



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:26 PM UTC

PDB ID : 8QU1 / pdb_00008qu1
EMDB ID : EMD-18460
Title : mt-LSU assembly intermediate in GTPBP8 knock-out cells, state 1
Authors : Valentin Gese, G.; Cipullo, M.; Rorbach, J.; Hallberg, B.M.
Deposited on : 2023-10-13
Resolution : 2.74 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

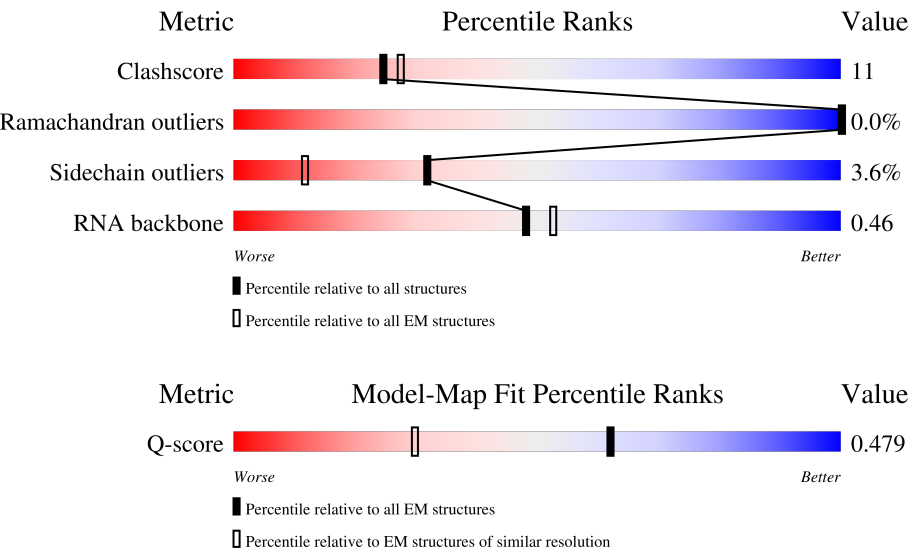
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.74 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	10492 (2.24 - 3.24)

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	A	1559	14% 33% 22% 5% 40%
2	B	69	32% 36% 35% 10% 19%
3	D	305	57% 40% 17% 43%

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Mol	Chain	Length	Quality of chain
4	E	348	
5	F	311	
6	H	267	
7	I	261	
8	J	192	
9	K	178	
10	L	145	
11	M	296	
12	N	251	
13	O	175	
14	P	180	
15	Q	292	
16	R	149	
17	S	205	
18	T	206	
19	U	153	
20	V	216	
21	W	148	
22	X	256	
23	Y	250	
24	Z	161	
25	0	188	
26	1	65	
27	2	92	
28	3	188	

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Mol	Chain	Length	Quality of chain
29	5	423	28% 52% 33% 12%
30	6	380	5% 7% 91%

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 57235 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	938	Total	C	N	O	P	0	0
			19916	8944	3614	6420	938		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3107	U	UNK	variant	GB 1025814679

- Molecule 2 is a RNA chain called mitochondrial tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	56	Total	C	N	O	P	0	0
			1191	534	214	387	56		

- Molecule 3 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	175	Total	C	N	O	S	0	0
			1363	848	262	245	8		

- Molecule 4 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	285	Total	C	N	O	S	0	0
			2258	1457	384	406	11		

- Molecule 5 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	240	Total	C	N	O	S	0	0
			1932	1244	346	336	6		

- Molecule 6 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	85	Total	C	N	O		
			713	457	138	118	0	0

- Molecule 7 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	158	Total	C	N	O	S		
			1283	828	235	210	10	0	0

- Molecule 8 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	140	Total	C	N	O	S		
			1061	680	192	187	2	0	0

- Molecule 9 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	177	Total	C	N	O	S		
			1451	934	259	251	7	0	0

- Molecule 10 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	115	Total	C	N	O	S		
			889	559	171	154	5	0	0

- Molecule 11 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	256	Total	C	N	O	S		
			2056	1329	358	364	5	0	0

- Molecule 12 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	173	Total	C	N	O	S		
			1412	907	255	241	9	0	0

- Molecule 13 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	152	Total	C	N	O	S	0	0
			1245	784	239	215	7		

- Molecule 14 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	141	Total	C	N	O	S	0	0
			1148	719	221	203	5		

- Molecule 15 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	217	Total	C	N	O	S	0	0
			1805	1159	317	320	9		

- Molecule 16 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	140	Total	C	N	O	S	0	0
			1153	732	231	186	4		

- Molecule 17 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	156	Total	C	N	O	S	0	0
			1251	806	222	219	4		

- Molecule 18 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	159	Total	C	N	O	S	0	0
			1305	835	239	224	7		

- Molecule 19 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	139	Total	C	N	O	S	0	0
			1154	734	220	197	3		

- Molecule 20 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	192	Total	C	N	O	S	0	0
			1575	1003	281	283	8		

- Molecule 21 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	101	Total	C	N	O	S	0	0
			805	520	151	131	3		

- Molecule 22 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	243	Total	C	N	O	S	0	0
			2035	1317	351	362	5		

- Molecule 23 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

- Molecule 24 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	120	Total	C	N	O	S	0	0
			978	626	183	166	3		

- Molecule 25 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 26 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	48	Total	C	N	O	S	0	0
			400	257	76	65	2		

- Molecule 27 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	38	Total	C	N	O	S	0	0
			309	193	69	46	1		

- Molecule 28 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 29 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	5	371	Total	C	N	O	S	0	0
			3022	1953	524	534	11		

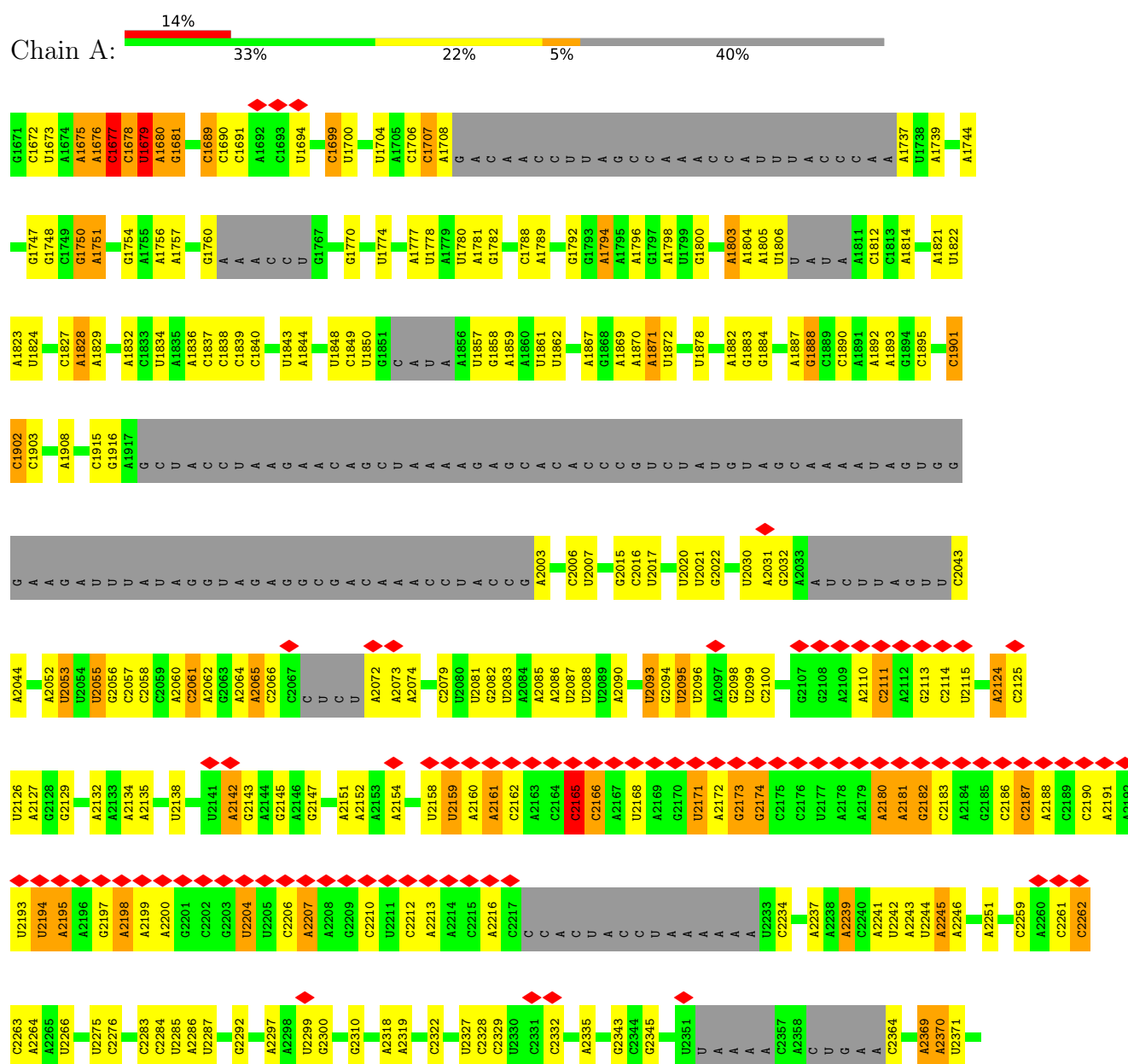
- Molecule 30 is a protein called 39S ribosomal protein L38, mitochondrial.

