



Full wwPDB EM Validation Report ⓘ

Jul 10, 2026 – 05:57 AM JST

PDB ID : 9XAE / pdb_00009xae
EMDB ID : EMD-66684
Title : Cryo-EM structure of the pre-40S ribosome (Enp1-Rrp12 WT) from *Chaetomium thermophilum*, state Rio2-C
Authors : Lau, B.; Li, Y.; Zhu, J.; Fischer, P.; Hong, X.; Yuan, R.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on : 2025-10-22
Resolution : 3.00 Å (reported)
Based on initial model : 6G18

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.dev133
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) : 2.50

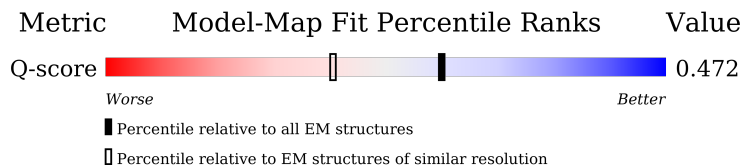
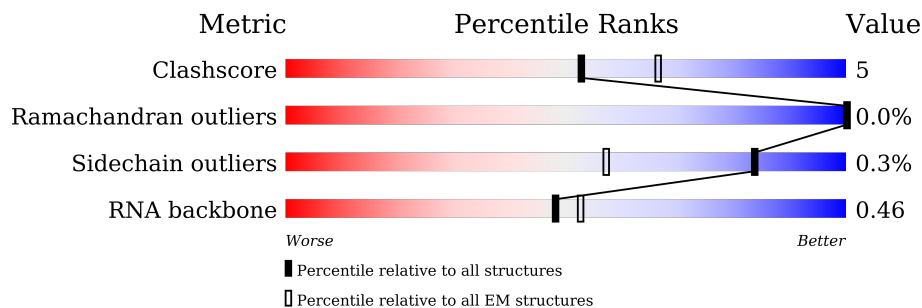
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



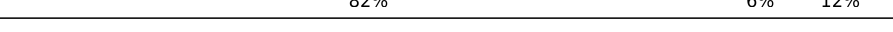
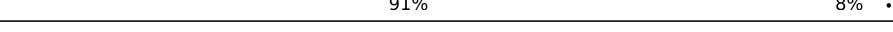
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	D	285	
2	E	255	
3	F	263	

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Mol	Chain	Length	Quality of chain
4	H	264	
5	I	212	
6	J	239	
7	K	203	
8	L	202	
9	M	190	
10	O	161	
11	P	144	
12	Q	151	
13	R	150	
14	S	153	
15	T	143	
16	U	143	
17	V	156	
18	W	153	
19	Y	98	
20	Z	130	
21	a	145	
22	b	136	
23	c	99	
24	e	82	
25	f	68	
26	h	62	
27	i	154	
28	A	1796	

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Mol	Chain	Length	Quality of chain
29	2	830	70%13%18%
30	3	259	60%11%29%
31	4	480	45%11%44%
32	5	445	16%82%

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 76910 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 Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	208	Total	C	N	O	S	0	0
			1641	1051	289	295	6		

- Molecule 2 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	213	Total	C	N	O	S	0	0
			1723	1096	319	303	5		

- Molecule 3 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	204	Total	C	N	O	S	0	0
			1573	1017	269	284	3		

- Molecule 4 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	261	Total	C	N	O	S	0	0
			2072	1314	389	362	7		

- Molecule 5 is a protein called 40S ribosomal protein s5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	199	Total	C	N	O	S	0	0
			1557	971	294	285	7		

- Molecule 6 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	232	Total	C	N	O	S	0	0
			1875	1171	376	323	5		

- Molecule 7 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	K	195	Total	C	N	O	0	0
			1562	983	300	279		

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	201	Total	C	N	O	S	0	0
			1621	1009	330	281	1		

- Molecule 9 is a protein called 40S ribosomal protein s9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	179	Total	C	N	O	S	0	0
			1466	933	290	241	2		

- Molecule 10 is a protein called 40S ribosomal protein S11-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	150	Total	C	N	O	S	0	0
			1222	780	236	201	5		

- Molecule 11 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	118	Total	C	N	O	S	0	0
			923	577	167	171	8		

- Molecule 12 is a protein called 40S ribosomal protein S13-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	150	Total	C	N	O	S	0	0
			1182	756	220	205	1		

- Molecule 13 is a protein called 40S ribosomal protein S14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	135	Total	C	N	O	S	0	0
			993	610	196	182	5		

- Molecule 14 is a protein called 40S ribosomal protein s15-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	123	Total	C	N	O	S	0	0
			986	628	184	171	3		

- Molecule 15 is a protein called 40S ribosomal protein S16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	120	Total	C	N	O	S	0	0
			935	603	168	163	1		

- Molecule 16 is a protein called 40S ribosomal protein S17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	109	Total	C	N	O	S	0	0
			876	552	161	160	3		

- Molecule 17 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	122	Total	C	N	O	S	0	0
			995	628	191	175	1		

- Molecule 18 is a protein called 40S ribosomal protein S19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	142	Total	C	N	O	S	0	0
			1117	694	221	201	1		

- Molecule 19 is a protein called 40S ribosomal protein S21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Y	86	Total	C	N	O	S	0	0
			664	408	124	128	4		

- Molecule 20 is a protein called 40S ribosomal protein S22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Z	129	Total	C	N	O	S	0	0
			1037	659	195	178	5		

- Molecule 21 is a protein called 40S ribosomal protein s23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	a	142	Total	C	N	O	S	0	0
			1099	694	215	188	2		

- Molecule 22 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	b	132	Total	C	N	O	S	0	0
			1061	668	209	182	2		

- Molecule 23 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	c	69	Total	C	N	O	S	0	0
			546	345	101	98	2		

- Molecule 24 is a protein called Ribosomal protein s27-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	81	Total	C	N	O	S	0	0
			611	386	111	107	7		

- Molecule 25 is a protein called 40S ribosomal protein S28-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	61	Total	C	N	O	S	0	0
			472	292	91	88	1		

- Molecule 26 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	h	21	Total	C	N	O	0	0
			173	112	37	24		

- Molecule 27 is a protein called 40S ribosomal protein S27a-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	i	65	Total	C	N	O	S	0	0
			528	332	97	93	6		

- Molecule 28 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A	1720	Total	C	N	O	P	0	0
			36686	16390	6537	12039	1720		

- Molecule 29 is a protein called Bms1-type G domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	683	Total	C	N	O	S	0	0
			5458	3445	991	1004	18		

- Molecule 30 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	184	Total	C	N	O	S	0	0
			1435	912	260	256	7		

- Molecule 31 is a protein called Bystin-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	270	Total	C	N	O	S	0	0
			2154	1401	377	366	10		

- Molecule 32 is a protein called Putative low-temperature viability protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	81	Total	C	N	O	S	0	0
			660	416	113	130	1		

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	a	1	Total	Mg	0
			1	1	
33	A	1	Total	Mg	0
			1	1	

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
34	e	1	Total	Zn	0
			1	1	

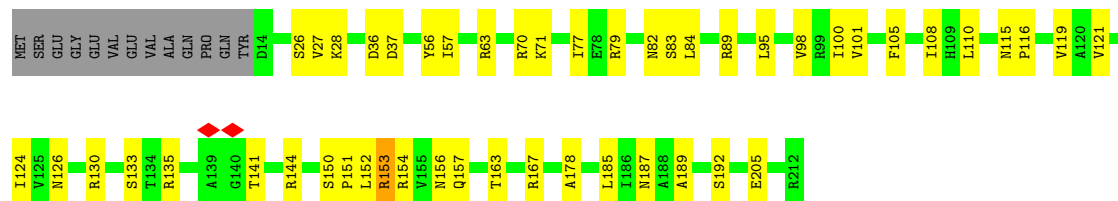
- Molecule 35 is water.

Mol	Chain	Residues	Atoms		AltConf
35	Q	1	Total 1	O 1	0
35	A	3	Total 3	O 3	0



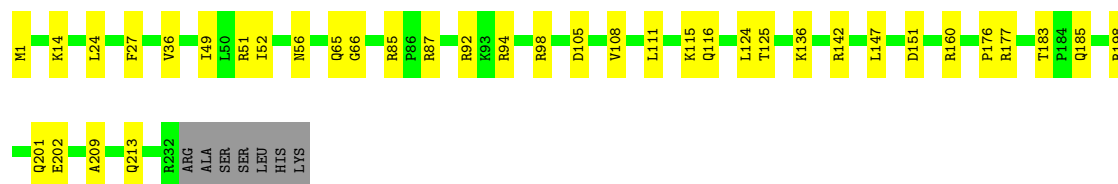
- Molecule 5: 40S ribosomal protein s5-like protein

Chain I: 71% 23% 6%



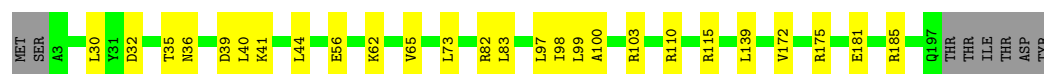
- Molecule 6: 40S ribosomal protein S6

Chain J: 82% 15% 3%



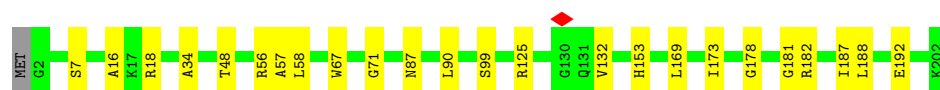
- Molecule 7: 40S ribosomal protein S7

Chain K: 83% 13% 4%



- Molecule 8: 40S ribosomal protein S8

Chain L: 88% 12% 0%



- Molecule 9: 40S ribosomal protein s9-like protein

Chain M: 83% 11% 6%



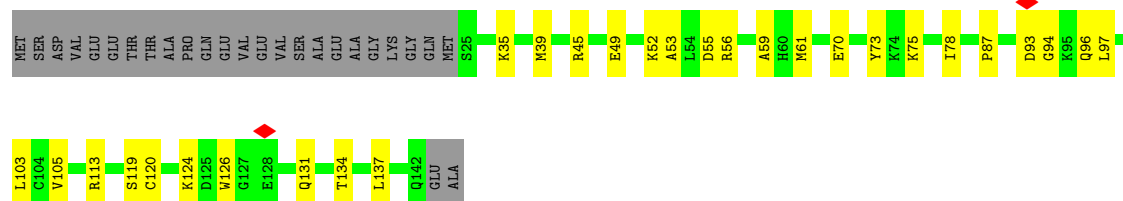
- Molecule 10: 40S ribosomal protein S11-like protein

Chain O:  87% 6% 7%



- Molecule 11: 40S ribosomal protein S12

Chain P:  62% 20% 18%



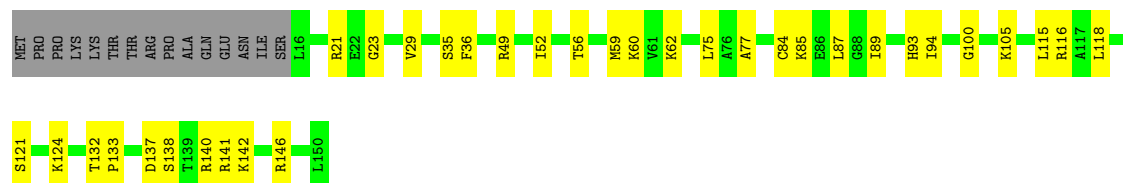
- Molecule 12: 40S ribosomal protein S13-like protein

Chain Q:  93% 7%



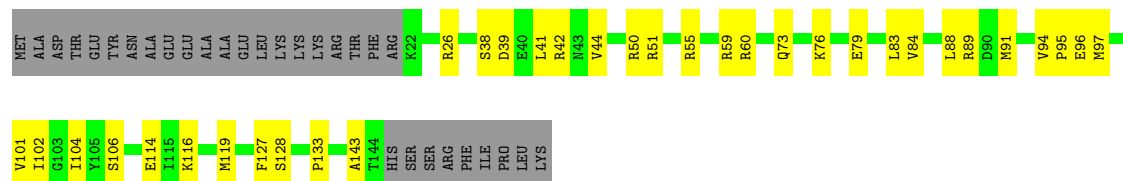
- Molecule 13: 40S ribosomal protein S14-like protein

Chain R:  67% 23% 10%



- Molecule 14: 40S ribosomal protein s15-like protein

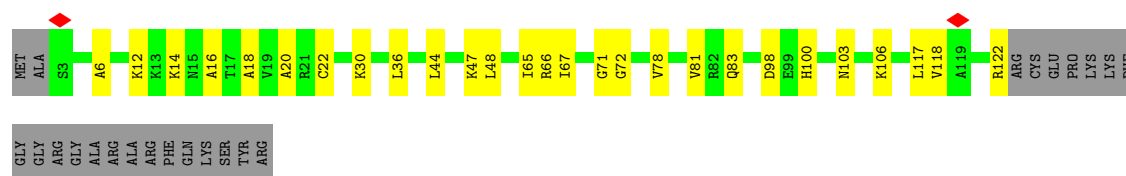
Chain S:  58% 22% 20%



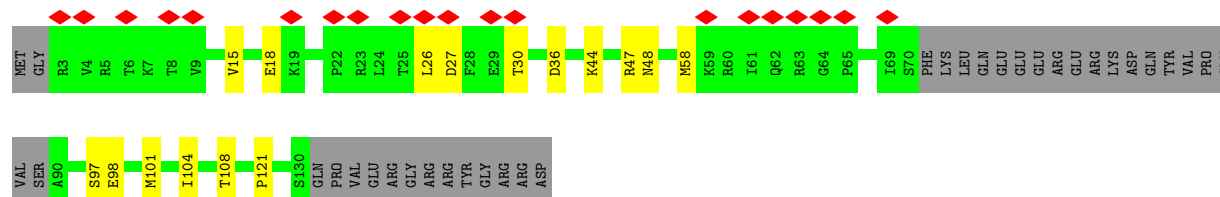
- Molecule 15: 40S ribosomal protein S16-like protein

Chain T:  65% 19% 16%

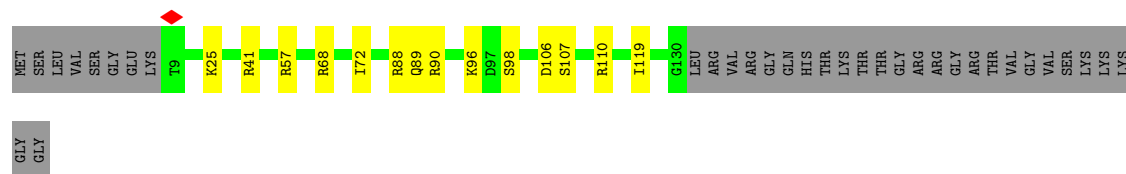




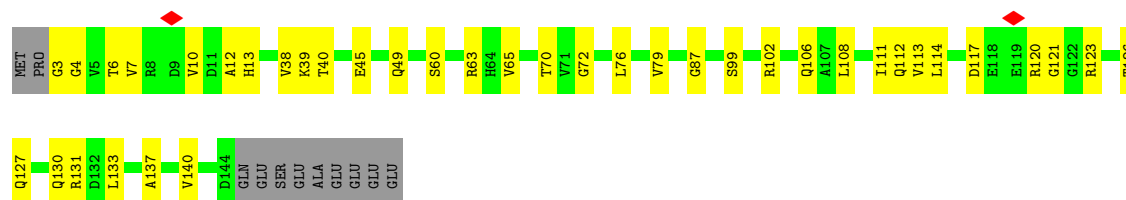
- Molecule 16: 40S ribosomal protein S17-like protein



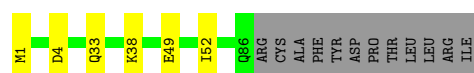
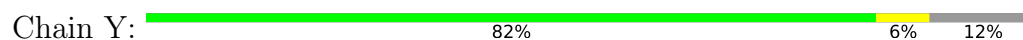
- Molecule 17: Putative ribosomal protein



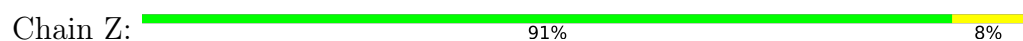
- Molecule 18: 40S ribosomal protein S19-like protein



- Molecule 19: 40S ribosomal protein S21-like protein



- Molecule 20: 40S ribosomal protein S22-like protein





- Molecule 21: 40S ribosomal protein s23-like protein

Chain a: 83% 15%



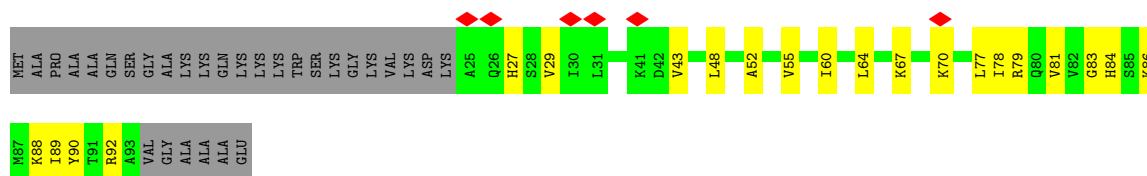
- Molecule 22: Small ribosomal subunit protein eS24

Chain b: 86% 11%



- Molecule 23: 40S ribosomal protein S25

Chain c: 6% 48% 21% 30%



- Molecule 24: Ribosomal protein s27-like protein

Chain e: 87% 12%



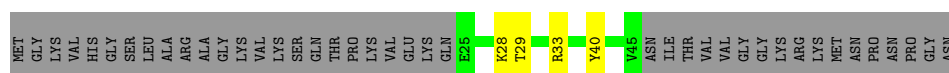
- Molecule 25: 40S ribosomal protein S28-like protein

