



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 05:10 PM UTC

PDB ID : 6G18 / pdb_00006g18
EMDB ID : EMD-4337
Title : Cryo-EM structure of a late human pre-40S ribosomal subunit - State C
Authors : Ameismeier, M.; Cheng, J.; Berninghausen, O.; Beckmann, R.
Deposited on : 2018-03-20
Resolution : 3.60 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:

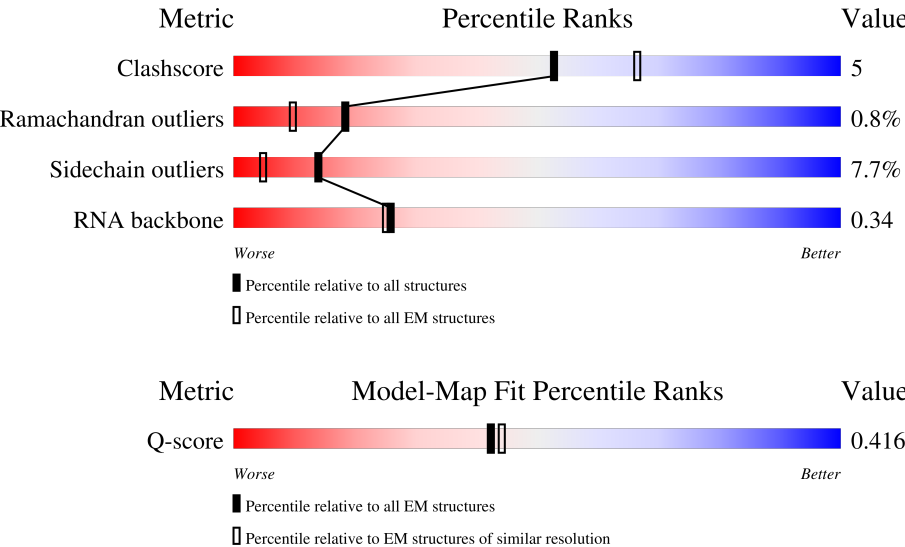
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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.



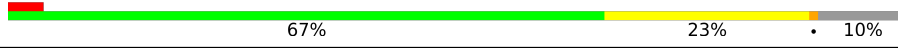
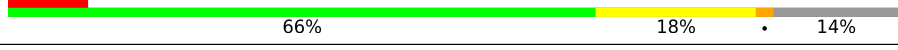
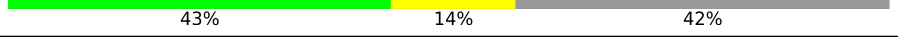
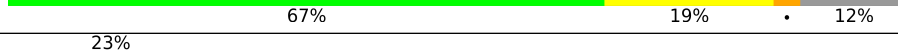
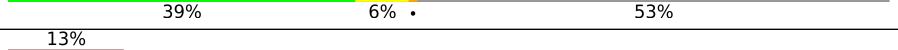
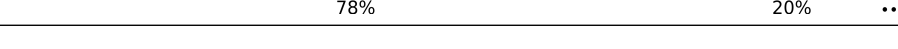
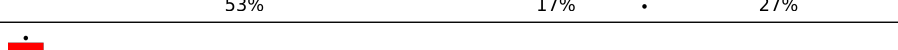
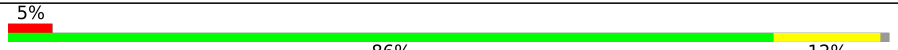
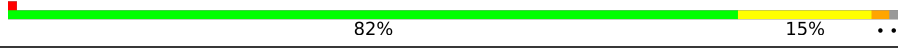
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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

Mol	Chain	Length	Quality of chain
1	2	1873	
2	F	204	
3	M	132	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	P	145	
5	Q	146	
6	R	135	
7	S	152	
8	T	145	
9	Z	125	
10	c	69	
11	f	156	
12	g	317	
13	A	295	
14	B	264	
15	C	293	
16	E	263	
17	G	249	
18	H	194	
19	I	208	
20	J	194	
21	L	158	
22	N	151	
23	O	151	
24	V	83	
25	W	130	
26	X	143	
27	Y	133	
28	b	84	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	e	59	24% 81% 12% 7%
30	x	252	55% 13% 29%
31	y	412	64% 14% 21%
32	u	804	64% 13% 22%
33	w	437	8% 50% 7% 43%
34	v	552	33% 56% 41%
35	t	475	5% 21% 5% 73%

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 83819 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called pre-18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1658	Total	C	N	O	P	0	0
			35407	15804	6362	11584	1657		

- Molecule 2 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 3 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 4 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	120	Total	C	N	O	S	0	0
			984	625	184	168	7		

- Molecule 5 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	122	Total	C	N	O	S	0	0
			969	616	180	170	3		

- Molecule 6 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	122	Total	C	N	O	S	0	0
			990	621	184	182	3		

- Molecule 7 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	130	Total	C	N	O	S	0	0
			1083	686	214	182	1		

- Molecule 8 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	144	Total	C	N	O	S	0	0
			1122	703	217	199	3		

- Molecule 9 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 10 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	c	61	Total	C	N	O	S	0	0
			471	288	95	86	2		

- Molecule 11 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	f	73	Total	C	N	O	S	0	0
			596	375	115	99	7		

- Molecule 12 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	g	313	Total	C	N	O	S	0	0
			2433	1533	424	464	12		

- Molecule 13 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	216	Total	C	N	O	S	0	0
			1705	1083	299	315	8		

- Molecule 14 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 15 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	218	Total	C	N	O	S	0	0
			1690	1094	289	297	10		

- Molecule 16 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 17 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 18 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	H	186	Total	C	N	O	S	0	0
			1501	957	276	267	1		

- Molecule 19 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 20 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 21 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 22 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 23 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	135	Total	C	N	O	S	0	0
			1009	618	198	187	6		

- Molecule 24 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 25 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 26 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 27 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 28 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 29 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	55	Total	C	N	O	S	0	0
			438	271	95	71	1		

- Molecule 30 is a protein called RNA-binding protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	x	178	Total	C	N	O	S	0	0
			1391	891	252	244	4		

- Molecule 31 is a protein called RNA-binding protein NOB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	y	325	Total	C	N	O	S	0	0
			2568	1622	473	463	10		

- Molecule 32 is a protein called Pre-rRNA-processing protein TSR1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	u	629	Total	C	N	O	S	0	0
			5062	3249	902	887	24		

- Molecule 33 is a protein called Bystin.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	w	249	Total	C	N	O	S	0	0
			2027	1322	354	342	9		

- Molecule 34 is a protein called Serine/threonine-protein kinase RIO2.

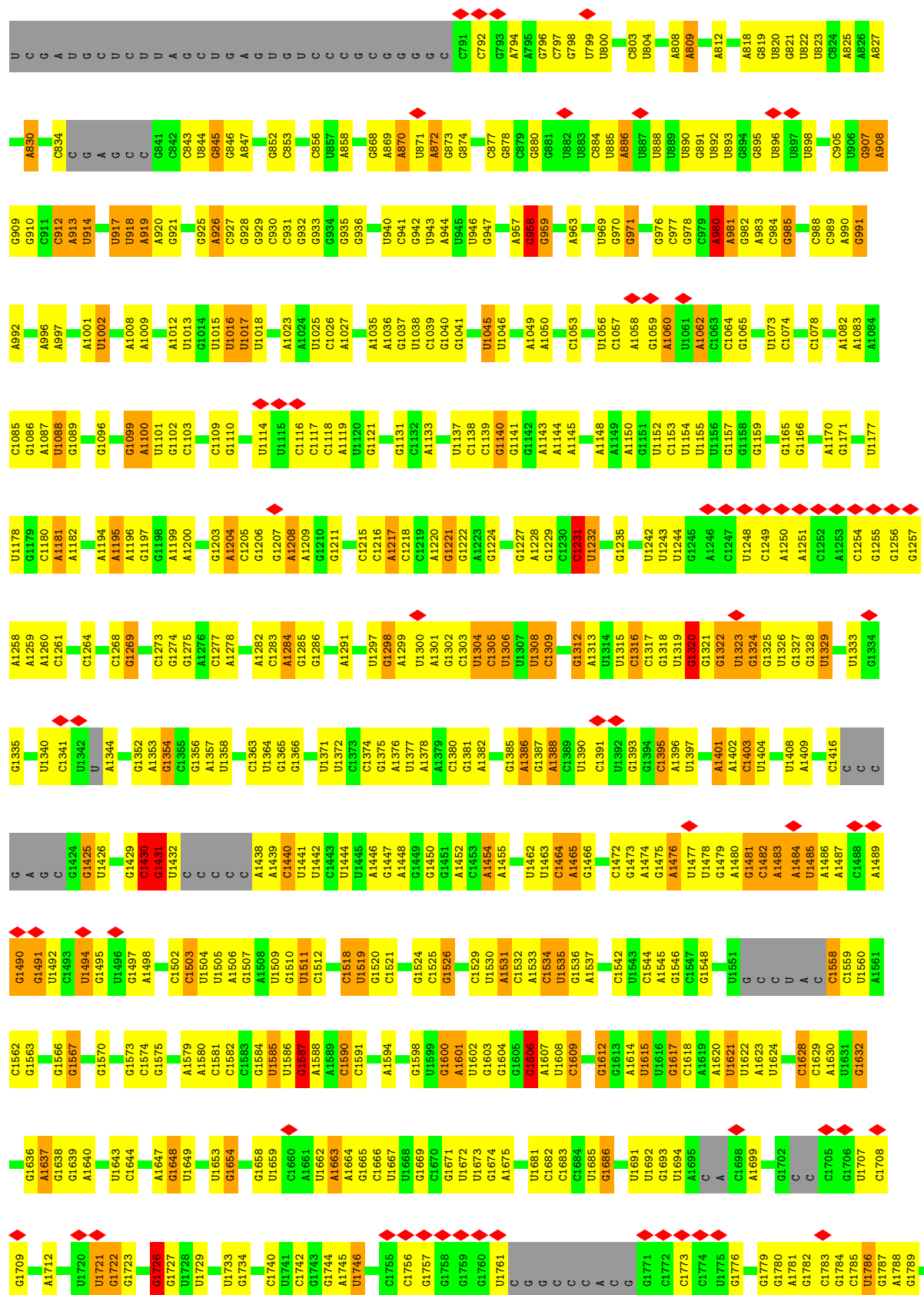
Mol	Chain	Residues	Atoms					AltConf	Trace
34	v	325	Total	C	N	O	S	0	0
			2593	1649	460	470	14		

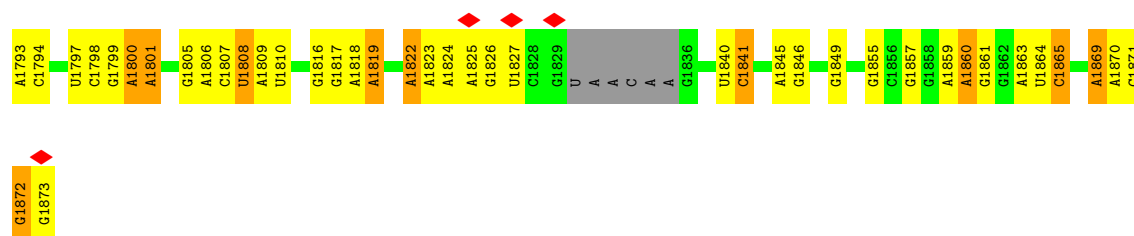
- Molecule 35 is a protein called Protein LTV1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	t	127	Total	C	N	O	S	0	0
			1066	661	204	199	2		

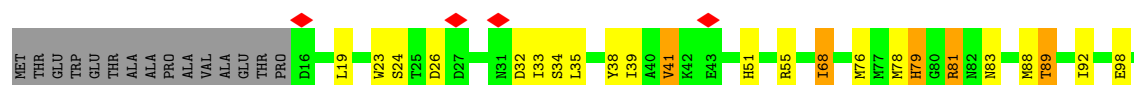
- Molecule 36 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
36	f	1	Total	Zn	0
			1	1	
36	y	1	Total	Zn	0
			1	1	

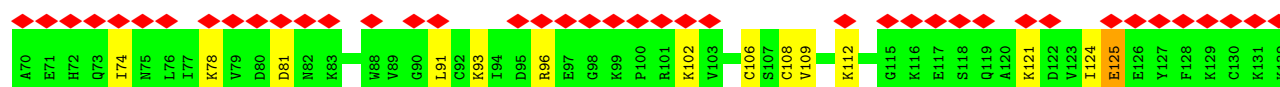
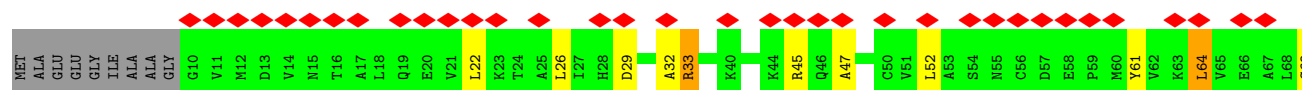
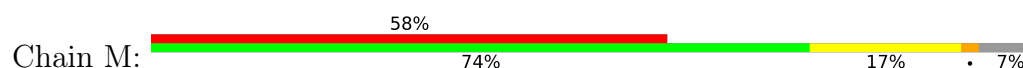




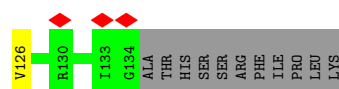
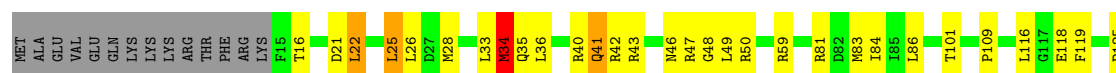
• Molecule 2: 40S ribosomal protein S5



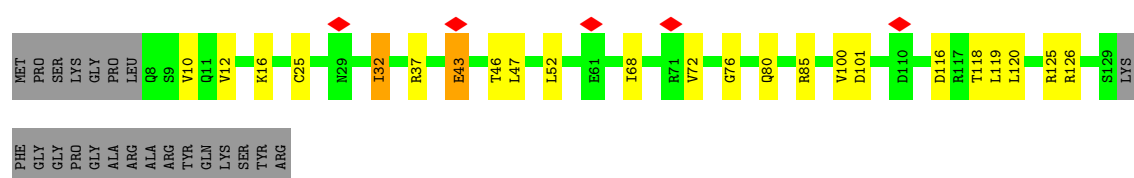
• Molecule 3: 40S ribosomal protein S12



• Molecule 4: 40S ribosomal protein S15

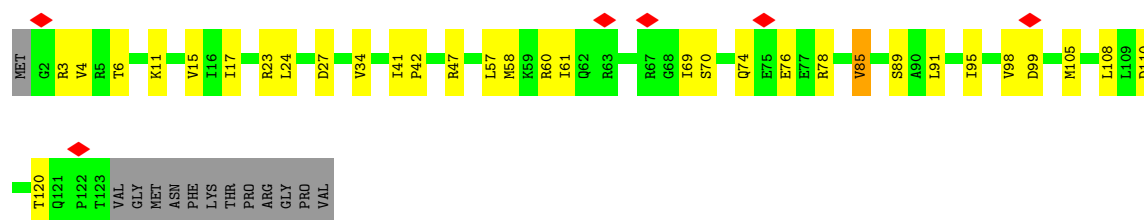


• Molecule 5: 40S ribosomal protein S16



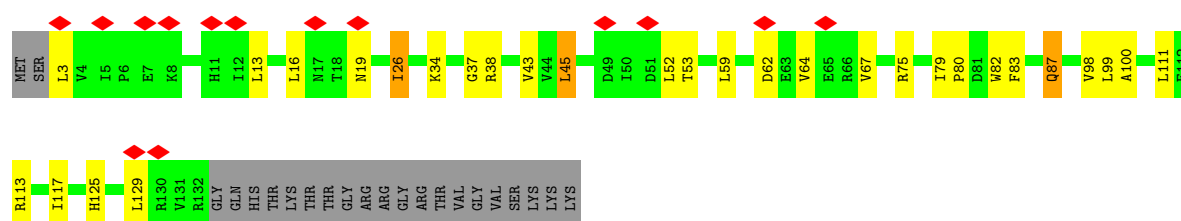
- Molecule 6: 40S ribosomal protein S17

Chain R: 



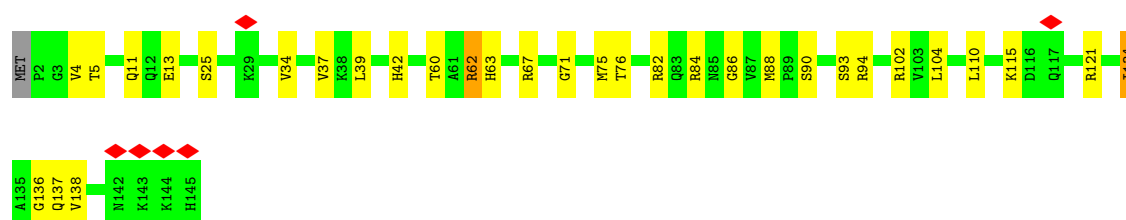
- Molecule 7: 40S ribosomal protein S18

Chain S: 

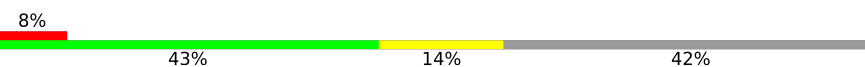


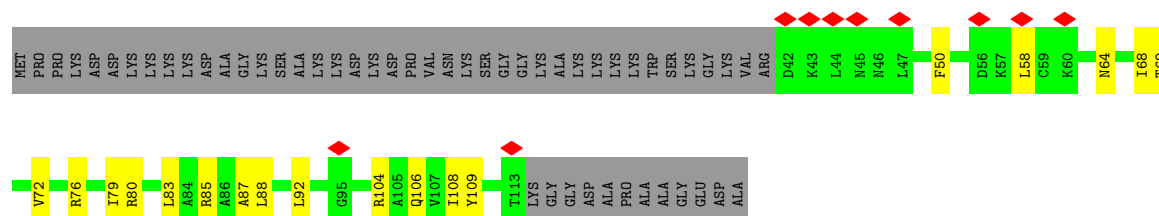
- Molecule 8: 40S ribosomal protein S19

Chain T: 



- Molecule 9: 40S ribosomal protein S25

Chain Z: 

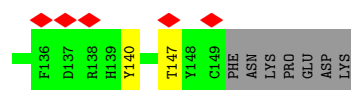
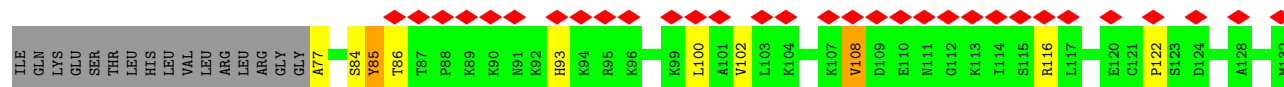
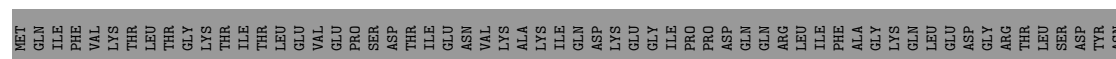
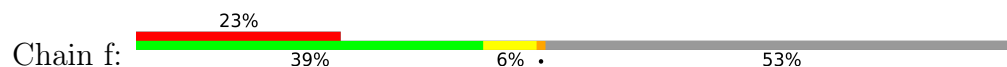


- Molecule 10: 40S ribosomal protein S28

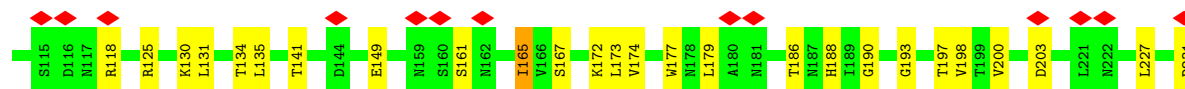
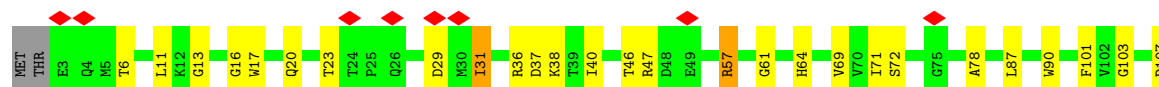
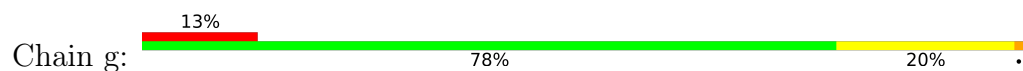
Chain c: 



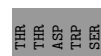
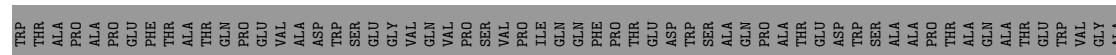
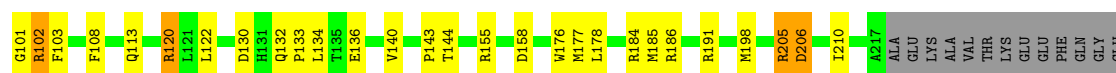
• Molecule 11: Ubiquitin-40S ribosomal protein S27a



• Molecule 12: Receptor of activated protein C kinase 1

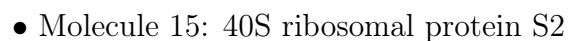


• Molecule 13: 40S ribosomal protein SA



• Molecule 14: 40S ribosomal protein S3a

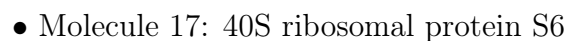
Frequency	Percentage
Daily	68%
Weekly	12%
Monthly	19%



Frequency	Percentage
Often	60%
Sometimes	13%
Never	26%



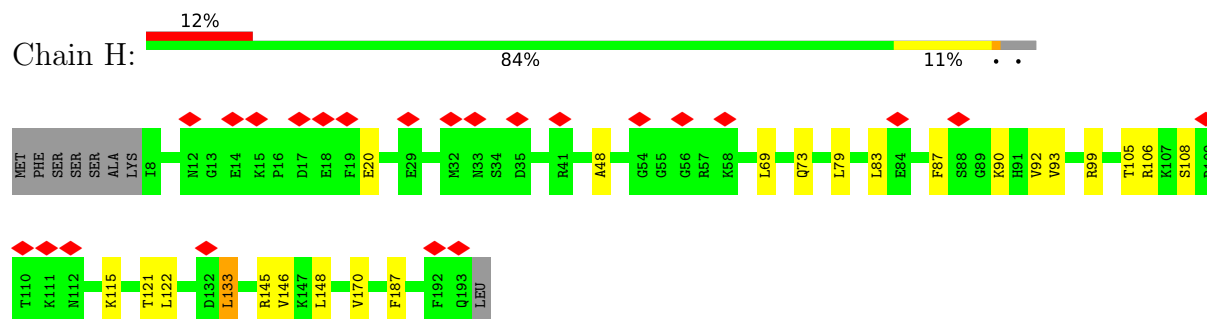
Response	Percentage
Doing a good job	83%
Not doing a good job	16%