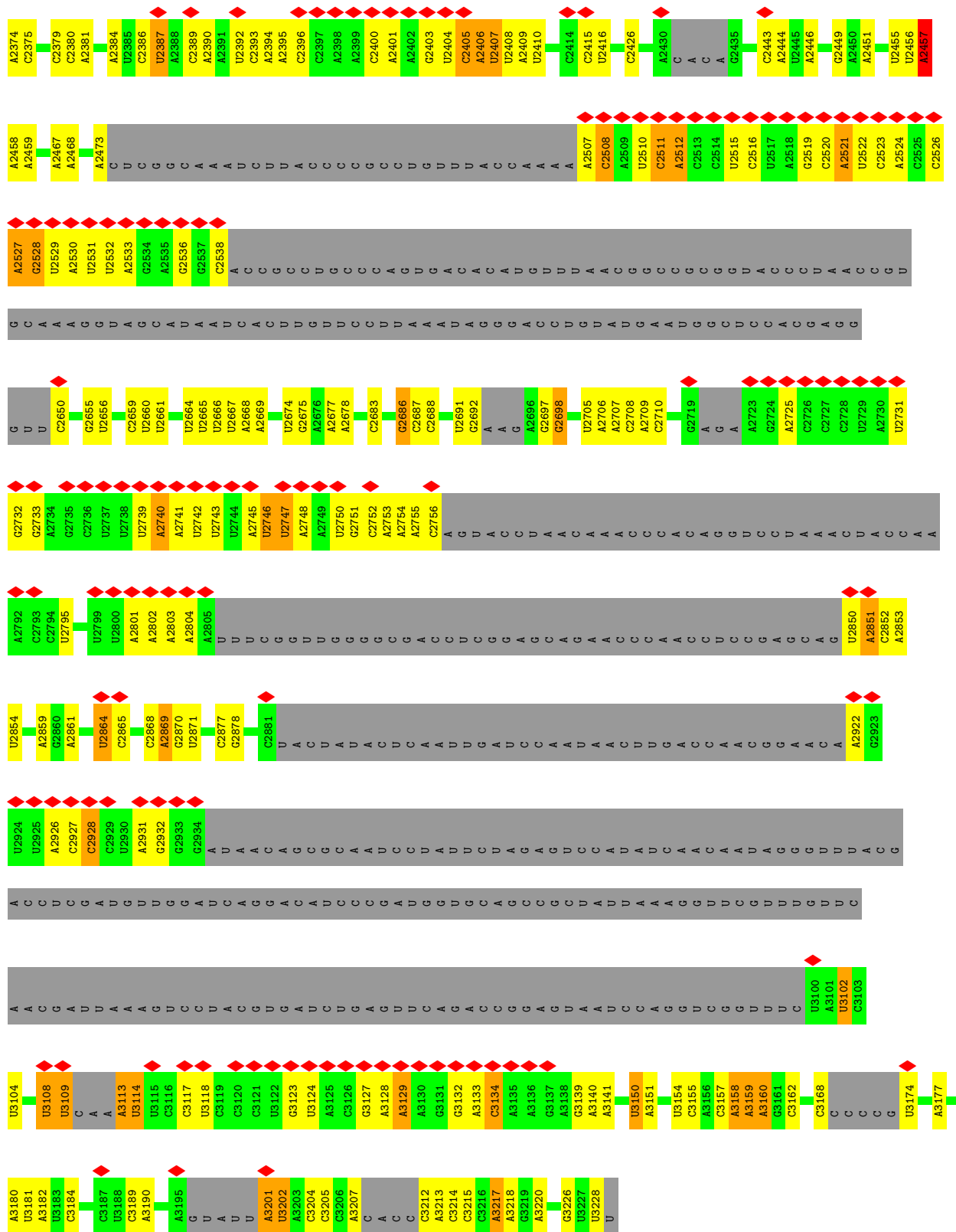
Mol	Chain	Residues	Atoms					AltConf	Trace
30	6	35	Total	C	N	O	S	0	1
			297	182	62	52	1		

