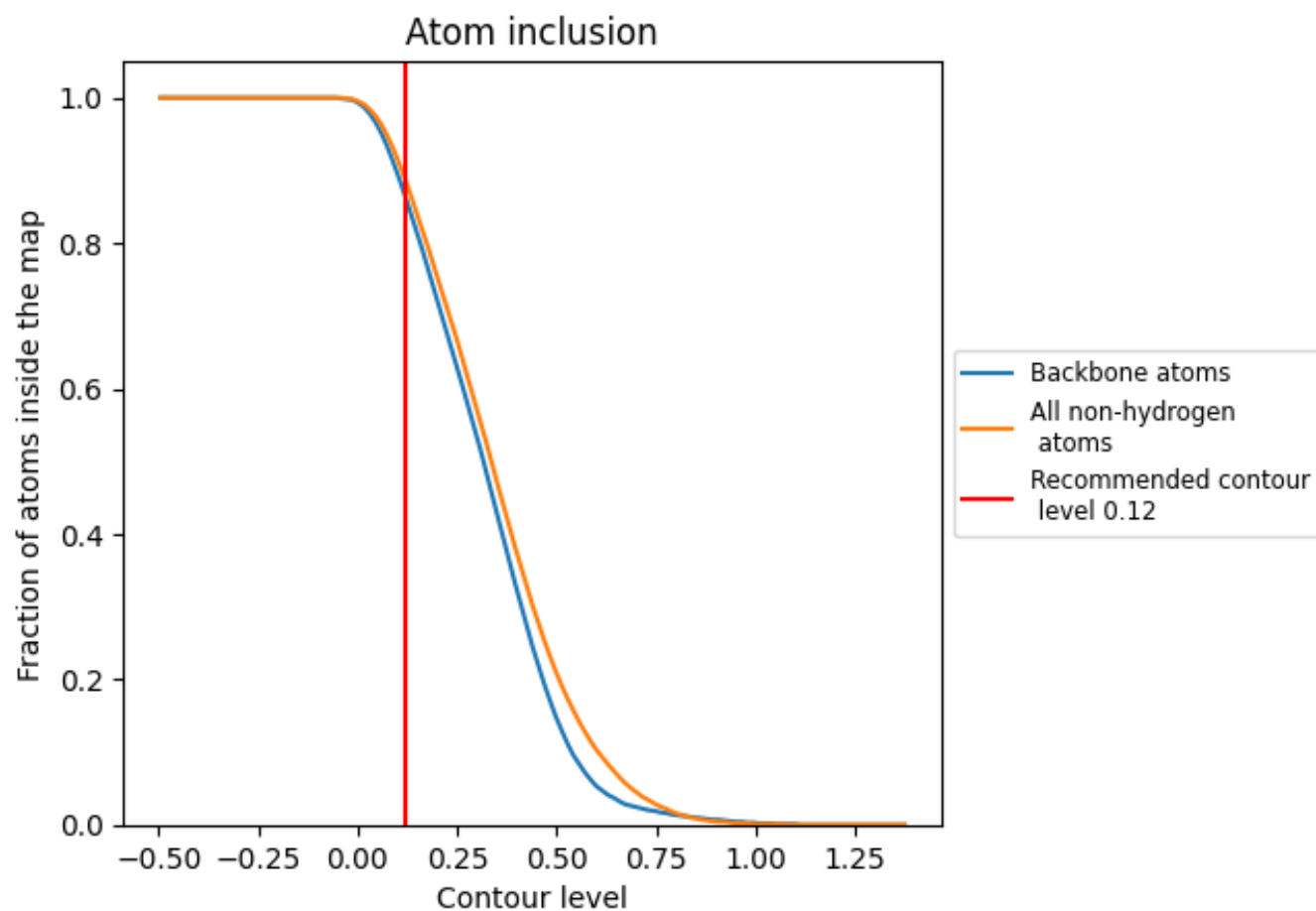
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 89% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8880	 0.5740
1e	 0.9180	 0.5820
2f	 0.9860	 0.6010
3n	 0.9790	 0.6360
AN	 0.5910	 0.4010
As	 0.7450	 0.4110
B4	 0.9850	 0.6430
Bt	 0.6590	 0.4380
CD	 0.9880	 0.6440
CW	 0.2200	 0.2930
DK	 0.1370	 0.2580
DO	 0.9740	 0.6330
EX	 0.0430	 0.2810
Ez	 0.9310	 0.5640
F8	 0.9380	 0.5930
FR	 0.0370	 0.2680
Gu	 0.9680	 0.6270
Hj	 0.9350	 0.5830
Ib	 0.9670	 0.6030
Jy	 0.8760	 0.5030
KM	 0.6760	 0.3940
LL	 0.9280	 0.6060
MQ	 0.9660	 0.6130
No	 0.9960	 0.6550
O6	 0.9780	 0.6400
Pv	 0.9700	 0.6380
Qk	 0.9890	 0.6430
RP	 0.8440	 0.5720
SZ	 0.9780	 0.6270
Tl	 0.9540	 0.6190
UF	 0.8930	 0.5970
V5	 0.9700	 0.6220
Wg	 0.8660	 0.4760
Xc	 0.9660	 0.6280
YU	 0.9510	 0.6300



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Chain	Atom inclusion	Q-score
Zq	 0.9440	 0.5930
aw	 0.9680	 0.6420
b3	 0.9730	 0.6000
cC	 0.9530	 0.6030
dG	 0.9400	 0.6240
eH	 0.9740	 0.6370
f7	 0.9900	 0.6580
g2	 0.9520	 0.6190
h1	 0.9670	 0.6180
ia	 0.9540	 0.5780
jh	 0.9770	 0.6530
kr	 0.9090	 0.5670
li	 0.9880	 0.6540
mS	 0.9740	 0.6170
nY	 0.9800	 0.6200
ox	 0.9240	 0.5880
pT	 0.8570	 0.5700
qJ	 0.8340	 0.5620
rA	 0.8800	 0.5630
sm	 0.5560	 0.4350
tB	 0.9250	 0.6080
v9	 0.7890	 0.4760
vV	 0.8850	 0.5370
xI	 0.8450	 0.5530
xd	 0.8810	 0.5530
yE	 0.9450	 0.5980
zp	 0.8660	 0.5440