Chain f: 84% 6% 10%

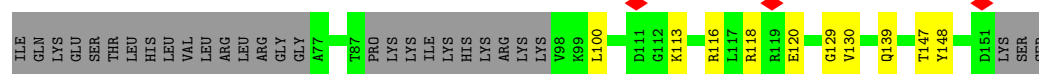


- Molecule 26: 40S ribosomal protein S30

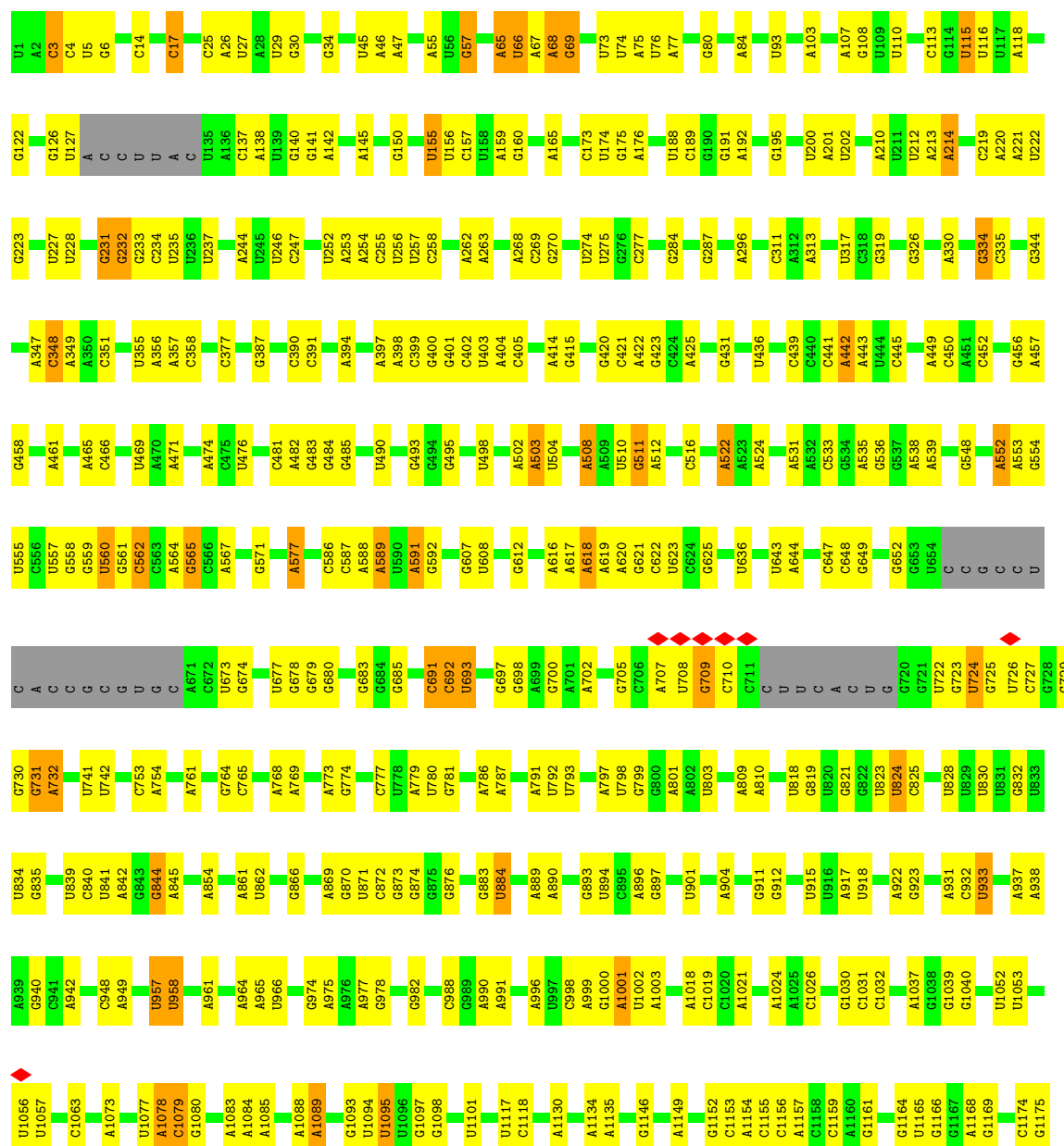
Chain h: 27% 6% 66%

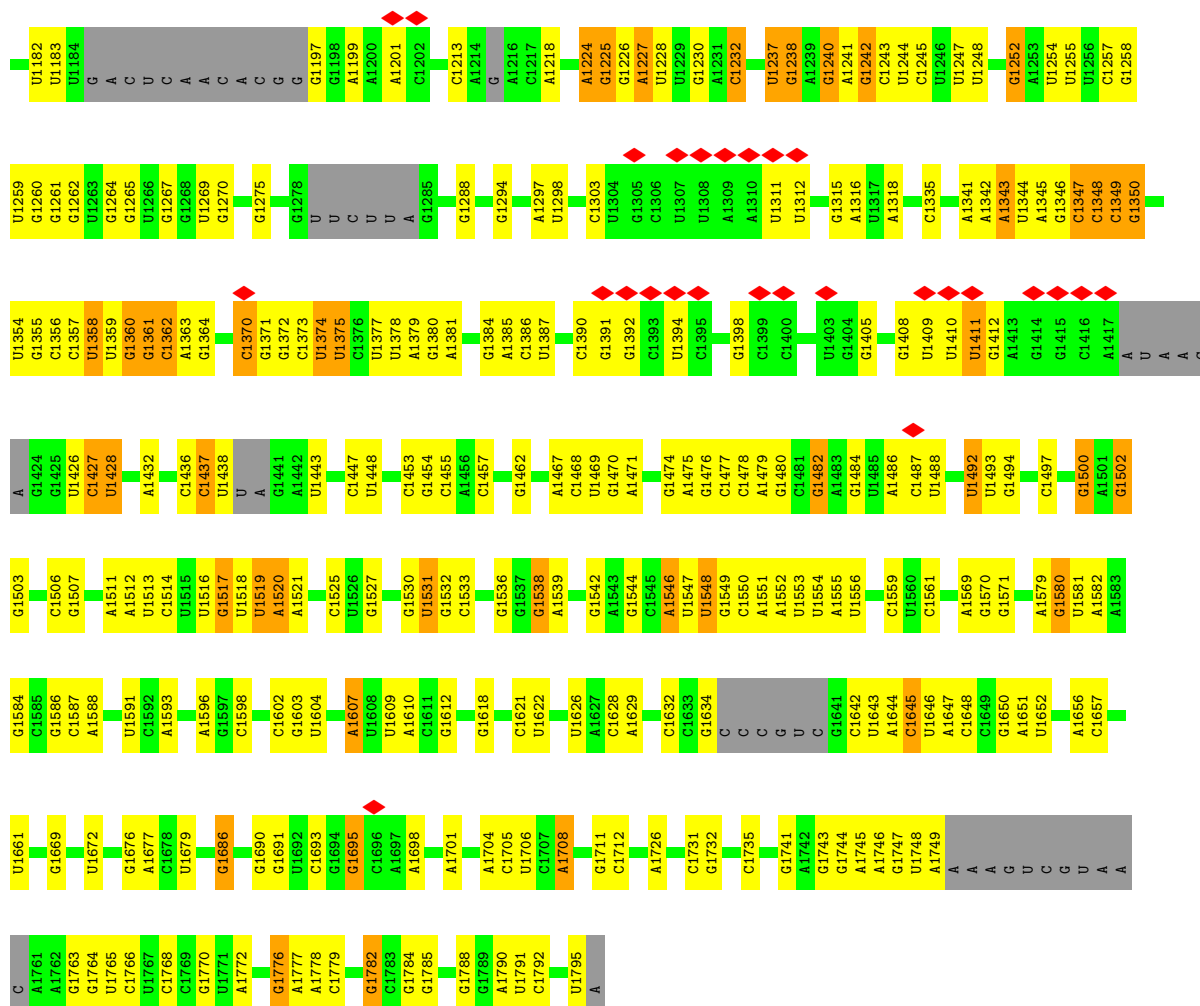


- Molecule 27: 40S ribosomal protein S27a-like protein



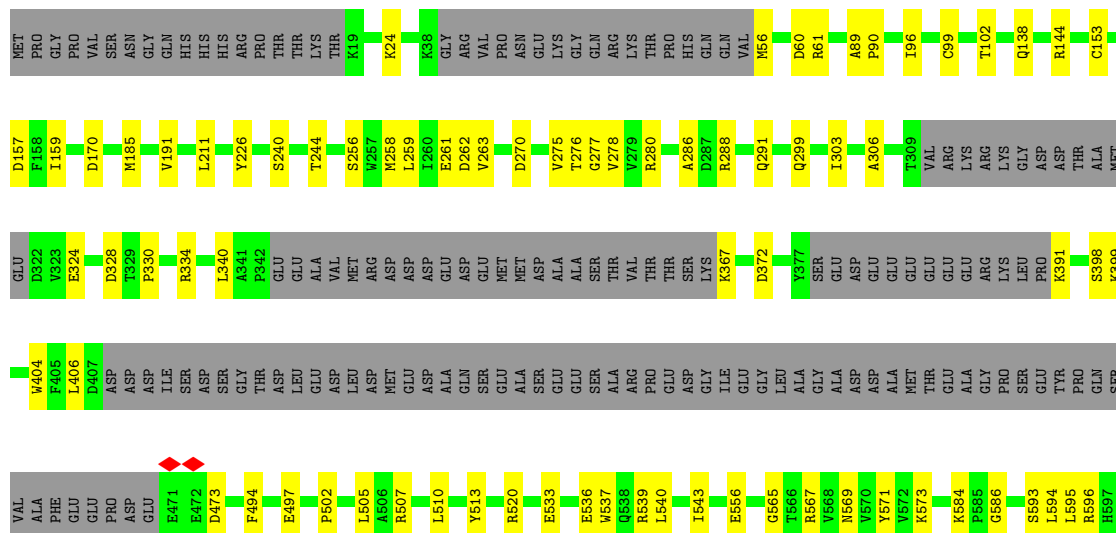
Chain A: 58% 33% 5%



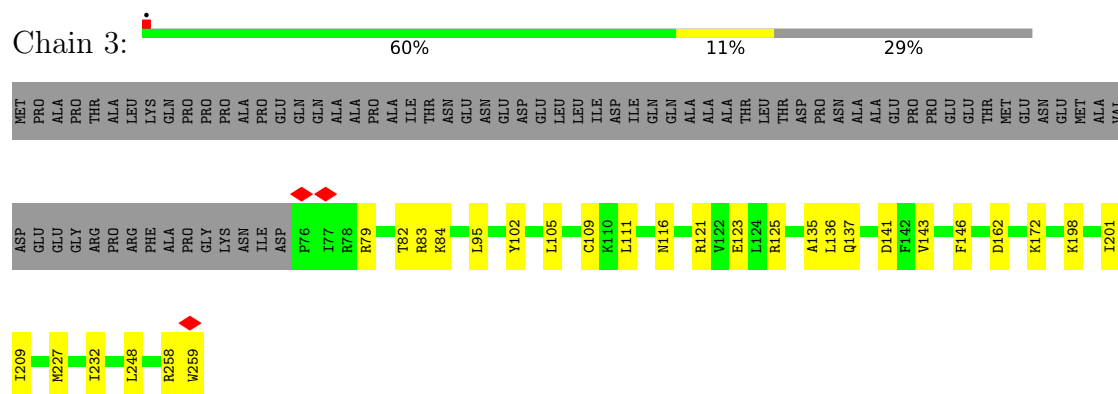


• Molecule 29: Bms1-type G domain-containing protein

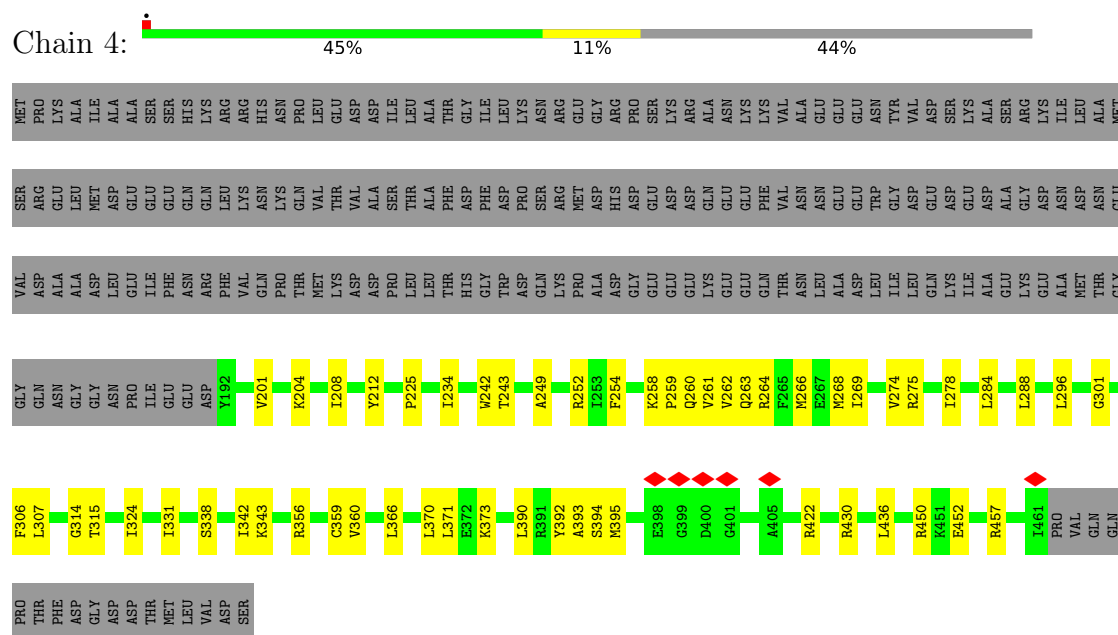
Chain 2: 70% 13% 18%



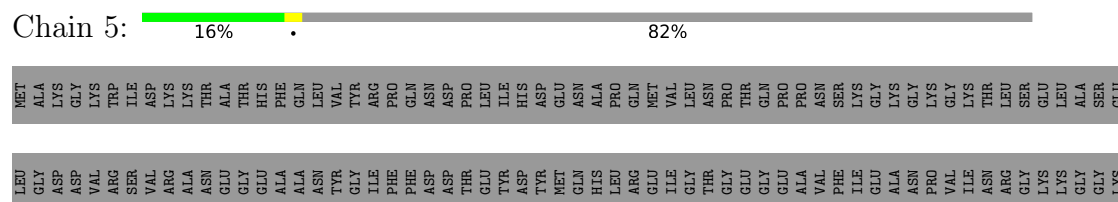
- Molecule 30: Pre-rRNA-processing protein PNO1



- Molecule 31: Bystin-like protein



- Molecule 32: Putative low-temperature viability protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85384	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Relion	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.752	Depositor
Minimum map value	-0.357	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	412.56, 412.56, 412.56	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.146, 1.146, 1.146	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	D	0.18	0/1683	0.47	0/2299
2	E	0.30	0/1752	0.59	1/2361 (0.0%)
3	F	0.18	0/1603	0.46	0/2169
4	H	0.22	0/2112	0.48	0/2842
5	I	0.32	0/1578	0.65	0/2130
6	J	0.27	0/1906	0.57	0/2547
7	K	0.23	0/1587	0.50	0/2140
8	L	0.20	0/1654	0.50	0/2213
9	M	0.19	0/1489	0.42	0/1993
10	O	0.23	0/1249	0.43	0/1678
11	P	0.22	0/934	0.63	0/1255
12	Q	0.17	0/1205	0.33	0/1627
13	R	0.35	0/1005	0.63	1/1350 (0.1%)
14	S	0.18	0/1003	0.53	0/1342
15	T	0.20	0/949	0.52	0/1278
16	U	0.21	0/887	0.45	0/1191
17	V	0.22	0/1009	0.63	0/1356
18	W	0.19	0/1137	0.54	0/1533
19	Y	0.16	0/671	0.36	0/900
20	Z	0.23	0/1055	0.53	0/1416
21	a	0.22	0/1116	0.49	0/1489
22	b	0.19	0/1075	0.43	0/1431
23	c	0.20	0/550	0.63	0/736
24	e	0.21	0/623	0.52	0/843
25	f	0.18	0/475	0.45	0/639
26	h	0.52	0/176	0.68	0/233
27	i	0.14	0/535	0.45	0/710
28	A	0.23	0/41025	0.39	1/63918 (0.0%)
29	2	0.16	0/5573	0.42	0/7533
30	3	0.21	0/1459	0.51	0/1964
31	4	0.24	0/2205	0.64	0/2990
32	5	0.25	0/670	0.75	0/896

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.22	0/81950	0.45	3/119002 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	I	0	1
14	S	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	150	ILE	N-CA-C	-6.02	107.63	113.53
28	A	1531	U	C2'-C3'-O3'	6.02	118.53	109.50
13	R	138	SER	N-CA-C	5.21	118.14	110.59

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	I	153	ARG	Sidechain
14	S	73	GLN	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	D	1641	0	1650	24	0
2	E	1723	0	1804	22	0
3	F	1573	0	1669	13	0
4	H	2072	0	2155	22	0
5	I	1557	0	1608	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	1875	0	1983	23	0
7	K	1562	0	1641	16	0
8	L	1621	0	1645	16	0
9	M	1466	0	1582	18	0
10	O	1222	0	1289	8	0
11	P	923	0	946	19	0
12	Q	1182	0	1264	9	0
13	R	993	0	1021	20	0
14	S	986	0	1045	27	0
15	T	935	0	997	17	0
16	U	876	0	921	9	0
17	V	995	0	1040	14	0
18	W	1117	0	1133	27	0
19	Y	664	0	662	5	0
20	Z	1037	0	1076	8	0
21	a	1099	0	1169	18	0
22	b	1061	0	1150	12	0
23	c	546	0	591	16	0
24	e	611	0	634	6	0
25	f	472	0	491	2	0
26	h	173	0	192	2	0
27	i	528	0	541	7	0
28	A	36686	0	18488	297	0
29	2	5458	0	5501	63	0
30	3	1435	0	1491	18	0
31	4	2154	0	2242	35	0
32	5	660	0	648	10	0
33	A	1	0	0	0	0
33	a	1	0	0	0	0
34	e	1	0	0	0	0
35	A	3	0	0	0	0
35	Q	1	0	0	0	0
All	All	76910	0	60269	702	0