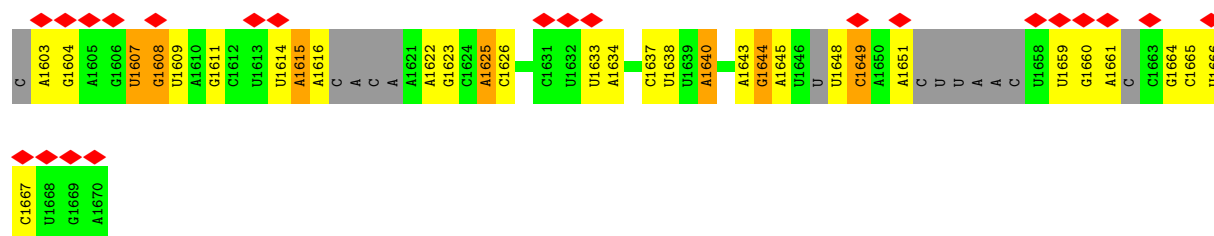
3 Residue-property plots

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

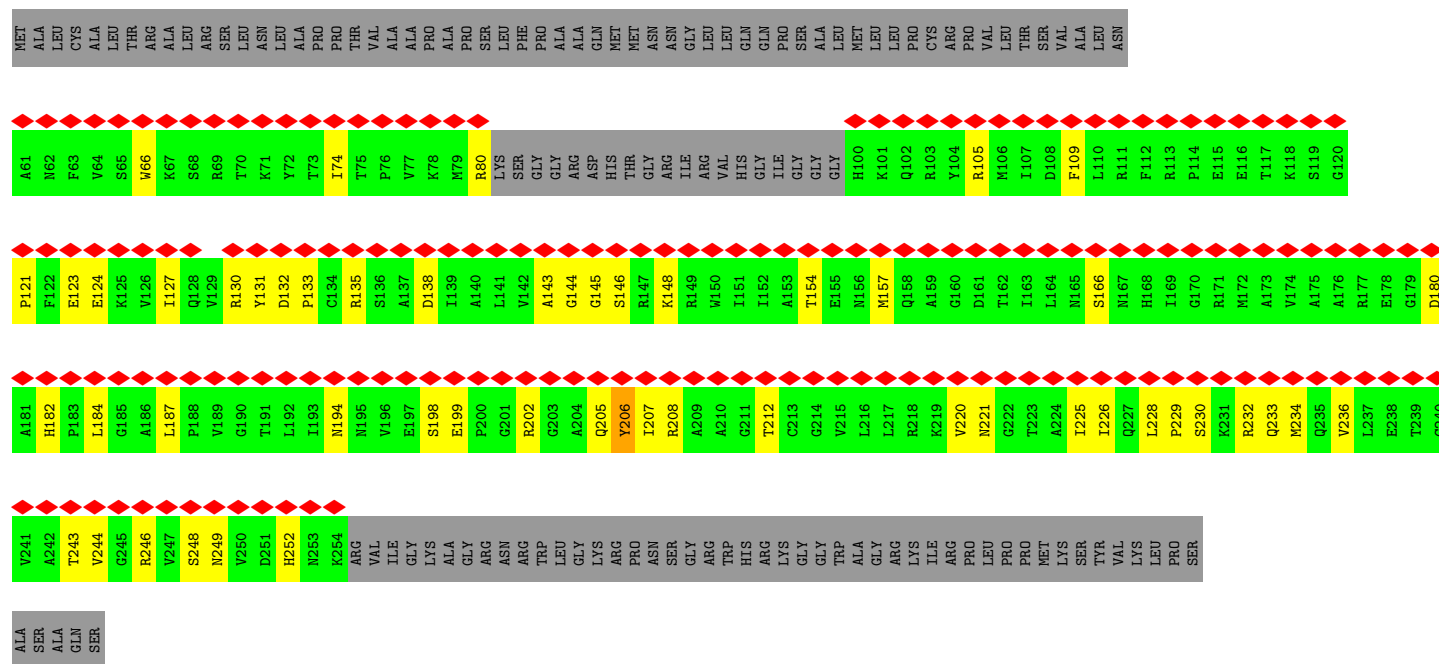
• Molecule 1: 16S ribosomal RNA



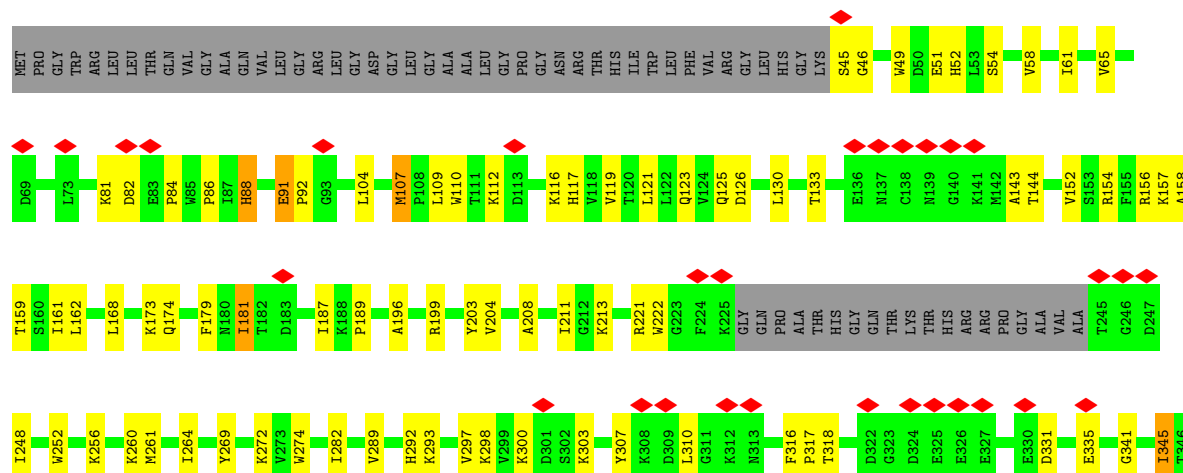


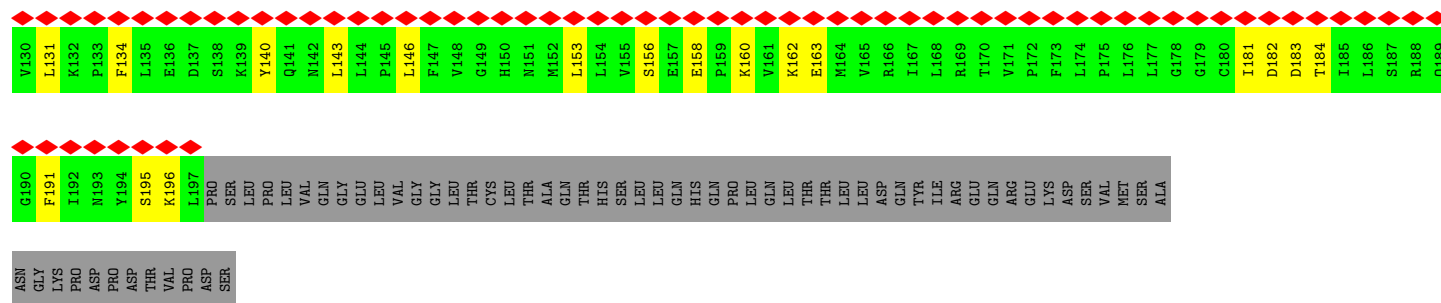


• Molecule 3: 39S ribosomal protein L2, mitochondrial

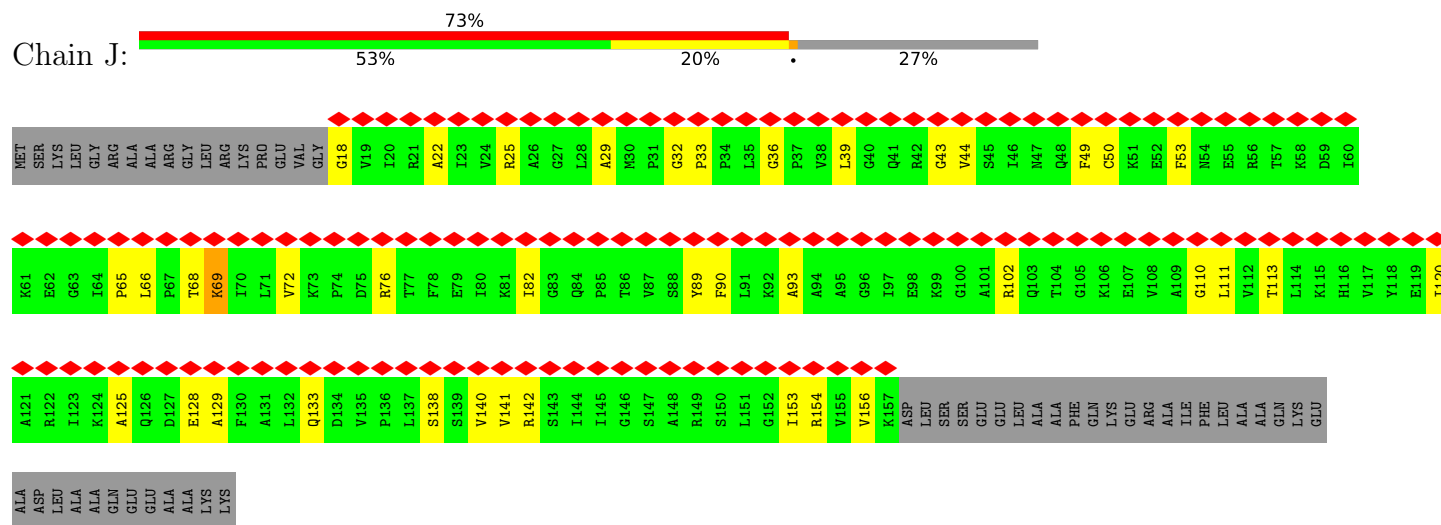


• Molecule 4: 39S ribosomal protein L3, mitochondrial