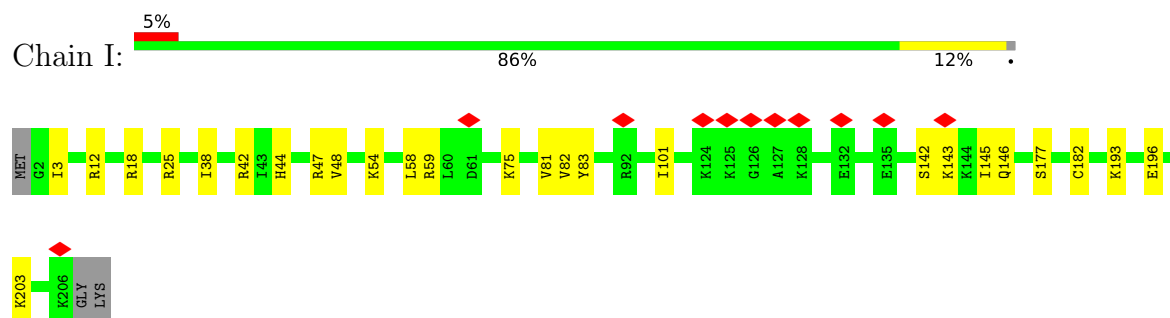
Frequency	Percentage
Daily	11%
Weekly	78%
Monthly	14%
Other	8%



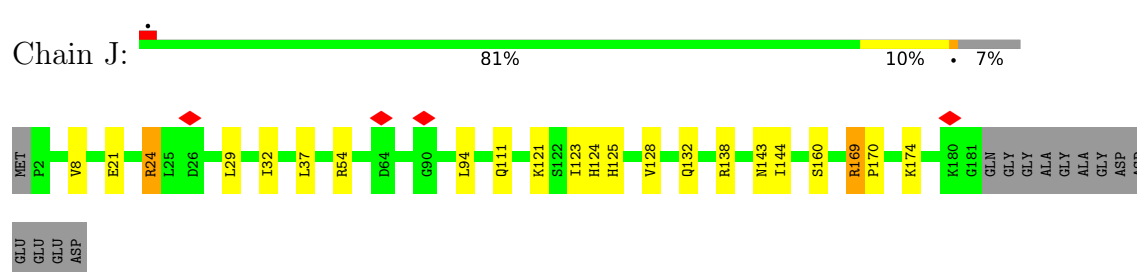
- Molecule 18: 40S ribosomal protein S7



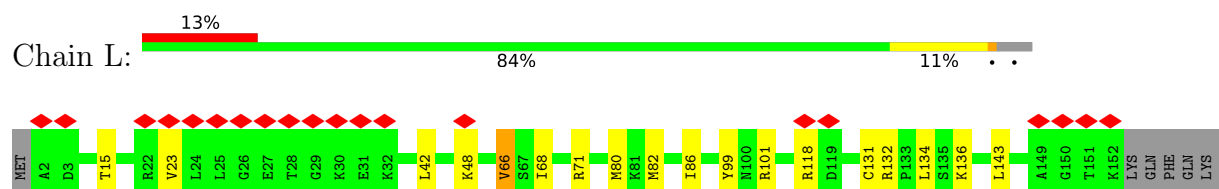
- Molecule 19: 40S ribosomal protein S8



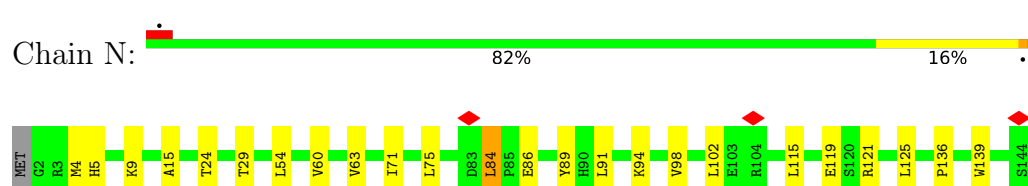
- Molecule 20: 40S ribosomal protein S9



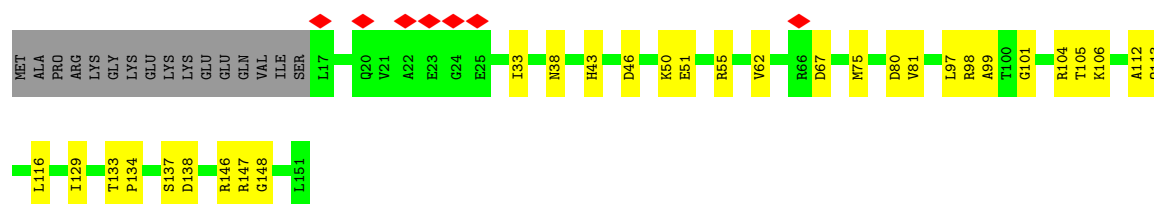
- Molecule 21: 40S ribosomal protein S11



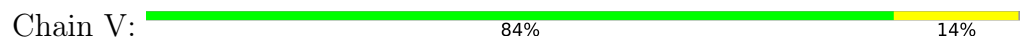
- Molecule 22: 40S ribosomal protein S13



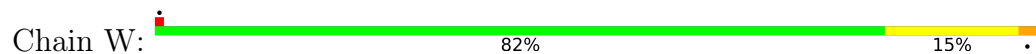
- Molecule 23: 40S ribosomal protein S14



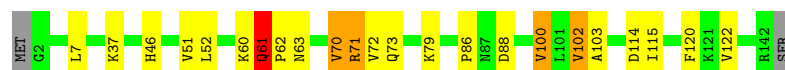
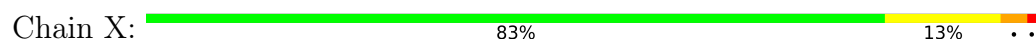
- Molecule 24: 40S ribosomal protein S21



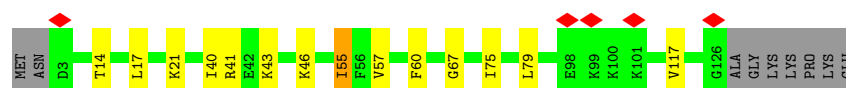
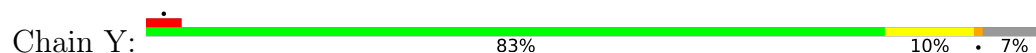
- Molecule 25: 40S ribosomal protein S15a



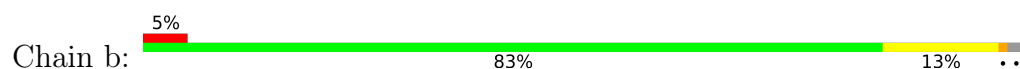
- Molecule 26: 40S ribosomal protein S23



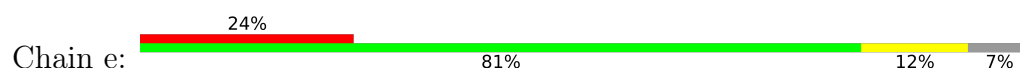
- Molecule 27: 40S ribosomal protein S24

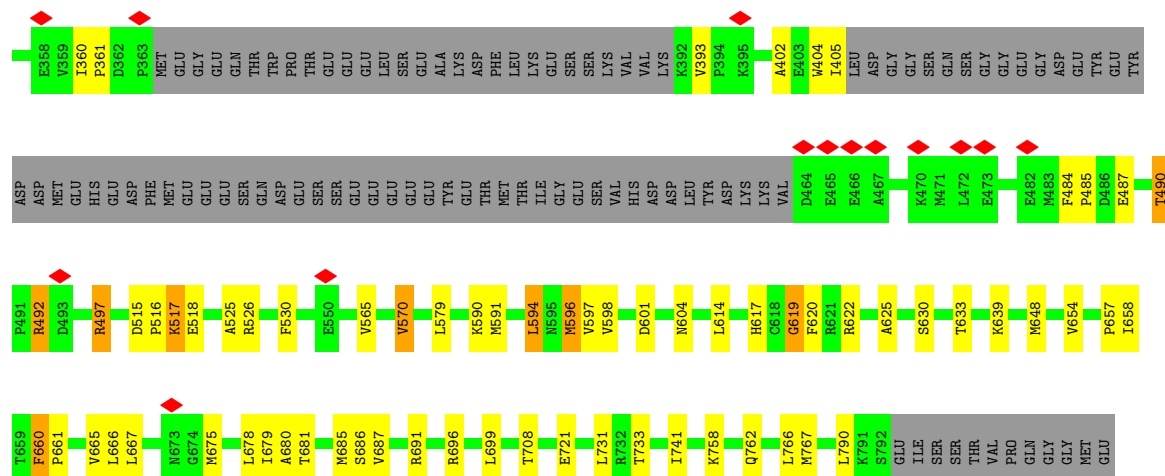


- Molecule 28: 40S ribosomal protein S27

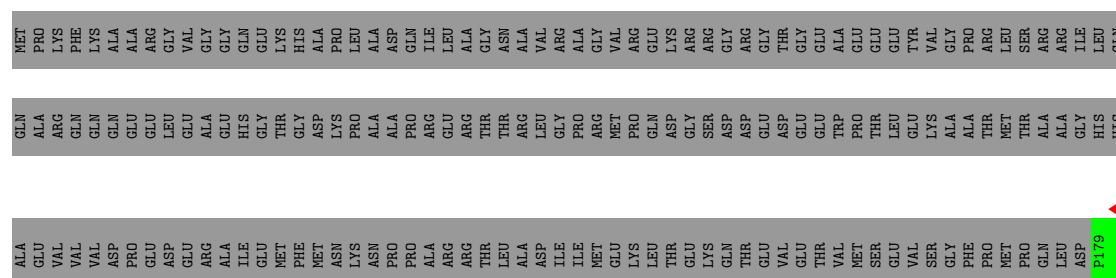


- Molecule 29: 40S ribosomal protein S30

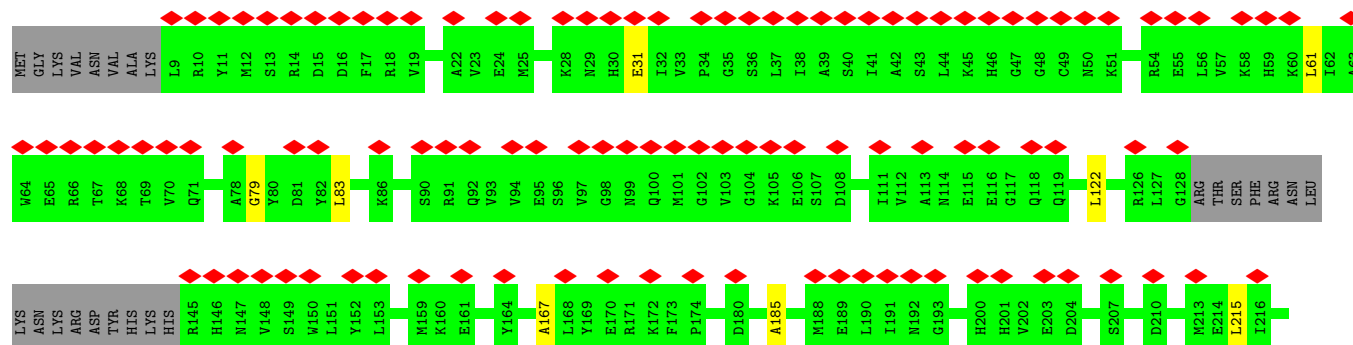




• Molecule 33: Bystin



• Molecule 34: Serine/threonine-protein kinase RIO2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	287847	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 ($e^-/\text{\AA}^2$)	2.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.470	Depositor
Minimum map value	-0.211	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.0583	Depositor
Map size (Å)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.40	0/39590	0.78	50/61690 (0.1%)
2	F	0.51	0/1516	1.05	3/2037 (0.1%)
3	M	0.56	0/963	0.98	0/1291
4	P	0.53	0/1003	0.95	0/1341
5	Q	0.56	0/982	1.01	1/1318 (0.1%)
6	R	0.56	0/1002	1.03	0/1345
7	S	0.51	0/1100	0.99	1/1475 (0.1%)
8	T	0.58	0/1142	1.06	0/1530
9	Z	0.51	0/580	0.93	0/780
10	c	0.47	0/473	0.84	0/633
11	f	0.53	0/607	0.86	0/802
12	g	0.49	0/2490	0.79	0/3389
13	A	0.56	0/1742	1.00	2/2367 (0.1%)
14	B	0.48	0/1756	0.90	1/2350 (0.0%)
15	C	0.58	0/1726	0.92	0/2332
16	E	0.47	0/2118	0.87	0/2849
17	G	0.51	0/1885	0.92	0/2510
18	H	0.51	0/1524	0.91	0/2042
19	I	0.47	0/1711	0.90	0/2282
20	J	0.54	0/1524	1.01	0/2035
21	L	0.51	0/1250	0.83	1/1673 (0.1%)
22	N	0.57	0/1226	1.04	0/1649
23	O	0.58	0/1022	1.03	1/1372 (0.1%)
24	V	0.50	0/631	0.90	0/844
25	W	0.55	0/1051	0.94	1/1406 (0.1%)
26	X	0.55	0/1116	0.94	1/1490 (0.1%)
27	Y	0.50	0/1031	0.88	0/1370
28	b	0.47	0/653	0.82	1/876 (0.1%)
29	e	0.57	0/443	0.88	0/582
30	x	0.56	0/1413	1.01	2/1906 (0.1%)
31	y	0.50	0/2618	0.91	2/3536 (0.1%)
32	u	0.49	0/5187	0.87	2/7011 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	w	0.52	0/2074	1.01	0/2806
34	v	0.51	0/2644	0.91	0/3562
35	t	0.48	0/1075	1.10	4/1424 (0.3%)
All	All	0.47	0/88868	0.86	73/127905 (0.1%)