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

All (702) 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)
28:A:1079:C:H42	28:A:1089:A:N6	1.48	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:1079:C:N4	28:A:1089:A:H62	1.50	1.09
28:A:214:A:N6	28:A:840:C:H42	1.55	1.03
28:A:1695:G:H21	28:A:1698:A:N6	1.57	1.03
28:A:214:A:H61	28:A:840:C:N4	1.60	0.99
28:A:443:A:N6	28:A:458:G:H21	1.62	0.97
28:A:1584:G:H1	28:A:1604:U:H3	0.98	0.95
28:A:652:G:H1	28:A:673:U:H3	0.98	0.95
28:A:866:G:H1	28:A:958:U:H3	1.14	0.94
28:A:1695:G:H21	28:A:1698:A:H62	1.05	0.94
28:A:1695:G:N2	28:A:1698:A:H62	1.65	0.93
28:A:1218:A:C2	28:A:1260:G:N1	2.36	0.93
28:A:1652:U:H3	28:A:1741:G:H1	1.23	0.83
28:A:1693:C:N4	28:A:1701:A:H61	1.77	0.81
28:A:219:C:N4	28:A:220:A:N6	2.29	0.80
15:T:6:ALA:HA	15:T:22:CYS:O	1.81	0.80
28:A:1693:C:H42	28:A:1701:A:N6	1.82	0.78
28:A:483:G:H1	28:A:498:U:H3	1.32	0.78
28:A:1686:G:N2	28:A:1708:A:N6	2.32	0.77
9:M:140:ASN:C	9:M:140:ASN:HD22	1.94	0.76
28:A:214:A:N1	28:A:840:C:N3	2.35	0.74
28:A:1695:G:N2	28:A:1698:A:N6	2.29	0.74
28:A:1686:G:N2	28:A:1708:A:C6	2.55	0.74
28:A:753:C:H42	28:A:791:A:N6	1.86	0.73
28:A:1078:A:H62	28:A:1088:A:H62	1.35	0.72
28:A:702:A:H62	28:A:731:G:N2	1.87	0.72
28:A:1686:G:C2	28:A:1708:A:N6	2.58	0.72
28:A:1693:C:H42	28:A:1701:A:H61	1.37	0.72
28:A:220:A:N1	28:A:835:G:C6	2.58	0.72
28:A:214:A:H61	28:A:840:C:H42	0.78	0.71
29:2:256:SER:HB3	29:2:593:SER:HB3	1.72	0.70
28:A:443:A:N6	28:A:458:G:N2	2.38	0.70
28:A:1427:C:H2'	28:A:1428:U:H2'	1.74	0.70
10:O:80:VAL:O	10:O:125:GLY:N	2.25	0.69
28:A:1237:U:H2'	28:A:1238:G:H2'	1.75	0.69
28:A:709:G:H1	28:A:722:U:H3	1.41	0.69
28:A:1218:A:N1	28:A:1260:G:O6	2.26	0.69
31:4:390:LEU:O	31:4:394:SER:HB3	1.93	0.69
28:A:1303:C:H42	28:A:1316:A:H61	1.37	0.68
15:T:20:ALA:HB1	15:T:65:ILE:HD11	1.75	0.68
4:H:140:VAL:HG22	4:H:146:THR:HG22	1.76	0.68
28:A:1242:G:H1	28:A:1247:U:H3	1.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:72:GLY:HA3	28:A:1494:G:H5'	1.75	0.67
3:F:172:SER:HB3	28:A:1083:A:H5'	1.76	0.67
28:A:893:G:H1	28:A:915:U:H3	1.43	0.67
28:A:753:C:N4	28:A:791:A:H61	1.92	0.67
15:T:67:ILE:HG12	15:T:81:VAL:HG23	1.76	0.67
20:Z:90:VAL:HG13	20:Z:94:LEU:HD12	1.76	0.66
28:A:753:C:N4	28:A:791:A:N6	2.43	0.66
15:T:71:GLY:HA2	28:A:1479:A:H4'	1.77	0.66
1:D:149:LEU:HD11	1:D:176:ILE:HG21	1.76	0.65
5:I:57:ILE:HD11	15:T:47:LYS:HG2	1.79	0.65
30:3:111:LEU:HD21	30:3:136:LEU:HA	1.79	0.65
21:a:17:ASN:OD1	21:a:20:ARG:NH2	2.29	0.65
15:T:44:LEU:HD21	15:T:78:VAL:HG21	1.77	0.65
12:Q:70:LYS:NZ	28:A:961:A:N7	2.44	0.64
13:R:21:ARG:HD3	13:R:23:GLY:H	1.62	0.64
7:K:73:LEU:HD22	7:K:100:ALA:HB2	1.80	0.64
28:A:442:A:H1'	28:A:522:A:H5''	1.79	0.64
29:2:191:VAL:HG12	29:2:226:TYR:HB2	1.80	0.64
1:D:85:GLY:O	1:D:88:ALA:HB3	1.97	0.64
25:f:26:VAL:HA	25:f:46:LYS:HA	1.80	0.64
29:2:291:GLN:HB2	29:2:594:LEU:HD11	1.80	0.63
8:L:99:SER:N	8:L:173:ILE:O	2.30	0.63
4:H:87:MET:HE3	4:H:123:LEU:HB2	1.80	0.63
15:T:30:LYS:NZ	28:A:1363:A:OP1	2.32	0.63
16:U:101:MET:HE1	16:U:121:PRO:HB2	1.80	0.62
21:a:69:ARG:NH2	28:A:565:G:N7	2.47	0.62
6:J:136:LYS:NZ	28:A:65:A:OP1	2.28	0.62
28:A:1201:A:N6	28:A:1550:C:C2	2.67	0.62
6:J:147:LEU:HD23	6:J:151:ASP:HB3	1.81	0.62
29:2:510:LEU:HD23	29:2:796:LEU:HD22	1.82	0.62
31:4:263:GLN:HB3	31:4:301:GLY:HA2	1.82	0.62
28:A:220:A:N1	28:A:835:G:O6	2.32	0.61
28:A:1580:G:N2	28:A:1607:A:OP2	2.34	0.61
14:S:116:LYS:H	14:S:119:MET:HE1	1.66	0.61
29:2:618:ILE:HB	29:2:656:LEU:HB3	1.83	0.61
18:W:12:ALA:HA	18:W:63:ARG:HH22	1.65	0.61
31:4:430:ARG:NH2	31:4:457:ARG:O	2.34	0.61
4:H:199:GLU:OE2	28:A:797:A:O2'	2.18	0.61
28:A:1693:C:N3	28:A:1701:A:N1	2.49	0.61
21:a:82:LYS:NZ	28:A:1645:C:OP2	2.34	0.60
28:A:443:A:H61	28:A:458:G:H21	1.43	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:1275:G:H1	28:A:1426:U:H3	1.50	0.60
20:Z:106:THR:HG22	20:Z:108:ALA:H	1.66	0.60
23:c:79:ARG:NH1	23:c:92:ARG:O	2.35	0.60
31:4:331:ILE:O	31:4:373:LYS:NZ	2.33	0.60
28:A:1227:A:H62	28:A:1252:G:H21	1.49	0.60
1:D:168:LYS:O	1:D:170:ARG:NH2	2.34	0.60
24:e:37:CYS:SG	24:e:61:ASN:ND2	2.74	0.60
11:P:59:ALA:HA	11:P:124:LYS:HZ3	1.67	0.60
8:L:58:LEU:HD21	28:A:1672:U:H5''	1.84	0.59
31:4:201:VAL:HG21	32:5:393:LEU:HG	1.84	0.59
8:L:7:SER:O	8:L:18:ARG:NH1	2.35	0.59
18:W:131:ARG:NH1	28:A:1356:C:OP1	2.34	0.59
21:a:56:LYS:HE3	21:a:93:LEU:HD22	1.84	0.59
28:A:443:A:H61	28:A:458:G:N2	2.00	0.59
15:T:18:ALA:HB1	15:T:67:ILE:HD11	1.84	0.59
3:F:150:GLY:HA2	19:Y:1:MET:HE1	1.85	0.59
30:3:201:ILE:HD13	30:3:248:LEU:HD11	1.83	0.59
28:A:1218:A:H2	28:A:1260:G:N1	1.97	0.59
32:5:395:GLU:OE2	32:5:399:ASN:ND2	2.36	0.59
21:a:103:LEU:HB3	21:a:126:LYS:HB2	1.85	0.58
28:A:1218:A:N1	28:A:1260:G:C6	2.71	0.58
3:F:160:HIS:ND1	3:F:203:ASP:OD2	2.36	0.58
28:A:1303:C:N3	28:A:1316:A:N1	2.50	0.58
29:2:772:LEU:O	29:2:777:TYR:HB2	2.03	0.58
28:A:702:A:N6	28:A:731:G:N2	2.51	0.58
28:A:1480:G:H21	28:A:1602:C:H1'	1.68	0.58
28:A:1493:U:O4	28:A:1506:C:N3	2.36	0.58
20:Z:2:VAL:N	28:A:1032:C:HO2'	1.99	0.58
24:e:20:LYS:NZ	28:A:957:U:OP2	2.36	0.58
1:D:19:GLN:HB3	1:D:175:LEU:HD11	1.85	0.58
8:L:56:ARG:NH2	8:L:178:GLY:O	2.35	0.58
31:4:274:VAL:HG12	31:4:288:LEU:HD23	1.85	0.58
28:A:1693:C:N4	28:A:1701:A:N6	2.44	0.58
14:S:89:ARG:NH2	28:A:1554:U:O4	2.36	0.58
22:b:91:ARG:NH2	22:b:101:ALA:O	2.35	0.58
14:S:38:SER:HA	14:S:41:LEU:HB2	1.86	0.58
3:F:126:SER:HB2	3:F:132:ALA:HB2	1.86	0.57
17:V:41:ARG:HG2	28:A:1561:C:H5''	1.86	0.57
8:L:48:THR:HG23	28:A:330:A:H5'	1.85	0.57
14:S:143:ALA:HB2	28:A:1175:G:H21	1.70	0.57
4:H:9:GLN:HB2	4:H:30:ARG:HD3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:57:ALA:HB2	8:L:181:GLY:HA2	1.87	0.57
30:3:209:ILE:HD13	30:3:232:ILE:HD11	1.87	0.57
18:W:7:VAL:HG11	18:W:133:LEU:HG	1.85	0.57
13:R:124:LYS:HD3	30:3:79:ARG:HD3	1.87	0.57
28:A:702:A:N6	28:A:731:G:C2	2.73	0.57
21:a:95:PHE:O	21:a:142:LYS:NZ	2.31	0.57
15:T:117:LEU:HG	15:T:118:VAL:HG23	1.87	0.57
5:I:151:PRO:HA	5:I:154:ARG:HG3	1.87	0.56
29:2:288:ARG:NH2	29:2:556:GLU:OE2	2.38	0.56
8:L:125:ARG:HE	8:L:132:VAL:HA	1.70	0.56
13:R:116:ARG:NH1	30:3:141:ASP:OD2	2.38	0.56
28:A:67:A:O2'	28:A:69:G:OP1	2.24	0.56
29:2:270:ASP:O	29:2:573:LYS:NZ	2.38	0.56
4:H:88:ASP:OD1	4:H:122:LYS:NZ	2.39	0.56
17:V:25:LYS:O	17:V:57:ARG:NH2	2.39	0.56
28:A:457:A:H3'	28:A:458:G:H8	1.70	0.56
29:2:367:LYS:NZ	29:2:751:GLU:OE2	2.38	0.56
31:4:204:LYS:HD3	32:5:408:VAL:HG11	1.86	0.56
13:R:29:VAL:HG12	13:R:93:HIS:HB2	1.88	0.56
17:V:88:ARG:NH2	28:A:1542:G:N3	2.54	0.56
21:a:65:ASN:ND2	21:a:116:ASP:OD2	2.36	0.56
31:4:242:TRP:HZ3	31:4:269:ILE:HG21	1.71	0.56
28:A:1500:G:N3	28:A:1559:C:O2'	2.39	0.56
28:A:869:A:H2'	28:A:870:G:C8	2.41	0.55
29:2:306:ALA:O	29:2:567:ARG:NH1	2.37	0.55
12:Q:99:ARG:NH2	12:Q:119:GLU:OE2	2.37	0.55
31:4:234:ILE:HD12	31:4:268:MET:HE3	1.88	0.55
5:I:82:ASN:ND2	28:A:1607:A:O3'	2.39	0.55
28:A:1294:G:N2	28:A:1297:A:OP2	2.34	0.55
28:A:1343:A:N1	28:A:1373:C:N4	2.55	0.55
5:I:63:ARG:O	5:I:70:ARG:NH2	2.40	0.55
11:P:61:MET:HE1	11:P:126:TRP:HZ2	1.71	0.55
12:Q:106:ARG:NH2	28:A:1018:A:OP1	2.40	0.55
28:A:1517:G:O2'	28:A:1519:U:OP2	2.24	0.55
14:S:50:ARG:NH1	28:A:1546:A:OP2	2.40	0.55
31:4:393:ALA:HB3	31:4:436:LEU:HD11	1.88	0.55
28:A:616:A:OP1	29:2:24:LYS:NZ	2.39	0.55
30:3:258:ARG:HE	30:3:259:TRP:HD1	1.55	0.55
8:L:182:ARG:NH1	28:A:202:U:O2	2.40	0.55
28:A:1690:G:H2'	28:A:1691:G:H8	1.72	0.55
30:3:84:LYS:HG2	30:3:123:GLU:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:LEU:HD13	1:D:163:ILE:HB	1.89	0.55
28:A:974:G:N1	28:A:1021:A:O2'	2.35	0.55
1:D:87:ARG:HA	1:D:90:LEU:HD12	1.88	0.54
10:O:60:ASP:HB3	10:O:63:CYS:HB2	1.88	0.54
27:i:116:ARG:NH2	27:i:130:VAL:O	2.40	0.54
28:A:1257:C:H2'	28:A:1258:G:C8	2.43	0.54
4:H:11:ARG:NH1	4:H:21:ASP:O	2.40	0.54
9:M:57:LEU:HD22	9:M:67:ARG:HA	1.87	0.54
15:T:66:ARG:NH2	28:A:1362:C:OP2	2.40	0.54
16:U:36:ASP:HB3	16:U:47:ARG:HD2	1.88	0.54
1:D:201:MET:HG3	1:D:203:ASP:H	1.73	0.54
2:E:146:ARG:NH2	28:A:1053:U:O2	2.41	0.54
7:K:110:ARG:NH2	28:A:803:U:O4	2.41	0.54
13:R:146:ARG:NH1	28:A:1782:G:OP2	2.39	0.54
28:A:557:U:H2'	28:A:558:G:H8	1.72	0.54
14:S:83:LEU:HA	14:S:101:VAL:HG23	1.90	0.54
23:c:81:VAL:HB	23:c:89:ILE:HG13	1.89	0.54
28:A:1358:U:O2'	28:A:1360:G:N1	2.40	0.54
5:I:83:SER:O	5:I:167:ARG:NH2	2.41	0.54
18:W:117:ASP:O	18:W:121:GLY:HA2	2.07	0.54
28:A:17:C:O2'	28:A:1134:A:N1	2.40	0.54
1:D:56:THR:HA	1:D:164:PRO:HD2	1.89	0.54
7:K:110:ARG:NH1	28:A:801:A:O2'	2.41	0.54
28:A:1686:G:N2	28:A:1708:A:C5	2.76	0.54
1:D:44:ARG:HB2	1:D:47:GLY:HA3	1.90	0.54
11:P:45:ARG:NH2	28:A:1252:G:O2'	2.41	0.54
28:A:1201:A:C6	28:A:1550:C:N3	2.76	0.54
29:2:303:ILE:HB	29:2:328:ASP:HB2	1.90	0.54
30:3:83:ARG:NH1	30:3:137:GLN:OE1	2.41	0.54
28:A:1484:G:H3'	28:A:1511:A:H61	1.73	0.53
7:K:83:LEU:HD22	7:K:98:ILE:HD11	1.90	0.53
32:5:422:ILE:O	32:5:426:LEU:HB2	2.08	0.53
29:2:262:ASP:OD1	29:2:276:THR:OG1	2.26	0.53
9:M:21:ARG:O	9:M:25:GLU:HG2	2.08	0.53
2:E:25:THR:O	2:E:50:ARG:NH2	2.40	0.53
7:K:30:LEU:HG	7:K:44:LEU:HD21	1.89	0.53
29:2:722:LYS:HB3	29:2:798:LYS:HG2	1.91	0.53
9:M:124:ARG:HD3	26:h:33:ARG:HD3	1.90	0.53
29:2:159:ILE:HD12	29:2:185:MET:HG3	1.91	0.53
29:2:584:LYS:NZ	29:2:586:GLY:O	2.39	0.53
30:3:109:CYS:HB3	30:3:135:ALA:HB1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:1168:A:H2'	28:A:1169:G:C8	2.44	0.53
13:R:84:CYS:HB2	13:R:89:ILE:HB	1.90	0.53
13:R:141:ARG:NH2	30:3:172:LYS:O	2.42	0.53
29:2:686:THR:HB	29:2:693:GLU:HG2	1.90	0.53
1:D:86:GLN:HG3	1:D:102:ALA:HB1	1.91	0.52
28:A:1587:C:H2'	28:A:1588:A:H8	1.74	0.52
11:P:131:GLN:O	11:P:134:THR:OG1	2.24	0.52
22:b:13:ARG:NH1	22:b:29:ASP:OD2	2.42	0.52
29:2:324:GLU:OE2	29:2:571:TYR:OH	2.27	0.52
27:i:100:LEU:HD21	28:A:1225:G:H4'	1.89	0.52
8:L:16:ALA:HB2	28:A:351:C:H5''	1.91	0.52
5:I:110:LEU:HB3	23:c:48:LEU:HD21	1.91	0.52
6:J:116:GLN:NE2	6:J:125:THR:OG1	2.43	0.52
18:W:10:VAL:HG21	18:W:140:VAL:HG23	1.90	0.52
28:A:841:U:H2'	28:A:842:A:H8	1.74	0.52
5:I:126:ASN:ND2	5:I:189:ALA:O	2.42	0.52
28:A:707:A:N1	28:A:724:U:O2'	2.43	0.52
29:2:138:GLN:NE2	29:2:261:GLU:OE2	2.40	0.52
6:J:66:GLY:HA2	28:A:1677:A:H1'	1.92	0.52
8:L:67:TRP:O	8:L:71:GLY:N	2.42	0.52
32:5:351:LEU:HA	32:5:354:ARG:HG2	1.92	0.52
5:I:135:ARG:NH1	5:I:141:THR:O	2.43	0.52
17:V:88:ARG:NH1	28:A:1542:G:O2'	2.38	0.51
29:2:513:TYR:HB3	29:2:796:LEU:HB3	1.91	0.51
31:4:390:LEU:O	31:4:394:SER:CB	2.57	0.51
31:4:392:TYR:HA	31:4:395:MET:HE3	1.92	0.51
4:H:95:THR:HG22	22:b:19:PRO:HD2	1.91	0.51
8:L:153:HIS:HB3	10:O:24:LYS:HE2	1.92	0.51
11:P:61:MET:HA	11:P:87:PRO:HB2	1.92	0.51
12:Q:124:ARG:NH2	28:A:965:A:OP2	2.42	0.51
28:A:1237:U:O2	28:A:1240:G:N1	2.43	0.51
6:J:56:ASN:HB2	6:J:108:VAL:HG12	1.92	0.51
6:J:142:ARG:HA	6:J:147:LEU:HD13	1.92	0.51
15:T:98:ASP:OD2	15:T:100:HIS:NE2	2.43	0.51
4:H:100:ARG:HH21	4:H:118:GLU:HG2	1.76	0.51
28:A:1584:G:O6	28:A:1604:U:O4	2.29	0.51
22:b:63:LEU:HD23	22:b:74:GLY:HA3	1.91	0.51
27:i:118:ARG:NH1	27:i:120:GLU:OE1	2.38	0.51
28:A:1117:U:H2'	28:A:1118:C:C6	2.45	0.51
11:P:94:GLY:HA2	11:P:97:LEU:HD23	1.93	0.51
14:S:26:ARG:HH12	17:V:90:ARG:HB3	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:115:LYS:NZ	28:A:57:G:OP1	2.39	0.51
28:A:219:C:C4	28:A:220:A:N6	2.79	0.51
29:2:595:LEU:H	29:2:598:GLU:HG3	1.75	0.51
3:F:43:TRP:O	3:F:54:LYS:NZ	2.41	0.51
28:A:1002:U:H5'	28:A:1003:A:H5''	1.92	0.51
28:A:1410:U:O2'	28:A:1412:G:OP2	2.28	0.51
2:E:180:THR:H	2:E:183:GLN:NE2	2.08	0.51
6:J:209:ALA:O	6:J:213:GLN:OE1	2.29	0.51