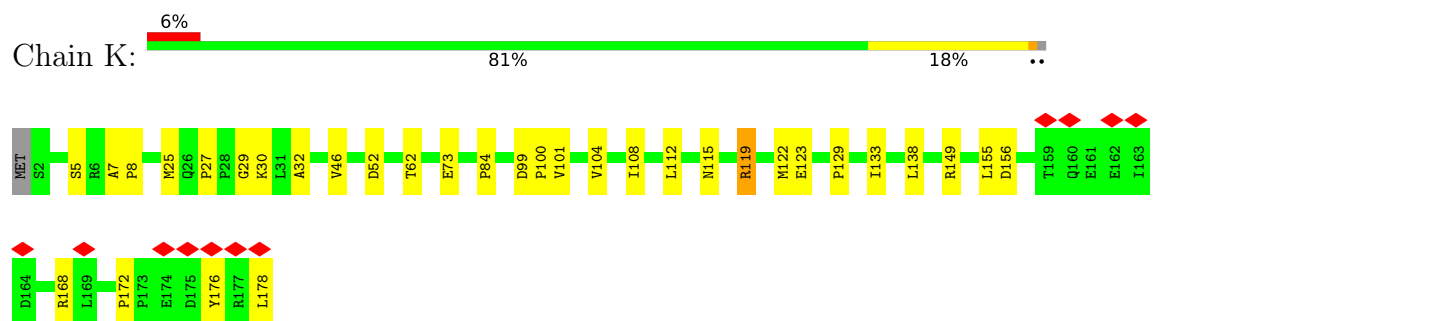




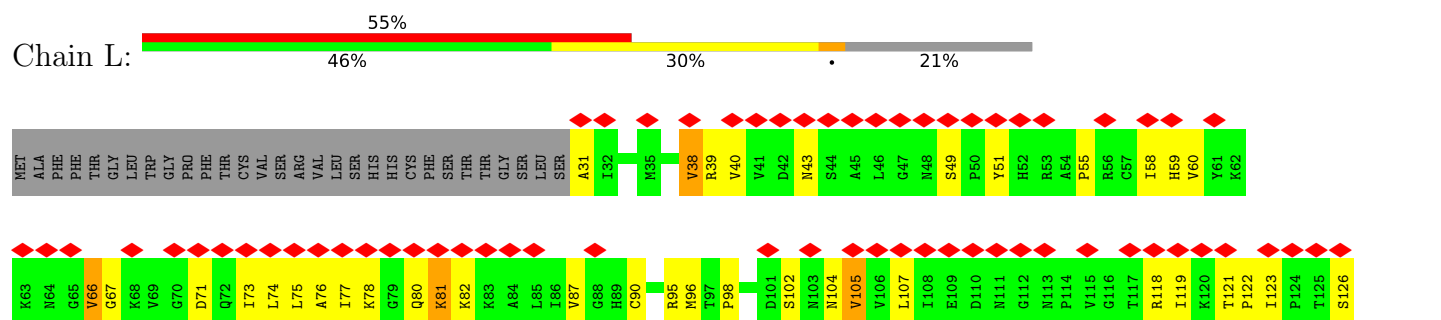
- Molecule 8: 39S ribosomal protein L11, mitochondrial



- Molecule 9: 39S ribosomal protein L13, mitochondrial

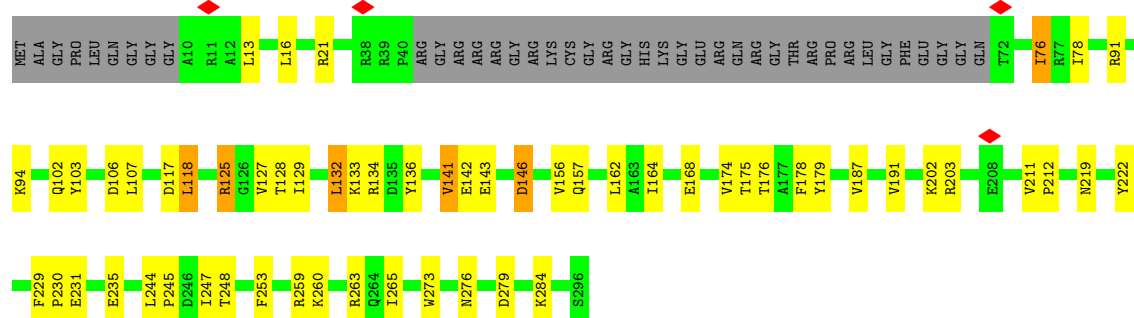


- Molecule 10: 39S ribosomal protein L14, mitochondrial

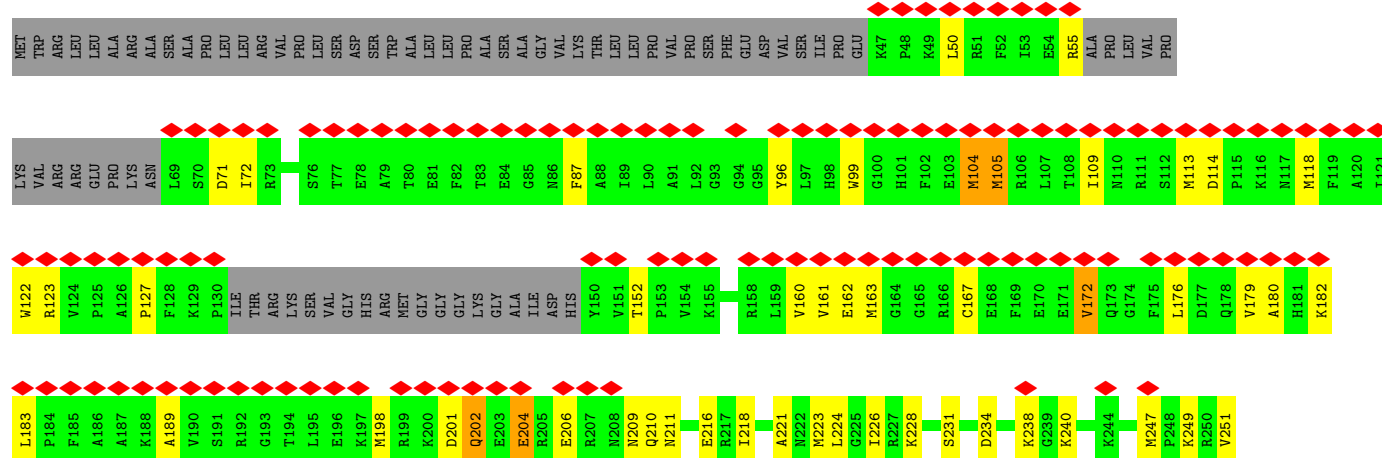




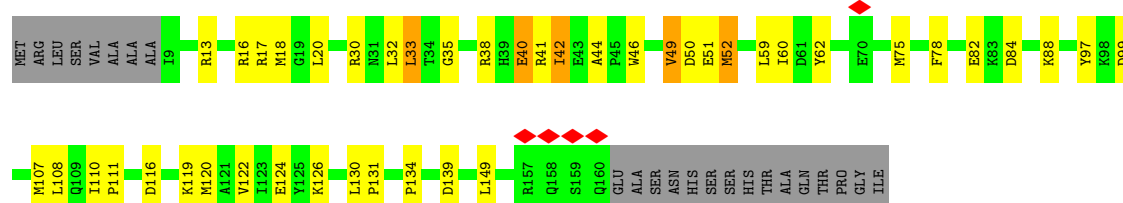
- Molecule 11: 39S ribosomal protein L15, mitochondrial