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	t	357	TYR	N-CA-C	-14.77	83.79	108.76
1	2	1494	U	C2'-C3'-O3'	11.15	126.22	109.50
35	t	357	TYR	CB-CA-C	-11.04	89.73	109.70
1	2	1648	G	C4'-C3'-O3'	9.49	123.64	109.40
1	2	547	G	C2'-C3'-O3'	9.16	123.24	109.50
1	2	1601	A	C2'-C3'-O3'	8.41	122.11	109.50
1	2	1430	C	C2'-C3'-O3'	8.03	121.54	109.50
1	2	102	A	C2'-C3'-O3'	7.96	121.43	109.50
1	2	114	G	C2'-C3'-O3'	7.72	121.09	109.50
1	2	594	A	C4'-C3'-O3'	7.54	120.71	109.40
1	2	1511	U	C2'-C3'-O3'	7.52	124.98	113.70
1	2	143	U	C2'-C3'-O3'	7.28	120.42	109.50
1	2	1587	G	C2'-C3'-O3'	7.16	120.24	109.50
1	2	604	A	C2'-C3'-O3'	7.12	124.37	113.70
1	2	1231	C	C2'-C3'-O3'	7.08	124.31	113.70
1	2	958	G	C2'-C3'-O3'	6.98	124.17	113.70
1	2	980	A	C2'-C3'-O3'	6.94	124.11	113.70
1	2	1534	C	C4'-C3'-O3'	6.93	119.80	109.40
1	2	465	A	C4'-C3'-O3'	6.89	119.74	109.40
1	2	1440	C	C4'-C3'-O3'	6.87	119.71	109.40
13	A	206	ASP	CA-C-N	6.72	128.24	119.84
13	A	206	ASP	C-N-CA	6.72	128.24	119.84
1	2	1476	A	C4'-C3'-O3'	6.69	119.44	109.40
1	2	1726	G	C2'-C3'-O3'	6.68	123.72	113.70
1	2	1558	C	C4'-C3'-O3'	6.67	119.40	109.40
35	t	358	SER	N-CA-CB	-6.55	100.68	110.90
1	2	1403	C	C4'-C3'-O3'	6.53	119.20	109.40
1	2	1431	G	C2'-C3'-O3'	6.45	123.38	113.70
26	X	61	GLN	N-CA-C	6.36	123.86	109.81
30	x	232	ASN	CA-C-N	6.33	124.22	119.66
30	x	232	ASN	C-N-CA	6.33	124.22	119.66
7	S	26	ILE	N-CA-C	6.32	116.99	110.36
1	2	1558	C	C2'-C3'-O3'	6.28	118.92	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1606	G	C4'-C3'-O3'	-6.18	103.73	113.00
1	2	1425	G	C2'-C3'-O3'	6.12	122.88	113.70
1	2	1587	G	C4'-C3'-O3'	6.09	118.53	109.40
1	2	314	U	C2'-C3'-O3'	6.06	122.79	113.70
31	y	370	VAL	N-CA-C	6.04	121.90	109.34
1	2	912	C	C2'-C3'-O3'	6.02	118.52	109.50
1	2	1871	C	C2'-C3'-O3'	-5.98	104.74	113.70
1	2	1430	C	C4'-C3'-O3'	5.83	118.15	109.40
1	2	1869	A	C4'-C3'-O3'	-5.78	104.33	113.00
2	F	169	ILE	CB-CA-C	-5.75	104.28	112.22
2	F	103	LEU	N-CA-C	5.69	117.17	110.97
1	2	1573	G	C4'-C3'-O3'	-5.61	104.59	113.00
1	2	1316	C	C2'-C3'-O3'	5.55	117.82	109.50
1	2	1601	A	C4'-C3'-O3'	5.52	117.68	109.40
1	2	1320	G	C4'-C3'-O3'	-5.51	104.73	113.00
1	2	114	G	C4'-C3'-O3'	5.49	117.64	109.40
5	Q	43	GLU	N-CA-C	5.49	120.39	113.25
31	y	214	ILE	N-CA-C	5.46	116.19	110.62
1	2	1617	G	C4'-C3'-O3'	-5.45	104.83	113.00
14	B	200	ALA	N-CA-C	5.44	119.64	112.89
1	2	8	U	C2'-C3'-O3'	5.44	117.65	109.50
1	2	180	G	C4'-C3'-O3'	-5.40	104.90	113.00
25	W	14	ILE	N-CA-CB	5.35	117.81	110.54
1	2	1403	C	C2'-C3'-O3'	5.33	117.49	109.50
23	O	148	GLY	N-CA-C	5.30	118.04	110.46
1	2	1304	U	C4'-C3'-O3'	-5.29	105.06	113.00
1	2	1316	C	C4'-C3'-O3'	5.29	117.33	109.40
21	L	66	VAL	N-CA-C	5.28	116.18	108.58
1	2	668	A	C4'-C3'-O3'	-5.27	105.10	113.00
1	2	102	A	C4'-C3'-O3'	5.26	117.29	109.40
35	t	359	ASN	N-CA-C	5.23	118.02	110.28
2	F	83	ASN	N-CA-C	5.21	118.74	112.38
1	2	991	G	C4'-C3'-O3'	-5.19	105.22	113.00
32	u	660	PHE	CA-C-N	5.14	123.41	119.66
32	u	660	PHE	C-N-CA	5.14	123.41	119.66
1	2	666	U	N1-C1'-C2'	5.11	119.66	112.00
1	2	870	A	C4'-C3'-O3'	5.04	116.96	109.40
1	2	332	G	C2'-C3'-O3'	5.02	121.24	113.70
1	2	1140	G	C4'-C3'-O3'	-5.02	105.46	113.00
28	b	20	LYS	N-CA-C	5.01	118.16	111.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	35407	0	17876	432	0
2	F	1495	0	1549	24	0
3	M	953	0	990	10	0
4	P	984	0	1028	17	0
5	Q	969	0	1030	7	0
6	R	990	0	1037	8	0
7	S	1083	0	1140	10	0
8	T	1122	0	1153	21	0
9	Z	574	0	627	6	0
10	c	471	0	499	7	0
11	f	596	0	627	4	0
12	g	2433	0	2389	16	0
13	A	1705	0	1706	29	0
14	B	1729	0	1803	10	0
15	C	1690	0	1777	19	0
16	E	2076	0	2177	19	0
17	G	1862	0	2018	20	0
18	H	1501	0	1593	14	0
19	I	1682	0	1769	15	0
20	J	1499	0	1618	12	0
21	L	1229	0	1302	6	0
22	N	1202	0	1289	10	0
23	O	1009	0	1034	16	0
24	V	625	0	628	9	0
25	W	1034	0	1080	9	0
26	X	1098	0	1167	12	0
27	Y	1014	0	1082	6	0
28	b	640	0	665	6	0
29	e	438	0	484	3	0
30	x	1391	0	1467	22	0
31	y	2568	0	2624	32	0
32	u	5062	0	5113	53	0
33	w	2027	0	2126	13	0
34	v	2593	0	2551	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	t	1066	0	1070	19	0
36	f	1	0	0	0	0
36	y	1	0	0	0	0
All	All	83819	0	68088	794	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 (794) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:872:A:N6	1:2:914:U:H3	1.01	1.43
1:2:830:A:N6	1:2:844:U:H3	0.85	1.32
1:2:1144:A:H2'	1:2:1145:A:C8	1.74	1.23
32:u:525:ALA:HB2	35:t:362:ASN:ND2	1.52	1.23
1:2:872:A:N1	1:2:914:U:O4	1.82	1.11
1:2:1542:C:H5''	8:T:62:ARG:NH2	1.68	1.07
1:2:1542:C:H5''	8:T:62:ARG:HH21	1.21	1.03
1:2:943:U:H2'	1:2:944:A:C8	1.96	1.00
1:2:1356:G:H2'	1:2:1357:A:C8	1.98	0.97
1:2:1335:G:H1	1:2:1492:U:H3	1.12	0.96
32:u:525:ALA:HB2	35:t:362:ASN:HD21	1.15	0.95
32:u:517:LYS:O	35:t:360:LEU:HD13	1.70	0.90
1:2:830:A:N1	1:2:844:U:O4	2.04	0.89
1:2:1144:A:H2'	1:2:1145:A:H8	1.34	0.84
1:2:981:A:H2'	1:2:982:G:C8	2.12	0.84
1:2:666:U:H2'	1:2:667:U:C6	2.12	0.84
1:2:830:A:N6	1:2:844:U:C2	2.42	0.84
1:2:1144:A:H1'	1:2:1199:A:O2'	1.78	0.83
32:u:625:ALA:HB1	32:u:654:VAL:HG21	1.59	0.83
1:2:1585:U:C5	8:T:67:ARG:HD2	2.15	0.81
1:2:1518:C:H5''	1:2:1519:U:H5''	1.61	0.81
20:J:128:VAL:O	20:J:132:GLN:HG2	1.81	0.80
23:O:43:HIS:HD2	23:O:55:ARG:HB2	1.49	0.77
32:u:272:LEU:HB2	32:u:565:VAL:HG11	1.67	0.76
1:2:913:A:H2	18:H:99:ARG:H	1.32	0.75
1:2:830:A:N6	1:2:844:U:N3	1.65	0.75
1:2:943:U:H2'	1:2:944:A:H8	1.46	0.75
1:2:145:G:H2'	1:2:146:G:C8	2.21	0.74
1:2:380:G:H22	1:2:382:C:H3'	1.51	0.74
8:T:76:THR:HG22	8:T:94:ARG:HB3	1.69	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:925:G:H1	1:2:1017:U:H3	1.35	0.73
1:2:1857:G:H3'	23:O:146:ARG:NH2	2.03	0.73
1:2:386:C:H2'	1:2:387:C:C6	2.23	0.73
1:2:1630:A:H5''	7:S:37:GLY:H	1.54	0.72
30:x:179:ALA:HB1	30:x:229:ILE:HG22	1.71	0.72
14:B:82:ARG:HH12	14:B:191:ASP:HB2	1.52	0.72
17:G:135:PRO:HG2	17:G:141:ILE:HD13	1.70	0.72
21:L:80:MET:HB3	21:L:86:ILE:HG22	1.71	0.72
1:2:380:G:N2	1:2:382:C:H3'	2.03	0.72
1:2:808:A:HO2'	1:2:809:A:H8	1.38	0.72
1:2:12:U:H2'	1:2:13:C:C6	2.24	0.71
1:2:1817:G:H2'	1:2:1818:A:C8	2.25	0.71
1:2:1857:G:H3'	23:O:146:ARG:HH22	1.55	0.71
12:g:87:LEU:HB3	12:g:101:PHE:HB2	1.73	0.70
1:2:1217:A:H2'	1:2:1218:C:C6	2.26	0.70
14:B:140:VAL:HG23	14:B:213:ARG:HG2	1.75	0.69
22:N:63:VAL:HG21	22:N:71:ILE:HD11	1.74	0.69
1:2:64:A:H2	1:2:83:A:H62	1.38	0.68
1:2:996:A:H2'	1:2:997:A:C8	2.29	0.68
1:2:552:G:H2'	1:2:553:U:C6	2.29	0.67
1:2:617:G:H4'	26:X:88:ASP:HB3	1.75	0.67
1:2:1545:A:H2'	1:2:1546:G:C8	2.29	0.67
32:u:91:HIS:HA	32:u:167:ASP:HB2	1.75	0.67
30:x:211:ILE:HD11	30:x:218:ILE:HG23	1.75	0.67
1:2:16:G:H2'	1:2:17:C:C6	2.29	0.67
1:2:1464:C:O2'	1:2:1465:A:C8	2.46	0.67
12:g:165:ILE:HG12	12:g:177:TRP:HB2	1.76	0.67
1:2:595:U:H2'	1:2:596:U:C6	2.30	0.67
1:2:931:C:H2'	1:2:932:G:C8	2.30	0.67
18:H:93:VAL:HG11	18:H:133:LEU:HD12	1.77	0.66
1:2:118:C:H1'	1:2:445:A:C5	2.30	0.66
19:I:12:ARG:HE	19:I:18:ARG:HD3	1.60	0.66
1:2:1231:C:H2'	1:2:1232:U:O4'	1.96	0.66
32:u:517:LYS:O	35:t:360:LEU:CD1	2.42	0.65
31:y:111:LYS:HG3	31:y:307:HIS:HB3	1.78	0.65
1:2:872:A:N6	1:2:914:U:N3	1.83	0.65
32:u:596:MET:HG2	32:u:665:VAL:HG21	1.76	0.65
1:2:624:C:H41	26:X:63:ASN:HD22	1.45	0.64
1:2:1374:C:H2'	1:2:1375:G:O4'	1.97	0.64
1:2:1726:G:H1	1:2:1808:U:H3	1.45	0.64
1:2:1797:U:H2'	1:2:1798:C:C6	2.32	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1530:U:H2'	1:2:1531:A:O4'	1.98	0.64
1:2:12:U:H2'	1:2:13:C:H6	1.63	0.64
13:A:5:LEU:HD21	24:V:41:LYS:HA	1.80	0.64
1:2:1628:C:H2'	1:2:1629:C:C6	2.33	0.64
1:2:619:A:N1	26:X:114:ASP:HB2	2.13	0.63
1:2:1600:G:H2'	1:2:1600:G:N3	2.13	0.63
1:2:1228:A:H2'	1:2:1229:G:C8	2.34	0.63
32:u:490:THR:HG23	32:u:699:LEU:HD22	1.81	0.63
1:2:1037:G:H4'	1:2:1845:A:H4'	1.79	0.63
1:2:926:A:H2'	1:2:927:C:O4'	1.98	0.63
1:2:872:A:N1	1:2:914:U:C4	2.66	0.62
1:2:297:A:H5'	16:E:132:GLY:HA2	1.82	0.62
1:2:1567:G:O2'	8:T:37:VAL:HG23	1.99	0.62
23:O:62:VAL:HG11	23:O:67:ASP:HB2	1.82	0.62
1:2:980:A:H2'	1:2:981:A:C8	2.35	0.61
1:2:1217:A:H2'	1:2:1218:C:H6	1.64	0.61
1:2:1196:A:O5'	1:2:1196:A:H8	1.83	0.61
23:O:99:ALA:H	23:O:133:THR:HG22	1.64	0.61
1:2:495:U:H2'	1:2:496:C:O4'	2.01	0.61
1:2:51:U:H2'	1:2:52:G:C8	2.35	0.61
13:A:84:GLN:HE22	13:A:101:GLY:H	1.49	0.61
1:2:983:A:H2'	1:2:984:C:O4'	2.01	0.61
24:V:20:SER:HB3	24:V:59:ILE:HD11	1.82	0.61
1:2:51:U:H2'	1:2:52:G:H8	1.66	0.60
12:g:11:LEU:HB2	12:g:307:VAL:HB	1.82	0.60
1:2:444:G:N2	1:2:446:G:H3'	2.17	0.60
12:g:57:ARG:HG2	12:g:57:ARG:HH11	1.67	0.60
1:2:1872:G:N2	31:y:122:PRO:HD2	2.16	0.60
19:I:83:TYR:HD2	19:I:101:ILE:HD13	1.67	0.60
1:2:1681:U:H2'	1:2:1682:C:C6	2.36	0.60
7:S:26:ILE:HD12	7:S:59:LEU:HD11	1.84	0.60
1:2:1587:G:N2	8:T:63:HIS:HD2	2.00	0.60
1:2:1585:U:H5	8:T:67:ARG:HD2	1.64	0.59
31:y:69:PHE:CZ	31:y:248:MET:HG3	2.37	0.59
1:2:1606:G:H22	1:2:1632:G:H2'	1.68	0.59
1:2:1692:U:H5'	31:y:384:THR:HG21	1.85	0.59
27:Y:41:ARG:HA	27:Y:55:ILE:HD11	1.83	0.59
1:2:29:G:H2'	1:2:30:C:C6	2.37	0.59
1:2:808:A:O2'	1:2:809:A:H8	1.85	0.59
1:2:1606:G:N2	1:2:1632:G:H2'	2.17	0.59
13:A:66:VAL:HG21	13:A:185:MET:HB3	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:84:LEU:HD13	22:N:89:TYR:HB2	1.84	0.59
1:2:441:C:H2'	1:2:442:C:C6	2.38	0.58
1:2:1480:A:H2'	1:2:1481:G:C8	2.37	0.58
6:R:105:MET:HE1	13:A:51:LEU:HD12	1.85	0.58
1:2:301:A:H2'	1:2:302:A:O4'	2.03	0.58
1:2:1520:G:N3	1:2:1520:G:H2'	2.18	0.58
3:M:32:ALA:HB2	3:M:112:LYS:HE3	1.85	0.58
1:2:293:C:O2	1:2:293:C:H2'	2.04	0.58
1:2:1639:G:H2'	1:2:1640:A:C8	2.39	0.58
1:2:220:U:H5'	19:I:177:SER:HB2	1.86	0.58
1:2:346:C:H5''	16:E:38:LEU:HD23	1.84	0.58
1:2:1502:C:H2'	1:2:1503:C:C6	2.39	0.58
32:u:639:LYS:HD2	32:u:696:ARG:HD2	1.86	0.58
32:u:157:LEU:HD11	32:u:232:LEU:HD21	1.86	0.57
6:R:58:MET:HA	6:R:61:ILE:HG22	1.85	0.57
14:B:136:ARG:HB3	14:B:216:LYS:HB2	1.86	0.57
1:2:171:A:C5'	17:G:177:GLN:HG2	2.33	0.57
1:2:1798:C:H2'	1:2:1799:G:O4'	2.04	0.57
1:2:639:C:H2'	1:2:640:A:C8	2.39	0.57
32:u:685:MET:HG2	32:u:686:SER:H	1.69	0.57
1:2:1268:C:H2'	1:2:1269:G:O4'	2.05	0.57
13:A:38:ILE:HD11	13:A:47:TYR:HB3	1.86	0.57
1:2:666:U:H2'	1:2:667:U:H6	1.65	0.57
1:2:1143:A:H2'	1:2:1144:A:C8	2.39	0.57
17:G:62:PRO:HG2	17:G:83:CYS:HB2	1.86	0.57
1:2:104:A:H62	1:2:356:C:H5	1.53	0.57
1:2:107:A:H2'	1:2:108:G:C8	2.39	0.57
22:N:15:ALA:HB2	28:b:21:LYS:HD3	1.87	0.57
1:2:441:C:H2'	1:2:442:C:H6	1.69	0.57
1:2:551:U:H2'	1:2:552:G:C8	2.40	0.57
1:2:1144:A:C2'	1:2:1145:A:C8	2.68	0.57
14:B:49:VAL:HG21	14:B:62:LEU:HD22	1.87	0.57
15:C:137:VAL:HG21	15:C:244:ILE:HD12	1.87	0.57
1:2:1628:C:H2'	1:2:1629:C:H6	1.69	0.56
1:2:1779:G:H2'	1:2:1780:G:C8	2.40	0.56
25:W:30:CYS:HB2	25:W:61:ILE:HD11	1.87	0.56
1:2:386:C:H2'	1:2:387:C:H6	1.70	0.56
32:u:594:LEU:HD23	32:u:596:MET:HE3	1.87	0.56
1:2:594:A:H61	1:2:643:A:H5''	1.70	0.56
10:c:12:ALA:HB1	10:c:32:VAL:HG13	1.87	0.56
1:2:928:G:H1	1:2:1013:U:H3	1.51	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Z:50:PHE:HZ	9:Z:87:ALA:HB2	1.70	0.56
1:2:1139:C:H2'	1:2:1140:G:O4'	2.05	0.56
12:g:16:GLY:H	12:g:37:ASP:HB3	1.70	0.56
1:2:1144:A:C2	1:2:1145:A:C6	2.94	0.56
13:A:77:ILE:HG12	13:A:99:ILE:HB	1.88	0.56
1:2:1746:U:H4'	17:G:65:GLN:HE21	1.71	0.56
16:E:182:MET:HE2	16:E:192:ILE:HD11	1.88	0.55
8:T:62:ARG:NH1	8:T:62:ARG:HG3	2.22	0.55
13:A:143:PRO:HG3	24:V:32:ILE:HG23	1.88	0.55
1:2:1144:A:H1'	1:2:1199:A:HO2'	1.71	0.55
4:P:43:ARG:O	4:P:47:ARG:HG2	2.07	0.55
14:B:121:ILE:HG12	14:B:161:VAL:HG13	1.88	0.55
19:I:143:LYS:O	19:I:146:GLN:HG2	2.06	0.55
1:2:332:G:H5'	17:G:193:ALA:HB2	1.89	0.55
1:2:1636:G:H1'	2:F:164:ARG:NH2	2.22	0.55
30:x:151:ALA:HA	31:y:361:VAL:HG21	1.89	0.55
1:2:375:U:H2'	1:2:376:A:C8	2.41	0.55
1:2:533:A:H61	1:2:550:C:H42	1.55	0.55
31:y:13:ALA:HB2	31:y:235:LEU:HB3	1.88	0.55
5:Q:100:VAL:HG12	5:Q:101:ASP:N	2.22	0.55
1:2:448:A:H4'	1:2:449:A:H5'	1.88	0.55
1:2:1319:U:H2'	1:2:1320:G:O4'	2.06	0.55
1:2:1781:A:H2'	1:2:1782:G:C8	2.41	0.55
31:y:30:ILE:HG22	31:y:32:GLU:H	1.72	0.55
32:u:223:LEU:HD11	32:u:232:LEU:HD22	1.89	0.55
1:2:14:C:H2'	1:2:15:U:C6	2.41	0.54
1:2:501:C:O2	1:2:501:C:H2'	2.08	0.54
1:2:1277:C:H2'	1:2:1278:A:C8	2.42	0.54
5:Q:100:VAL:HG12	5:Q:101:ASP:H	1.72	0.54
30:x:224:ALA:HB2	30:x:241:ILE:HD13	1.89	0.54
1:2:93:U:H1'	16:E:7:LYS:HE2	1.89	0.54
1:2:1144:A:C2'	1:2:1145:A:H8	2.15	0.54
1:2:1196:A:O5'	1:2:1196:A:C8	2.60	0.54
15:C:94:ILE:HG13	15:C:159:LYS:O	2.08	0.54
13:A:56:GLU:HG2	24:V:79:VAL:HG13	1.89	0.54
30:x:99:ILE:HD11	30:x:136:PHE:CD2	2.42	0.54
1:2:1322:G:N2	1:2:1324:G:O4'	2.40	0.54
1:2:1408:U:H2'	1:2:1409:A:C8	2.42	0.54
28:b:49:HIS:CD2	28:b:70:LYS:HG2	2.42	0.54
1:2:1222:G:H5''	2:F:78:MET:HE3	1.89	0.54
15:C:202:THR:HG23	20:J:54:ARG:HH22	1.71	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:4:MET:HE3	22:N:121:ARG:HG2	1.89	0.54
1:2:103:A:OP2	1:2:356:C:N4	2.41	0.54
1:2:913:A:H2	18:H:99:ARG:N	2.04	0.54
4:P:34:MET:HE3	4:P:46:ASN:HA	1.89	0.54
28:b:64:CYS:HB3	28:b:73:LEU:HD23	1.89	0.54
1:2:575:A:H2'	1:2:576:A:O4'	2.08	0.54
1:2:1788:A:H2'	1:2:1789:G:O4'	2.08	0.54
32:u:484:PHE:HB3	32:u:487:GLU:HG3	1.88	0.54
15:C:131:GLY:HA3	15:C:216:MET:HB3	1.90	0.54
1:2:1865:C:O4'	1:2:1865:C:O2	2.24	0.54
4:P:33:LEU:C	4:P:35:GLN:H	2.16	0.54
26:X:71:ARG:NH2	35:t:470:VAL:H	2.05	0.54
33:w:394:ALA:H	33:w:397:GLN:HE21	1.54	0.54
1:2:1099:G:O2'	1:2:1100:A:H8	1.91	0.53
1:2:1502:C:H2'	1:2:1503:C:H6	1.72	0.53
1:2:1872:G:H22	31:y:122:PRO:HD2	1.73	0.53
32:u:614:LEU:HD13	32:u:667:LEU:HD23	1.91	0.53
1:2:501:C:O2	1:2:501:C:C2'	2.56	0.53
1:2:595:U:H2'	1:2:596:U:H6	1.72	0.53
1:2:15:U:H2'	1:2:16:G:O4'	2.08	0.53
1:2:45:A:N6	1:2:481:C:H4'	2.23	0.53
1:2:370:G:H4'	1:2:371:A:OP1	2.09	0.53
7:S:80:PRO:HB2	7:S:82:TRP:CZ3	2.44	0.53
2:F:154:LEU:HD22	2:F:177:LEU:HD12	1.91	0.53
12:g:107:ASP:HB2	12:g:125:ARG:HD2	1.90	0.53
27:Y:57:VAL:HB	27:Y:60:PHE:HE2	1.73	0.53
1:2:349:A:H2'	1:2:350:C:C6	2.44	0.53
15:C:209:VAL:HB	15:C:210:PRO:CD	2.38	0.53
1:2:57:U:H1'	1:2:499:G:O2'	2.08	0.53
13:A:120:ARG:HH21	15:C:267:GLN:HA	1.72	0.53
1:2:528:A:H2'	1:2:529:A:C8	2.44	0.53
33:w:309:GLY:HA2	33:w:312:ILE:HD12	1.91	0.53
1:2:1203:G:H22	1:2:1694:U:H2'	1.72	0.53
1:2:1502:C:H5'	11:f:77:ALA:HB3	1.91	0.53
1:2:1608:U:H2'	1:2:1609:C:O4'	2.09	0.53
1:2:1860:A:H2'	30:x:178:ARG:NH1	2.24	0.53
6:R:74:GLN:O	6:R:78:ARG:HB2	2.09	0.53
6:R:85:VAL:HG22	13:A:198:MET:HE2	1.89	0.53
1:2:44:U:O2'	1:2:45:A:H2'	2.08	0.53
3:M:33:ARG:H	3:M:33:ARG:HD3	1.74	0.53
8:T:11:GLN:HB3	8:T:62:ARG:HH22	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:853:C:O4'	1:2:853:C:O2	2.28	0.52
1:2:1485:U:H2'	1:2:1486:A:H8	1.74	0.52
1:2:1536:G:H2'	1:2:1537:A:C8	2.45	0.52
12:g:172:LYS:HE2	12:g:193:GLY:H	1.75	0.52
32:u:81:PRO:HB2	32:u:82:PRO:CD	2.39	0.52
33:w:184:VAL:HG21	35:t:298:LEU:HG	1.90	0.52
1:2:1045:U:H2'	1:2:1046:U:C6	2.45	0.52
16:E:42:LEU:HD13	16:E:47:PHE:HB2	1.92	0.52
1:2:1204:A:N3	1:2:1204:A:H2'	2.25	0.52
2:F:81:ARG:HG3	2:F:81:ARG:HH11	1.75	0.52
3:M:93:LYS:H	3:M:102:LYS:HB3	1.73	0.52
25:W:42:MET:HE2	25:W:49:GLU:HA	1.90	0.52
1:2:1137:U:H5''	31:y:328:THR:HG23	1.92	0.52
8:T:62:ARG:HG3	8:T:62:ARG:HH11	1.74	0.52
2:F:76:MET:HB3	2:F:89:THR:CG2	2.39	0.52
35:t:363:HIS:HB3	35:t:364:PRO:HD2	1.92	0.52
1:2:980:A:H2'	1:2:981:A:H8	1.72	0.52
35:t:360:LEU:N	35:t:360:LEU:CD2	2.73	0.52
1:2:4:C:H4'	15:C:207:ALA:HB2	1.90	0.52
1:2:1228:A:H2'	1:2:1229:G:H8	1.74	0.52
1:2:1305:C:C2	1:2:1306:U:H5	2.28	0.52
9:Z:79:ILE:HG23	9:Z:83:LEU:HD23	1.91	0.52
1:2:171:A:H5''	17:G:177:GLN:HG2	1.92	0.52
20:J:121:LYS:H	20:J:125:HIS:HD2	1.58	0.52
32:u:525:ALA:CB	35:t:362:ASN:HD21	2.05	0.52
1:2:639:C:H2'	1:2:640:A:H8	1.75	0.51
3:M:96:ARG:HB3	33:w:388:ARG:NH1	2.25	0.51
12:g:23:THR:HG22	12:g:31:ILE:HG12	1.91	0.51
1:2:212:C:H2'	1:2:213:G:C8	2.45	0.51
1:2:291:G:H2'	1:2:292:A:C8	2.46	0.51
1:2:1195:A:H2'	1:2:1196:A:C8	2.45	0.51
23:O:50:LYS:HB3	23:O:51:GLU:OE1	2.09	0.51
1:2:928:G:H2'	1:2:929:G:C8	2.45	0.51
1:2:1025:U:H2'	1:2:1026:C:O4'	2.10	0.51
1:2:1779:G:H2'	1:2:1780:G:H8	1.75	0.51
1:2:126:G:OP1	17:G:198:ARG:NH1	2.44	0.51
1:2:1860:A:H2'	30:x:178:ARG:HH11	1.75	0.51
2:F:38:TYR:HD2	2:F:143:PRO:HB2	1.76	0.51
23:O:97:LEU:HD11	23:O:112:ALA:HB1	1.92	0.51
1:2:1102:G:H2'	1:2:1103:C:C6	2.45	0.51
1:2:1353:A:N6	1:2:1354:G:C6	2.79	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1797:U:H2'	1:2:1798:C:H6	1.73	0.51
19:I:193:LYS:O	19:I:196:GLU:HG2	2.11	0.51
1:2:483:C:H2'	1:2:484:A:C8	2.46	0.51
1:2:1587:G:H22	8:T:63:HIS:HD2	1.57	0.51
1:2:1291:A:O2'	11:f:140:TYR:OH	2.29	0.51
8:T:60:THR:HG23	8:T:75:MET:SD	2.51	0.51
16:E:19:MET:SD	16:E:108:ARG:HD2	2.51	0.51
1:2:946:U:H2'	1:2:947:G:O4'	2.11	0.50
1:2:1322:G:H21	1:2:1323:U:H2'	1.76	0.50
1:2:1365:G:H2'	1:2:1366:G:C8	2.45	0.50
1:2:1017:U:H2'	1:2:1018:U:C6	2.46	0.50
10:c:13:ARG:HD3	10:c:35:MET:HE3	1.94	0.50
33:w:365:LEU:HD21	33:w:400:ALA:HB1	1.93	0.50
1:2:685:A:N6	1:2:917:U:N3	2.58	0.50
1:2:808:A:H5''	16:E:219:ALA:O	2.11	0.50
13:A:132:GLN:N	13:A:133:PRO:HD2	2.26	0.50
31:y:118:HIS:HD2	31:y:120:GLU:H	1.58	0.50
32:u:604:ASN:HD22	32:u:679:ILE:HG22	1.74	0.50
16:E:87:MET:HE1	16:E:236:ILE:HG21	1.92	0.50
10:c:43:ILE:HD13	31:y:368:ALA:HB2	1.93	0.50
30:x:169:LYS:HD2	30:x:230:LEU:HA	1.94	0.50
1:2:1390:U:H2'	1:2:1391:C:O4'	2.12	0.50
1:2:1659:U:N3	1:2:1664:A:N6	2.60	0.50
2:F:128:ILE:HD12	2:F:137:GLN:HB3	1.93	0.50
21:L:66:VAL:HG11	21:L:134:LEU:HD21	1.94	0.50
1:2:1397:U:H3	5:Q:12:VAL:HA	1.76	0.50
1:2:1600:G:N3	1:2:1600:G:C2'	2.75	0.50
7:S:26:ILE:HD13	7:S:45:LEU:HD21	1.92	0.50
15:C:68:ARG:HD3	15:C:276:THR:HG21	1.93	0.50
15:C:88:ILE:HD13	15:C:94:ILE:HD11	1.93	0.50
21:L:66:VAL:HB	21:L:131:CYS:SG	2.51	0.50
1:2:957:A:H3'	1:2:958:G:H21	1.77	0.50
1:2:1143:A:H5'	15:C:190:SER:HB3	1.93	0.50
30:x:97:THR:HB	30:x:98:PRO:HD3	1.93	0.50
1:2:1474:A:H2'	1:2:1475:G:C8	2.47	0.50
1:2:1733:U:H2'	1:2:1734:G:O4'	2.12	0.50
10:c:13:ARG:HB2	10:c:33:GLU:HB3	1.92	0.50
18:H:83:LEU:HD23	18:H:92:VAL:HG11	1.92	0.50
1:2:446:G:OP2	19:I:47:ARG:NH2	2.44	0.49
1:2:640:A:H2'	1:2:641:A:C8	2.47	0.49
1:2:798:G:H4'	18:H:108:SER:HB2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1606:G:H5'	8:T:86:GLY:HA2	1.93	0.49
22:N:54:LEU:HB3	22:N:60:VAL:HB	1.94	0.49
1:2:830:A:N1	1:2:844:U:C4	2.80	0.49
1:2:1298:G:H2'	1:2:1298:G:N3	2.28	0.49
1:2:1308:U:H1'	1:2:1309:C:C5	2.48	0.49
1:2:1818:A:H2'	1:2:1819:A:O4'	2.11	0.49
1:2:1395:C:H2'	1:2:1396:A:N3	2.27	0.49
1:2:1478:U:H2'	1:2:1479:G:C8	2.48	0.49
31:y:395:GLY:HA2	31:y:398:ARG:HE	1.77	0.49
1:2:26:U:H2'	1:2:27:A:O4'	2.12	0.49
1:2:145:G:H2'	1:2:146:G:H8	1.71	0.49
1:2:1045:U:H2'	1:2:1046:U:H6	1.78	0.49
1:2:1535:U:H5'	2:F:169:ILE:HD11	1.94	0.49
2:F:92:ILE:HG12	2:F:169:ILE:HD13	1.95	0.49
1:2:508:A:H3'	1:2:509:G:H8	1.78	0.49
8:T:42:HIS:HB3	8:T:93:SER:HB2	1.94	0.49
27:Y:55:ILE:HG22	27:Y:75:ILE:HG23	1.94	0.49
34:v:167:ALA:HB1	34:v:296:LEU:HD22	1.94	0.49
10:c:12:ALA:HB3	10:c:56:LEU:HB2	1.94	0.49
16:E:124:CYS:HA	16:E:142:HIS:HE1	1.78	0.49
1:2:443:U:H2'	1:2:444:G:O4'	2.12	0.49
17:G:98:ARG:HH22	17:G:103:ASP:HB2	1.78	0.49
20:J:111:GLN:HE21	20:J:123:ILE:HG13	1.78	0.49
1:2:349:A:H2'	1:2:350:C:H6	1.76	0.48
1:2:1653:U:H2'	1:2:1654:G:C8	2.48	0.48
32:u:138:ALA:HB2	32:u:149:MET:HE2	1.94	0.48
32:u:259:ASP:HB2	32:u:273:LYS:HB2	1.94	0.48
1:2:58:C:H5''	1:2:499:G:N2	2.28	0.48
1:2:591:U:O2'	1:2:592:C:H3'	2.13	0.48
1:2:1464:C:O2'	1:2:1465:A:H8	1.93	0.48
22:N:5:HIS:CE1	22:N:121:ARG:HG3	2.48	0.48
30:x:225:ILE:O	30:x:229:ILE:HG12	2.13	0.48
1:2:1845:A:H2'	1:2:1846:G:C8	2.48	0.48
13:A:140:VAL:O	13:A:140:VAL:CG1	2.61	0.48
1:2:1691:U:H2'	1:2:1692:U:O4'	2.13	0.48
8:T:134:ILE:O	8:T:138:VAL:HG23	2.13	0.48
23:O:43:HIS:CD2	23:O:55:ARG:HB2	2.39	0.48
30:x:106:GLN:HG2	31:y:210:THR:HG22	1.93	0.48
1:2:1324:G:N2	1:2:1504:U:H2'	2.28	0.48
13:A:44:ASP:HB3	31:y:271:HIS:CD2	2.48	0.48
35:t:360:LEU:N	35:t:360:LEU:HD22	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:212:C:H2'	1:2:213:G:H8	1.77	0.48
1:2:399:C:H3'	1:2:400:C:H5'	1.95	0.48
1:2:1073:U:H2'	1:2:1074:C:C6	2.48	0.48
1:2:213:G:H2'	1:2:214:U:O4'	2.14	0.48
30:x:168:VAL:HG21	30:x:229:ILE:HG13	1.96	0.48
1:2:49:C:H41	1:2:472:C:H2'	1.78	0.48
1:2:1377:U:H3'	13:A:102:ARG:HH21	1.78	0.48
32:u:617:HIS:HB2	32:u:666:LEU:HB2	1.96	0.48
1:2:942:G:H2'	1:2:943:U:C6	2.49	0.48
1:2:1454:A:C8	6:R:3:ARG:HD2	2.49	0.48
29:e:8:ARG:HG2	32:u:633:THR:HG22	1.95	0.48
1:2:673:G:H2'	1:2:674:C:C6	2.49	0.48
1:2:1143:A:H2'	1:2:1144:A:O4'	2.14	0.48
1:2:1385:G:OP1	1:2:1484:A:H5'	2.14	0.48
30:x:120:THR:HG23	30:x:130:LEU:HD12	1.96	0.48
35:t:362:ASN:ND2	35:t:362:ASN:C	2.72	0.48
1:2:70:G:O5'	1:2:70:G:H8	1.97	0.47
1:2:985:G:H1'	23:O:138:ASP:CG	2.38	0.47
1:2:1324:G:H22	1:2:1504:U:H2'	1.79	0.47
16:E:44:LEU:HD13	16:E:72:ILE:HD11	1.95	0.47
23:O:98:ARG:HH21	23:O:134:PRO:HG3	1.78	0.47
33:w:288:LYS:HE2	35:t:266:PHE:HA	1.95	0.47
1:2:219:U:H4'	19:I:182:CYS:SG	2.54	0.47
1:2:940:U:H3	1:2:1002:U:H3	1.60	0.47
1:2:1430:C:HO2'	1:2:1431:G:H8	1.61	0.47
2:F:35:LEU:HD21	2:F:146:ARG:HD3	1.96	0.47
10:c:12:ALA:HB2	10:c:58:LEU:HD11	1.95	0.47
1:2:941:C:H2'	1:2:942:G:C8	2.49	0.47
1:2:1536:G:H2'	1:2:1537:A:H8	1.79	0.47
4:P:83:MET:HB3	4:P:116:LEU:HD12	1.96	0.47
22:N:136:PRO:HG2	22:N:139:TRP:HB2	1.95	0.47
30:x:200:THR:HG22	30:x:213:GLY:HA3	1.96	0.47
1:2:434:G:H2'	1:2:435:A:C8	2.49	0.47
1:2:872:A:N6	1:2:914:U:C2	2.65	0.47
4:P:49:LEU:O	35:t:309:CYS:HA	2.14	0.47
5:Q:116:ASP:HB3	5:Q:119:LEU:HD12	1.96	0.47
1:2:29:G:H2'	1:2:30:C:H6	1.79	0.47
1:2:106:C:H5''	1:2:431:G:O2'	2.15	0.47
1:2:337:C:H3'	1:2:338:G:H5''	1.96	0.47
1:2:798:G:O2'	18:H:106:ARG:HA	2.14	0.47
1:2:1139:C:O4'	1:2:1139:C:O2	2.32	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1220:A:H2'	1:2:1221:G:O4'	2.15	0.47
1:2:1707:U:H2'	1:2:1708:C:C6	2.50	0.47
27:Y:43:LYS:O	27:Y:46:LYS:HG2	2.15	0.47
1:2:996:A:H2'	1:2:997:A:H8	1.77	0.47
1:2:1532:C:H4'	1:2:1604:G:H21	1.79	0.47
1:2:1624:U:O2	1:2:1624:U:O4'	2.30	0.47
1:2:427:U:O4'	1:2:427:U:O2	2.32	0.47
1:2:872:A:N3	1:2:872:A:H2'	2.28	0.47
1:2:925:G:H2'	1:2:926:A:H5''	1.97	0.47
1:2:1016:U:OP2	28:b:20:LYS:NZ	2.48	0.47
1:2:1614:A:P	4:P:42:ARG:HH22	2.38	0.47
1:2:1630:A:H5''	7:S:37:GLY:N	2.26	0.47
12:g:174:VAL:HB	12:g:188:HIS:HB2	1.97	0.47
26:X:100:VAL:HG13	26:X:122:VAL:HG13	1.95	0.47
32:u:125:LEU:HD11	32:u:311:LEU:HA	1.96	0.47
1:2:352:U:H2'	1:2:353:C:C6	2.50	0.47
1:2:374:G:H2'	1:2:375:U:C6	2.50	0.47
1:2:415:A:H2'	1:2:416:U:O4'	2.15	0.47
1:2:886:A:N3	1:2:886:A:H2'	2.30	0.47
1:2:1181:A:H2'	1:2:1182:A:C8	2.50	0.47
30:x:150:LEU:HD23	30:x:153:ILE:HD12	1.97	0.47
1:2:25:A:N6	1:2:26:U:O4	2.48	0.47
1:2:560:A:H5'	20:J:174:LYS:HE3	1.96	0.47
1:2:587:A:H5'	1:2:592:C:H41	1.79	0.47
1:2:1144:A:H2'	1:2:1145:A:N7	2.22	0.47
1:2:1542:C:H5''	8:T:62:ARG:HH22	1.71	0.47
18:H:20:GLU:HG2	18:H:48:ALA:HB3	1.97	0.47
19:I:48:VAL:HG11	19:I:54:LYS:HD2	1.96	0.47
1:2:433:A:N6	1:2:434:G:O6	2.48	0.46
1:2:433:A:H5''	19:I:25:ARG:HH22	1.80	0.46
1:2:1662:U:H2'	1:2:1663:A:O4'	2.15	0.46
1:2:1781:A:H2'	1:2:1782:G:H8	1.80	0.46
2:F:34:SER:HA	10:c:55:VAL:HG13	1.97	0.46
32:u:258:VAL:HG21	32:u:579:LEU:HD12	1.97	0.46
13:A:103:PHE:HE2	13:A:136:GLU:HG3	1.80	0.46
18:H:121:THR:HG23	18:H:122:LEU:N	2.30	0.46
18:H:145:ARG:HD3	25:W:51:GLU:HG3	1.97	0.46
21:L:68:ILE:HG13	21:L:143:LEU:HD21	1.97	0.46
23:O:116:LEU:HD11	23:O:129:ILE:HD12	1.97	0.46
34:v:61:LEU:HD23	34:v:79:GLY:HA2	1.97	0.46
1:2:556:U:H2'	1:2:557:U:O4'	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1590:C:H5'	1:2:1591:C:OP2	2.16	0.46
6:R:17:ILE:HG13	6:R:57:LEU:HD23	1.96	0.46
33:w:185:TYR:HA	33:w:188:VAL:HG12	1.98	0.46
1:2:1038:U:O2'	1:2:1180:C:N3	2.49	0.46
1:2:1447:G:H2'	1:2:1448:A:C8	2.51	0.46
1:2:1612:G:H1'	7:S:87:GLN:HG3	1.96	0.46
6:R:23:ARG:HB3	6:R:34:VAL:HG21	1.96	0.46
17:G:64:LYS:HB2	17:G:97:VAL:HG11	1.97	0.46
24:V:71:ARG:HH22	25:W:23:ARG:HH21	1.63	0.46
1:2:303:C:H5''	19:I:75:LYS:HD3	1.98	0.46
1:2:823:U:H5	20:J:143:ASN:HB3	1.79	0.46
1:2:918:U:O2'	1:2:919:A:O4'	2.34	0.46
1:2:1614:A:OP2	4:P:42:ARG:NH2	2.48	0.46
16:E:44:LEU:HD11	16:E:70:ILE:HG21	1.97	0.46
19:I:42:ARG:HH12	19:I:59:ARG:HE	1.64	0.46
32:u:675:MET:HE3	32:u:790:LEU:H	1.80	0.46
1:2:223:C:H2'	1:2:224:A:C8	2.50	0.46
1:2:680:G:H2'	1:2:681:U:C6	2.50	0.46
4:P:41:GLN:H	4:P:41:GLN:HG2	1.50	0.46
31:y:243:ASN:O	31:y:247:GLN:HG2	2.15	0.46
1:2:674:C:H2'	1:2:675:U:C6	2.50	0.46
1:2:1064:C:H2'	1:2:1065:G:H8	1.80	0.46
1:2:1632:G:OP2	7:S:34:LYS:HG3	2.16	0.46
1:2:1806:A:H2'	1:2:1807:C:C6	2.51	0.46
4:P:25:LEU:HA	4:P:28:MET:HE3	1.97	0.46
18:H:69:LEU:O	18:H:73:GLN:HG2	2.16	0.46
30:x:111:LEU:HD11	31:y:128:PHE:HB3	1.97	0.46
1:2:171:A:H5'	17:G:177:GLN:HG2	1.97	0.46
11:f:85:TYR:CD1	32:u:492:ARG:HD2	2.51	0.46
28:b:33:MET:HE3	28:b:48:SER:HA	1.97	0.46
1:2:115:U:H2'	1:2:116:U:C6	2.51	0.46
1:2:340:C:H2'	1:2:341:C:O4'	2.16	0.46
1:2:594:A:H1'	1:2:595:U:C6	2.51	0.46
1:2:1447:G:H2'	1:2:1448:A:H8	1.81	0.46
2:F:76:MET:CE	2:F:173:LEU:HD13	2.46	0.46
20:J:124:HIS:NE2	29:e:35:ARG:HG3	2.31	0.46
1:2:27:A:H2'	1:2:28:U:O4'	2.16	0.46
1:2:199:C:H3'	1:2:200:G:H8	1.81	0.46
1:2:1073:U:H2'	1:2:1074:C:H6	1.81	0.46
13:A:140:VAL:O	13:A:140:VAL:HG12	2.16	0.46
1:2:5:U:H2'	1:2:6:G:H8	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:155:G:H21	17:G:56:ASN:HD21	1.65	0.45
1:2:375:U:H2'	1:2:376:A:H8	1.79	0.45
1:2:941:C:H2'	1:2:942:G:H8	1.82	0.45
19:I:142:SER:HB2	19:I:145:ILE:HD12	1.97	0.45
1:2:215:G:H2'	1:2:216:C:C6	2.52	0.45
1:2:376:A:H2'	1:2:377:G:O4'	2.16	0.45
13:A:68:ILE:HG23	13:A:120:ARG:NH1	2.31	0.45
26:X:51:VAL:HG13	26:X:70:VAL:HG13	1.99	0.45
32:u:89:PRO:HA	32:u:159:LEU:HB2	1.99	0.45
1:2:498:C:H2'	1:2:499:G:O4'	2.17	0.45
1:2:616:A:H2'	1:2:617:G:O4'	2.15	0.45
1:2:1284:A:O4'	1:2:1312:G:N2	2.50	0.45
1:2:1793:A:C2	1:2:1794:C:C5	3.05	0.45
3:M:121:LYS:O	3:M:125:GLU:HB2	2.17	0.45
1:2:524:U:H5''	1:2:525:A:O4'	2.16	0.45
1:2:1088:U:H4'	1:2:1089:G:OP2	2.17	0.45
5:Q:32:ILE:HG12	5:Q:68:ILE:HD12	1.99	0.45
18:H:170:VAL:HG13	18:H:187:PHE:HB2	1.99	0.45
32:u:262:PRO:HA	32:u:270:GLY:HA3	1.98	0.45
28:b:49:HIS:HD2	28:b:70:LYS:HA	1.82	0.45
29:e:14:GLY:HA3	32:u:648:MET:HG3	1.98	0.45
33:w:308:VAL:HA	33:w:311:ILE:HD12	1.98	0.45
1:2:307:G:C2	19:I:44:HIS:HB3	2.51	0.45
1:2:520:A:O2'	1:2:825:A:N3	2.47	0.45
1:2:926:A:H5''	1:2:926:A:H8	1.82	0.45
1:2:1060:A:O2'	1:2:1062:A:N6	2.40	0.45
1:2:1598:G:H3'	9:Z:80:ARG:HG2	1.98	0.45
2:F:155:CYS:O	2:F:159:ARG:HD2	2.16	0.45
17:G:216:ARG:HA	17:G:219:GLU:HG2	1.97	0.45
20:J:32:ILE:HA	20:J:37:LEU:HD12	1.99	0.45
1:2:146:G:H2'	1:2:147:A:O4'	2.17	0.45
1:2:548:C:H2'	1:2:549:C:H6	1.82	0.45
1:2:1203:G:H21	1:2:1204:A:H62	1.65	0.45
13:A:42:LYS:HE3	13:A:46:ILE:HB	1.99	0.45
31:y:210:THR:H	31:y:213:ASN:HB2	1.82	0.45
32:u:591:MET:HA	32:u:657:PRO:HA	1.97	0.45
13:A:122:LEU:HB3	13:A:144:THR:HG23	1.99	0.45
16:E:126:VAL:HG11	16:E:139:LEU:HD22	1.98	0.45
17:G:88:ARG:HB2	17:G:91:GLU:HG2	1.99	0.45
31:y:69:PHE:HZ	31:y:248:MET:HG3	1.81	0.45
31:y:267:ILE:HD11	31:y:308:MET:HE3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:845:G:H3'	1:2:846:G:H8	1.82	0.45
1:2:1786:U:H2'	1:2:1787:G:C8	2.52	0.45
2:F:89:THR:HA	2:F:92:ILE:HD12	1.99	0.45
12:g:78:ALA:HB3	12:g:90:TRP:HB2	1.98	0.45
1:2:1485:U:H2'	1:2:1486:A:C8	2.51	0.45
1:2:1637:A:H4'	1:2:1638:G:O5'	2.17	0.45
1:2:1672:U:H2'	1:2:1673:U:C6	2.52	0.45
2:F:19:LEU:HB3	2:F:23:TRP:HB2	1.99	0.45
3:M:64:LEU:HA	11:f:108:VAL:HG21	1.99	0.45
33:w:327:LEU:HD12	33:w:356:VAL:HG22	1.99	0.45
1:2:527:C:O3'	20:J:121:LYS:HD2	2.18	0.44
1:2:1636:G:H1'	2:F:164:ARG:HH22	1.82	0.44
16:E:11:ARG:HA	16:E:28:ALA:HB2	1.99	0.44
25:W:75:ILE:HD13	25:W:125:ILE:HG12	1.99	0.44
1:2:673:G:H2'	1:2:674:C:H6	1.81	0.44
2:F:179:ASN:HB3	2:F:187:SER:HB2	1.99	0.44
3:M:47:ALA:HA	3:M:112:LYS:HA	2.00	0.44
14:B:47:THR:HG23	23:O:46:ASP:OD2	2.17	0.44
22:N:91:LEU:HD12	22:N:125:LEU:HD12	1.99	0.44
30:x:92:TRP:HE1	31:y:127:GLY:HA3	1.82	0.44
30:x:137:VAL:O	30:x:141:ILE:HG12	2.16	0.44
32:u:144:HIS:HA	32:u:622:ARG:NH2	2.32	0.44
32:u:530:PHE:CE2	32:u:658:ILE:HD13	2.52	0.44
1:2:511:U:H2'	1:2:512:A:O4'	2.17	0.44
1:2:909:G:H2'	1:2:910:G:H8	1.83	0.44
1:2:1482:C:H2'	1:2:1482:C:O2	2.16	0.44
2:F:142:SER:HB2	2:F:145:ARG:HB3	1.98	0.44
9:Z:69:THR:HG23	9:Z:106:GLN:HE22	1.81	0.44
1:2:343:A:H2'	1:2:343:A:N3	2.31	0.44
1:2:528:A:H2'	1:2:529:A:H8	1.81	0.44
1:2:1177:U:H2'	1:2:1178:U:C6	2.53	0.44
1:2:1639:G:H2'	1:2:1640:A:H8	1.82	0.44
15:C:102:LEU:HD22	15:C:130:ILE:HG12	1.99	0.44
1:2:122:G:H1	1:2:342:C:H42	1.66	0.44
4:P:119:PHE:HE1	7:S:117:ILE:HG23	1.83	0.44
22:N:115:LEU:O	22:N:119:GLU:HG2	2.17	0.44
1:2:388:U:H2'	1:2:389:A:C8	2.52	0.44
1:2:442:C:H2'	1:2:443:U:C6	2.52	0.44
1:2:907:G:H2'	1:2:908:A:C8	2.52	0.44
1:2:983:A:H2'	1:2:984:C:C6	2.52	0.44
1:2:1356:G:H2'	1:2:1357:A:H8	1.72	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1685:U:C4	1:2:1686:G:N7	2.86	0.44
4:P:22:LEU:HD11	4:P:109:PRO:HB3	1.98	0.44
12:g:303:THR:C	12:g:305:ASN:H	2.25	0.44
31:y:253:LEU:HB3	31:y:259:LEU:HA	1.98	0.44
33:w:354:TYR:HB3	35:t:252:ARG:HB3	2.00	0.44
1:2:659:G:HO2'	1:2:662:G:HO2'	1.63	0.44
1:2:659:G:H2'	1:2:663:C:C5	2.53	0.44
7:S:99:LEU:HB3	7:S:100:ALA:H	1.61	0.44
14:B:168:MET:O	14:B:172:MET:HG2	2.18	0.44
20:J:21:GLU:HG3	20:J:24:ARG:HB2	2.00	0.44
25:W:66:THR:C	25:W:68:ARG:H	2.26	0.44
26:X:72:VAL:HG21	26:X:102:VAL:HG21	1.99	0.44
32:u:159:LEU:HD22	32:u:190:GLN:HE21	1.81	0.44
1:2:803:C:H2'	1:2:804:U:C6	2.53	0.44
13:A:158:ASP:OD1	24:V:32:ILE:HG21	2.18	0.44
16:E:11:ARG:HH21	16:E:21:ASP:H	1.65	0.44
31:y:80:SER:H	31:y:83:ASP:HB2	1.82	0.44
31:y:321:GLY:HA3	31:y:400:ASN:HB2	2.00	0.44
34:v:219:LEU:HD22	34:v:250:MET:HE1	1.99	0.44
1:2:152:U:H2'	1:2:153:G:O4'	2.18	0.44
1:2:493:A:N6	1:2:509:G:N2	2.66	0.44
1:2:685:A:N6	1:2:917:U:H3	2.16	0.44
15:C:90:GLU:HB2	15:C:93:ILE:HD12	1.99	0.44
31:y:321:GLY:HA3	31:y:400:ASN:CB	2.48	0.44
32:u:147:LEU:HD22	32:u:180:GLN:HG2	2.00	0.44
34:v:290:ILE:HA	34:v:291:ARG:HA	1.72	0.44
1:2:1012:A:H2'	1:2:1013:U:O4'	2.17	0.43
1:2:1275:G:H22	1:2:1324:G:H1'	1.82	0.43
2:F:35:LEU:HD22	2:F:147:VAL:HG23	2.00	0.43
8:T:4:VAL:HG21	8:T:136:GLY:HA2	2.00	0.43
21:L:99:TYR:O	21:L:101:ARG:HD2	2.18	0.43
1:2:96:C:H2'	1:2:97:U:O4'	2.18	0.43
1:2:1017:U:H2'	1:2:1018:U:H6	1.83	0.43
32:u:598:VAL:HG22	32:u:680:ALA:HB1	1.99	0.43
1:2:590:A:N3	1:2:590:A:H2'	2.33	0.43
1:2:1365:G:H2'	1:2:1366:G:H8	1.83	0.43
7:S:79:ILE:HA	7:S:80:PRO:HD3	1.89	0.43
22:N:94:LYS:O	22:N:98:VAL:HG23	2.18	0.43
1:2:548:C:H2'	1:2:549:C:C6	2.54	0.43
1:2:823:U:O2	1:2:823:U:O4'	2.36	0.43
6:R:17:ILE:HD13	6:R:24:LEU:HD13	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:g:291:TRP:HE1	12:g:295:GLY:HA2	1.84	0.43
15:C:108:LYS:HE3	15:C:110:MET:HB3	2.01	0.43
32:u:708:THR:HA	32:u:758:LYS:HG3	2.01	0.43
33:w:181:VAL:HG13	35:t:298:LEU:HD11	2.01	0.43
1:2:5:U:H2'	1:2:6:G:C8	2.53	0.43
1:2:53:C:O2'	1:2:507:G:N7	2.43	0.43
1:2:977:C:H2'	1:2:978:G:O4'	2.18	0.43
1:2:1562:C:H5''	8:T:71:GLY:HA3	2.00	0.43
2:F:79:HIS:H	2:F:159:ARG:HH22	1.66	0.43
2:F:103:LEU:HD22	2:F:178:ILE:HD13	2.01	0.43
2:F:150:ALA:HA	2:F:153:LEU:HD12	2.00	0.43
13:A:63:ARG:NH1	24:V:78:ILE:HG23	2.33	0.43
17:G:215:LYS:O	17:G:218:LYS:HG2	2.19	0.43
1:2:25:A:C6	1:2:26:U:C4	3.06	0.43
1:2:843:C:H2'	1:2:844:U:O4'	2.18	0.43
1:2:959:G:H5''	23:O:38:ASN:HD21	1.83	0.43
15:C:130:ILE:HG23	15:C:162:ILE:HD11	2.00	0.43
1:2:909:G:H2'	1:2:910:G:C8	2.52	0.43
1:2:1734:G:O2'	1:2:1800:A:N6	2.52	0.43
1:2:1872:G:H21	31:y:121:THR:HG22	1.83	0.43
16:E:46:ILE:HG23	16:E:50:ASN:HD22	1.83	0.43
17:G:57:ASP:HA	17:G:106:LEU:HA	1.99	0.43
3:M:52:LEU:HD23	3:M:78:LYS:HE3	2.00	0.43
3:M:61:TYR:OH	3:M:108:CYS:HB2	2.19	0.43
16:E:35:PRO:HG2	16:E:36:HIS:CD2	2.54	0.43
34:v:122:LEU:HD11	34:v:185:ALA:HB1	2.01	0.43
1:2:1387:G:C2	1:2:1388:A:H1'	2.54	0.43
23:O:33:ILE:HB	23:O:97:LEU:HD12	2.00	0.43
31:y:18:ALA:HB2	31:y:255:VAL:HG23	2.01	0.43
1:2:126:G:C6	17:G:196:LYS:HG2	2.53	0.43
1:2:1621:U:O2'	4:P:118:GLU:HB3	2.19	0.43
1:2:1840:U:H2'	1:2:1841:C:O4'	2.19	0.43
12:g:17:TRP:CE2	12:g:303:THR:HG23	2.54	0.43
24:V:51:LYS:HD2	24:V:78:ILE:HD11	2.01	0.43
32:u:525:ALA:HB2	35:t:362:ASN:HD22	1.65	0.43
1:2:110:U:O2	1:2:110:U:H2'	2.19	0.42
1:2:823:U:C5	20:J:143:ASN:HB3	2.53	0.42
1:2:1386:A:C2	1:2:1387:G:H1'	2.54	0.42
12:g:130:LYS:HD3	12:g:141:THR:HG23	2.01	0.42
1:2:65:C:H4'	17:G:172:LYS:HD3	2.02	0.42
1:2:417:C:H2'	1:2:418:A:H5''	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:480:G:H2'	1:2:481:C:O4'	2.19	0.42
1:2:1208:A:H2'	1:2:1209:A:C8	2.54	0.42
1:2:1532:C:H4'	1:2:1604:G:N2	2.34	0.42
4:P:125:PRO:HD3	32:u:404:TRP:NE1	2.33	0.42
13:A:71:PRO:HB3	13:A:186:ARG:HH22	1.84	0.42
26:X:52:LEU:HD11	26:X:73:GLN:HB2	2.01	0.42
31:y:28:TYR:HE1	31:y:54:ARG:HD3	1.84	0.42
32:u:678:LEU:HD11	32:u:681:THR:HG22	2.01	0.42
1:2:176:U:H2'	1:2:177:G:O4'	2.18	0.42
1:2:552:G:H2'	1:2:553:U:H6	1.78	0.42
1:2:929:G:H2'	1:2:930:C:O4'	2.19	0.42
1:2:1380:C:H2'	1:2:1381:G:O4'	2.19	0.42
1:2:1482:C:H3'	1:2:1483:A:C8	2.54	0.42
31:y:294:LYS:HD3	31:y:316:VAL:HG12	2.00	0.42
1:2:126:G:H21	1:2:180:G:H21	1.68	0.42
1:2:681:U:H2'	1:2:682:U:O4'	2.19	0.42
1:2:1328:G:H2'	1:2:1329:U:O4'	2.20	0.42
1:2:1401:A:H2'	1:2:1402:A:C8	2.54	0.42
30:x:178:ARG:HH21	30:x:178:ARG:HB2	1.83	0.42
31:y:110:VAL:HG23	31:y:306:LEU:HB3	2.01	0.42
32:u:731:LEU:HD23	32:u:767:MET:HB3	2.02	0.42
1:2:680:G:H2'	1:2:681:U:H6	1.83	0.42
1:2:1408:U:H2'	1:2:1409:A:H8	1.82	0.42
1:2:1525:C:H2'	1:2:1526:G:O4'	2.19	0.42
4:P:50:ARG:HA	4:P:50:ARG:HD3	1.91	0.42
14:B:82:ARG:NH1	14:B:191:ASP:HB2	2.28	0.42
16:E:248:ILE:H	16:E:248:ILE:HG13	1.71	0.42
32:u:260:PHE:HB2	32:u:570:VAL:HG21	2.00	0.42
33:w:222:PRO:HA	33:w:225:TRP:CD2	2.55	0.42
1:2:1620:A:H2'	4:P:40:ARG:CZ	2.49	0.42
2:F:39:ILE:HG23	2:F:68:ILE:HD13	2.02	0.42
17:G:7:PHE:HA	17:G:8:PRO:HD3	1.84	0.42
30:x:209:VAL:HG11	30:x:225:ILE:HG21	2.01	0.42
1:2:88:G:H2'	1:2:89:C:O4'	2.20	0.42
1:2:1277:C:H2'	1:2:1278:A:H8	1.85	0.42
1:2:1490:G:H2'	1:2:1491:G:H4'	2.02	0.42
9:Z:58:LEU:HD21	9:Z:87:ALA:HB1	2.00	0.42
14:B:23:ASP:HA	14:B:24:PRO:HD3	1.88	0.42
31:y:231:ARG:NH2	31:y:232:VAL:HB	2.34	0.42
1:2:976:G:H2'	1:2:977:C:C6	2.55	0.42
4:P:48:GLY:HA3	35:t:309:CYS:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:114:LYS:HD2	15:C:123:ARG:HH11	1.85	0.42
26:X:102:VAL:HG12	26:X:120:PHE:HB3	2.02	0.42
27:Y:14:THR:HG22	27:Y:21:LYS:HG2	2.02	0.42
32:u:84:GLN:HG3	32:u:134:PHE:HD2	1.84	0.42
32:u:272:LEU:HD22	32:u:565:VAL:HG21	2.01	0.42
1:2:17:C:C2	1:2:18:C:C5	3.08	0.42
1:2:1100:A:H2'	1:2:1101:U:O4'	2.20	0.42
1:2:1102:G:H2'	1:2:1103:C:H6	1.83	0.42
13:A:108:PHE:HB2	13:A:136:GLU:HB3	2.02	0.42
16:E:31:PRO:HG2	16:E:38:LEU:HB2	2.02	0.42
27:Y:57:VAL:HB	27:Y:60:PHE:CE2	2.54	0.42
1:2:1822:A:H2'	1:2:1823:A:C8	2.55	0.41
3:M:69:CYS:HA	3:M:74:ILE:HB	2.02	0.41
5:Q:100:VAL:CG1	5:Q:101:ASP:H	2.31	0.41
12:g:20:GLN:HG2	12:g:69:VAL:H	1.85	0.41
12:g:36:ARG:C	12:g:38:LYS:H	2.27	0.41
15:C:191:VAL:HG11	15:C:236:PHE:HA	2.02	0.41
19:I:38:ILE:HD11	19:I:81:VAL:HG23	2.01	0.41
26:X:46:HIS:CD2	26:X:103:ALA:HB2	2.55	0.41
32:u:619:GLY:O	32:u:620:PHE:HB2	2.20	0.41
1:2:178:C:H2'	1:2:178:C:O2	2.20	0.41
1:2:926:A:H61	1:2:1015:U:H3	1.68	0.41
1:2:969:U:H1'	1:2:971:G:C2	2.55	0.41
1:2:1666:C:H2'	1:2:1667:U:C6	2.55	0.41
1:2:1740:C:H5''	19:I:58:LEU:HD11	2.01	0.41
1:2:1809:A:H2'	1:2:1810:U:O4'	2.20	0.41
13:A:24:HIS:HB3	13:A:51:LEU:HD11	2.03	0.41
13:A:184:ARG:HD3	13:A:191:ARG:HG2	2.02	0.41
1:2:407:G:N3	1:2:407:G:H2'	2.35	0.41
1:2:462:C:H2'	1:2:463:C:O4'	2.21	0.41
1:2:475:C:C4	1:2:476:A:N7	2.88	0.41
1:2:493:A:C8	1:2:574:A:C8	3.08	0.41
1:2:943:U:H1'	23:O:137:SER:CB	2.50	0.41
1:2:14:C:OP1	15:C:189:GLY:O	2.37	0.41
1:2:818:A:H2'	1:2:819:G:O4'	2.21	0.41
1:2:868:G:C4	18:H:115:LYS:HB3	2.54	0.41
1:2:1643:U:H2'	1:2:1644:C:C6	2.55	0.41
1:2:1672:U:O3'	5:Q:76:GLY:HA3	2.20	0.41
1:2:1721:U:H3'	1:2:1722:G:H5'	2.02	0.41
1:2:493:A:H61	1:2:509:G:N2	2.18	0.41
1:2:1529:C:H2'	1:2:1530:U:C6	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1563:G:H4'	8:T:115:LYS:HE3	2.02	0.41
1:2:1607:A:N6	1:2:1632:G:O2'	2.53	0.41
32:u:126:CYS:HA	32:u:127:PRO:HD3	1.92	0.41
32:u:360:ILE:HG22	32:u:526:ARG:HA	2.02	0.41
1:2:935:G:H2'	1:2:936:G:H8	1.85	0.41
1:2:49:C:N4	1:2:472:C:H2'	2.36	0.41
1:2:373:G:C2	1:2:374:G:C8	3.08	0.41
1:2:1817:G:H2'	1:2:1818:A:H8	1.83	0.41
25:W:76:SER:HA	25:W:77:PRO:C	2.46	0.41
32:u:402:ALA:HA	32:u:405:ILE:HD12	2.03	0.41
1:2:1152:U:H2'	25:W:12:LYS:NZ	2.36	0.41
16:E:100:ARG:HD2	16:E:102:ILE:HD11	2.02	0.41
20:J:169:ARG:HA	20:J:170:PRO:HD2	1.94	0.41
23:O:101:GLY:HA3	23:O:134:PRO:HD2	2.03	0.41
31:y:219:GLN:HB3	31:y:220:GLU:H	1.70	0.41
31:y:340:LEU:H	31:y:344:GLN:HE21	1.67	0.41
34:v:215:LEU:HD13	34:v:244:MET:HE2	2.01	0.41
1:2:654:A:H5'	1:2:655:A:H3'	2.02	0.41
1:2:1472:C:H2'	1:2:1473:G:O4'	2.21	0.41
1:2:1639:G:H1'	34:v:230:ASN:HD22	1.86	0.41
1:2:1845:A:H2'	1:2:1846:G:H8	1.86	0.41
8:T:75:MET:HG3	8:T:104:LEU:HD11	2.03	0.41
14:B:38:MET:HE3	14:B:182:LYS:HA	2.01	0.41
18:H:87:PHE:HB3	18:H:90:LYS:HE2	2.02	0.41
26:X:61:GLN:HB3	26:X:62:PRO:HD3	2.02	0.41
30:x:202:ILE:HB	30:x:211:ILE:HG22	2.02	0.41
32:u:515:ASP:HA	32:u:516:PRO:HD3	1.95	0.41
32:u:660:PHE:HA	32:u:661:PRO:HD3	1.94	0.41
33:w:241:LEU:HB3	33:w:242:LYS:H	1.78	0.41
1:2:310:C:H2'	1:2:311:C:O4'	2.20	0.41
1:2:344:U:H2'	1:2:345:U:C6	2.56	0.41
1:2:345:U:H2'	1:2:346:C:C6	2.56	0.41
9:Z:68:ILE:HB	9:Z:109:TYR:HB2	2.03	0.41
13:A:176:TRP:HZ3	13:A:177:MET:HE3	1.86	0.41
30:x:80:VAL:HA	30:x:81:PRO:HD3	1.87	0.41
1:2:67:C:H5''	17:G:162:LEU:HD11	2.03	0.40
1:2:353:C:H1'	21:L:71:ARG:NE	2.36	0.40
1:2:454:U:C2	1:2:455:A:C8	3.10	0.40
1:2:1674:G:OP1	2:F:51:HIS:NE2	2.53	0.40
1:2:1708:C:H2'	1:2:1709:G:C8	2.56	0.40
1:2:1800:A:C2	1:2:1801:A:H1'	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:89:LYS:HD3	13:A:89:LYS:HA	1.79	0.40
1:2:1035:A:H2'	1:2:1036:A:O4'	2.21	0.40
1:2:1614:A:H2'	1:2:1615:U:C6	2.55	0.40
17:G:67:VAL:HB	17:G:99:GLY:HA2	2.03	0.40
32:u:78:LYS:H	32:u:78:LYS:HG2	1.76	0.40
32:u:630:SER:HB2	32:u:691:ARG:HH22	1.84	0.40
1:2:217:A:H2'	1:2:217:A:N3	2.37	0.40
1:2:1177:U:H2'	1:2:1178:U:H6	1.85	0.40
1:2:1849:G:P	35:t:441:ARG:HH22	2.44	0.40
13:A:205:ARG:HG3	13:A:210:ILE:HG12	2.03	0.40
1:2:320:G:H2'	1:2:321:C:C6	2.57	0.40
1:2:648:A:H2'	1:2:649:U:O4'	2.22	0.40
1:2:1036:A:H4'	1:2:1855:G:N2	2.35	0.40
1:2:1340:U:H2'	1:2:1341:C:C6	2.57	0.40
1:2:1479:G:H2'	1:2:1480:A:H8	1.85	0.40
1:2:1614:A:H2'	1:2:1615:U:H6	1.87	0.40
1:2:1787:G:H2'	1:2:1788:A:C8	2.56	0.40
15:C:251:LEU:HD12	24:V:23:ILE:HG13	2.03	0.40
18:H:146:VAL:O	25:W:49:GLU:HB2	2.22	0.40
32:u:497:ARG:NH2	32:u:721:GLU:HG2	2.36	0.40
1:2:674:C:H2'	1:2:675:U:H6	1.85	0.40
1:2:1520:G:H21	4:P:126:VAL:HG21	1.86	0.40
8:T:104:LEU:HD22	8:T:121:ARG:HD3	2.03	0.40
13:A:34:MET:HE3	13:A:34:MET:HB3	1.92	0.40
15:C:65:LYS:HB2	15:C:266:TYR:HE1	1.86	0.40
26:X:71:ARG:HH21	35:t:469:ASN:HB2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	187/204 (92%)	173 (92%)	13 (7%)	1 (0%)	24	57
3	M	121/132 (92%)	112 (93%)	9 (7%)	0	100	100
4	P	118/145 (81%)	111 (94%)	6 (5%)	1 (1%)	16	49
5	Q	120/146 (82%)	115 (96%)	5 (4%)	0	100	100
6	R	120/135 (89%)	110 (92%)	9 (8%)	1 (1%)	16	49
7	S	128/152 (84%)	118 (92%)	9 (7%)	1 (1%)	16	49
8	T	142/145 (98%)	131 (92%)	11 (8%)	0	100	100
9	Z	70/125 (56%)	65 (93%)	5 (7%)	0	100	100
10	c	59/69 (86%)	54 (92%)	4 (7%)	1 (2%)	7	35
11	f	71/156 (46%)	58 (82%)	10 (14%)	3 (4%)	2	19
12	g	311/317 (98%)	282 (91%)	23 (7%)	6 (2%)	6	33
13	A	214/295 (72%)	201 (94%)	12 (6%)	1 (0%)	24	57
14	B	211/264 (80%)	198 (94%)	12 (6%)	1 (0%)	24	57
15	C	216/293 (74%)	203 (94%)	11 (5%)	2 (1%)	14	46
16	E	260/263 (99%)	246 (95%)	13 (5%)	1 (0%)	30	61
17	G	228/249 (92%)	218 (96%)	9 (4%)	1 (0%)	30	61
18	H	184/194 (95%)	175 (95%)	9 (5%)	0	100	100
19	I	203/208 (98%)	195 (96%)	8 (4%)	0	100	100
20	J	178/194 (92%)	164 (92%)	11 (6%)	3 (2%)	7	35
21	L	149/158 (94%)	144 (97%)	5 (3%)	0	100	100
22	N	147/151 (97%)	139 (95%)	8 (5%)	0	100	100
23	O	133/151 (88%)	123 (92%)	10 (8%)	0	100	100
24	V	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
25	W	127/130 (98%)	120 (94%)	6 (5%)	1 (1%)	16	49
26	X	139/143 (97%)	131 (94%)	6 (4%)	2 (1%)	9	38
27	Y	122/133 (92%)	115 (94%)	6 (5%)	1 (1%)	16	49
28	b	80/84 (95%)	73 (91%)	7 (9%)	0	100	100
29	e	53/59 (90%)	47 (89%)	5 (9%)	1 (2%)	6	33
30	x	176/252 (70%)	170 (97%)	6 (3%)	0	100	100
31	y	319/412 (77%)	295 (92%)	20 (6%)	4 (1%)	9	39
32	u	619/804 (77%)	573 (93%)	38 (6%)	8 (1%)	9	39
33	w	247/437 (56%)	236 (96%)	10 (4%)	1 (0%)	30	61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	v	317/552 (57%)	297 (94%)	17 (5%)	3 (1%)	14	46
35	t	119/475 (25%)	101 (85%)	15 (13%)	3 (2%)	4	28
All	All	5968/7710 (77%)	5572 (93%)	349 (6%)	47 (1%)	18	49