23:c:88:LYS:HB3	23:c:90:TYR:HE1	1.75	0.51
24:e:67:THR:OG1	24:e:70:LYS:O	2.26	0.51
28:A:1349:C:H2'	28:A:1350:G:H8	1.75	0.51
28:A:1371:G:H2'	28:A:1372:G:C8	2.45	0.51
28:A:1520:A:N3	28:A:1586:G:O2'	2.42	0.51
30:3:102:TYR:HE2	30:3:143:VAL:HG22	1.76	0.51
28:A:1039:G:H2'	28:A:1040:G:C8	2.45	0.51
29:2:754:LYS:NZ	29:2:769:LYS:O	2.44	0.51
31:4:314:GLY:O	31:4:356:ARG:NH2	2.44	0.51
1:D:110:PHE:HE2	1:D:124:ILE:HD11	1.76	0.50
16:U:97:SER:OG	16:U:98:GLU:N	2.42	0.50
2:E:223:PHE:HD2	2:E:225:LEU:HD22	1.76	0.50
8:L:34:ALA:HB2	8:L:56:ARG:HD3	1.93	0.50
14:S:88:LEU:HD11	14:S:91:MET:HE3	1.93	0.50
28:A:1380:G:H2'	28:A:1381:A:H8	1.77	0.50
29:2:543:ILE:HD13	29:2:714:PRO:HG2	1.94	0.50
6:J:177:ARG:NH1	28:A:65:A:OP2	2.44	0.50
6:J:183:THR:HG22	6:J:185:GLN:H	1.77	0.50
14:S:39:ASP:OD1	14:S:42:ARG:NH2	2.43	0.50
15:T:103:ASN:HA	15:T:106:LYS:HZ3	1.76	0.50
28:A:510:U:H2'	28:A:511:G:C8	2.46	0.50
19:Y:4:ASP:OD1	19:Y:4:ASP:N	2.45	0.50
28:A:1257:C:H2'	28:A:1258:G:H8	1.75	0.50
28:A:1303:C:N4	28:A:1316:A:H61	2.06	0.50
31:4:278:ILE:HD11	31:4:284:LEU:HB2	1.94	0.50
5:I:36:ASP:OD1	5:I:37:ASP:N	2.44	0.50
18:W:38:VAL:HG12	18:W:40:THR:H	1.76	0.50
28:A:1260:G:H2'	28:A:1261:G:H8	1.77	0.50
29:2:263:VAL:HG22	29:2:275:VAL:HG12	1.92	0.50
5:I:77:ILE:HD12	5:I:105:PHE:HZ	1.77	0.50
12:Q:62:GLN:NE2	28:A:958:U:OP1	2.45	0.50
17:V:25:LYS:HB3	23:c:29:VAL:HG11	1.93	0.50
28:A:159:A:H3'	28:A:160:G:H21	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:30:PRO:HB3	12:Q:67:THR:HA	1.94	0.50
11:P:53:ALA:O	11:P:56:ARG:NH1	2.44	0.50
22:b:108:ARG:NH2	28:A:456:G:OP2	2.41	0.50
23:c:84:HIS:HD1	23:c:86:LYS:H	1.60	0.50
28:A:1502:G:H2'	28:A:1503:G:H8	1.77	0.50
28:A:1492:U:O2	28:A:1507:G:O6	2.29	0.50
29:2:502:PRO:HA	29:2:745:PHE:HD2	1.77	0.50
2:E:65:ILE:HD11	28:A:918:U:H5''	1.93	0.49
6:J:27:PHE:HE1	6:J:36:VAL:HG21	1.77	0.49
9:M:107:LEU:HB2	9:M:144:PHE:HB3	1.94	0.49
28:A:700:G:N2	28:A:732:A:C2	2.74	0.49
3:F:42:GLU:OE2	3:F:44:GLN:NE2	2.45	0.49
4:H:19:LEU:HD22	28:A:786:A:H2'	1.94	0.49
14:S:104:ILE:HD11	14:S:127:PHE:HB2	1.93	0.49
18:W:130:GLN:NE2	28:A:1354:U:O2'	2.45	0.49
31:4:338:SER:O	31:4:342:ILE:HD12	2.13	0.49
2:E:90:GLU:HB3	2:E:97:LEU:HB2	1.93	0.49
7:K:115:ARG:HD2	28:A:741:U:H1'	1.93	0.49
23:c:64:LEU:HA	23:c:67:LYS:HG2	1.94	0.49
1:D:10:PHE:O	1:D:57:TRP:NE1	2.31	0.49
8:L:182:ARG:NH1	28:A:255:C:O2	2.45	0.49
13:R:52:ILE:HG23	13:R:87:LEU:HD13	1.93	0.49
13:R:77:ALA:HB1	13:R:118:LEU:HD22	1.94	0.49
24:e:56:CYS:HB3	24:e:63:LEU:HD11	1.94	0.49
1:D:82:ARG:NH1	1:D:128:ASP:OD2	2.45	0.49
4:H:146:THR:HG21	28:A:122:G:H21	1.78	0.49
17:V:106:ASP:OD1	17:V:106:ASP:N	2.45	0.49
18:W:108:LEU:HA	18:W:111:ILE:HG22	1.95	0.49
28:A:1405:G:N2	28:A:1408:G:OP2	2.44	0.49
2:E:126:THR:HG22	2:E:136:ARG:HE	1.77	0.49
22:b:9:THR:HB	22:b:31:LEU:HB2	1.93	0.49
23:c:43:VAL:HG22	23:c:92:ARG:HD3	1.95	0.49
23:c:83:GLY:HA2	23:c:88:LYS:HG2	1.94	0.49
28:A:839:U:H2'	28:A:840:C:H6	1.78	0.49
29:2:610:LEU:HD12	29:2:611:PRO:HD2	1.95	0.49
5:I:98:VAL:HA	5:I:101:VAL:HG22	1.95	0.49
7:K:103:ARG:NE	28:A:854:A:OP1	2.40	0.49
13:R:49:ARG:HH21	28:A:917:A:H2	1.61	0.49
21:a:14:LYS:NZ	28:A:1101:U:OP1	2.46	0.49
28:A:824:U:O4	28:A:844:G:O6	2.30	0.49
30:3:82:THR:HG22	30:3:125:ARG:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4:296:LEU:HD22	31:4:331:ILE:HG21	1.94	0.49
20:Z:86:LEU:HD21	20:Z:104:LEU:HD11	1.93	0.49
28:A:834:U:H2'	28:A:835:G:C8	2.47	0.49
28:A:220:A:C2	28:A:835:G:C6	3.01	0.49
9:M:167:PRO:HB3	9:M:171:ARG:HD2	1.95	0.48
29:2:604:MET:HE1	29:2:711:THR:HB	1.95	0.48
4:H:19:LEU:HD11	4:H:108:ARG:HD2	1.95	0.48
7:K:65:VAL:HG12	7:K:97:LEU:HB2	1.95	0.48
13:R:56:THR:H	13:R:59:MET:HE2	1.78	0.48
30:3:95:LEU:HB3	30:3:146:PHE:HE2	1.77	0.48
18:W:106:GLN:OE1	18:W:123:ARG:NH2	2.47	0.48
23:c:67:LYS:HA	23:c:70:LYS:HG2	1.95	0.48
28:A:560:U:H3	28:A:577:A:H62	1.60	0.48
31:4:254:PHE:HE2	31:4:262:VAL:HA	1.77	0.48
5:I:121:VAL:HA	5:I:124:ILE:HG12	1.96	0.48
21:a:86:PHE:HB3	21:a:107:PHE:HZ	1.77	0.48
29:2:505:LEU:HD23	29:2:507:ARG:HH22	1.78	0.48
12:Q:108:ASP:OD1	28:A:876:G:O2'	2.28	0.48
14:S:84:VAL:O	14:S:102:ILE:HA	2.12	0.48
18:W:70:THR:OG1	18:W:120:ARG:NH2	2.46	0.48
28:A:874:G:O6	28:A:933:U:C4	2.67	0.48
27:i:147:THR:HG1	28:A:1232:C:HO2'	1.60	0.48
28:A:84:A:N3	28:A:145:A:O2'	2.45	0.48
28:A:1174:C:H2'	28:A:1175:G:H8	1.79	0.48
4:H:44:LEU:HB3	4:H:65:MET:HE1	1.95	0.48
11:P:35:LYS:O	11:P:39:MET:HG2	2.13	0.48
18:W:49:GLN:OE1	28:A:1527:G:N2	2.44	0.48
1:D:182:ARG:O	1:D:186:ARG:HB3	2.14	0.48
13:R:85:LYS:NZ	13:R:121:SER:O	2.38	0.48
28:A:469:U:O2'	28:A:768:A:N3	2.42	0.48
18:W:99:SER:N	28:A:1500:G:OP1	2.47	0.47
23:c:55:VAL:HG12	23:c:60:ILE:HG13	1.95	0.47
27:i:139:GLN:HB2	27:i:148:TYR:HB2	1.96	0.47
11:P:55:ASP:OD2	27:i:129:GLY:N	2.47	0.47
28:A:347:A:OP1	28:A:348:C:O2'	2.26	0.47
28:A:673:U:H2'	28:A:674:G:C8	2.49	0.47
28:A:893:G:H2'	28:A:894:U:C6	2.50	0.47
31:4:258:LYS:NZ	31:4:260:GLN:OE1	2.47	0.47
8:L:87:ASN:HB3	8:L:90:LEU:HG	1.94	0.47
22:b:117:ARG:O	22:b:120:THR:OG1	2.31	0.47
28:A:1374:U:H4'	28:A:1375:U:H5'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:a:109:ARG:HB3	21:a:112:LYS:HB2	1.97	0.47
28:A:220:A:C6	28:A:835:G:O6	2.67	0.47
28:A:612:G:O2'	28:A:618:A:N1	2.45	0.47
3:F:178:ILE:HB	3:F:205:TYR:HB2	1.96	0.47
6:J:51:ARG:NH2	28:A:1679:U:OP1	2.48	0.47
7:K:40:LEU:HD21	7:K:82:ARG:HD3	1.97	0.47
28:A:484:G:H2'	28:A:485:G:C8	2.49	0.47
29:2:276:THR:HG22	29:2:569:ASN:HB3	1.96	0.47
4:H:97:GLU:OE2	4:H:113:ARG:NH1	2.37	0.47
11:P:75:LYS:HA	11:P:78:ILE:HG12	1.97	0.47
18:W:60:SER:HB3	28:A:1475:A:H5''	1.97	0.47
21:a:67:ALA:HB3	21:a:69:ARG:HH21	1.79	0.47
1:D:41:TRP:HD1	1:D:50:ILE:HD11	1.80	0.47
18:W:112:GLN:O	18:W:126:THR:OG1	2.31	0.47
28:A:5:U:H2'	28:A:6:G:H8	1.80	0.47
28:A:140:G:H2'	28:A:141:G:C8	2.49	0.47
28:A:355:U:OP1	29:2:61:ARG:NH2	2.39	0.47
4:H:128:ARG:HB3	4:H:140:VAL:HB	1.97	0.47
15:T:12:LYS:NZ	15:T:14:LYS:O	2.48	0.47
28:A:978:G:H4'	28:A:1772:A:H4'	1.97	0.47
3:F:46:VAL:HG13	3:F:47:THR:HG23	1.95	0.47
4:H:180:LEU:HD23	4:H:233:PRO:HB3	1.97	0.47
5:I:79:ARG:NH2	28:A:1609:U:OP1	2.47	0.47
6:J:94:ARG:NH2	28:A:1669:G:OP1	2.42	0.47
28:A:874:G:O6	28:A:933:U:O4	2.33	0.47
28:A:1462:G:O2'	28:A:1598:C:OP1	2.33	0.47
6:J:176:PRO:O	28:A:77:A:O2'	2.24	0.47
5:I:130:ARG:N	5:I:205:GLU:OE2	2.42	0.46
6:J:85:ARG:O	6:J:87:ARG:NH1	2.47	0.46
20:Z:76:SER:HB2	28:A:1098:G:H5''	1.97	0.46
21:a:31:LYS:NZ	28:A:1130:A:OP1	2.48	0.46
28:A:588:A:H2'	28:A:589:A:C8	2.50	0.46
28:A:1776:G:H3'	28:A:1777:A:H8	1.80	0.46
30:3:116:ASN:HB3	30:3:121:ARG:HG2	1.96	0.46
1:D:178:TRP:HD1	1:D:205:TYR:HE2	1.62	0.46
31:4:259:PRO:O	31:4:262:VAL:HG22	2.14	0.46
2:E:134:LEU:HB3	2:E:219:LYS:HB2	1.98	0.46
14:S:119:MET:HE3	17:V:119:ILE:HD11	1.96	0.46
17:V:88:ARG:HH21	28:A:1542:G:H21	1.63	0.46
18:W:65:VAL:HG21	18:W:114:LEU:HD21	1.96	0.46
29:2:398:SER:OG	29:2:399:LYS:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:87:MET:HE1	4:H:235:ILE:HD13	1.97	0.46
6:J:98:ARG:NH2	6:J:105:ASP:OD1	2.46	0.46
8:L:188:LEU:HD12	8:L:192:GLU:HG2	1.96	0.46
10:O:82:SER:OG	28:A:344:G:OP1	2.30	0.46
28:A:708:U:O2	28:A:723:G:O6	2.33	0.46
23:c:27:HIS:ND1	23:c:60:ILE:O	2.49	0.46
28:A:1391:G:H2'	28:A:1392:G:H8	1.81	0.46
31:4:356:ARG:NH2	31:4:359:CYS:SG	2.77	0.46
9:M:77:ARG:NH1	28:A:761:A:OP1	2.35	0.46
10:O:31:ARG:NH1	28:A:210:A:H5''	2.30	0.46
21:a:144:ARG:HH22	29:2:710:THR:HG22	1.80	0.46
28:A:937:A:H2'	28:A:938:A:C8	2.51	0.46
1:D:106:THR:HG23	1:D:109:SER:HB3	1.98	0.46
2:E:88:VAL:HG12	2:E:98:THR:HG22	1.97	0.46
18:W:102:ARG:NH1	28:A:1497:C:OP2	2.48	0.46
29:2:330:PRO:HB3	29:2:334:ARG:HD3	1.98	0.46
29:2:670:VAL:HG23	29:2:714:PRO:HG3	1.98	0.46
28:A:1358:U:HO2'	28:A:1360:G:H1	1.63	0.46
18:W:87:GLY:HA2	28:A:1538:G:H5'	1.98	0.46
28:A:1077:U:O2'	28:A:1078:A:O4'	2.24	0.46
28:A:1479:A:H2	28:A:1603:G:H1'	1.81	0.46
28:A:709:G:O6	28:A:722:U:O4	2.33	0.46
28:A:1519:U:H5''	28:A:1520:A:H5'	1.97	0.46
31:4:275:ARG:NH2	31:4:315:THR:OG1	2.49	0.45
2:E:144:LYS:HB3	2:E:206:PRO:HB2	1.98	0.45
7:K:181:GLU:O	7:K:185:ARG:HG2	2.15	0.45
16:U:27:ASP:HB3	16:U:30:THR:HG22	1.97	0.45
28:A:29:U:H2'	28:A:30:G:H8	1.81	0.45
28:A:1260:G:H2'	28:A:1261:G:C8	2.52	0.45
28:A:1355:G:C6	28:A:1363:A:N1	2.84	0.45
28:A:1390:C:H2'	28:A:1391:G:H8	1.81	0.45
14:S:41:LEU:HA	14:S:44:VAL:HG12	1.99	0.45
28:A:889:A:H2'	28:A:890:A:H8	1.81	0.45
28:A:1001:A:H62	30:3:227:MET:HG2	1.81	0.45
28:A:1084:A:H2'	28:A:1085:A:C8	2.51	0.45
29:2:144:ARG:HH22	29:2:170:ASP:HB2	1.82	0.45
2:E:56:ASN:ND2	2:E:58:ASN:OD1	2.50	0.45
9:M:15:ARG:NH2	28:A:3:C:O2	2.32	0.45
11:P:119:SER:OG	11:P:120:CYS:N	2.39	0.45
22:b:115:LYS:NZ	28:A:55:A:OP1	2.45	0.45
28:A:107:A:H2'	28:A:108:G:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:1581:U:H2'	28:A:1582:A:H8	1.81	0.45
32:5:418:GLN:O	32:5:422:ILE:HG12	2.16	0.45
2:E:168:MET:HG2	2:E:197:ILE:HD13	1.99	0.45
14:S:95:PRO:HG2	32:5:423:ARG:HH22	1.81	0.45
28:A:552:A:N3	28:A:587:C:O2'	2.42	0.45
28:A:798:U:H2'	28:A:799:G:H8	1.81	0.45
29:2:473:ASP:N	29:2:473:ASP:OD1	2.50	0.45
5:I:37:ASP:OD1	5:I:115:ASN:ND2	2.50	0.45
5:I:156:ASN:OD1	5:I:157:GLN:N	2.50	0.45
9:M:118:LYS:HD2	28:A:476:U:H4'	1.98	0.45
15:T:16:ALA:HB2	15:T:72:GLY:HA3	1.99	0.45
17:V:68:ARG:O	17:V:72:ILE:HG12	2.17	0.45
28:A:841:U:H2'	28:A:842:A:C8	2.52	0.45
28:A:844:G:H2'	28:A:845:A:H8	1.80	0.45
2:E:61:LEU:HD23	2:E:64:ARG:HD3	1.99	0.45
10:O:138:LYS:HB2	28:A:334:G:H3'	1.99	0.45
11:P:93:ASP:OD2	11:P:96:GLN:NE2	2.48	0.45
28:A:652:G:O6	28:A:673:U:O4	2.35	0.45
28:A:1587:C:H2'	28:A:1588:A:C8	2.52	0.45
2:E:52:THR:OG1	2:E:53:GLY:N	2.50	0.45
5:I:152:LEU:HD12	5:I:153:ARG:HD3	1.98	0.45
16:U:26:LEU:HA	16:U:58:MET:HE3	1.98	0.45
28:A:481:C:O3'	31:4:450:ARG:NH2	2.44	0.45
28:A:697:G:H2'	28:A:698:G:H8	1.81	0.45
28:A:1197:G:OP1	28:A:1591:U:O2'	2.35	0.45
29:2:99:CYS:HB2	29:2:102:THR:HG23	1.99	0.45
29:2:259:LEU:O	29:2:277:GLY:HA3	2.17	0.45
1:D:78:VAL:HG12	1:D:125:VAL:HB	1.99	0.45
14:S:76:LYS:HE3	14:S:79:GLU:HG2	1.98	0.45
28:A:648:C:H2'	28:A:649:G:C8	2.52	0.45
30:3:105:LEU:O	30:3:109:CYS:N	2.39	0.45
1:D:23:ALA:HB2	1:D:175:LEU:HD13	1.99	0.44
9:M:142:PRO:HD2	28:A:471:A:H5''	1.99	0.44
11:P:134:THR:HA	11:P:137:LEU:HG	2.00	0.44
14:S:119:MET:HG3	14:S:127:PHE:HZ	1.81	0.44
28:A:29:U:H2'	28:A:30:G:C8	2.52	0.44
31:4:261:VAL:O	31:4:264:ARG:HB2	2.17	0.44
23:c:52:ALA:HA	23:c:55:VAL:HG22	1.98	0.44
28:A:118:A:H1'	28:A:394:A:C5	2.53	0.44
11:P:103:LEU:HD21	28:A:1224:A:C6	2.52	0.44
28:A:561:G:N1	28:A:577:A:OP1	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:1354:U:H2'	28:A:1355:G:C8	2.52	0.44
4:H:22:LYS:HG3	4:H:23:LEU:HD12	1.98	0.44
18:W:4:GLY:HA2	28:A:1357:C:H1'	2.00	0.44
6:J:1:MET:HE3	6:J:24:LEU:HD22	1.99	0.44
11:P:53:ALA:HB1	11:P:124:LYS:HZ2	1.82	0.44
15:T:36:LEU:HD23	15:T:48:LEU:HB3	1.98	0.44
16:U:48:ASN:HB3	28:A:1386:C:H1'	2.00	0.44
18:W:39:LYS:HD2	18:W:45:GLU:HA	1.99	0.44
21:a:144:ARG:HD3	29:2:676:PRO:HB3	2.00	0.44
9:M:51:ARG:NH1	9:M:97:LEU:O	2.47	0.44
14:S:133:PRO:HG3	29:2:404:TRP:CD2	2.52	0.44
28:A:1380:G:H2'	28:A:1381:A:C8	2.53	0.44
31:4:343:LYS:HD2	32:5:355:PHE:HZ	1.83	0.44
14:S:94:VAL:H	14:S:97:MET:HE2	1.81	0.44
14:S:106:SER:HB2	14:S:128:SER:HB2	1.99	0.44
28:A:975:A:H61	28:A:1770:G:H1'	1.82	0.44
29:2:533:GLU:OE2	29:2:537:TRP:HB3	2.17	0.44
3:F:133:ILE:O	3:F:137:ILE:HG12	2.18	0.44
4:H:176:ASP:OD1	4:H:177:THR:N	2.46	0.44
28:A:231:G:H2'	28:A:232:G:C8	2.53	0.44
28:A:1581:U:H2'	28:A:1582:A:C8	2.53	0.44
18:W:13:HIS:HE1	28:A:1525:C:H1'	1.83	0.44