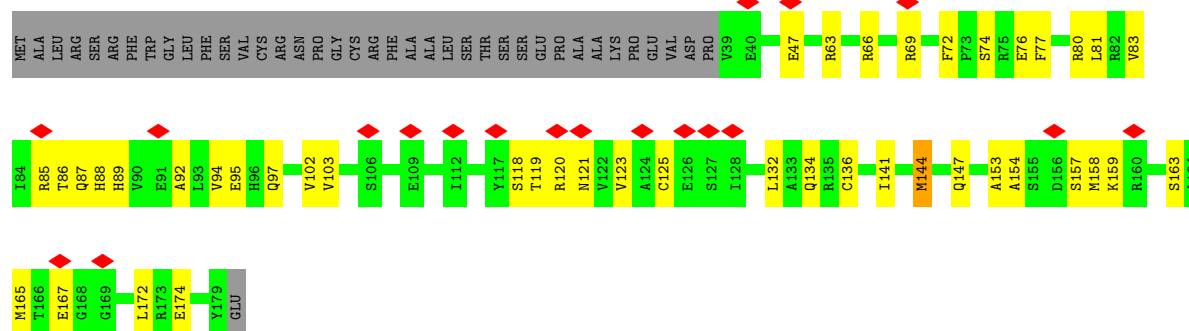
- Molecule 12: 39S ribosomal protein L16, mitochondrial



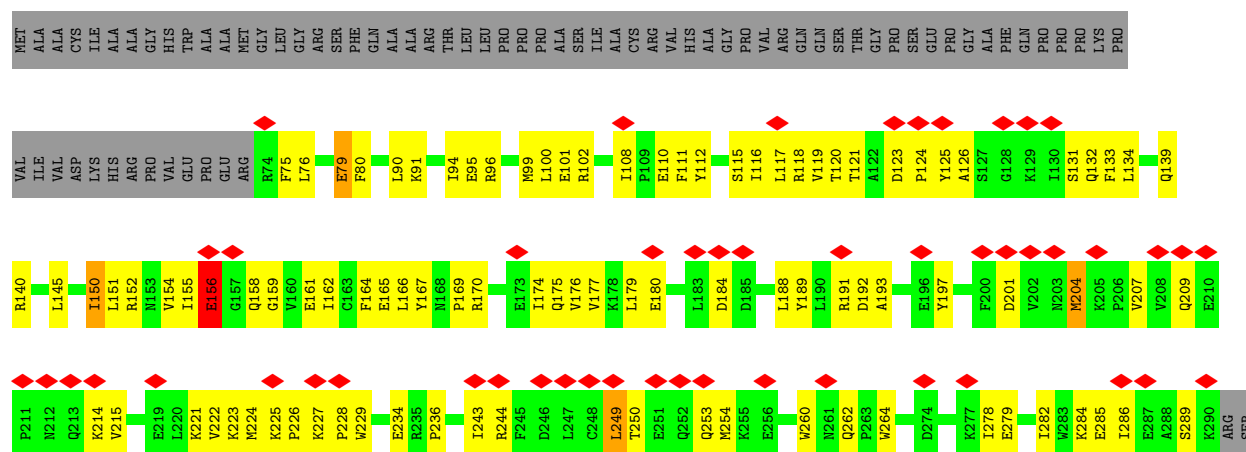
- Molecule 13: 39S ribosomal protein L17, mitochondrial



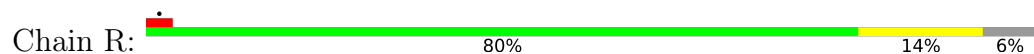
- Molecule 14: 39S ribosomal protein L18, mitochondrial



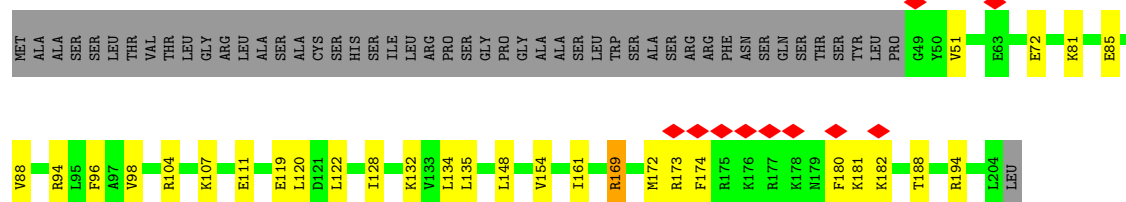
- Molecule 15: 39S ribosomal protein L19, mitochondrial



- Molecule 16: 39S ribosomal protein L20, mitochondrial

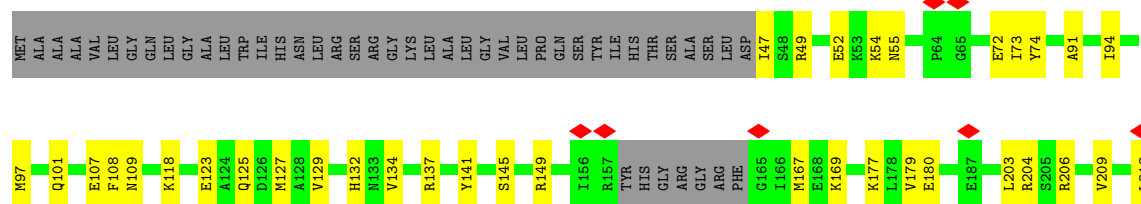


- Molecule 17: 39S ribosomal protein L21, mitochondrial



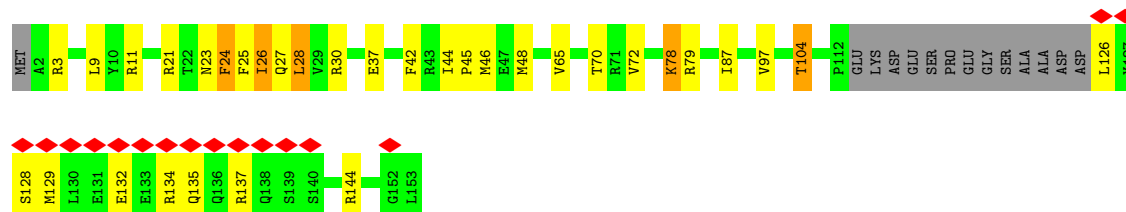
- Molecule 18: 39S ribosomal protein L22, mitochondrial

Chain T: 



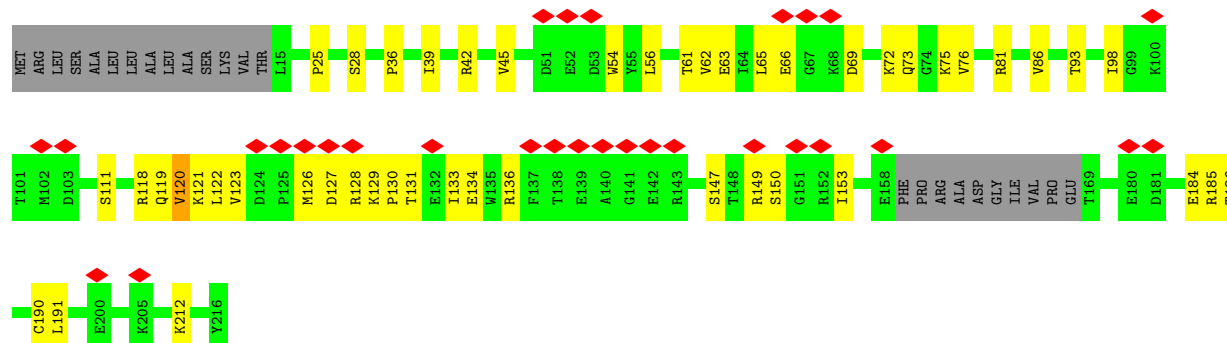
- Molecule 19: 39S ribosomal protein L23, mitochondrial