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	c	66	ARG
26	X	61	GLN
26	X	86	PRO
31	y	370	VAL
12	g	190	GLY
20	J	160	SER
32	u	81	PRO
32	u	183	PRO
32	u	518	GLU
32	u	619	GLY
34	v	31	GLU
4	P	34	MET
11	f	84	SER
11	f	85	TYR
15	C	72	ASP
16	E	133	THR
17	G	133	LEU
31	y	106	GLU
31	y	219	GLN
32	u	49	SER
35	t	256	LEU
12	g	161	SER
13	A	206	ASP
15	C	135	GLY
20	J	138	ARG
29	e	51	LYS
34	v	246	ASP
6	R	42	PRO
12	g	13	GLY
12	g	103	GLY
33	w	242	LYS
35	t	253	ASN
35	t	255	GLN
2	F	41	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	S	87	GLN
20	J	169	ARG
27	Y	67	GLY
34	v	248	PRO
31	y	107	PRO
12	g	61	GLY
14	B	93	GLY
25	W	67	GLY
11	f	122	PRO
32	u	76	GLY
32	u	361	PRO
32	u	485	PRO
12	g	253	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	159/170 (94%)	135 (85%)	24 (15%)	3	17
3	M	104/108 (96%)	92 (88%)	12 (12%)	5	25
4	P	107/130 (82%)	94 (88%)	13 (12%)	5	23
5	Q	103/121 (85%)	87 (84%)	16 (16%)	2	16
6	R	110/122 (90%)	90 (82%)	20 (18%)	2	11
7	S	114/132 (86%)	95 (83%)	19 (17%)	2	14
8	T	114/115 (99%)	100 (88%)	14 (12%)	4	23
9	Z	64/103 (62%)	56 (88%)	8 (12%)	4	22
10	c	52/62 (84%)	45 (86%)	7 (14%)	4	21
11	f	65/140 (46%)	58 (89%)	7 (11%)	6	28
12	g	271/275 (98%)	237 (88%)	34 (12%)	4	22
13	A	180/243 (74%)	155 (86%)	25 (14%)	3	19
14	B	194/231 (84%)	179 (92%)	15 (8%)	12	38
15	C	184/225 (82%)	172 (94%)	12 (6%)	15	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	E	224/225 (100%)	208 (93%)	16 (7%)	13	40
17	G	200/218 (92%)	191 (96%)	9 (4%)	24	51
18	H	167/174 (96%)	163 (98%)	4 (2%)	43	63
19	I	178/180 (99%)	175 (98%)	3 (2%)	53	69
20	J	160/168 (95%)	155 (97%)	5 (3%)	35	59
21	L	135/142 (95%)	127 (94%)	8 (6%)	18	45
22	N	130/131 (99%)	122 (94%)	8 (6%)	16	44
23	O	105/119 (88%)	97 (92%)	8 (8%)	12	39
24	V	66/67 (98%)	63 (96%)	3 (4%)	24	51
25	W	112/113 (99%)	103 (92%)	9 (8%)	11	37
26	X	113/115 (98%)	104 (92%)	9 (8%)	11	37
27	Y	108/115 (94%)	103 (95%)	5 (5%)	24	51
28	b	74/76 (97%)	70 (95%)	4 (5%)	20	47
29	e	45/48 (94%)	42 (93%)	3 (7%)	15	42
30	x	150/208 (72%)	136 (91%)	14 (9%)	8	32
31	y	285/367 (78%)	273 (96%)	12 (4%)	26	53
32	u	550/705 (78%)	522 (95%)	28 (5%)	21	49
33	w	217/370 (59%)	203 (94%)	14 (6%)	15	43
34	v	274/489 (56%)	272 (99%)	2 (1%)	76	78
35	t	113/434 (26%)	102 (90%)	11 (10%)	8	31
All	All	5227/6641 (79%)	4826 (92%)	401 (8%)	14	38