24:e:20:LYS:HG3	24:e:21:LEU:HD12	1.99	0.44
28:A:1347:C:H2'	28:A:1348:C:C6	2.53	0.44
28:A:1474:G:H2'	28:A:1475:A:C8	2.53	0.44
29:2:89:ALA:HB2	29:2:565:GLY:HA2	2.00	0.44
29:2:652:TYR:HB3	29:2:722:LYS:HA	2.00	0.44
28:A:1474:G:H2'	28:A:1475:A:H8	1.83	0.43
29:2:157:ASP:OD1	29:2:280:ARG:NH2	2.51	0.43
29:2:340:LEU:HB3	29:2:539:ARG:HB3	2.00	0.43
29:2:618:ILE:HD12	29:2:681:MET:HE1	1.99	0.43
29:2:769:LYS:H	29:2:780:ALA:HA	1.82	0.43
28:A:1411:U:H2'	28:A:1412:G:H8	1.82	0.43
29:2:96:ILE:HD11	29:2:153:CYS:SG	2.58	0.43
7:K:35:THR:O	7:K:41:LYS:NZ	2.42	0.43
13:R:62:LYS:NZ	28:A:897:G:OP2	2.52	0.43
14:S:59:ARG:HE	14:S:60:ARG:H	1.65	0.43
28:A:1792:C:O2	30:3:198:LYS:NZ	2.45	0.43
17:V:107:SER:O	17:V:110:ARG:N	2.52	0.43
20:Z:101:TYR:HB3	20:Z:112:ASP:HB2	2.00	0.43
28:A:966:U:OP1	28:A:1031:C:O2'	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:71:LYS:HD3	5:I:79:ARG:HH22	1.83	0.43
23:c:78:ILE:HD13	23:c:92:ARG:HA	2.00	0.43
28:A:1168:A:H2'	28:A:1169:G:H8	1.83	0.43
31:4:266:MET:HB3	31:4:306:PHE:HB2	2.00	0.43
4:H:94:LYS:HG2	22:b:19:PRO:HB2	2.00	0.43
17:V:96:LYS:HZ2	17:V:98:SER:HG	1.59	0.43
21:a:66:SER:OG	28:A:562:C:O3'	2.37	0.43
23:c:64:LEU:HA	23:c:67:LYS:HZ2	1.84	0.43
29:2:536:GLU:O	29:2:540:LEU:N	2.44	0.43
29:2:556:GLU:OE2	29:2:596:ARG:NH2	2.51	0.43
3:F:176:ARG:NE	28:A:1095:U:OP2	2.46	0.43
9:M:144:PHE:HD2	9:M:146:VAL:HG22	1.84	0.43
13:R:35:SER:OG	13:R:36:PHE:N	2.52	0.43
18:W:3:GLY:O	28:A:1361:G:N2	2.49	0.43
25:f:28:GLN:NE2	25:f:44:ASN:OD1	2.52	0.43
28:A:798:U:H2'	28:A:799:G:C8	2.54	0.43
31:4:422:ARG:NH1	31:4:452:GLU:OE2	2.44	0.43
6:J:49:ILE:HG12	6:J:115:LYS:HE3	2.01	0.43
6:J:65:GLN:HG3	28:A:1677:A:H8	1.84	0.43
10:O:42:ASP:O	28:A:244:A:O2'	2.25	0.43
11:P:49:GLU:HA	11:P:52:LYS:HB3	2.01	0.43
28:A:155:U:O2'	28:A:157:C:OP2	2.32	0.43
28:A:622:C:H2'	28:A:623:U:C6	2.53	0.43
1:D:171:HIS:HA	1:D:206:PHE:CE1	2.54	0.43
6:J:52:ILE:HA	6:J:111:LEU:HD23	2.01	0.43
19:Y:33:GLN:HE21	19:Y:52:ILE:HG21	1.84	0.43
28:A:115:U:H2'	28:A:116:U:C6	2.53	0.43
28:A:404:A:H2'	28:A:405:C:C6	2.54	0.43
28:A:692:C:H4'	28:A:693:U:H5''	2.00	0.43
28:A:1482:G:N2	28:A:1518:U:O4	2.52	0.43
28:A:1520:A:H2'	28:A:1521:A:C8	2.54	0.43
21:a:144:ARG:HH12	29:2:710:THR:HG22	1.85	0.42
28:A:227:U:O2	28:A:231:G:C6	2.72	0.42
29:2:261:GLU:OE1	29:2:277:GLY:HA2	2.19	0.42
5:I:84:LEU:O	5:I:167:ARG:NH1	2.46	0.42
6:J:92:ARG:O	28:A:402:C:O2'	2.25	0.42
9:M:38:ARG:NH2	28:A:591:A:OP1	2.52	0.42
13:R:142:LYS:HB2	28:A:988:C:H5'	2.01	0.42
14:S:96:GLU:OE1	32:5:423:ARG:NH1	2.52	0.42
21:a:109:ARG:O	21:a:112:LYS:NZ	2.43	0.42
22:b:109:GLN:NE2	28:A:439:C:OP2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:77:LEU:HG	23:c:78:ILE:HG12	2.00	0.42
28:A:1549:G:H4'	28:A:1593:A:H1'	2.01	0.42
29:2:90:PRO:HD2	29:2:278:VAL:HG11	2.01	0.42
31:4:249:ALA:HA	31:4:252:ARG:HG2	2.01	0.42
31:4:307:LEU:HD11	31:4:366:LEU:HD21	2.01	0.42
2:E:65:ILE:HA	2:E:86:LEU:O	2.19	0.42
3:F:134:ARG:O	3:F:138:ILE:HG12	2.19	0.42
9:M:140:ASN:C	9:M:140:ASN:ND2	2.66	0.42
27:i:113:LYS:HB2	27:i:113:LYS:HE2	1.89	0.42
5:I:108:ILE:HG21	5:I:185:LEU:HD11	2.00	0.42
9:M:171:ARG:HB2	28:A:508:A:H5''	2.02	0.42
13:R:140:ARG:NH1	28:A:1784:G:OP1	2.52	0.42
28:A:1247:U:N3	28:A:1248:U:C4	2.87	0.42
1:D:74:SER:OG	1:D:99:GLN:NE2	2.52	0.42
9:M:30:GLY:HA3	26:h:40:TYR:CG	2.55	0.42
16:U:44:LYS:NZ	28:A:1384:G:N7	2.68	0.42
16:U:104:ILE:HD12	16:U:108:THR:HB	2.00	0.42
28:A:872:C:H2'	28:A:873:G:C8	2.54	0.42
28:A:1244:U:H2'	28:A:1245:C:H6	1.83	0.42
29:2:494:PHE:HB3	29:2:497:GLU:HG3	2.02	0.42
5:I:163:THR:O	5:I:167:ARG:HG3	2.19	0.42
7:K:99:LEU:HD21	7:K:139:LEU:HD23	2.02	0.42
30:3:162:ASP:OD1	30:3:162:ASP:N	2.50	0.42
2:E:185:VAL:O	2:E:189:ILE:HD12	2.20	0.42
5:I:116:PRO:HA	5:I:119:VAL:HG12	2.02	0.42
7:K:56:GLU:HA	7:K:62:LYS:HD3	2.01	0.42
13:R:105:LYS:HA	13:R:132:THR:HG21	2.02	0.42
28:A:768:A:H2'	28:A:769:A:C8	2.55	0.42
28:A:883:G:H2'	28:A:884:U:C6	2.55	0.42
3:F:244:ILE:O	19:Y:33:GLN:NE2	2.51	0.42
14:S:26:ARG:HH22	17:V:90:ARG:HG2	1.85	0.42
28:A:643:U:H2'	28:A:644:A:H8	1.83	0.42
28:A:691:C:H4'	28:A:692:C:H5'	2.01	0.42
28:A:1153:C:H2'	28:A:1154:A:C8	2.54	0.42
28:A:1394:U:O2	28:A:1398:G:C6	2.73	0.42
1:D:171:HIS:HA	1:D:206:PHE:HE1	1.85	0.42
2:E:180:THR:HG23	2:E:183:GLN:HE22	1.84	0.42
4:H:141:THR:OG1	4:H:143:ASP:OD1	2.31	0.42
5:I:26:SER:HB2	5:I:28:LYS:HE3	2.02	0.42
9:M:47:LEU:HD13	9:M:102:PHE:HE2	1.85	0.42
18:W:76:LEU:HA	18:W:79:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:948:C:H2'	28:A:949:A:C8	2.55	0.42
28:A:1370:C:O2'	28:A:1372:G:OP1	2.36	0.42
7:K:39:ASP:OD1	7:K:39:ASP:N	2.52	0.41
12:Q:20:ARG:HH21	20:Z:56:HIS:CG	2.38	0.41
28:A:1227:A:H62	28:A:1252:G:N2	2.17	0.41
17:V:89:GLN:HE21	28:A:1544:G:H1'	1.84	0.41
28:A:200:U:H2'	28:A:201:A:H8	1.86	0.41
28:A:390:C:H2'	28:A:391:C:C6	2.55	0.41
29:2:240:SER:O	29:2:244:THR:HG22	2.20	0.41
29:2:286:ALA:HB2	29:2:303:ILE:HD12	2.02	0.41
16:U:15:VAL:HA	16:U:18:GLU:HG2	2.02	0.41
28:A:403:U:H2'	28:A:404:A:C8	2.56	0.41
31:4:370:LEU:HD12	31:4:371:LEU:HD12	2.02	0.41
2:E:151:LYS:HE2	28:A:1063:C:H5'	2.02	0.41
9:M:129:GLN:HB3	28:A:510:U:H4'	2.02	0.41
10:O:107:LYS:O	21:a:13:ARG:NH2	2.43	0.41
11:P:45:ARG:H	11:P:45:ARG:HD3	1.86	0.41
14:S:51:ARG:HE	14:S:55:ARG:HD2	1.85	0.41
15:T:20:ALA:HB2	15:T:67:ILE:HD13	2.01	0.41
28:A:1436:C:H2'	28:A:1437:C:C6	2.56	0.41
4:H:49:ARG:NH2	28:A:445:C:OP1	2.34	0.41
5:I:27:VAL:HG23	5:I:56:TYR:CZ	2.55	0.41
6:J:160:ARG:NE	28:A:66:U:O2	2.38	0.41
6:J:160:ARG:HH12	28:A:68:A:H5'	1.85	0.41
12:Q:124:ARG:NH1	28:A:625:G:OP1	2.48	0.41
29:2:520:ARG:HH21	29:2:646:PRO:HD3	1.85	0.41
3:F:84:LEU:HD12	3:F:114:ASP:HB3	2.03	0.41
5:I:187:ASN:OD1	5:I:192:SER:OG	2.29	0.41
14:S:26:ARG:HG3	14:S:44:VAL:HG22	2.03	0.41
14:S:89:ARG:NH1	14:S:128:SER:O	2.38	0.41
18:W:111:ILE:HG23	18:W:113:VAL:HG23	2.01	0.41
18:W:127:GLN:OE1	28:A:1354:U:O2'	2.27	0.41
22:b:32:HIS:O	22:b:32:HIS:ND1	2.51	0.41
28:A:1166:G:N1	28:A:1571:G:OP2	2.53	0.41
31:4:212:TYR:O	31:4:243:THR:OG1	2.35	0.41
2:E:26:ARG:H	2:E:26:ARG:HG2	1.62	0.41
5:I:150:SER:HB3	5:I:153:ARG:HH21	1.86	0.41
28:A:1259:U:H2'	28:A:1260:G:C8	2.56	0.41
1:D:36:MET:HG2	1:D:152:THR:HA	2.01	0.41
7:K:172:VAL:HG23	7:K:175:ARG:HD3	2.01	0.41
28:A:824:U:H2'	28:A:825:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:2:391:LYS:NZ	29:2:406:LEU:O	2.41	0.41
2:E:87:ARG:NH2	2:E:89:ASP:OD2	2.54	0.41
5:I:133:SER:HB2	5:I:144:ARG:HB3	2.02	0.41
6:J:14:LYS:HB3	6:J:124:LEU:HD12	2.01	0.41
7:K:32:ASP:OD1	7:K:36:ASN:ND2	2.53	0.41
20:Z:76:SER:OG	28:A:1098:G:O3'	2.32	0.41
28:A:503:A:H2'	28:A:504:U:C6	2.56	0.41
28:A:834:U:H2'	28:A:835:G:H8	1.85	0.41
28:A:1621:C:H2'	28:A:1622:U:H6	1.85	0.41
29:2:258:MET:HG2	29:2:278:VAL:O	2.21	0.41
29:2:299:GLN:OE1	29:2:334:ARG:NH2	2.54	0.41
29:2:682:ARG:NH2	29:2:817:GLU:OE1	2.53	0.41
2:E:192:VAL:HG12	2:E:195:ARG:HH12	1.85	0.41
13:R:60:LYS:HB3	13:R:75:LEU:HD12	2.02	0.41
19:Y:38:LYS:HD3	19:Y:49:GLU:HB3	2.03	0.41
24:e:18:LYS:O	24:e:29:ARG:NH2	2.53	0.41
28:A:252:U:H2'	28:A:253:A:C8	2.56	0.41
28:A:1390:C:H2'	28:A:1391:G:C8	2.56	0.41
28:A:1391:G:H2'	28:A:1392:G:C8	2.55	0.41
13:R:100:GLY:HA3	13:R:133:PRO:HG2	2.03	0.40
15:T:122:ARG:HG3	28:A:1580:G:H5''	2.02	0.40
28:A:922:A:H2'	28:A:923:G:C8	2.56	0.40
31:4:208:ILE:HD13	31:4:208:ILE:HA	1.94	0.40
31:4:208:ILE:HD11	32:5:408:VAL:HB	2.03	0.40
31:4:360:VAL:HB	31:4:392:TYR:HE2	1.86	0.40
5:I:100:ILE:HG13	5:I:178:ALA:HB2	2.03	0.40
11:P:105:VAL:HG13	11:P:113:ARG:HB3	2.04	0.40
13:R:94:ILE:HG21	13:R:115:LEU:HD12	2.03	0.40
18:W:6:THR:OG1	18:W:7:VAL:N	2.53	0.40
29:2:56:MET:HE3	29:2:60:ASP:HB3	2.02	0.40
31:4:225:PRO:HG3	31:4:254:PHE:CD1	2.56	0.40
1:D:86:GLN:O	1:D:89:VAL:HG12	2.21	0.40
5:I:95:LEU:HA	5:I:98:VAL:HG22	2.03	0.40
11:P:70:GLU:HB3	11:P:73:TYR:HD2	1.86	0.40
14:S:51:ARG:HH12	28:A:1548:U:H5	1.70	0.40
28:A:587:C:H2'	28:A:588:A:C8	2.57	0.40
2:E:65:ILE:HG22	2:E:87:ARG:HA	2.03	0.40
4:H:71:LYS:HB2	4:H:91:THR:HB	2.03	0.40
8:L:169:LEU:HD13	8:L:187:ILE:HD13	2.03	0.40
14:S:101:VAL:HG12	14:S:114:GLU:HB2	2.02	0.40
18:W:7:VAL:HG12	18:W:137:ALA:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:889:A:H2'	28:A:890:A:C8	2.57	0.40
28:A:977:A:H4'	28:A:1782:G:N2	2.37	0.40
29:2:211:LEU:HD23	29:2:211:LEU:HA	1.94	0.40
31:4:324:ILE:HD11	31:4:366:LEU:HD11	2.02	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	D	206/285 (72%)	197 (96%)	9 (4%)	0	100	100
2	E	211/255 (83%)	199 (94%)	12 (6%)	0	100	100
3	F	200/263 (76%)	194 (97%)	6 (3%)	0	100	100
4	H	259/264 (98%)	250 (96%)	9 (4%)	0	100	100
5	I	197/212 (93%)	182 (92%)	15 (8%)	0	100	100
6	J	230/239 (96%)	222 (96%)	8 (4%)	0	100	100
7	K	193/203 (95%)	184 (95%)	9 (5%)	0	100	100
8	L	199/202 (98%)	188 (94%)	11 (6%)	0	100	100
9	M	177/190 (93%)	173 (98%)	4 (2%)	0	100	100
10	O	148/161 (92%)	143 (97%)	5 (3%)	0	100	100
11	P	116/144 (81%)	103 (89%)	13 (11%)	0	100	100
12	Q	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
13	R	133/150 (89%)	124 (93%)	8 (6%)	1 (1%)	16	50
14	S	121/153 (79%)	118 (98%)	3 (2%)	0	100	100
15	T	118/143 (82%)	111 (94%)	7 (6%)	0	100	100
16	U	105/143 (73%)	102 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	V	120/156 (77%)	112 (93%)	8 (7%)	0	100	100
18	W	140/153 (92%)	131 (94%)	9 (6%)	0	100	100
19	Y	84/98 (86%)	82 (98%)	2 (2%)	0	100	100
20	Z	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
21	a	140/145 (97%)	132 (94%)	8 (6%)	0	100	100
22	b	130/136 (96%)	126 (97%)	4 (3%)	0	100	100
23	c	67/99 (68%)	65 (97%)	2 (3%)	0	100	100
24	e	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
25	f	59/68 (87%)	59 (100%)	0	0	100	100
26	h	19/62 (31%)	19 (100%)	0	0	100	100
27	i	61/154 (40%)	57 (93%)	4 (7%)	0	100	100
29	2	671/830 (81%)	651 (97%)	19 (3%)	1 (0%)	48	80
30	3	182/259 (70%)	178 (98%)	4 (2%)	0	100	100
31	4	268/480 (56%)	255 (95%)	13 (5%)	0	100	100
32	5	77/445 (17%)	75 (97%)	2 (3%)	0	100	100
All	All	4985/6455 (77%)	4775 (96%)	208 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	R	137	ASP
29	2	372	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	178/225 (79%)	178 (100%)	0	100	100
2	E	187/223 (84%)	182 (97%)	5 (3%)	39	71
3	F	171/206 (83%)	171 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	219/221 (99%)	219 (100%)	0	100	100
5	I	167/178 (94%)	166 (99%)	1 (1%)	78	88
6	J	198/204 (97%)	195 (98%)	3 (2%)	57	80
7	K	169/177 (96%)	169 (100%)	0	100	100
8	L	163/164 (99%)	163 (100%)	0	100	100
9	M	154/162 (95%)	153 (99%)	1 (1%)	78	88
10	O	133/143 (93%)	133 (100%)	0	100	100
11	P	101/121 (84%)	101 (100%)	0	100	100
12	Q	129/130 (99%)	129 (100%)	0	100	100
13	R	100/117 (86%)	100 (100%)	0	100	100
14	S	106/132 (80%)	106 (100%)	0	100	100
15	T	98/115 (85%)	97 (99%)	1 (1%)	68	84
16	U	100/131 (76%)	100 (100%)	0	100	100
17	V	107/135 (79%)	107 (100%)	0	100	100
18	W	114/124 (92%)	114 (100%)	0	100	100
19	Y	69/80 (86%)	69 (100%)	0	100	100
20	Z	112/113 (99%)	112 (100%)	0	100	100
21	a	113/116 (97%)	113 (100%)	0	100	100
22	b	112/115 (97%)	112 (100%)	0	100	100
23	c	60/80 (75%)	60 (100%)	0	100	100
24	e	70/71 (99%)	70 (100%)	0	100	100
25	f	52/61 (85%)	52 (100%)	0	100	100
26	h	17/52 (33%)	15 (88%)	2 (12%)	5	22
27	i	57/139 (41%)	57 (100%)	0	100	100
29	2	589/714 (82%)	589 (100%)	0	100	100
30	3	152/215 (71%)	152 (100%)	0	100	100
31	4	229/411 (56%)	229 (100%)	0	100	100
32	5	70/373 (19%)	70 (100%)	0	100	100
All	All	4296/5448 (79%)	4283 (100%)	13 (0%)	84	91