Chain U: 



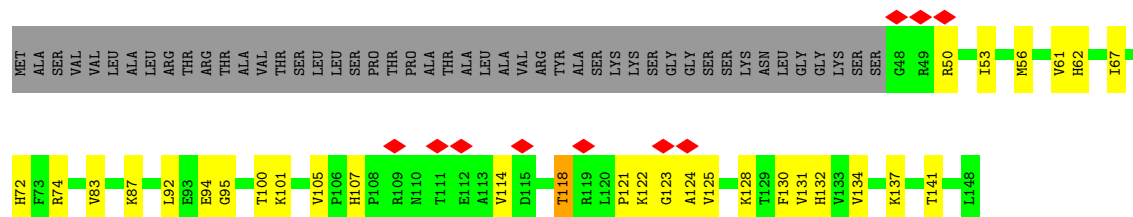
- Molecule 20: 39S ribosomal protein L24, mitochondrial

Chain V: 



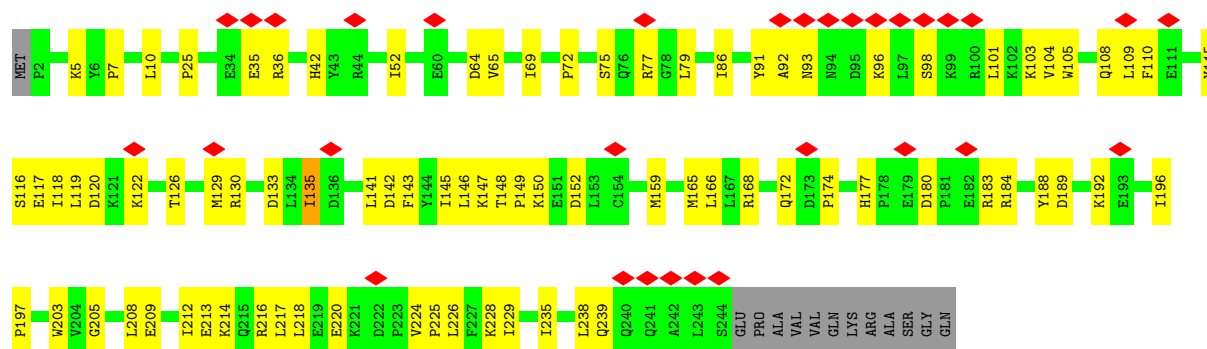
- Molecule 21: 39S ribosomal protein L27, mitochondrial

Chain W: 



- Molecule 22: 39S ribosomal protein L28, mitochondrial

Chain X: 



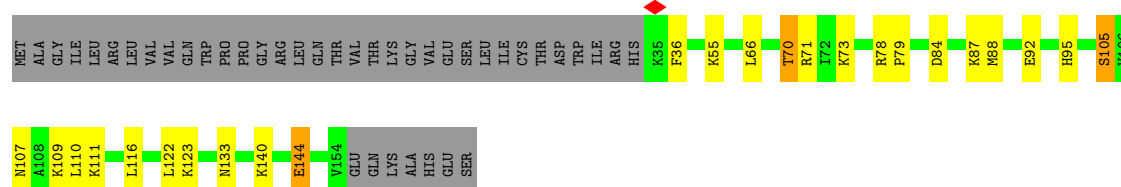
- Molecule 23: 39S ribosomal protein L47, mitochondrial

Chain Y: 57% 13% 30%



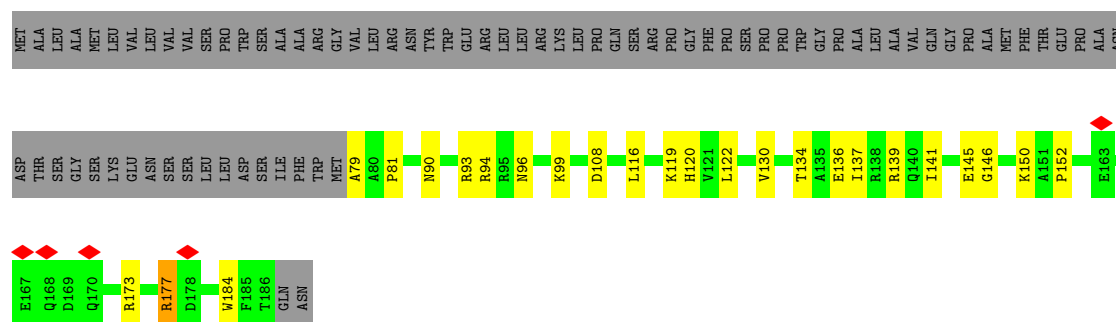
- Molecule 24: 39S ribosomal protein L30, mitochondrial