All (401) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	24	SER
2	F	26	ASP
2	F	32	ASP
2	F	33	ILE
2	F	41	VAL
2	F	55	ARG
2	F	68	ILE
2	F	79	HIS
2	F	81	ARG
2	F	88	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	89	THR
2	F	98	GLU
2	F	102	LEU
2	F	103	LEU
2	F	122	ARG
2	F	136	ARG
2	F	146	ARG
2	F	147	VAL
2	F	159	ARG
2	F	166	ILE
2	F	169	ILE
2	F	177	LEU
2	F	194	ASP
2	F	196	LEU
3	M	22	LEU
3	M	26	LEU
3	M	29	ASP
3	M	33	ARG
3	M	45	ARG
3	M	64	LEU
3	M	81	ASP
3	M	91	LEU
3	M	106	CYS
3	M	109	VAL
3	M	124	ILE
3	M	125	GLU
4	P	16	THR
4	P	21	ASP
4	P	22	LEU
4	P	25	LEU
4	P	26	LEU
4	P	34	MET
4	P	36	LEU
4	P	41	GLN
4	P	59	ARG
4	P	81	ARG
4	P	84	ILE
4	P	86	LEU
4	P	101	THR
5	Q	10	VAL
5	Q	16	LYS
5	Q	25	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	Q	32	ILE
5	Q	37	ARG
5	Q	43	GLU
5	Q	46	THR
5	Q	47	LEU
5	Q	52	LEU
5	Q	72	VAL
5	Q	80	GLN
5	Q	85	ARG
5	Q	118	THR
5	Q	120	LEU
5	Q	125	ARG
5	Q	126	ARG
6	R	4	VAL
6	R	6	THR
6	R	11	LYS
6	R	15	VAL
6	R	27	ASP
6	R	41	ILE
6	R	47	ARG
6	R	60	ARG
6	R	69	ILE
6	R	70	SER
6	R	76	GLU
6	R	85	VAL
6	R	89	SER
6	R	91	LEU
6	R	95	ILE
6	R	98	VAL
6	R	99	ASP
6	R	108	LEU
6	R	110	ASP
6	R	120	THR
7	S	3	LEU
7	S	13	LEU
7	S	16	LEU
7	S	19	ASN
7	S	38	ARG
7	S	43	VAL
7	S	45	LEU
7	S	52	LEU
7	S	53	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	S	62	ASP
7	S	64	VAL
7	S	67	VAL
7	S	75	ARG
7	S	83	PHE
7	S	98	VAL
7	S	111	LEU
7	S	113	ARG
7	S	125	HIS
7	S	129	LEU
8	T	5	THR
8	T	13	GLU
8	T	25	SER
8	T	34	VAL
8	T	39	LEU
8	T	62	ARG
8	T	82	ARG
8	T	84	ARG
8	T	88	MET
8	T	90	SER
8	T	102	ARG
8	T	110	LEU
8	T	134	ILE
8	T	137	GLN
9	Z	64	ASN
9	Z	72	VAL
9	Z	76	ARG
9	Z	85	ARG
9	Z	88	LEU
9	Z	92	LEU
9	Z	104	ARG
9	Z	108	ILE
10	c	21	THR
10	c	26	GLN
10	c	30	VAL
10	c	37	ASP
10	c	55	VAL
10	c	58	LEU
10	c	63	ARG
11	f	86	THR
11	f	93	HIS
11	f	100	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	f	102	VAL
11	f	108	VAL
11	f	116	ARG
11	f	147	THR
12	g	6	THR
12	g	29	ASP
12	g	31	ILE
12	g	40	ILE
12	g	46	THR
12	g	47	ARG
12	g	57	ARG
12	g	64	HIS
12	g	71	ILE
12	g	72	SER
12	g	118	ARG
12	g	131	LEU
12	g	134	THR
12	g	135	LEU
12	g	149	GLU
12	g	165	ILE
12	g	167	SER
12	g	173	LEU
12	g	179	LEU
12	g	186	THR
12	g	197	THR
12	g	198	VAL
12	g	200	VAL
12	g	203	ASP
12	g	227	LEU
12	g	231	ASP
12	g	240	CYS
12	g	252	THR
12	g	257	LYS
12	g	258	ILE
12	g	265	ILE
12	g	297	THR
12	g	298	LEU
12	g	306	LEU
13	A	7	VAL
13	A	8	LEU
13	A	11	LYS
13	A	16	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	A	23	THR
13	A	28	THR
13	A	38	ILE
13	A	41	ARG
13	A	56	GLU
13	A	57	LYS
13	A	60	LEU
13	A	66	VAL
13	A	68	ILE
13	A	73	ASP
13	A	82	THR
13	A	87	VAL
13	A	97	THR
13	A	102	ARG
13	A	113	GLN
13	A	120	ARG
13	A	130	ASP
13	A	134	LEU
13	A	155	ARG
13	A	178	LEU
13	A	205	ARG
14	B	33	VAL
14	B	50	THR
14	B	57	ILE
14	B	62	LEU
14	B	79	VAL
14	B	98	THR
14	B	125	VAL
14	B	151	ARG
14	B	163	GLN
14	B	166	LYS
14	B	178	THR
14	B	207	LEU
14	B	212	VAL
14	B	225	LEU
14	B	231	LEU
15	C	66	LEU
15	C	68	ARG
15	C	116	THR
15	C	132	ASP
15	C	137	VAL
15	C	156	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	C	202	THR
15	C	213	LEU
15	C	221	ASP
15	C	233	LEU
15	C	255	LEU
15	C	262	THR
16	E	10	LYS
16	E	12	VAL
16	E	22	LYS
16	E	23	LEU
16	E	38	LEU
16	E	48	LEU
16	E	105	THR
16	E	114	ILE
16	E	160	ILE
16	E	173	ILE
16	E	191	ARG
16	E	220	THR
16	E	236	ILE
16	E	238	LEU
16	E	244	ILE
16	E	248	ILE
17	G	67	VAL
17	G	69	THR
17	G	72	ARG
17	G	92	ARG
17	G	127	THR
17	G	141	ILE
17	G	171	THR
17	G	181	THR
17	G	201	LYS
18	H	79	LEU
18	H	105	THR
18	H	133	LEU
18	H	148	LEU
19	I	3	ILE
19	I	82	VAL
19	I	203	LYS
20	J	8	VAL
20	J	24	ARG
20	J	29	LEU
20	J	94	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	J	144	ILE
21	L	15	THR
21	L	23	VAL
21	L	42	LEU
21	L	48	LYS
21	L	82	MET
21	L	118	ARG
21	L	132	ARG
21	L	136	LYS
22	N	9	LYS
22	N	24	THR
22	N	29	THR
22	N	75	LEU
22	N	84	LEU
22	N	86	GLU
22	N	102	LEU
22	N	145	THR
23	O	75	MET
23	O	80	ASP
23	O	81	VAL
23	O	104	ARG
23	O	105	THR
23	O	106	LYS
23	O	113	GLN
23	O	147	ARG
24	V	9	VAL
24	V	43	THR
24	V	70	LEU
25	W	2	VAL
25	W	6	VAL
25	W	7	LEU
25	W	33	VAL
25	W	63	VAL
25	W	66	THR
25	W	75	ILE
25	W	78	ARG
25	W	104	LEU
26	X	7	LEU
26	X	37	LYS
26	X	60	LYS
26	X	70	VAL
26	X	71	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	X	79	LYS
26	X	100	VAL
26	X	102	VAL
26	X	115	ILE
27	Y	17	LEU
27	Y	40	ILE
27	Y	55	ILE
27	Y	79	LEU
27	Y	117	VAL
28	b	25	VAL
28	b	37	CYS
28	b	59	CYS
28	b	67	THR
29	e	12	VAL
29	e	26	LYS
29	e	58	ASN
30	x	78	ILE
30	x	86	THR
30	x	102	HIS
30	x	111	LEU
30	x	118	ILE
30	x	120	THR
30	x	127	VAL
30	x	146	VAL
30	x	155	LEU
30	x	160	LEU
30	x	178	ARG
30	x	202	ILE
30	x	229	ILE
30	x	241	ILE
31	y	52	GLU
31	y	89	LEU
31	y	98	VAL
31	y	100	VAL
31	y	219	GLN
31	y	221	LEU
31	y	253	LEU
31	y	256	ASN
31	y	306	LEU
31	y	356	ARG
31	y	367	ILE
31	y	378	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	u	51	VAL
32	u	136	THR
32	u	166	TRP
32	u	180	GLN
32	u	189	VAL
32	u	207	LEU
32	u	222	LEU
32	u	225	THR
32	u	253	LEU
32	u	288	LEU
32	u	297	PHE
32	u	299	MET
32	u	393	VAL
32	u	490	THR
32	u	492	ARG
32	u	497	ARG
32	u	517	LYS
32	u	570	VAL
32	u	590	LYS
32	u	594	LEU
32	u	596	MET
32	u	597	VAL
32	u	601	ASP
32	u	687	VAL
32	u	733	THR
32	u	741	ILE
32	u	762	GLN
32	u	766	LEU
33	w	181	VAL
33	w	199	LYS
33	w	226	THR
33	w	240	ASN
33	w	242	LYS
33	w	251	ASN
33	w	254	LEU
33	w	313	THR
33	w	327	LEU
33	w	355	ARG
33	w	395	THR
33	w	405	LEU
33	w	418	ARG
33	w	427	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	v	83	LEU
34	v	290	ILE
35	t	250	MET
35	t	257	THR
35	t	261	GLU
35	t	262	ARG
35	t	305	LYS
35	t	314	THR
35	t	360	LEU
35	t	362	ASN
35	t	363	HIS
35	t	473	LEU
35	t	474	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	101	HIS
2	F	203	ASN
4	P	24	GLN
4	P	46	ASN
4	P	114	HIS
5	Q	8	GLN
6	R	83	ASN
6	R	116	ASN
7	S	10	GLN
7	S	19	ASN
8	T	63	HIS
8	T	83	GLN
8	T	105	GLN
9	Z	103	HIS
9	Z	106	GLN
10	c	26	GLN
10	c	45	ASN
12	g	119	GLN
12	g	178	ASN
12	g	226	HIS
12	g	237	ASN
13	A	70	ASN
13	A	84	GLN
14	B	40	ASN
14	B	76	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	B	158	HIS
14	B	202	GLN
15	C	113	GLN
15	C	235	ASN
15	C	267	GLN
16	E	50	ASN
16	E	138	HIS
16	E	157	ASN
16	E	161	GLN
16	E	179	ASN
16	E	201	HIS
16	E	209	HIS
16	E	224	ASN
16	E	232	ASN
17	G	56	ASN
17	G	65	GLN
17	G	81	HIS
17	G	105	ASN
17	G	197	GLN
18	H	25	GLN
18	H	73	GLN
18	H	76	GLN
18	H	97	GLN
18	H	112	ASN
18	H	114	GLN
18	H	126	HIS
18	H	157	HIS
19	I	52	ASN
19	I	84	ASN
19	I	116	HIS
19	I	165	GLN
20	J	143	ASN
20	J	156	HIS
21	L	18	GLN
21	L	65	ASN
21	L	106	HIS
21	L	141	ASN
22	N	5	HIS
22	N	49	GLN
22	N	58	HIS
22	N	62	GLN
23	O	38	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	O	43	HIS
24	V	21	ASN
25	W	24	GLN
25	W	64	ASN
26	X	16	HIS
26	X	26	GLN
26	X	63	ASN
28	b	49	HIS
28	b	51	GLN
29	e	37	GLN
30	x	102	HIS
30	x	210	HIS
31	y	21	GLN
31	y	124	HIS
31	y	129	HIS
31	y	219	GLN
31	y	271	HIS
31	y	290	ASN
31	y	309	HIS
31	y	318	ASN
31	y	344	GLN
31	y	402	ASN
32	u	55	HIS
32	u	120	GLN
32	u	190	GLN
32	u	200	GLN
32	u	286	ASN
32	u	501	GLN
32	u	702	HIS
32	u	762	GLN
33	w	215	GLN
33	w	232	GLN
33	w	240	ASN
33	w	251	ASN
33	w	397	GLN
33	w	422	GLN
34	v	46	HIS
34	v	222	HIS
34	v	226	HIS
34	v	230	ASN
34	v	233	ASN
34	v	241	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	v	503	GLN
35	t	269	GLN
35	t	362	ASN
35	t	365	GLN
35	t	421	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1646/1873 (87%)	542 (32%)	61 (3%)