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	148	ASN
2	E	150	ILE
2	E	213	ARG
2	E	214	LYS
2	E	217	LEU
5	I	89	ARG
6	J	198	ARG
6	J	201	GLN
6	J	202	GLU
9	M	140	ASN
15	T	83	GLN
26	h	28	LYS
26	h	29	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	95	HIS
2	E	56	ASN
2	E	149	GLN
2	E	202	GLN
3	F	197	GLN
4	H	9	GLN
4	H	67	GLN
4	H	216	ASN
5	I	91	ASN
5	I	109	HIS
6	J	13	GLN
6	J	81	HIS
6	J	129	HIS
6	J	201	GLN
7	K	95	HIS
7	K	132	HIS
8	L	52	ASN
10	O	22	ASN
10	O	97	HIS
11	P	40	HIS
12	Q	69	ASN
12	Q	78	ASN
14	S	43	ASN
15	T	77	GLN
17	V	44	ASN
18	W	42	ASN

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Mol	Chain	Res	Type
21	a	99	ASN
27	i	139	GLN
29	2	63	ASN
29	2	112	ASN
29	2	609	ASN
29	2	650	HIS
31	4	290	ASN
31	4	419	GLN
31	4	429	GLN
32	5	382	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	A	1709/1796 (95%)	413 (24%)	23 (1%)

All (413) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
28	A	3	C
28	A	4	C
28	A	14	C
28	A	17	C
28	A	25	C
28	A	26	A
28	A	27	U
28	A	34	G
28	A	45	U
28	A	46	A
28	A	47	A
28	A	57	G
28	A	65	A
28	A	66	U
28	A	68	A
28	A	69	G
28	A	73	U
28	A	74	U
28	A	75	A
28	A	76	U
28	A	80	G
28	A	93	U

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Mol	Chain	Res	Type
28	A	103	A
28	A	110	U
28	A	113	C
28	A	115	U
28	A	126	G
28	A	127	U
28	A	137	C
28	A	138	A
28	A	142	A
28	A	150	G
28	A	155	U
28	A	156	U
28	A	165	A
28	A	173	C
28	A	175	G
28	A	176	A
28	A	188	U
28	A	189	C
28	A	191	G
28	A	192	A
28	A	195	G
28	A	212	U
28	A	213	A
28	A	214	A
28	A	221	A
28	A	222	U
28	A	223	G
28	A	228	U
28	A	231	G
28	A	232	G
28	A	234	C
28	A	235	U
28	A	237	U
28	A	246	U
28	A	247	C
28	A	254	A
28	A	256	U
28	A	257	U
28	A	258	C
28	A	262	A
28	A	263	A
28	A	268	A

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Mol	Chain	Res	Type
28	A	269	C
28	A	270	G
28	A	274	U
28	A	275	U
28	A	277	C
28	A	284	G
28	A	287	G
28	A	296	A
28	A	311	C
28	A	313	A
28	A	317	U
28	A	319	G
28	A	326	G
28	A	334	G
28	A	335	C
28	A	348	C
28	A	349	A
28	A	356	A
28	A	357	A
28	A	358	C
28	A	377	C
28	A	387	G
28	A	397	A
28	A	398	A
28	A	399	C
28	A	400	G
28	A	401	G
28	A	414	A
28	A	415	G
28	A	420	G
28	A	421	C
28	A	422	A
28	A	423	G
28	A	425	A
28	A	431	G
28	A	436	U
28	A	441	C
28	A	442	A
28	A	449	A
28	A	450	C
28	A	452	C
28	A	461	A

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Mol	Chain	Res	Type
28	A	465	A
28	A	466	C
28	A	474	A
28	A	482	A
28	A	490	U
28	A	493	G
28	A	495	G
28	A	502	A
28	A	503	A
28	A	508	A
28	A	511	G
28	A	512	A
28	A	516	C
28	A	522	A
28	A	524	A
28	A	531	A
28	A	533	C
28	A	535	A
28	A	536	G
28	A	538	A
28	A	539	A
28	A	548	G
28	A	552	A
28	A	553	A
28	A	554	G
28	A	555	U
28	A	560	U
28	A	562	C
28	A	564	A
28	A	565	G
28	A	567	A
28	A	571	G
28	A	577	A
28	A	586	C
28	A	589	A
28	A	591	A
28	A	592	G
28	A	607	G
28	A	608	U
28	A	617	A
28	A	618	A
28	A	619	A

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Mol	Chain	Res	Type
28	A	620	A
28	A	621	G
28	A	636	U
28	A	647	C
28	A	677	U
28	A	678	G
28	A	679	G
28	A	680	G
28	A	683	G
28	A	685	G
28	A	691	C
28	A	692	C
28	A	693	U
28	A	705	G
28	A	709	G
28	A	710	C
28	A	724	U
28	A	725	G
28	A	726	U
28	A	727	C
28	A	729	G
28	A	730	G
28	A	731	G
28	A	732	A
28	A	742	U
28	A	754	A
28	A	764	G
28	A	765	C
28	A	773	A
28	A	774	G
28	A	777	C
28	A	779	A
28	A	780	U
28	A	781	G
28	A	787	A
28	A	792	U
28	A	793	U
28	A	809	A
28	A	810	A
28	A	818	U
28	A	819	G
28	A	821	G

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Mol	Chain	Res	Type
28	A	823	U
28	A	824	U
28	A	828	U
28	A	830	U
28	A	832	G
28	A	844	G
28	A	861	A
28	A	862	U
28	A	871	U
28	A	884	U
28	A	896	A
28	A	901	U
28	A	904	A
28	A	911	G
28	A	912	G
28	A	931	A
28	A	932	C
28	A	933	U
28	A	940	G
28	A	942	A
28	A	957	U
28	A	958	U
28	A	964	A
28	A	982	G
28	A	990	A
28	A	991	A
28	A	996	A
28	A	998	C
28	A	999	A
28	A	1000	G
28	A	1001	A
28	A	1019	C
28	A	1024	A
28	A	1026	C
28	A	1030	G
28	A	1037	A
28	A	1052	U
28	A	1056	U
28	A	1057	U
28	A	1073	A
28	A	1078	A
28	A	1079	C

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Mol	Chain	Res	Type
28	A	1080	G
28	A	1089	A
28	A	1093	G
28	A	1094	U
28	A	1095	U
28	A	1097	G
28	A	1135	A
28	A	1146	G
28	A	1149	A
28	A	1152	G
28	A	1155	C
28	A	1156	C
28	A	1157	A
28	A	1159	C
28	A	1161	G
28	A	1164	G
28	A	1165	U
28	A	1182	U
28	A	1183	U
28	A	1199	A
28	A	1213	C
28	A	1224	A
28	A	1225	G
28	A	1226	G
28	A	1227	A
28	A	1228	U
28	A	1230	G
28	A	1232	C
28	A	1237	U
28	A	1238	G
28	A	1240	G
28	A	1241	A
28	A	1242	G
28	A	1243	C
28	A	1252	G
28	A	1254	U
28	A	1255	U
28	A	1262	G
28	A	1265	G
28	A	1267	G
28	A	1269	U
28	A	1270	G

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Mol	Chain	Res	Type
28	A	1288	G
28	A	1298	U
28	A	1311	U
28	A	1312	U
28	A	1315	G
28	A	1318	A
28	A	1335	C
28	A	1341	A
28	A	1342	A
28	A	1343	A
28	A	1344	U
28	A	1345	A
28	A	1346	G
28	A	1347	C
28	A	1348	C
28	A	1349	C
28	A	1350	G
28	A	1358	U
28	A	1359	U
28	A	1360	G
28	A	1362	C
28	A	1364	G
28	A	1370	C
28	A	1374	U
28	A	1375	U
28	A	1377	U
28	A	1379	A
28	A	1385	A
28	A	1387	U
28	A	1409	U
28	A	1411	U
28	A	1427	C
28	A	1428	U
28	A	1432	A
28	A	1437	C
28	A	1438	U
28	A	1443	U
28	A	1447	C
28	A	1448	U
28	A	1453	C
28	A	1454	G
28	A	1455	C

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Mol	Chain	Res	Type
28	A	1457	C
28	A	1467	A
28	A	1469	U
28	A	1470	G
28	A	1471	A
28	A	1476	G
28	A	1477	C
28	A	1478	C
28	A	1482	G
28	A	1486	A
28	A	1487	C
28	A	1488	U
28	A	1492	U
28	A	1500	G
28	A	1502	G
28	A	1512	A
28	A	1513	U
28	A	1514	C
28	A	1516	U
28	A	1517	G
28	A	1519	U
28	A	1520	A
28	A	1530	G
28	A	1531	U
28	A	1532	G
28	A	1533	C
28	A	1536	G
28	A	1538	G
28	A	1539	A
28	A	1546	A
28	A	1547	U
28	A	1548	U
28	A	1551	A
28	A	1552	A
28	A	1553	U
28	A	1555	A
28	A	1556	U
28	A	1569	A
28	A	1570	G
28	A	1579	A
28	A	1580	G
28	A	1596	A

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Mol	Chain	Res	Type
28	A	1607	A
28	A	1610	A
28	A	1612	G
28	A	1618	G
28	A	1626	U
28	A	1628	C
28	A	1629	A
28	A	1632	C
28	A	1634	G
28	A	1642	C
28	A	1643	U
28	A	1644	A
28	A	1645	C
28	A	1646	U
28	A	1647	A
28	A	1648	C
28	A	1650	G
28	A	1651	A
28	A	1656	A
28	A	1657	C
28	A	1661	U
28	A	1676	G
28	A	1686	G
28	A	1695	G
28	A	1704	A
28	A	1705	C
28	A	1706	U
28	A	1708	A
28	A	1711	G
28	A	1712	C
28	A	1726	A
28	A	1731	C
28	A	1732	G
28	A	1735	C
28	A	1743	G
28	A	1744	G
28	A	1745	A
28	A	1746	A
28	A	1747	G
28	A	1748	U
28	A	1749	A
28	A	1763	G

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Mol	Chain	Res	Type
28	A	1764	G
28	A	1765	U
28	A	1766	C
28	A	1768	C
28	A	1776	G
28	A	1778	A
28	A	1779	C
28	A	1782	G
28	A	1785	G
28	A	1788	G
28	A	1790	A
28	A	1791	U
28	A	1795	U

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
28	A	126	G
28	A	174	U
28	A	222	U
28	A	231	G
28	A	233	G
28	A	269	C
28	A	414	A
28	A	449	A
28	A	552	A
28	A	559	G
28	A	678	G
28	A	792	U
28	A	1094	U
28	A	1182	U
28	A	1264	G
28	A	1361	G
28	A	1378	U
28	A	1468	C
28	A	1469	U
28	A	1477	C
28	A	1531	U
28	A	1569	A
28	A	1645	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

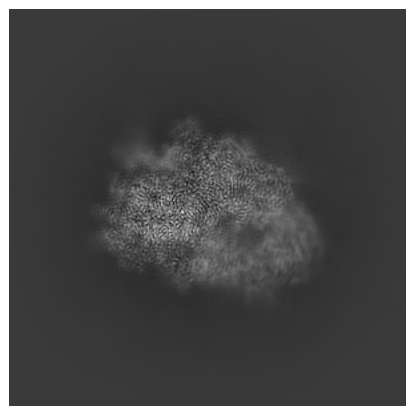
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66684. These allow visual inspection of the internal detail of the map and identification of artifacts.

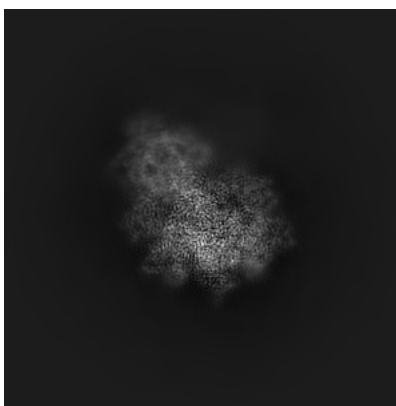
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

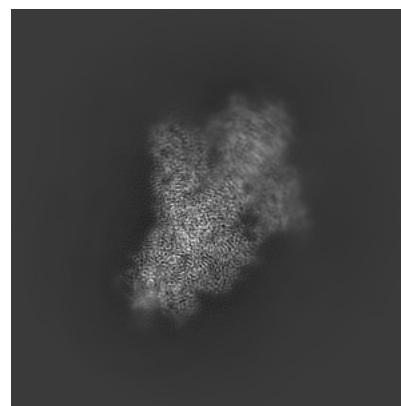
6.1.1 Primary map



X

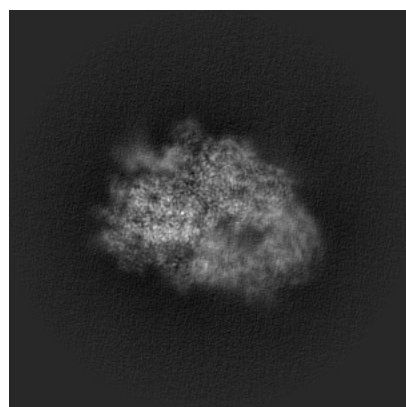


Y

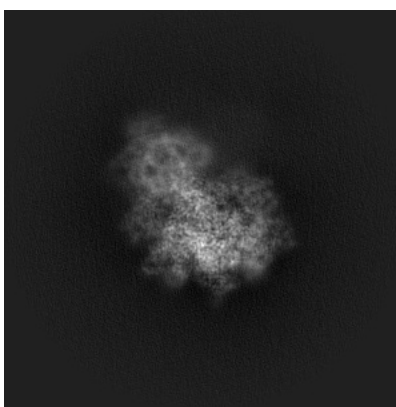


Z

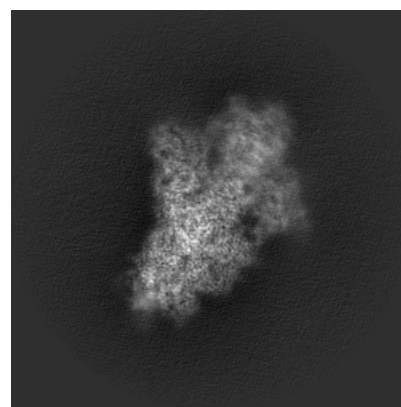
6.1.2 Raw map



X



Y

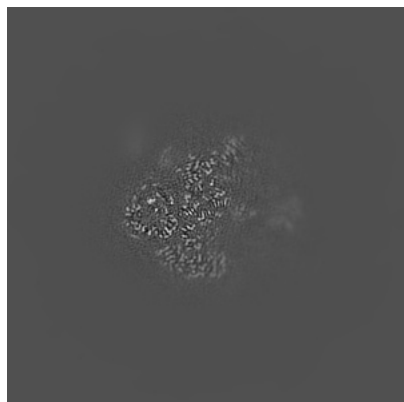


Z

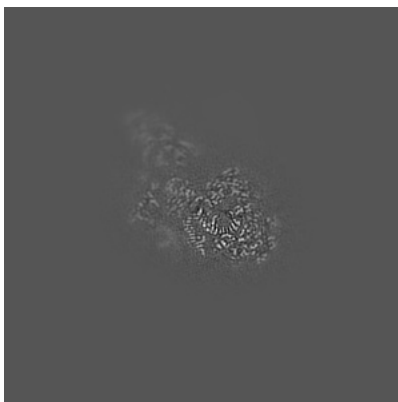
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