Chain Z: 60% 13% 25%

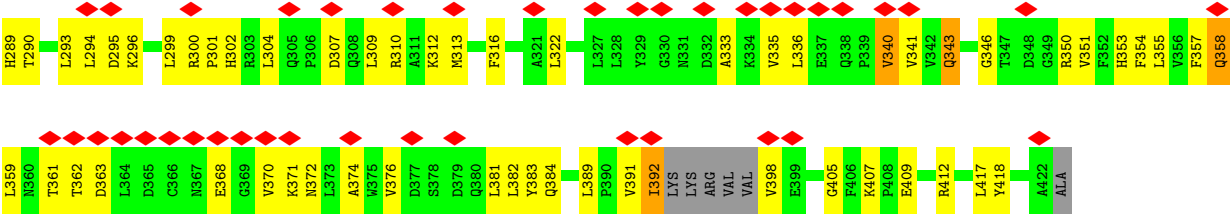


- Molecule 25: 39S ribosomal protein L32, mitochondrial

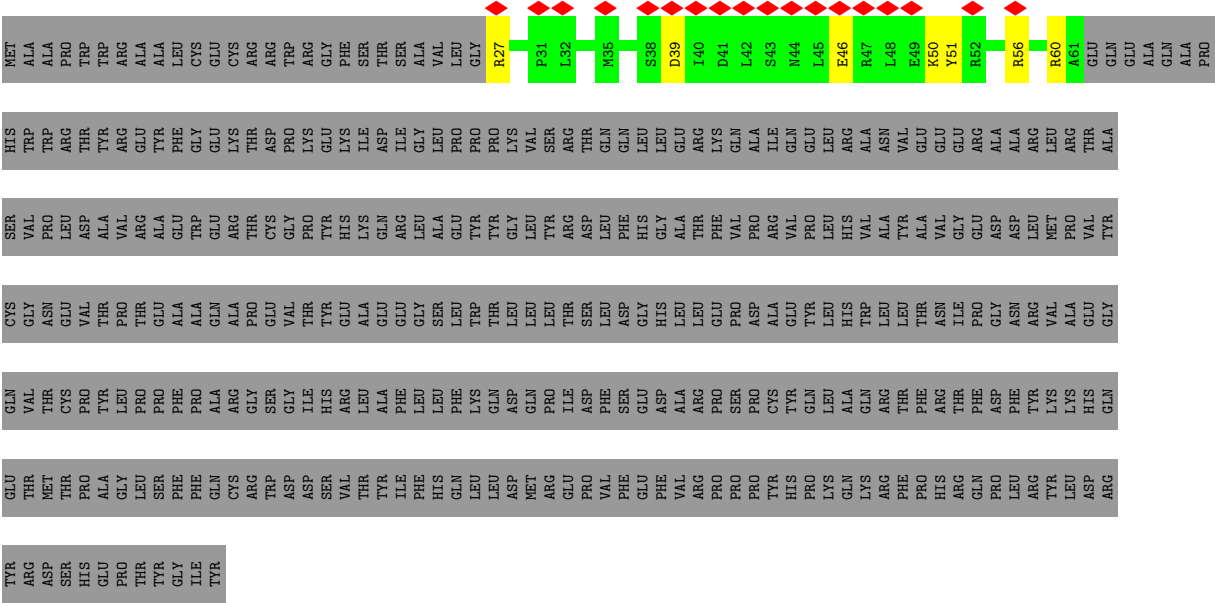
Chain 0: 44% 13% 43%



- Molecule 26: 39S ribosomal protein L33, mitochondrial



• Molecule 30: 39S ribosomal protein L38, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41197	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.126	Depositor
Minimum map value	-0.839	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	606.0, 606.0, 606.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.60	0/22270	0.81	17/34610 (0.0%)
2	B	0.50	0/1328	0.59	0/2056
3	D	0.47	0/1385	0.81	0/1867
4	E	0.45	0/2322	0.55	0/3148
5	F	0.62	0/1986	0.69	0/2701
6	H	0.42	0/726	0.58	0/974
7	I	0.45	0/1308	0.76	3/1761 (0.2%)
8	J	0.45	0/1077	0.67	1/1452 (0.1%)
9	K	0.56	0/1495	0.62	0/2029
10	L	0.41	0/904	0.54	0/1218
11	M	0.55	0/2106	0.67	0/2855
12	N	0.41	0/1448	0.49	0/1945
13	O	0.54	0/1269	0.65	0/1708
14	P	0.44	0/1173	0.56	0/1588
15	Q	0.40	0/1846	0.61	0/2487
16	R	0.71	1/1174 (0.1%)	0.80	1/1572 (0.1%)
17	S	0.61	0/1276	0.70	0/1729
18	T	0.63	0/1335	0.67	0/1796
19	U	0.54	0/1183	0.73	0/1600
20	V	0.44	0/1616	0.57	0/2189
21	W	0.51	0/827	0.57	0/1118
22	X	0.42	0/2090	0.59	0/2825
23	Y	0.50	0/1552	0.60	0/2079
24	Z	0.57	0/1003	0.67	0/1354
25	0	0.53	0/895	0.64	0/1201
26	1	0.37	0/405	0.56	0/539
27	2	0.63	0/314	0.70	0/416
28	3	0.56	0/852	0.64	0/1136
29	5	0.42	0/3110	0.59	0/4237
30	6	0.41	0/303	0.61	0/406
All	All	0.54	1/60578 (0.0%)	0.71	22/86596 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	F	0	1
8	J	0	1
9	K	0	1
11	M	0	1
17	S	0	1
18	T	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	R	12	ASN	C-O	-5.09	1.18	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2527	A	OP2-P-O3'	-9.80	78.60	108.00
1	A	2165	C	C2'-C3'-O3'	7.98	121.47	109.50
1	A	1675	A	O3'-P-O5'	-7.20	93.20	104.00
1	A	2162	C	O3'-P-O5'	6.83	114.24	104.00
1	A	2527	A	C4'-C3'-O3'	-6.82	102.77	113.00
1	A	2457	A	C2'-C3'-O3'	6.55	119.33	109.50
1	A	2162	C	C4'-C3'-O3'	-6.55	103.18	113.00
1	A	2369	A	P-O5'-C5'	-6.49	111.16	120.90
1	A	2162	C	OP2-P-O3'	-6.38	88.85	108.00
7	I	102	VAL	N-CA-C	-6.09	107.32	113.47
1	A	2159	U	O3'-P-O5'	-6.00	95.00	104.00
1	A	2869	A	O3'-P-O5'	-5.97	95.05	104.00
7	I	182	ASP	CA-CB-CG	5.92	118.52	112.60
7	I	183	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	2527	A	O3'-P-O5'	5.69	112.53	104.00
8	J	33	PRO	N-CA-C	5.63	117.57	110.70
1	A	1679	U	O3'-P-O5'	-5.54	95.70	104.00
1	A	1678	C	P-O5'-C5'	-5.51	112.64	120.90
1	A	1677	C	O3'-P-O5'	-5.45	95.82	104.00
16	R	12	ASN	OD1-CG-ND2	5.38	127.98	122.60
1	A	1680	A	P-O5'-C5'	-5.32	112.93	120.90
1	A	2527	A	OP1-P-O3'	5.09	123.26	108.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	F	281	ARG	Sidechain
8	J	69	LYS	Peptide
9	K	119	ARG	Sidechain
11	M	125	ARG	Sidechain
17	S	169	ARG	Sidechain
18	T	204	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	19916	0	10138	302	0
2	B	1191	0	607	22	0
3	D	1363	0	1393	90	0
4	E	2258	0	2264	57	0
5	F	1932	0	1961	52	0
6	H	713	0	764	27	0
7	I	1283	0	1370	23	0
8	J	1061	0	1141	22	0
9	K	1451	0	1448	22	0
10	L	889	0	941	36	0
11	M	2056	0	2120	39	0
12	N	1412	0	1418	36	0
13	O	1245	0	1283	32	0
14	P	1148	0	1148	29	0
15	Q	1805	0	1841	75	0
16	R	1153	0	1214	13	0
17	S	1251	0	1322	21	0
18	T	1305	0	1352	28	0
19	U	1154	0	1154	23	0
20	V	1575	0	1583	29	0
21	W	805	0	829	25	0
22	X	2035	0	2054	65	0
23	Y	1517	0	1561	27	0
24	Z	978	0	1030	16	0
25	0	880	0	906	24	0
26	1	400	0	435	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	2	309	0	344	8	0
28	3	831	0	883	18	0
29	5	3022	0	3007	117	0
30	6	297	0	297	17	0
All	All	57235	0	47808	1105	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 11.