All (542) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	C
1	2	4	C
1	2	5	U
1	2	9	U
1	2	14	C
1	2	17	C
1	2	23	G
1	2	25	A
1	2	26	U
1	2	33	G
1	2	41	G
1	2	44	U
1	2	45	A
1	2	46	A
1	2	49	C
1	2	50	A
1	2	56	G
1	2	58	C
1	2	60	A
1	2	61	A
1	2	62	G
1	2	65	C
1	2	66	G
1	2	67	C
1	2	68	A
1	2	69	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	70	G
1	2	72	C
1	2	73	C
1	2	74	G
1	2	75	G
1	2	76	U
1	2	77	A
1	2	79	A
1	2	92	A
1	2	97	U
1	2	102	A
1	2	103	A
1	2	104	A
1	2	110	U
1	2	111	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	127	C
1	2	128	U
1	2	129	C
1	2	130	G
1	2	143	U
1	2	144	U
1	2	155	G
1	2	167	G
1	2	168	C
1	2	171	A
1	2	172	U
1	2	181	A
1	2	182	C
1	2	184	G
1	2	187	G
1	2	191	A
1	2	214	U
1	2	215	G
1	2	217	A
1	2	220	U
1	2	221	A
1	2	290	U
1	2	291	G
1	2	292	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	293	C
1	2	294	U
1	2	295	C
1	2	302	A
1	2	305	U
1	2	306	C
1	2	308	G
1	2	309	G
1	2	310	C
1	2	312	G
1	2	315	C
1	2	318	A
1	2	319	C
1	2	332	G
1	2	333	G
1	2	338	G
1	2	342	C
1	2	343	A
1	2	347	G
1	2	351	G
1	2	356	C
1	2	357	C
1	2	360	A
1	2	362	C
1	2	364	A
1	2	370	G
1	2	371	A
1	2	377	G
1	2	381	C
1	2	385	G
1	2	386	C
1	2	387	C
1	2	392	A
1	2	400	C
1	2	407	G
1	2	408	A
1	2	409	C
1	2	411	G
1	2	413	G
1	2	418	A
1	2	421	G
1	2	426	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	428	U
1	2	429	C
1	2	438	G
1	2	441	C
1	2	445	A
1	2	448	A
1	2	449	A
1	2	450	C
1	2	455	A
1	2	465	A
1	2	466	G
1	2	471	G
1	2	472	C
1	2	473	A
1	2	474	G
1	2	482	G
1	2	487	U
1	2	492	C
1	2	496	C
1	2	500	A
1	2	502	C
1	2	503	C
1	2	508	A
1	2	517	C
1	2	531	A
1	2	534	G
1	2	537	C
1	2	539	C
1	2	542	U
1	2	544	G
1	2	545	A
1	2	547	G
1	2	548	C
1	2	552	G
1	2	554	A
1	2	555	A
1	2	556	U
1	2	559	G
1	2	560	A
1	2	564	A
1	2	568	C
1	2	576	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	583	A
1	2	587	A
1	2	588	G
1	2	589	G
1	2	590	A
1	2	591	U
1	2	593	C
1	2	594	A
1	2	595	U
1	2	598	G
1	2	604	A
1	2	605	A
1	2	606	G
1	2	608	C
1	2	614	C
1	2	617	G
1	2	627	U
1	2	628	A
1	2	629	A
1	2	630	U
1	2	632	C
1	2	643	A
1	2	644	G
1	2	655	A
1	2	660	C
1	2	664	A
1	2	666	U
1	2	668	A
1	2	669	A
1	2	670	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	684	G
1	2	685	A
1	2	687	C
1	2	688	U
1	2	748	C
1	2	749	U
1	2	750	C
1	2	751	G
1	2	792	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	794	A
1	2	796	G
1	2	797	C
1	2	799	U
1	2	800	U
1	2	809	A
1	2	812	A
1	2	821	G
1	2	822	U
1	2	827	A
1	2	830	A
1	2	834	C
1	2	845	G
1	2	847	A
1	2	852	G
1	2	856	C
1	2	858	A
1	2	869	A
1	2	870	A
1	2	871	U
1	2	872	A
1	2	873	G
1	2	874	G
1	2	877	C
1	2	878	G
1	2	880	G
1	2	884	C
1	2	885	U
1	2	886	A
1	2	888	U
1	2	890	U
1	2	891	G
1	2	892	U
1	2	893	U
1	2	895	G
1	2	896	U
1	2	898	U
1	2	905	C
1	2	907	G
1	2	908	A
1	2	912	C
1	2	913	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	914	U
1	2	917	U
1	2	918	U
1	2	919	A
1	2	920	A
1	2	921	G
1	2	926	A
1	2	933	G
1	2	958	G
1	2	959	G
1	2	963	A
1	2	970	G
1	2	971	G
1	2	980	A
1	2	981	A
1	2	985	G
1	2	988	C
1	2	989	C
1	2	990	A
1	2	991	G
1	2	992	A
1	2	1001	A
1	2	1002	U
1	2	1008	A
1	2	1009	A
1	2	1016	U
1	2	1017	U
1	2	1023	A
1	2	1027	A
1	2	1039	C
1	2	1040	G
1	2	1041	G
1	2	1045	U
1	2	1049	A
1	2	1050	A
1	2	1053	C
1	2	1056	U
1	2	1057	C
1	2	1058	A
1	2	1059	G
1	2	1060	A
1	2	1062	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1078	C
1	2	1082	A
1	2	1083	A
1	2	1085	C
1	2	1086	G
1	2	1087	A
1	2	1088	U
1	2	1096	G
1	2	1099	G
1	2	1100	A
1	2	1109	C
1	2	1110	G
1	2	1114	U
1	2	1116	C
1	2	1117	C
1	2	1118	C
1	2	1119	A
1	2	1121	G
1	2	1131	G
1	2	1133	A
1	2	1138	C
1	2	1141	G
1	2	1148	A
1	2	1150	A
1	2	1153	C
1	2	1154	U
1	2	1155	U
1	2	1157	G
1	2	1159	G
1	2	1165	G
1	2	1166	G
1	2	1170	A
1	2	1171	G
1	2	1181	A
1	2	1194	A
1	2	1195	A
1	2	1197	G
1	2	1200	A
1	2	1204	A
1	2	1205	C
1	2	1206	G
1	2	1207	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1208	A
1	2	1211	G
1	2	1215	C
1	2	1216	C
1	2	1217	A
1	2	1221	G
1	2	1224	G
1	2	1227	G
1	2	1231	C
1	2	1232	U
1	2	1235	G
1	2	1242	U
1	2	1243	U
1	2	1244	U
1	2	1248	U
1	2	1249	C
1	2	1250	A
1	2	1251	A
1	2	1254	C
1	2	1255	G
1	2	1256	G
1	2	1257	G
1	2	1258	A
1	2	1259	A
1	2	1260	A
1	2	1261	C
1	2	1264	C
1	2	1269	G
1	2	1273	C
1	2	1274	G
1	2	1282	A
1	2	1283	C
1	2	1284	A
1	2	1285	G
1	2	1286	G
1	2	1297	U
1	2	1298	G
1	2	1299	A
1	2	1300	U
1	2	1301	A
1	2	1302	G
1	2	1303	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1304	U
1	2	1305	C
1	2	1306	U
1	2	1308	U
1	2	1309	C
1	2	1313	A
1	2	1315	U
1	2	1316	C
1	2	1317	C
1	2	1318	G
1	2	1320	G
1	2	1321	G
1	2	1322	G
1	2	1323	U
1	2	1324	G
1	2	1325	G
1	2	1326	U
1	2	1327	G
1	2	1329	U
1	2	1333	U
1	2	1344	A
1	2	1354	G
1	2	1358	U
1	2	1363	C
1	2	1364	U
1	2	1371	U
1	2	1372	U
1	2	1376	A
1	2	1378	A
1	2	1382	A
1	2	1386	A
1	2	1388	A
1	2	1393	G
1	2	1395	C
1	2	1401	A
1	2	1403	C
1	2	1404	U
1	2	1416	C
1	2	1425	G
1	2	1426	U
1	2	1429	G
1	2	1430	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1431	G
1	2	1432	U
1	2	1439	A
1	2	1440	C
1	2	1441	U
1	2	1442	U
1	2	1444	U
1	2	1446	A
1	2	1450	G
1	2	1452	A
1	2	1454	A
1	2	1455	A
1	2	1462	U
1	2	1463	U
1	2	1464	C
1	2	1465	A
1	2	1466	G
1	2	1477	U
1	2	1481	G
1	2	1482	C
1	2	1483	A
1	2	1484	A
1	2	1485	U
1	2	1487	A
1	2	1489	A
1	2	1490	G
1	2	1491	G
1	2	1494	U
1	2	1495	G
1	2	1498	A
1	2	1503	C
1	2	1505	U
1	2	1506	A
1	2	1507	G
1	2	1509	U
1	2	1510	G
1	2	1511	U
1	2	1512	C
1	2	1518	C
1	2	1519	U
1	2	1521	C
1	2	1524	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1526	G
1	2	1531	A
1	2	1533	A
1	2	1534	C
1	2	1535	U
1	2	1544	C
1	2	1548	G
1	2	1559	C
1	2	1560	U
1	2	1566	G
1	2	1567	G
1	2	1570	G
1	2	1574	C
1	2	1575	G
1	2	1579	A
1	2	1580	A
1	2	1581	C
1	2	1582	C
1	2	1584	G
1	2	1585	U
1	2	1586	U
1	2	1587	G
1	2	1588	A
1	2	1590	C
1	2	1594	A
1	2	1600	G
1	2	1601	A
1	2	1602	U
1	2	1606	G
1	2	1609	C
1	2	1612	G
1	2	1615	U
1	2	1617	G
1	2	1618	C
1	2	1621	U
1	2	1622	U
1	2	1623	A
1	2	1628	C
1	2	1632	G
1	2	1637	A
1	2	1647	A
1	2	1648	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1649	U
1	2	1654	G
1	2	1658	G
1	2	1663	A
1	2	1665	G
1	2	1669	G
1	2	1671	G
1	2	1675	A
1	2	1683	C
1	2	1686	G
1	2	1693	G
1	2	1699	A
1	2	1712	A
1	2	1721	U
1	2	1722	G
1	2	1723	G
1	2	1726	G
1	2	1727	G
1	2	1729	U
1	2	1742	C
1	2	1744	G
1	2	1745	A
1	2	1746	U
1	2	1756	C
1	2	1757	G
1	2	1761	U
1	2	1773	C
1	2	1776	G
1	2	1783	C
1	2	1784	G
1	2	1785	C
1	2	1786	U
1	2	1800	A
1	2	1801	A
1	2	1805	G
1	2	1808	U
1	2	1816	G
1	2	1819	A
1	2	1822	A
1	2	1824	A
1	2	1825	A
1	2	1826	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1827	U
1	2	1841	C
1	2	1859	A
1	2	1861	G
1	2	1863	A
1	2	1864	U
1	2	1865	C
1	2	1869	A
1	2	1870	A
1	2	1872	G
1	2	1873	G