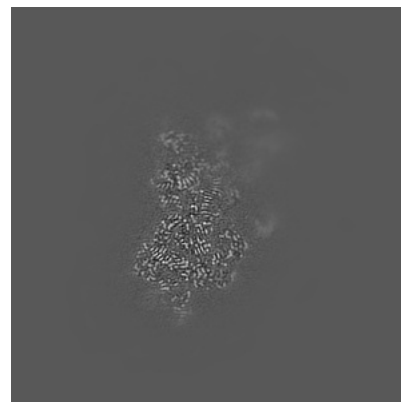
6.2.1 Primary map



X Index: 180

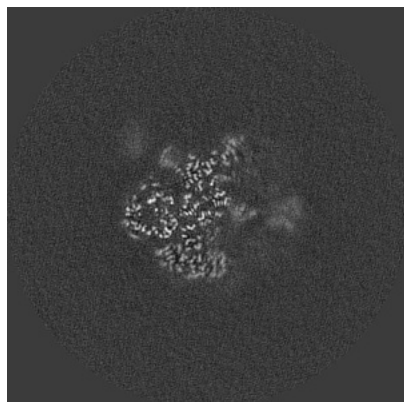


Y Index: 180

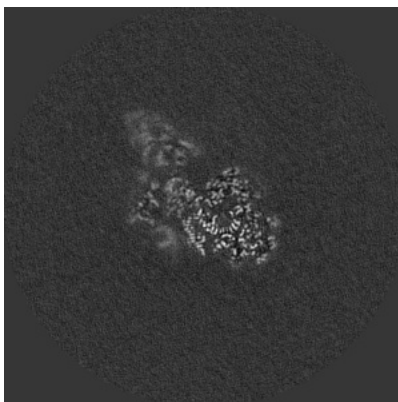


Z Index: 180

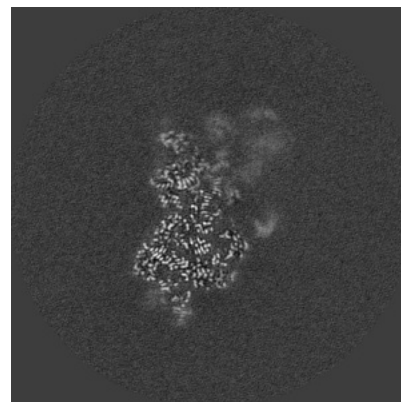
6.2.2 Raw map



X Index: 180



Y Index: 180

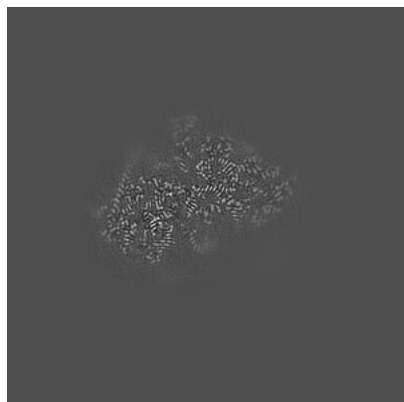


Z Index: 180

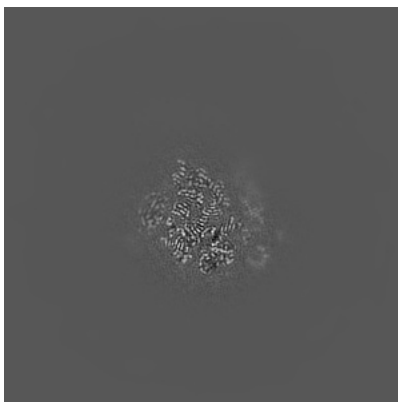
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

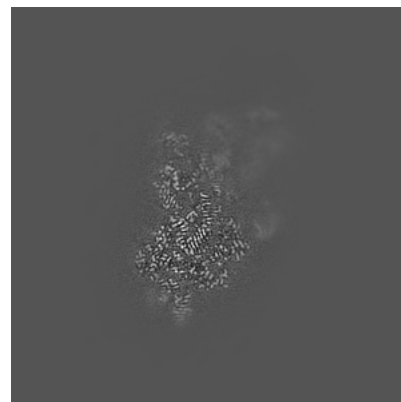
6.3.1 Primary map



X Index: 147

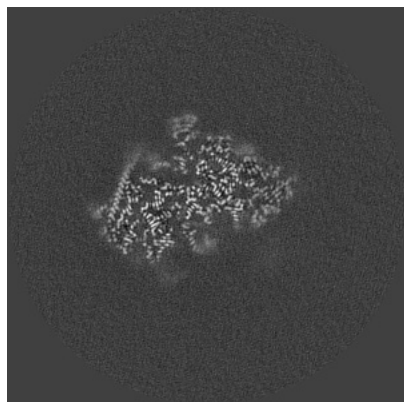


Y Index: 144

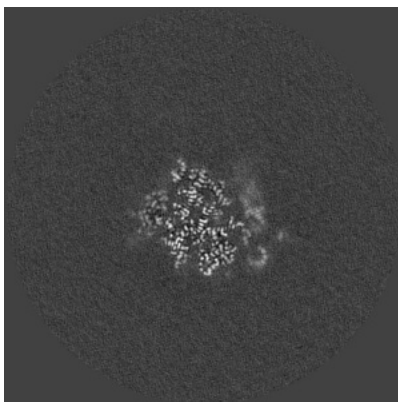


Z Index: 178

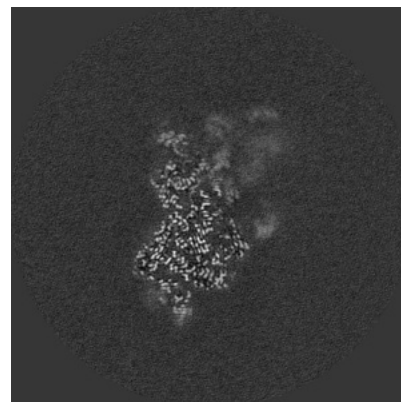
6.3.2 Raw map



X Index: 148



Y Index: 145

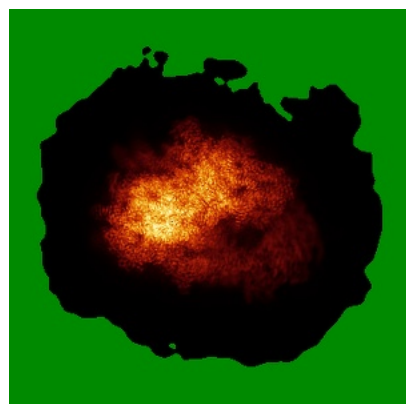


Z Index: 179

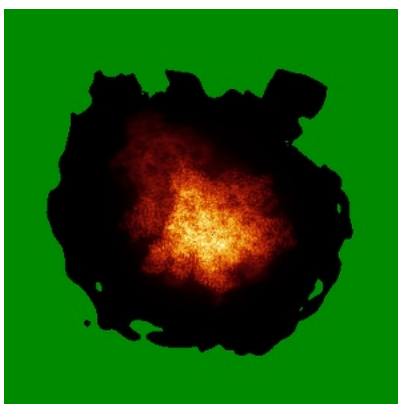
The images above show the largest variance slices of the map in three orthogonal directions.

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

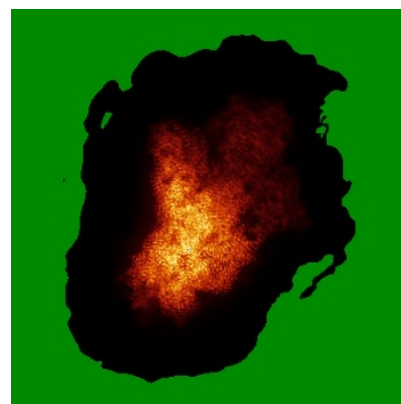
6.4.1 Primary map



X

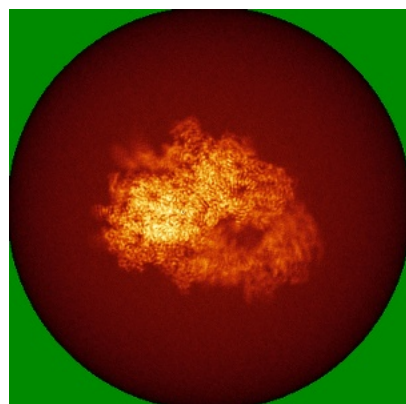


Y

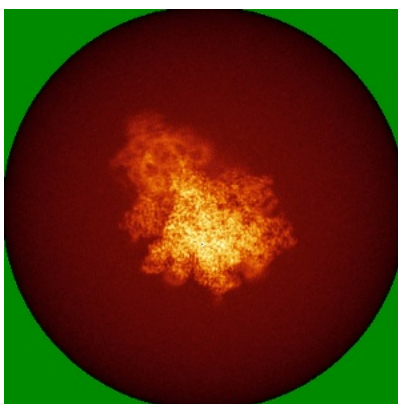


Z

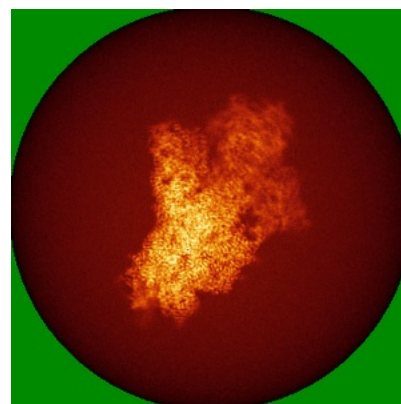
6.4.2 Raw map



X



Y

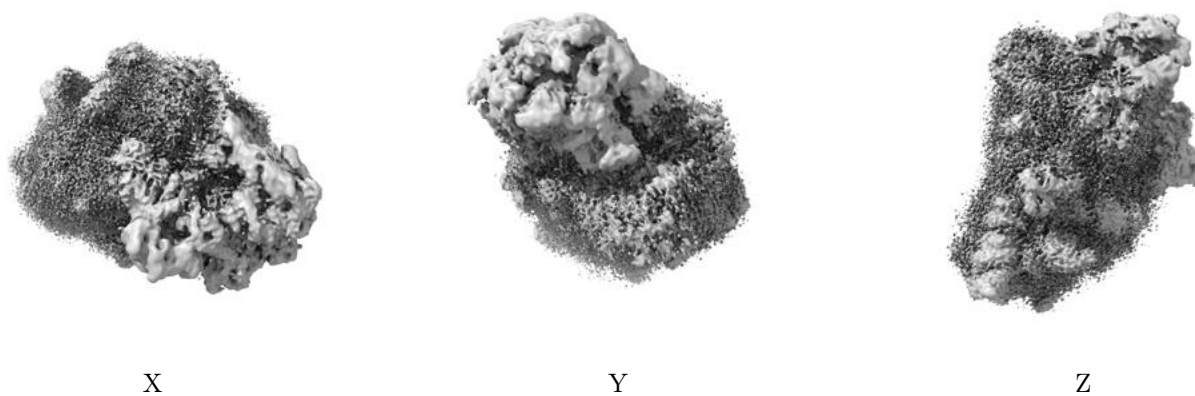


Z

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.

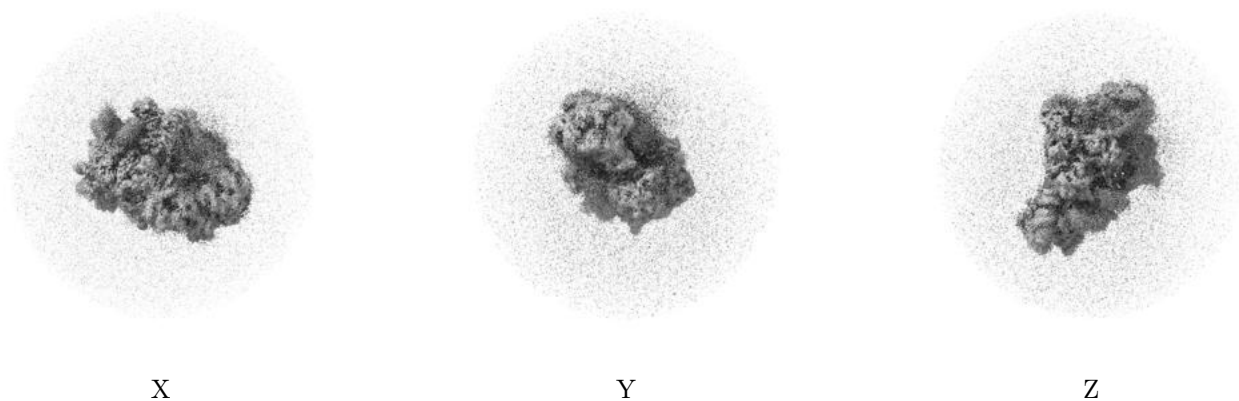
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

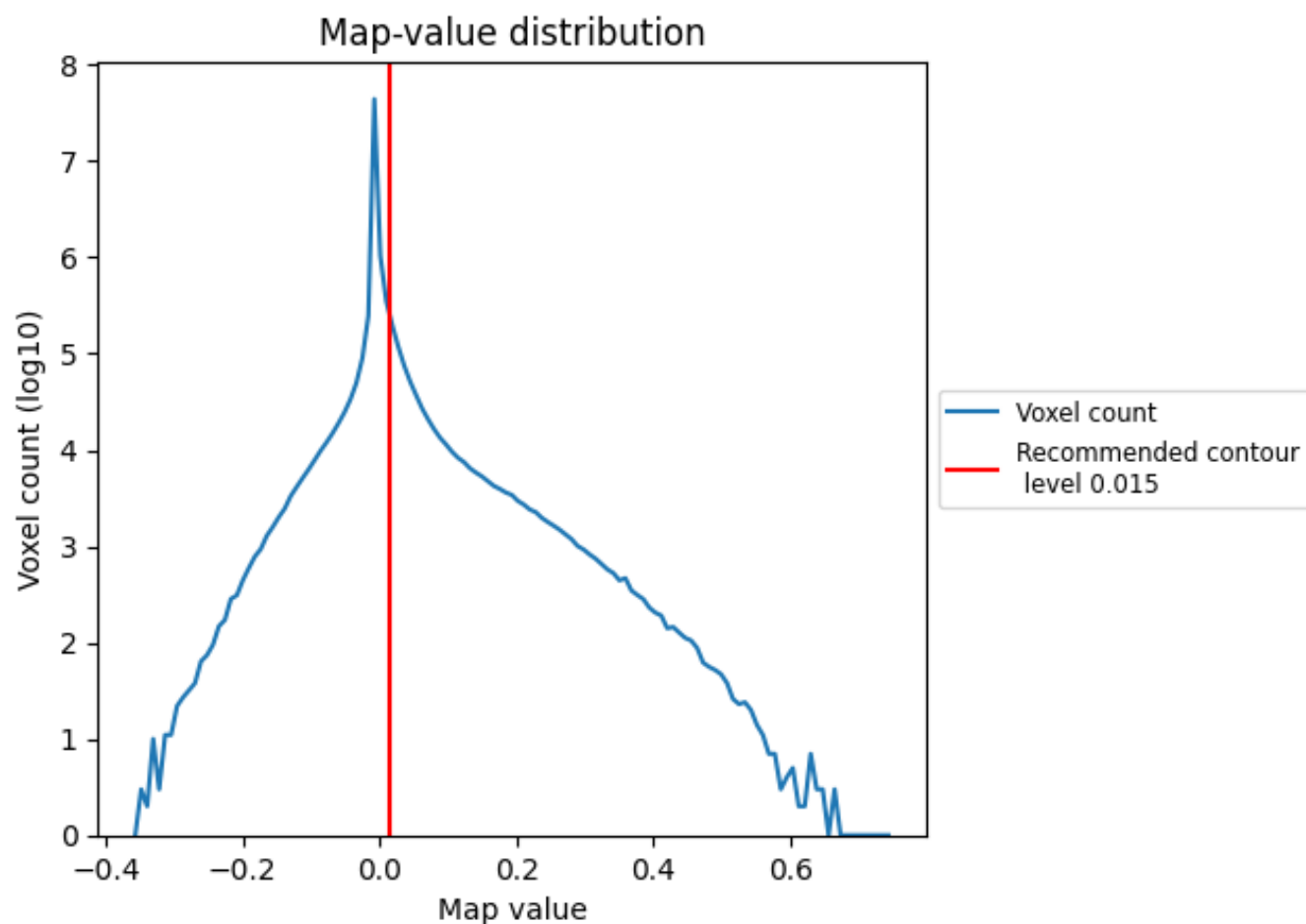
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

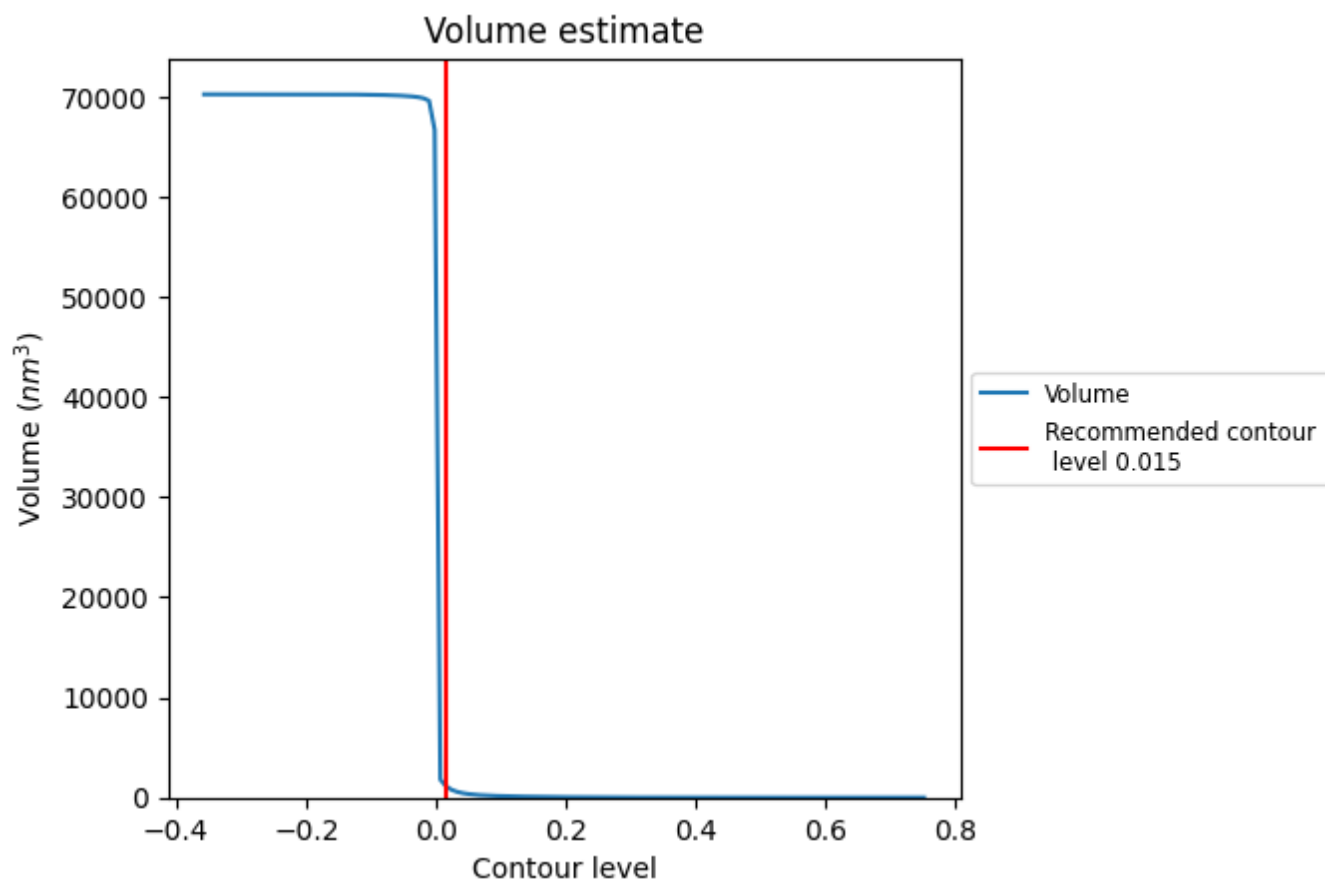
This section contains the results of statistical analysis of the map.

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.

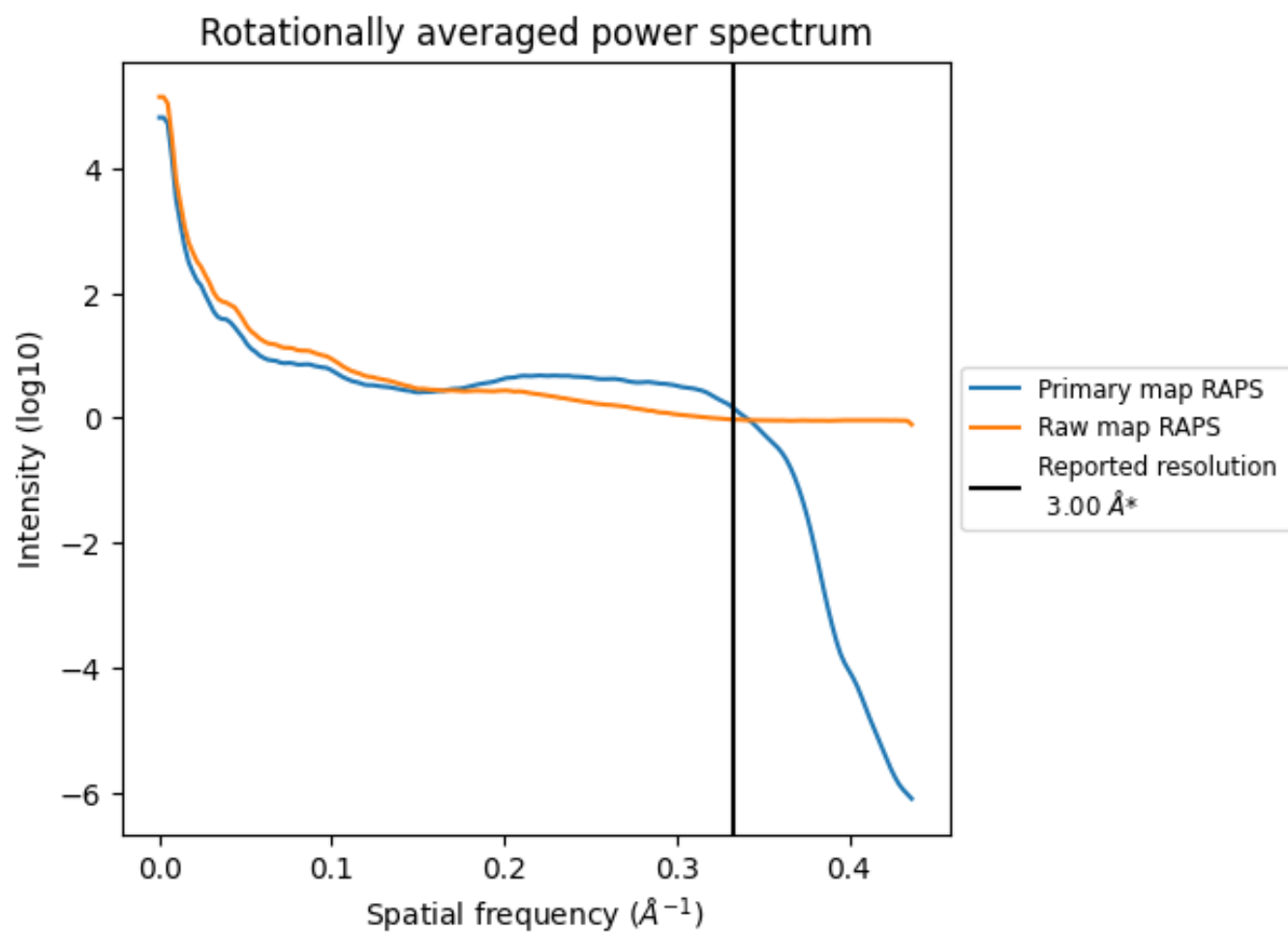
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1189 nm^3 ; this corresponds to an approximate mass of 1074 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 ⓘ

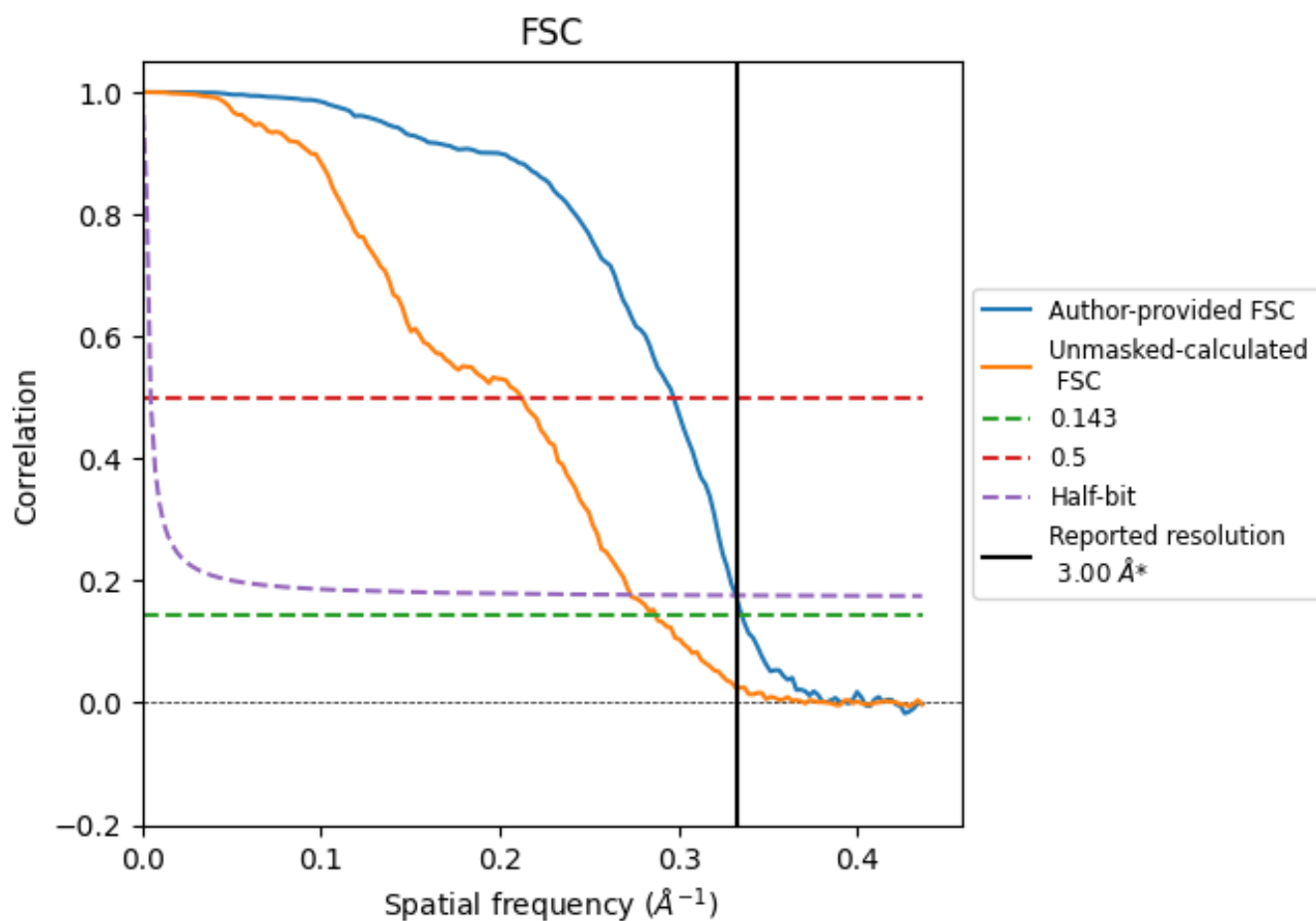


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

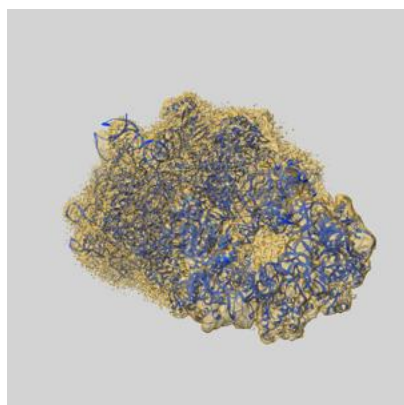
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.98	3.36	3.01
Unmasked-calculated*	3.48	4.72	3.66

*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 3.48 differs from the reported value 3.0 by more than 10 %

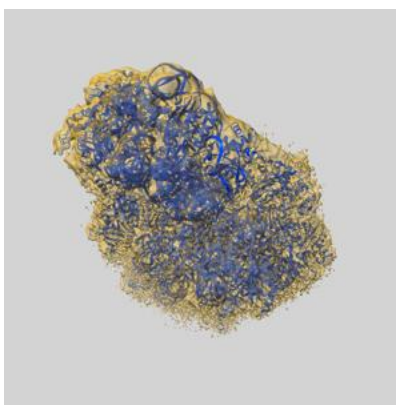
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66684 and PDB model 9XAE. Per-residue inclusion information can be found in section 3 on page 11.

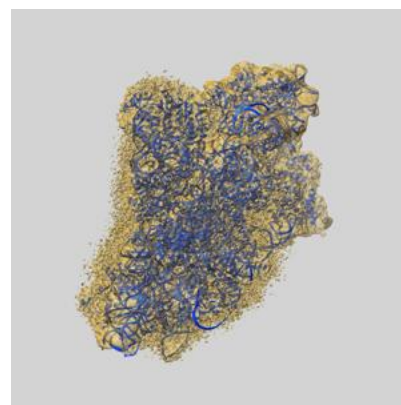
9.1 Map-model overlay [i](#)



X



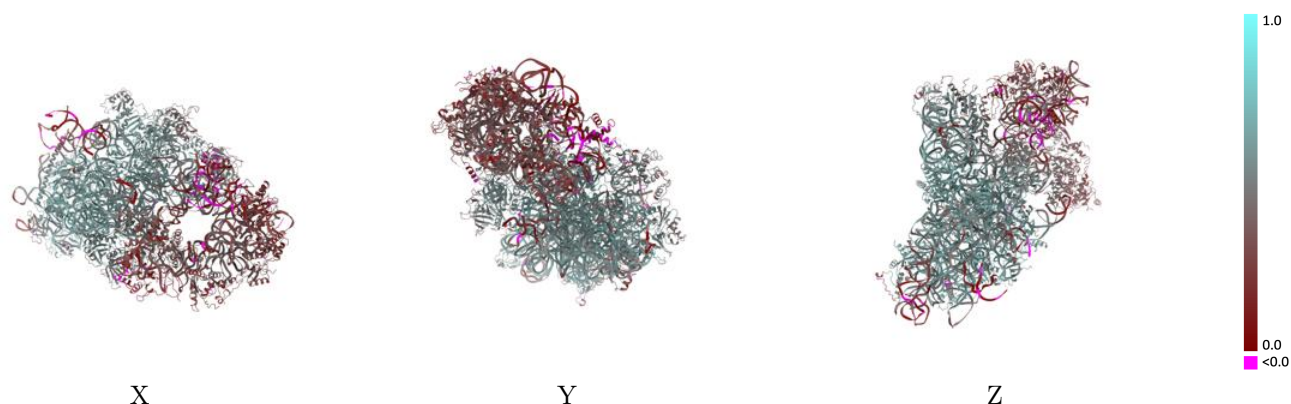
Y



Z

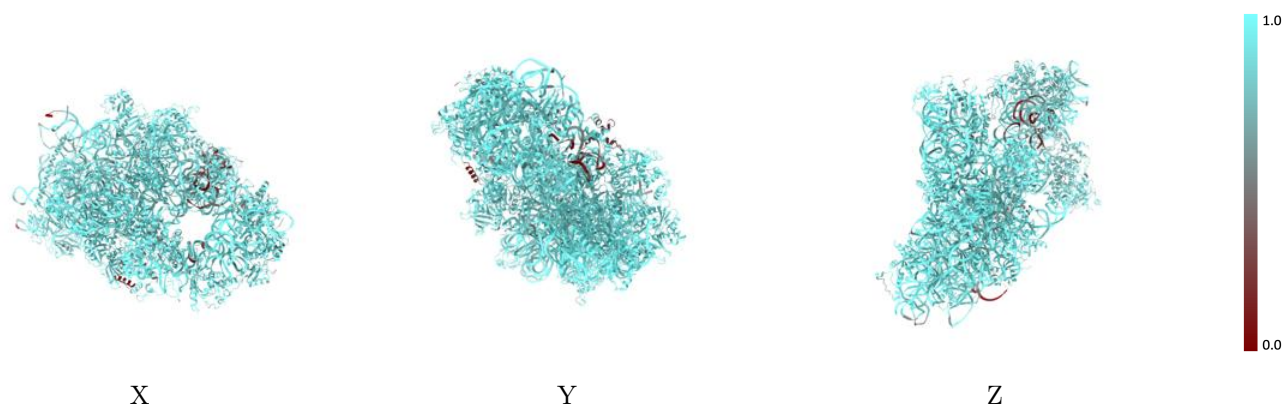
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



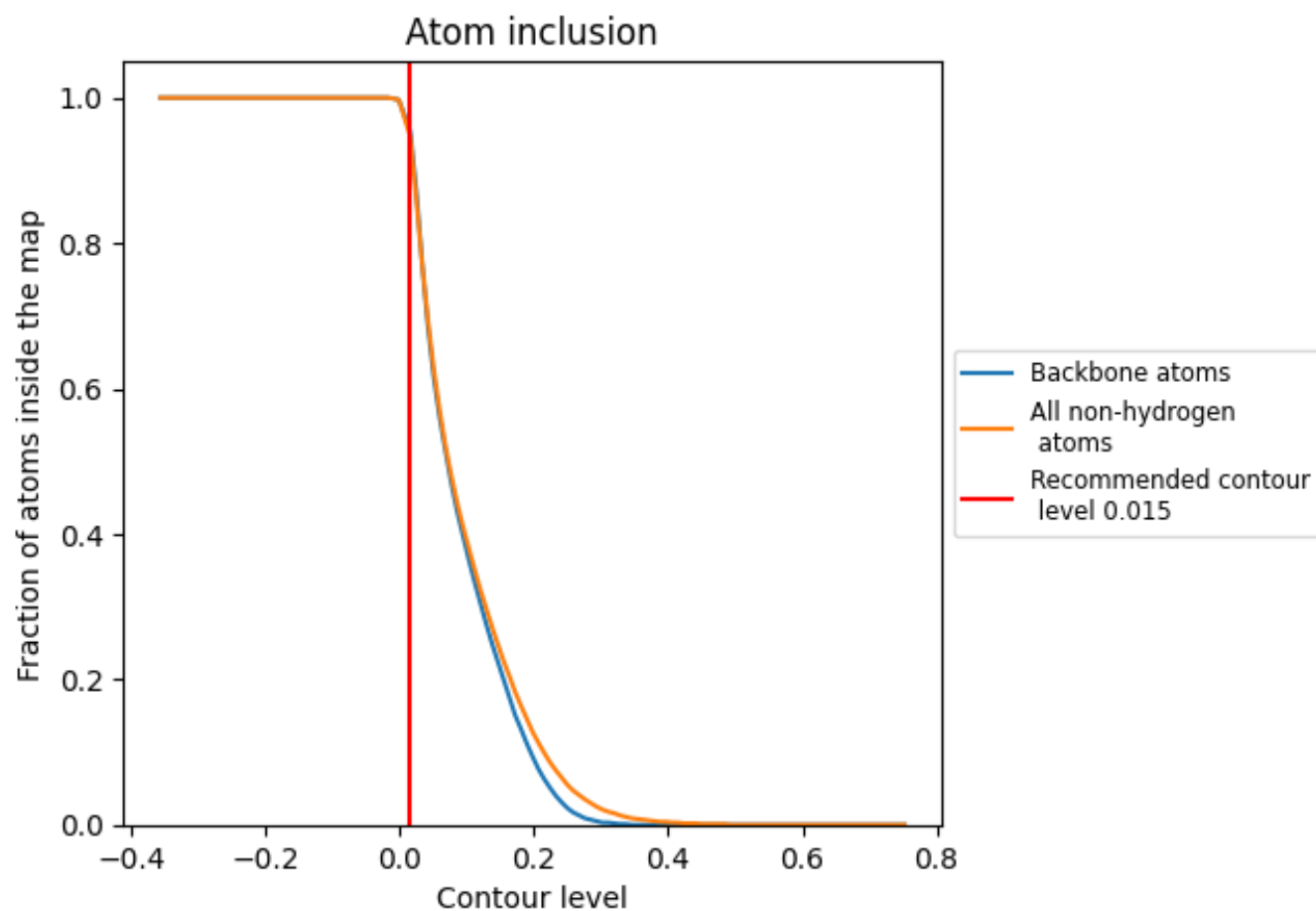
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9480	 0.4720
2	 0.9320	 0.4850
3	 0.9440	 0.4860
4	 0.9030	 0.3490
5	 0.8970	 0.2540
A	 0.9550	 0.4750
D	 0.9580	 0.4800
E	 0.9740	 0.5270
F	 0.9790	 0.5730
H	 0.9880	 0.6210
I	 0.8980	 0.2610
J	 0.9730	 0.5500
K	 0.9760	 0.5240
L	 0.9710	 0.5750
M	 0.9840	 0.6080
O	 0.9810	 0.6170
P	 0.9040	 0.2200
Q	 0.9820	 0.6010
R	 0.9600	 0.5060
S	 0.9330	 0.3410
T	 0.8780	 0.2420
U	 0.7490	 0.1890
V	 0.9000	 0.3160
W	 0.9200	 0.2900
Y	 0.9860	 0.5760
Z	 0.9940	 0.6390
a	 0.9760	 0.5950
b	 0.9610	 0.5760
c	 0.7950	 0.2000
e	 0.9880	 0.5800
f	 0.9060	 0.2240
h	 0.9820	 0.5780
i	 0.9060	 0.2140