All (61) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	8	U
1	2	43	U
1	2	44	U
1	2	72	C
1	2	102	A
1	2	114	G
1	2	142	C
1	2	143	U
1	2	171	A
1	2	180	G
1	2	220	U
1	2	291	G
1	2	293	C
1	2	314	U
1	2	332	G
1	2	407	G
1	2	447	A
1	2	465	A
1	2	516	A
1	2	547	G
1	2	554	A
1	2	559	G
1	2	594	A
1	2	604	A
1	2	656	G
1	2	820	U
1	2	870	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	912	C
1	2	918	U
1	2	958	G
1	2	980	A
1	2	1016	U
1	2	1165	G
1	2	1207	G
1	2	1231	C
1	2	1308	U
1	2	1312	G
1	2	1316	C
1	2	1325	G
1	2	1352	G
1	2	1403	C
1	2	1425	G
1	2	1430	C
1	2	1431	G
1	2	1438	A
1	2	1440	C
1	2	1476	A
1	2	1494	U
1	2	1497	G
1	2	1511	U
1	2	1534	C
1	2	1558	C
1	2	1581	C
1	2	1587	G
1	2	1601	A
1	2	1603	G
1	2	1648	G
1	2	1726	G
1	2	1744	G
1	2	1785	C
1	2	1860	A

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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.

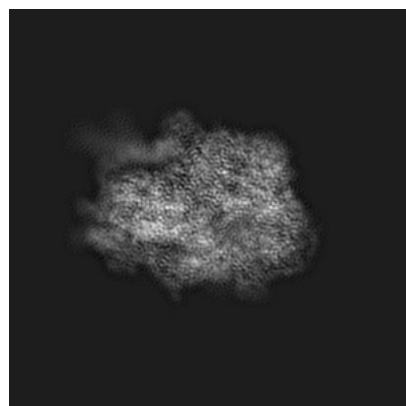
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4337. These allow visual inspection of the internal detail of the map and identification of artifacts.

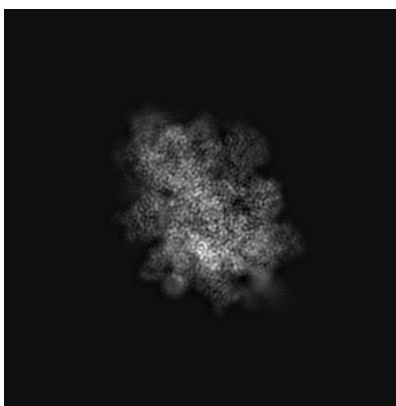
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

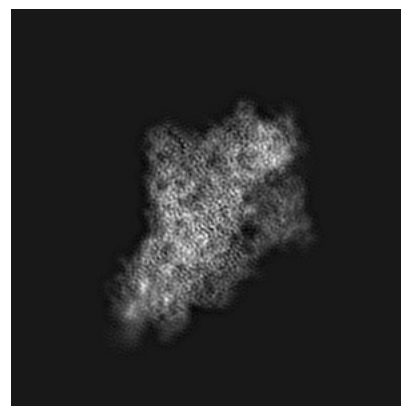
6.1.1 Primary map



X

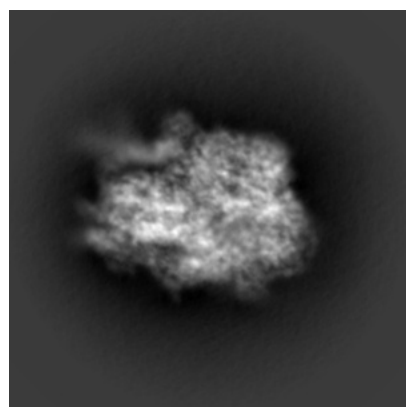


Y

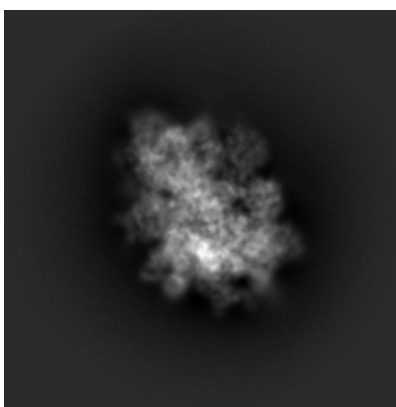


Z

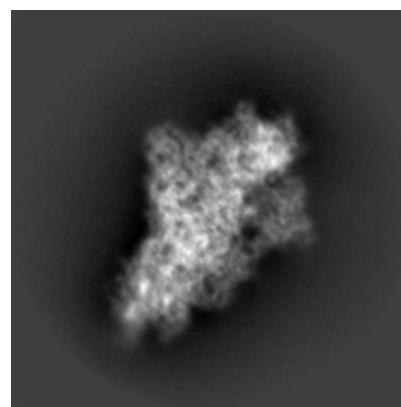
6.1.2 Raw map



X



Y

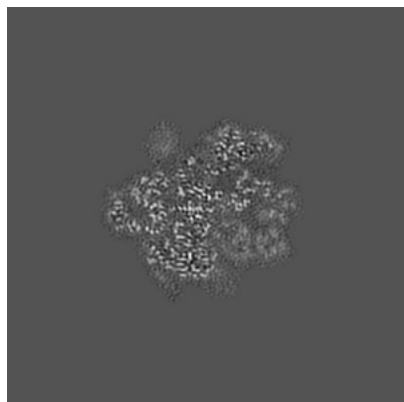


Z

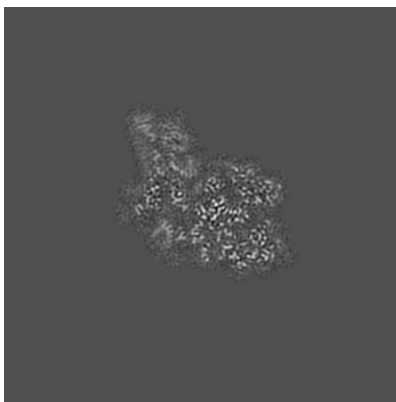
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

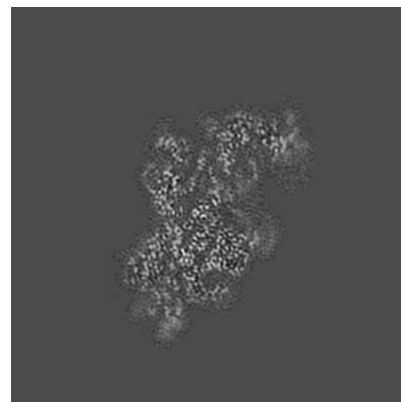
6.2.1 Primary map



X Index: 180

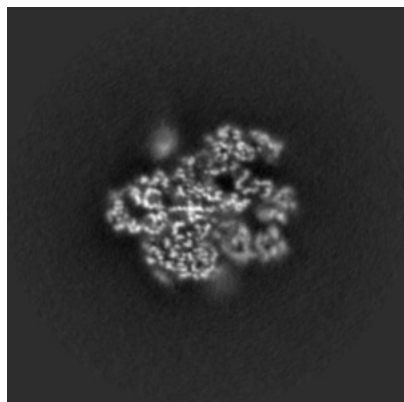


Y Index: 180

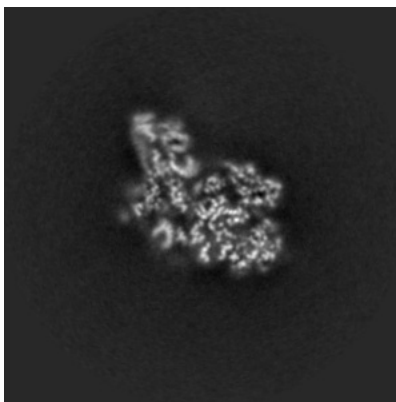


Z Index: 180

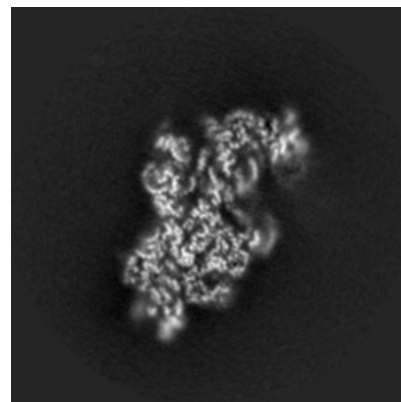
6.2.2 Raw map



X Index: 180



Y Index: 180

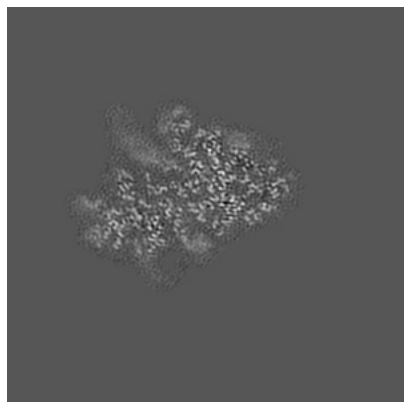


Z Index: 180

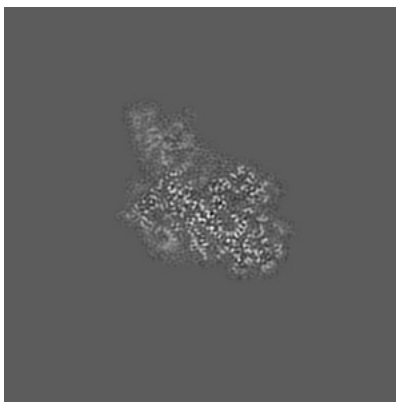
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

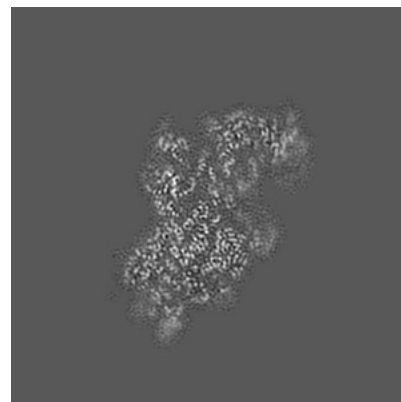
6.3.1 Primary map



X Index: 145

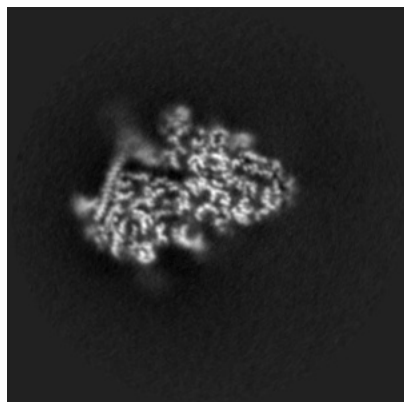


Y Index: 174

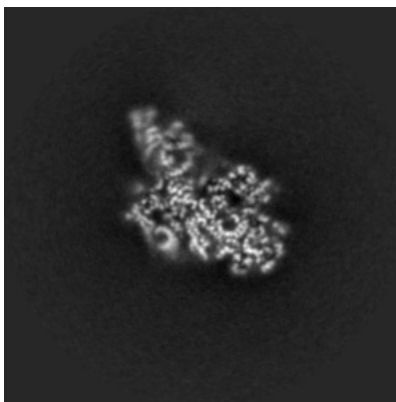


Z Index: 181

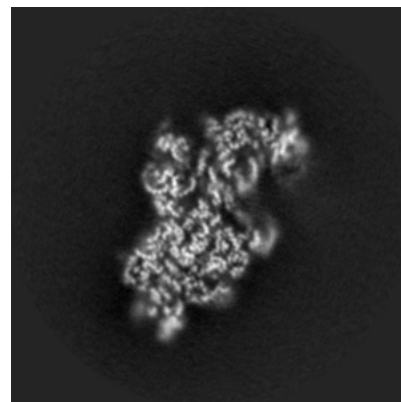
6.3.2 Raw map



X Index: 141



Y Index: 174

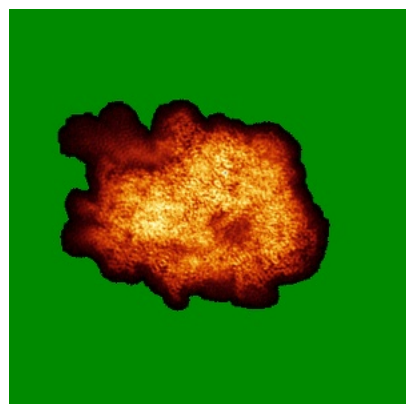


Z Index: 181

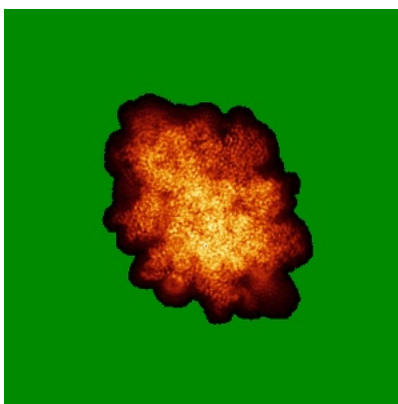
The images above show the largest variance slices of the map in three orthogonal directions.

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

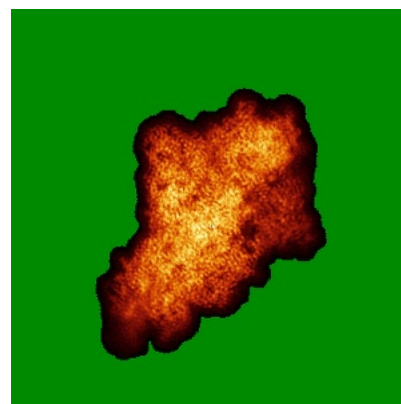
6.4.1 Primary map



X



Y

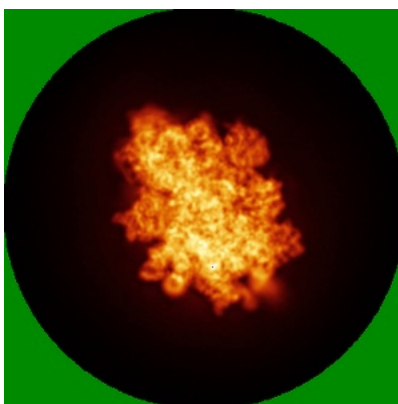


Z

6.4.2 Raw map



X



Y

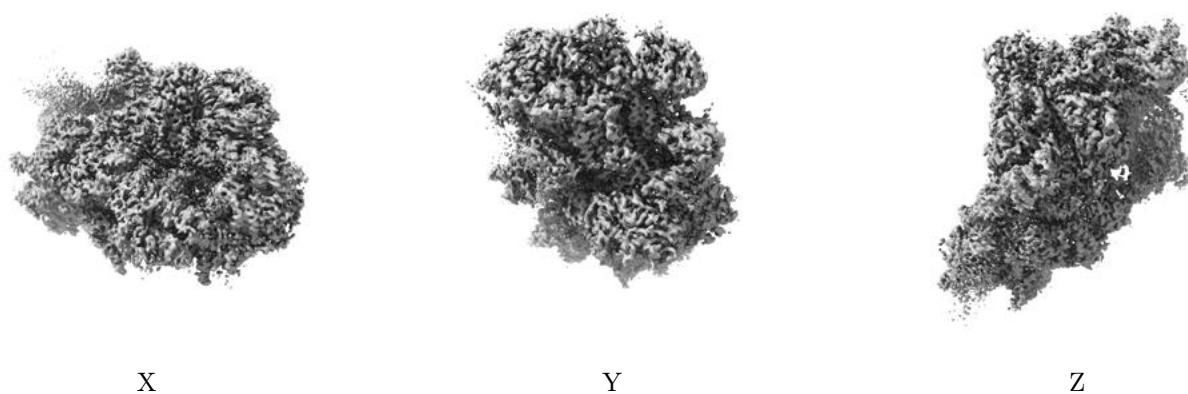


Z

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.

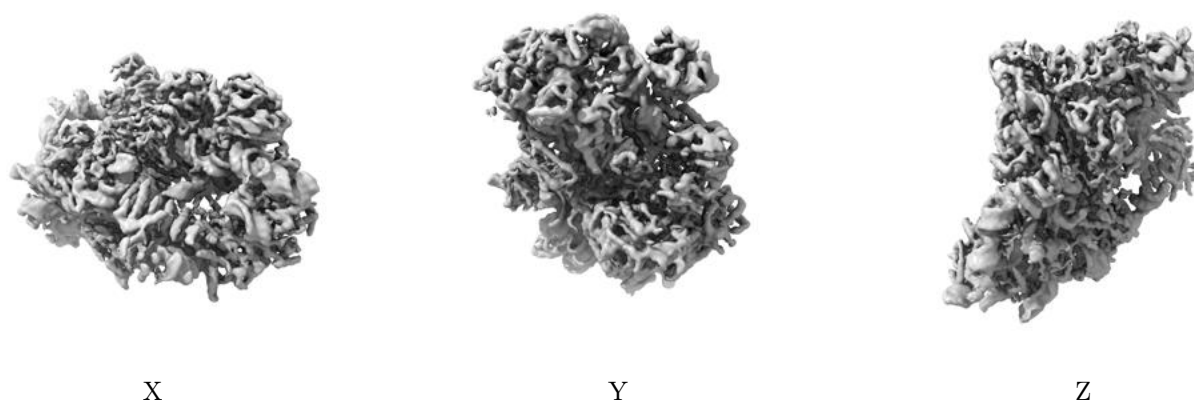
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0583. 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.

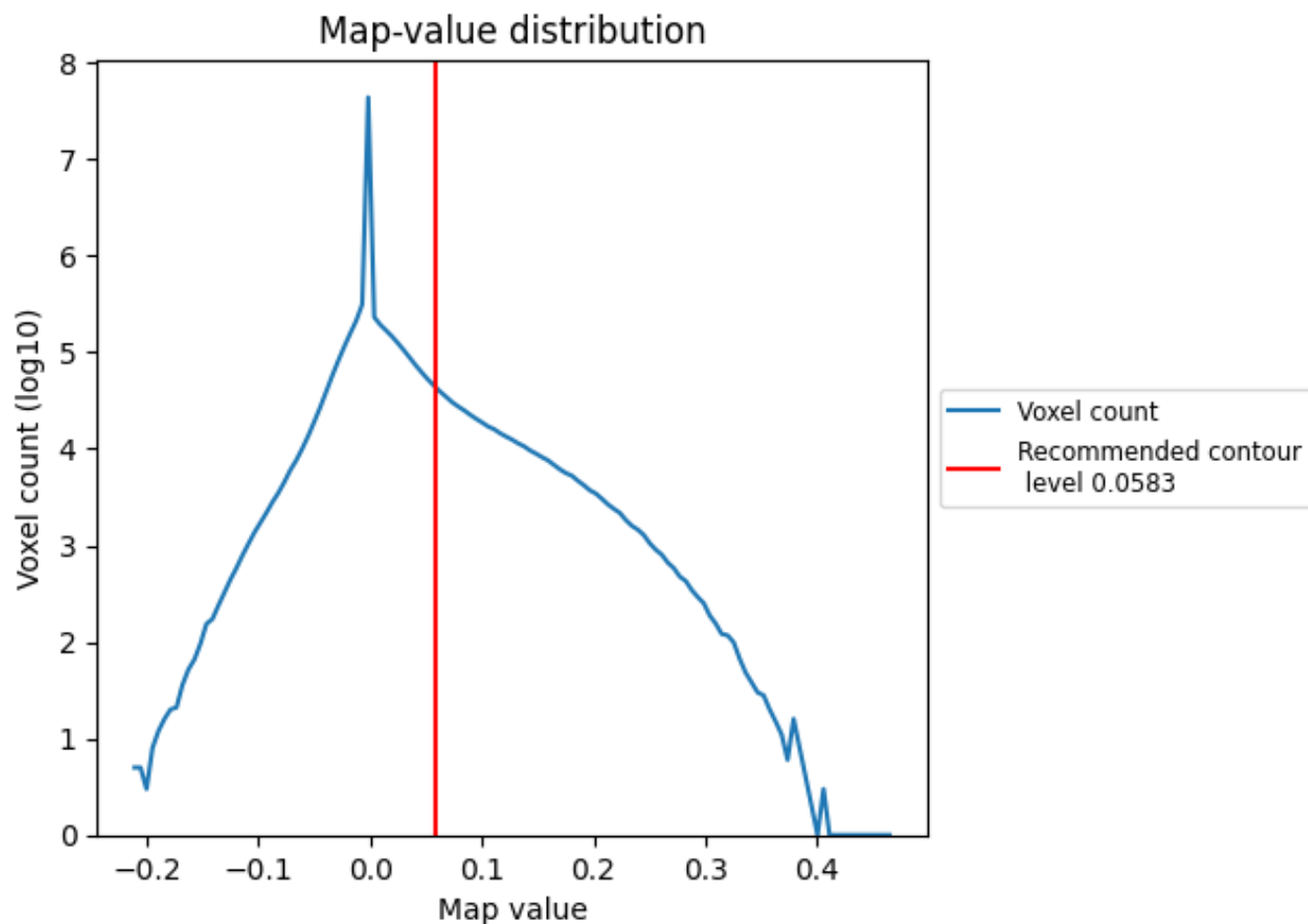
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

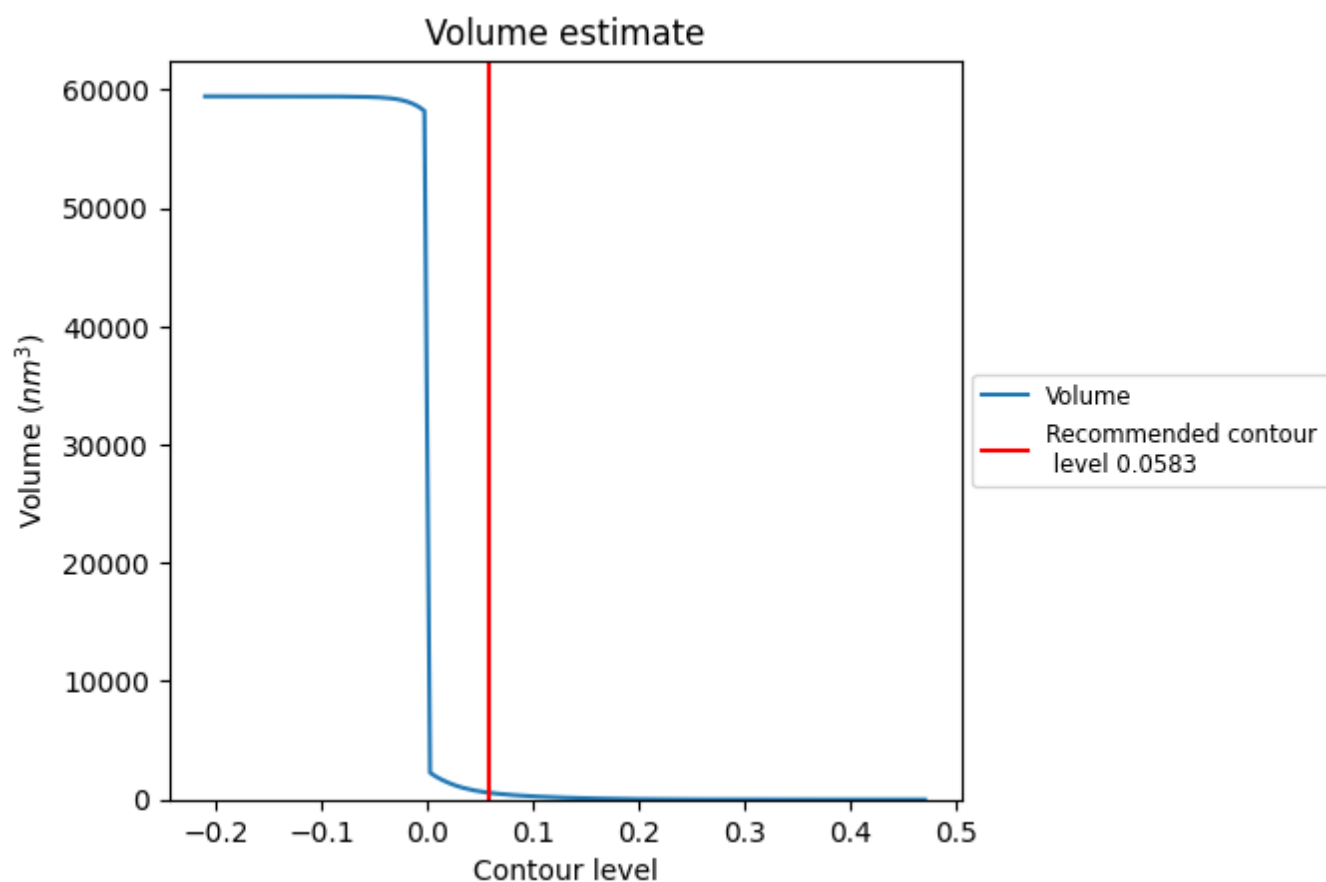
This section contains the results of statistical analysis of the map.

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.

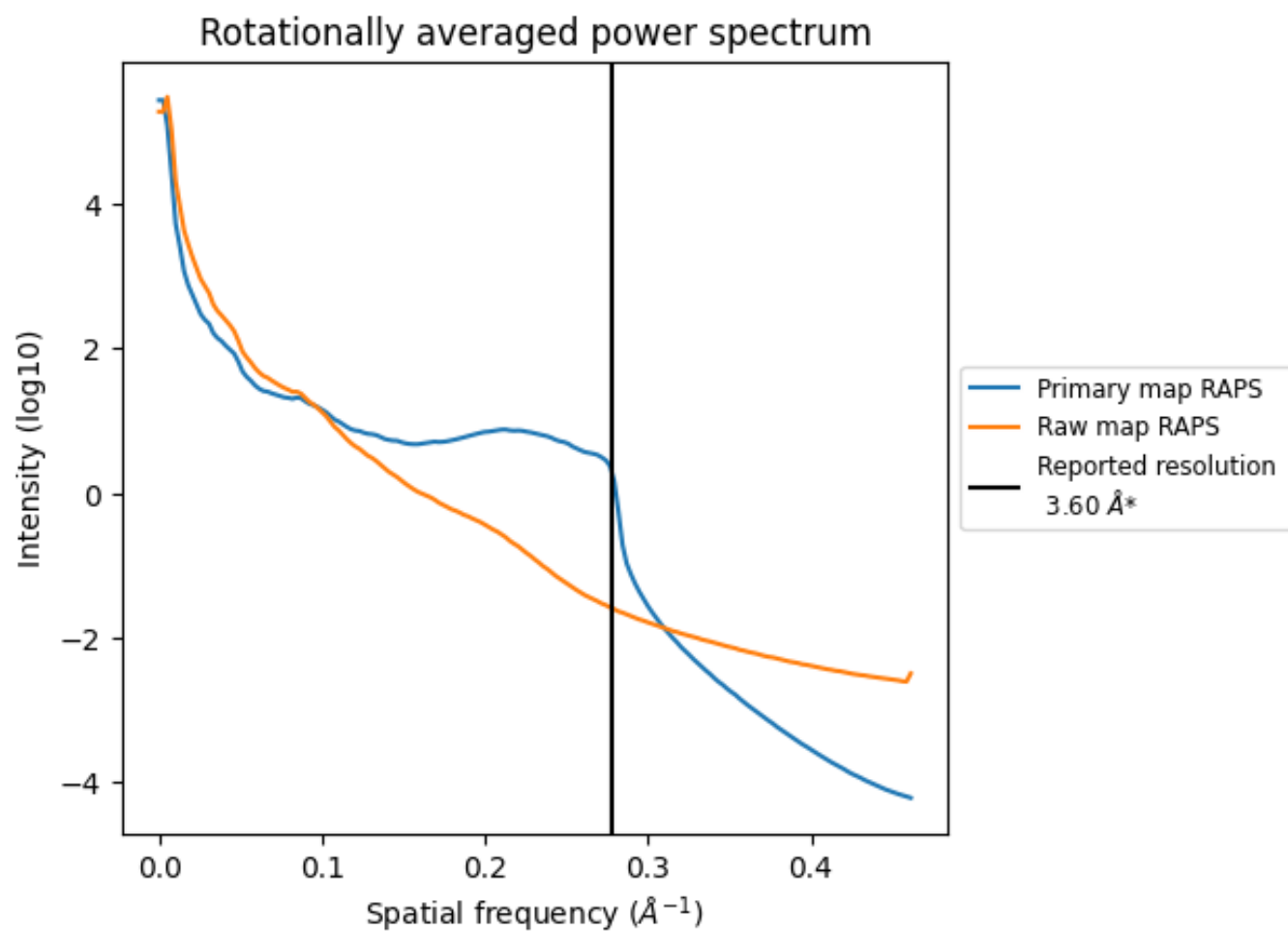
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 573 nm³; this corresponds to an approximate mass of 518 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 ⓘ

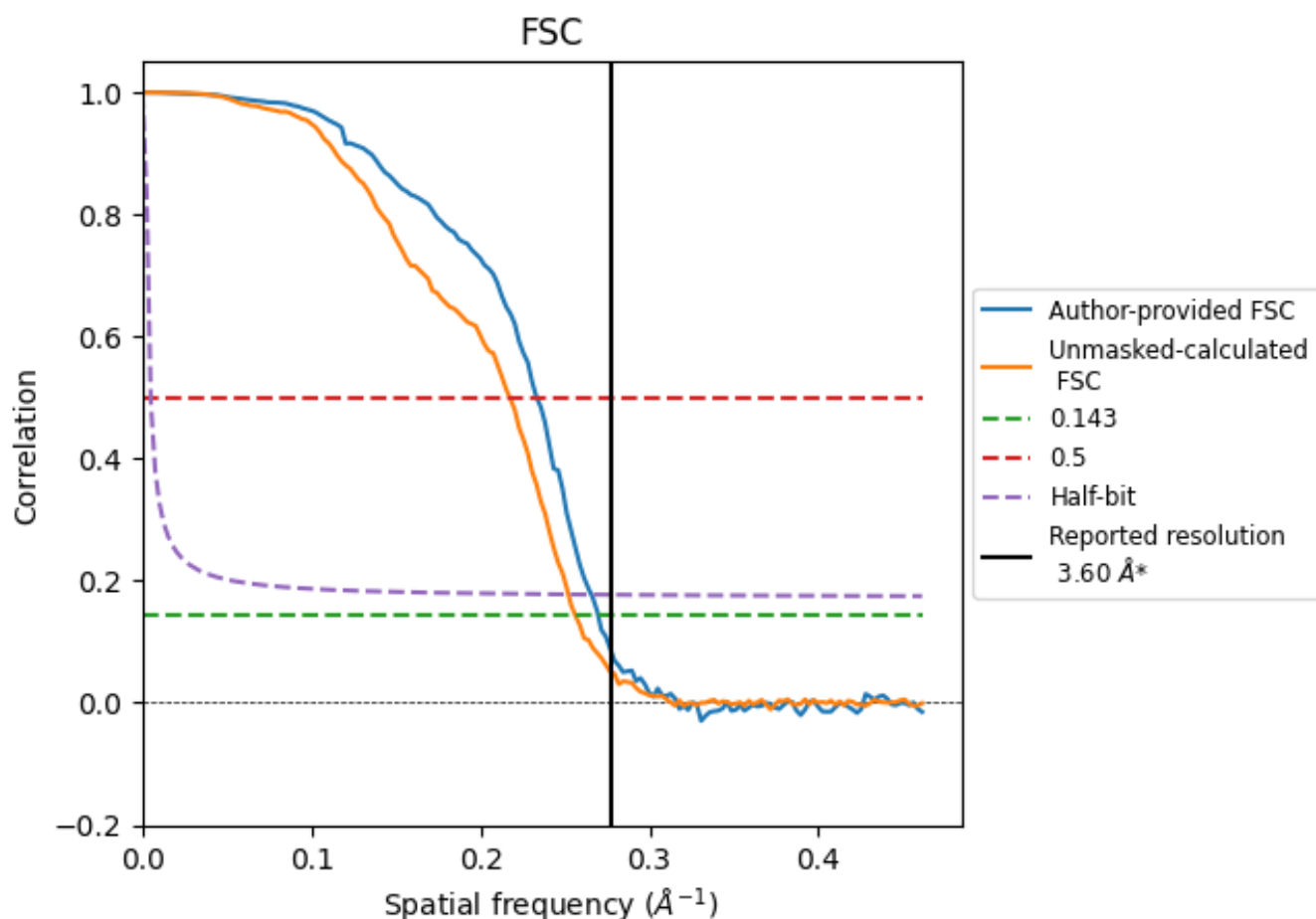


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

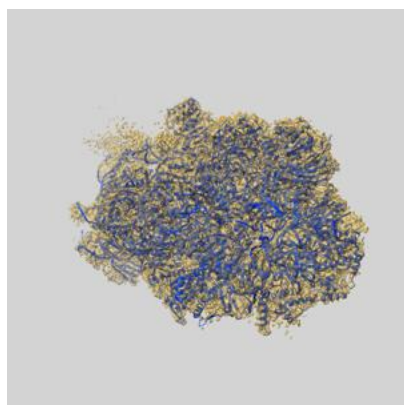
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.71	4.29	3.76
Unmasked-calculated*	3.90	4.60	3.97

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

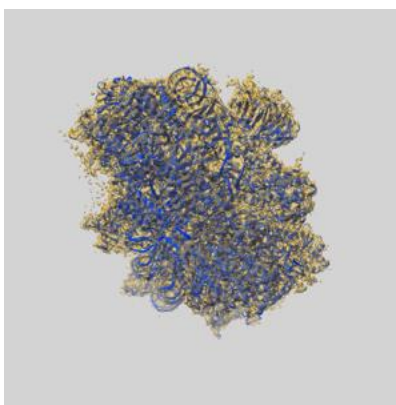
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4337 and PDB model 6G18. Per-residue inclusion information can be found in section [3](#) on page [11](#).

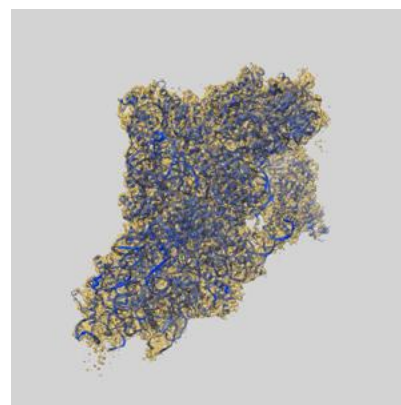
9.1 Map-model overlay [i](#)



X



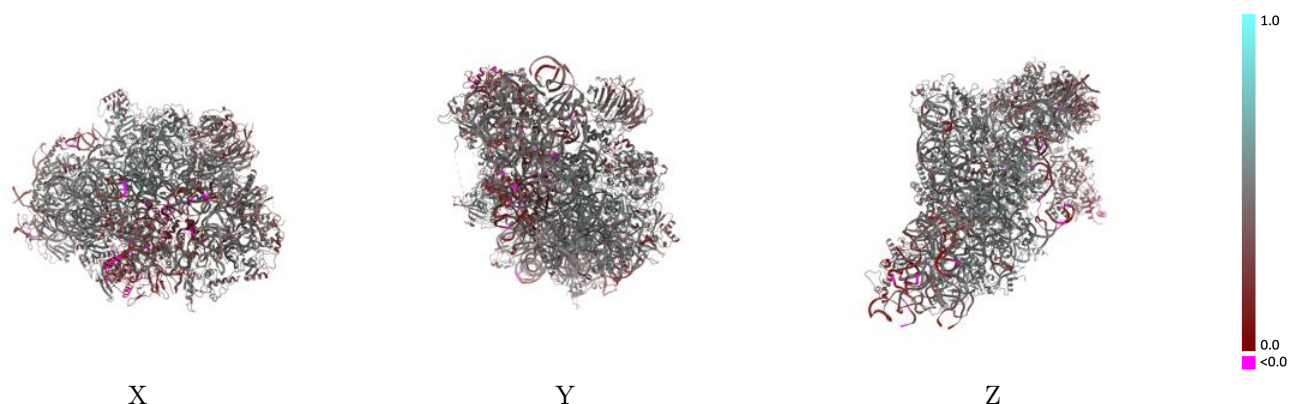
Y



Z

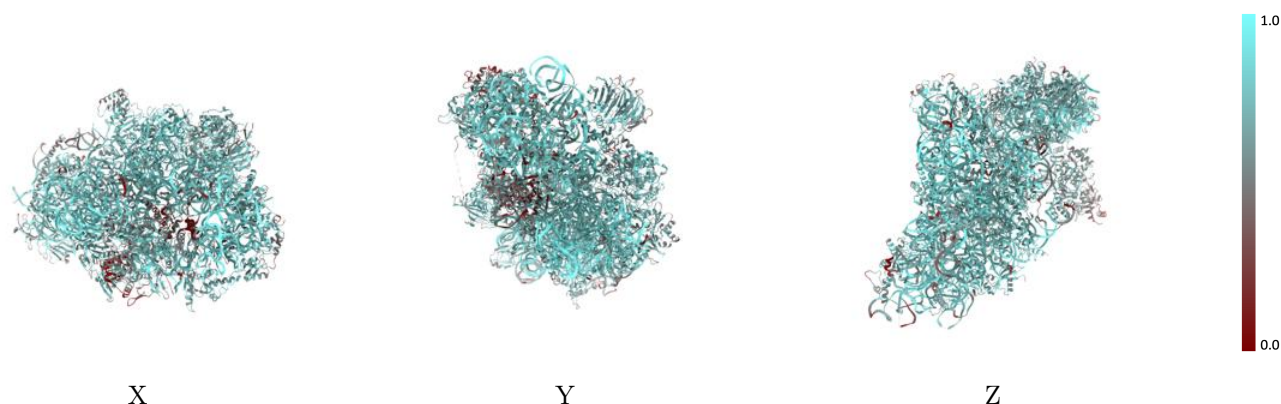
The images above show the 3D surface view of the map at the recommended contour level 0.0583 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



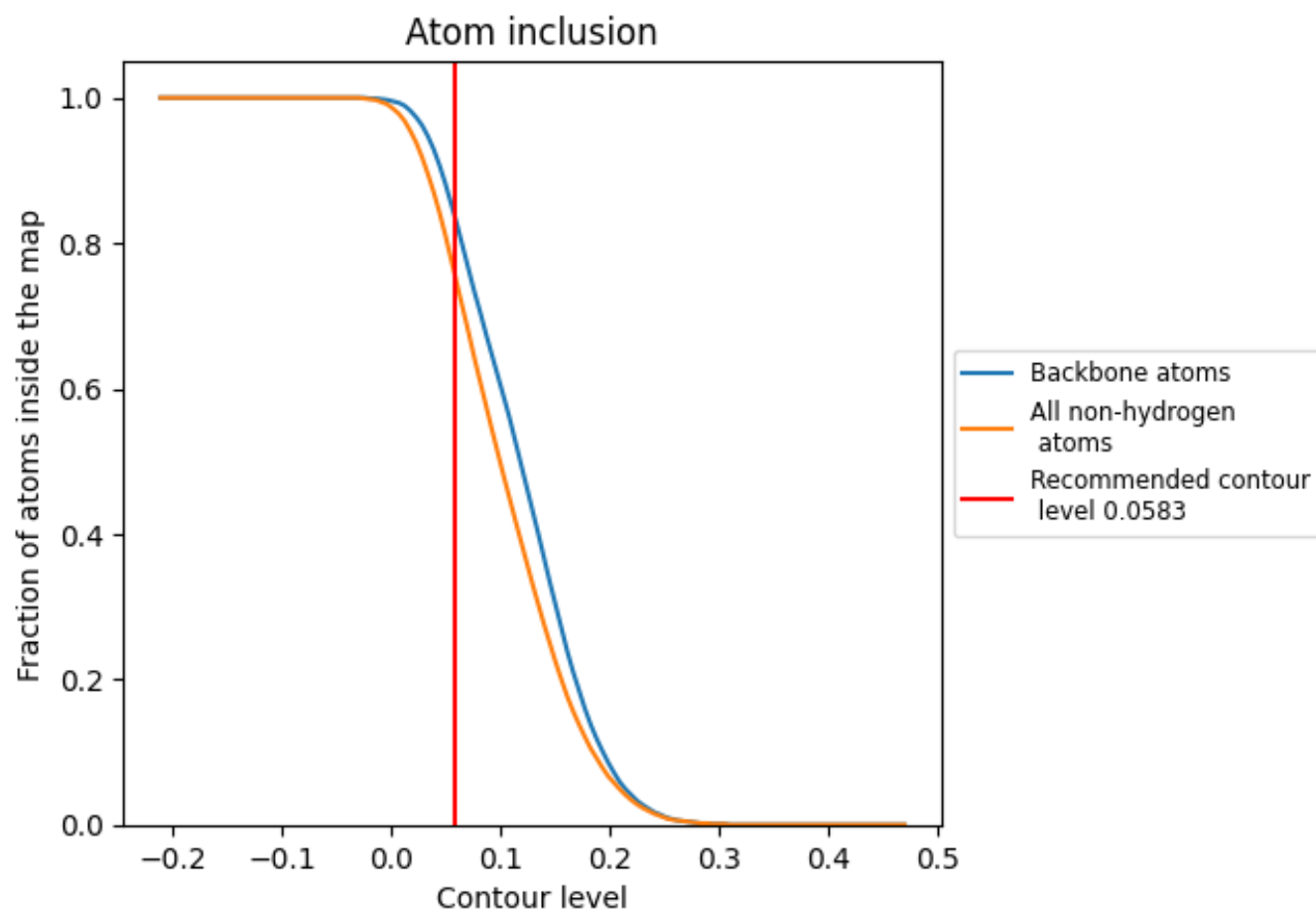
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0583).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 76% 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 (0.0583) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7590	 0.4160
2	 0.8440	 0.4090
A	 0.8090	 0.4940
B	 0.7510	 0.4600
C	 0.7660	 0.4910
E	 0.7450	 0.4680
F	 0.7270	 0.4420
G	 0.6930	 0.3970
H	 0.6580	 0.3950
I	 0.7410	 0.4350
J	 0.7880	 0.4820
L	 0.7270	 0.4580
M	 0.3300	 0.1480
N	 0.7830	 0.4590
O	 0.7350	 0.4600
P	 0.7470	 0.4540
Q	 0.7300	 0.4380
R	 0.6800	 0.4020
S	 0.6820	 0.4030
T	 0.7450	 0.4290
V	 0.7760	 0.4800
W	 0.7920	 0.4960
X	 0.7980	 0.5010
Y	 0.7570	 0.4650
Z	 0.6060	 0.3680
b	 0.7550	 0.4570
c	 0.7090	 0.4600
e	 0.6080	 0.4170
f	 0.4150	 0.2360
g	 0.6580	 0.3690
t	 0.6270	 0.3700
u	 0.7430	 0.4570
v	 0.3770	 0.2450
w	 0.6250	 0.3510
x	 0.7720	 0.4910
y	 0.7170	 0.4240