All (1105) 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:A:2521:A:N6	3:D:202:ARG:O	1.65	1.27
3:D:143:ALA:O	29:5:259:ILE:HD11	1.36	1.22
1:A:2015:G:N2	1:A:2931:A:O2'	1.79	1.14
1:A:2528:G:OP1	3:D:109:PHE:HE2	1.32	1.11
1:A:2528:G:OP1	3:D:109:PHE:CE2	2.06	1.08
1:A:2528:G:H3'	3:D:208:ARG:HH21	1.18	1.03
1:A:2015:G:H21	1:A:2931:A:C2'	1.73	1.00
13:O:38:ARG:HH12	13:O:82:GLU:HG3	1.25	0.98
16:R:141:ILE:HD12	17:S:72:GLU:HG2	1.48	0.93
1:A:1908:A:H2	1:A:2733:G:C4'	1.84	0.90
2:B:1607:U:H3	2:B:1664:G:H1	0.90	0.90
1:A:3174:U:H6	1:A:3174:U:P	1.96	0.89
21:W:122:LYS:O	30:6:60:ARG:NH1	2.06	0.87
1:A:2111:C:OP1	7:I:35:ARG:NH2	2.07	0.87
1:A:2161:A:C2	1:A:3182:A:C2	2.63	0.87
1:A:1679:U:H5'	20:V:42:ARG:HD3	1.55	0.86
1:A:3174:U:OP1	1:A:3174:U:C6	2.29	0.85
25:O:119:LYS:O	25:O:120:HIS:ND1	2.09	0.85
1:A:2529:U:C6	3:D:205:GLN:O	2.30	0.85
1:A:1908:A:C2	1:A:2733:G:H4'	2.13	0.84
1:A:1908:A:H2	1:A:2733:G:O4'	1.60	0.83
3:D:143:ALA:O	29:5:259:ILE:CD1	2.25	0.82
4:E:61:ILE:HD11	13:O:149:LEU:HD22	1.61	0.82
1:A:2406:A:O2'	29:5:110:ARG:NH2	2.13	0.82
7:I:123:MET:HA	7:I:153:LEU:O	1.80	0.82
1:A:1778:U:C5	5:F:121:ARG:HD2	2.14	0.82
1:A:2161:A:C2	1:A:3182:A:N3	2.49	0.81
1:A:1908:A:C2	1:A:2733:G:C4'	2.64	0.81
3:D:143:ALA:C	29:5:259:ILE:HD11	2.04	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2521:A:C2	3:D:202:ARG:CZ	2.65	0.80
5:F:281:ARG:NH2	11:M:128:THR:OG1	2.14	0.79
1:A:2526:C:P	1:A:2533:A:H4'	2.22	0.79
1:A:3174:U:P	1:A:3174:U:C6	2.77	0.78
1:A:2528:G:H5''	3:D:135:ARG:NH2	1.99	0.78
1:A:2528:G:H5''	3:D:135:ARG:HH21	1.48	0.78
1:A:2743:U:H5''	22:X:93:ASN:HD21	1.48	0.78
1:A:2521:A:C8	3:D:205:GLN:HG2	2.19	0.77
13:O:108:LEU:HD13	25:O:122:LEU:HD11	1.67	0.77
1:A:3174:U:H6	1:A:3174:U:OP1	1.65	0.77
10:L:87:VAL:HG11	10:L:123:ILE:HG12	1.67	0.76
15:Q:224:MET:HE1	15:Q:243:ILE:HD12	1.66	0.76
29:5:242:ARG:HA	29:5:242:ARG:NH1	2.00	0.76
1:A:2529:U:O2'	3:D:206:TYR:HA	1.86	0.76
1:A:2521:A:C4	3:D:205:GLN:OE1	2.38	0.75
1:A:2529:U:C5	3:D:205:GLN:O	2.39	0.75
6:H:86:THR:HG23	6:H:89:ARG:HH21	1.49	0.75
1:A:2073:A:OP2	30:6:27:ARG:N	2.20	0.75
5:F:262:THR:HG22	5:F:264:PRO:HD2	1.68	0.75
1:A:2521:A:N7	3:D:205:GLN:HG2	2.01	0.75
30:6:46:GLU:OE1	30:6:46:GLU:N	2.19	0.74
1:A:2528:G:H3'	3:D:208:ARG:NH2	2.00	0.74
29:5:313:MET:HE1	29:5:353:HIS:HB2	1.67	0.74
3:D:143:ALA:C	29:5:259:ILE:CD1	2.61	0.73
1:A:2521:A:C5	3:D:205:GLN:OE1	2.41	0.73
4:E:133:THR:OG1	4:E:144:THR:OG1	2.06	0.73
19:U:46:MET:HE1	19:U:72:VAL:HG13	1.71	0.73
21:W:123:GLY:C	30:6:60:ARG:HH22	1.96	0.73
1:A:1777:A:N6	1:A:1780:U:OP2	2.22	0.72
1:A:1782:G:O6	5:F:121:ARG:HD3	1.89	0.72
1:A:2528:G:C8	1:A:2528:G:OP2	2.42	0.72
29:5:341:VAL:HG22	29:5:358:GLN:HG2	1.70	0.72
1:A:1916:G:N2	1:A:2003:A:N1	2.38	0.72
15:Q:108:ILE:HD12	15:Q:166:LEU:HD22	1.71	0.72
21:W:122:LYS:C	30:6:60:ARG:HH12	1.98	0.72
22:X:142:ASP:O	22:X:146:LEU:HD12	1.89	0.71
1:A:1916:G:H22	1:A:2003:A:H2	1.36	0.71
5:F:83:HIS:HB3	5:F:86:VAL:HG12	1.72	0.71
7:I:140:TYR:HB3	7:I:143:LEU:HB2	1.72	0.71
22:X:166:LEU:HD23	22:X:196:ILE:HG21	1.72	0.71
3:D:144:GLY:HA2	29:5:259:ILE:CD1	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2529:U:OP2	3:D:208:ARG:NE	2.23	0.71
6:H:131:TYR:O	6:H:136:ASN:ND2	2.23	0.71
12:N:218:ILE:HA	12:N:223:MET:HG3	1.73	0.70
14:P:94:VAL:HG22	14:P:144:MET:HE1	1.73	0.70
19:U:128:SER:OG	19:U:129:MET:SD	2.49	0.70
1:A:2161:A:C2	1:A:3182:A:C4	2.79	0.70
22:X:224:VAL:HG13	22:X:229:ILE:HD11	1.73	0.70
14:P:81:LEU:HB2	14:P:144:MET:HE2	1.74	0.69
1:A:2161:A:N3	1:A:3182:A:C2	2.61	0.69
1:A:1890:C:OP2	28:3:168:ARG:NH1	2.24	0.69
22:X:118:ILE:HG21	22:X:165:MET:HG2	1.75	0.69
3:D:132:ASP:OD2	3:D:135:ARG:NH1	2.26	0.69
19:U:24:PHE:HB2	19:U:45:PRO:HG3	1.73	0.69
4:E:345:ILE:HD12	4:E:347:PHE:HE1	1.58	0.69
1:A:2015:G:H21	1:A:2931:A:C1'	2.06	0.69
15:Q:95:GLU:O	15:Q:99:MET:HG2	1.93	0.69
1:A:2143:G:OP1	17:S:173:ARG:NH2	2.25	0.68
2:B:1607:U:O4	2:B:1664:G:O6	2.11	0.68
23:Y:198:ARG:NH2	27:2:70:LEU:O	2.27	0.68
1:A:2292:G:C8	16:R:11:ARG:HB2	2.29	0.68
1:A:2262:C:OP1	17:S:173:ARG:NH1	2.27	0.68
1:A:2530:A:H5''	3:D:212:THR:HG21	1.75	0.68
1:A:2529:U:HO2'	3:D:206:TYR:HA	1.59	0.67
15:Q:254:MET:HE3	15:Q:254:MET:HA	1.75	0.67
29:5:122:TRP:O	29:5:215:ARG:NH1	2.27	0.67
1:A:1908:A:N3	1:A:2733:G:O2'	2.25	0.67
5:F:76:ARG:HG3	5:F:76:ARG:HH11	1.59	0.67
22:X:225:PRO:HD2	22:X:228:LYS:NZ	2.09	0.67
29:5:147:ILE:HG23	29:5:191:GLN:NE2	2.09	0.67
11:M:157:GLN:OE1	11:M:157:GLN:N	2.27	0.67
29:5:147:ILE:HG23	29:5:191:GLN:HE22	1.58	0.67
1:A:2521:A:N6	3:D:202:ARG:HG3	2.09	0.67
13:O:110:ILE:HD11	13:O:122:VAL:HB	1.77	0.67
29:5:95:GLU:N	29:5:95:GLU:OE1	2.29	0.66
1:A:2521:A:N1	3:D:202:ARG:HD2	2.10	0.66
4:E:213:LYS:HG3	4:E:261:MET:HE2	1.75	0.66
1:A:2801:A:H2'	1:A:2802:A:C8	2.30	0.66
22:X:119:LEU:HD22	29:5:53:PRO:HD2	1.76	0.66
20:V:131:THR:HG22	20:V:149:ARG:HD3	1.77	0.66
8:J:89:TYR:O	8:J:93:ALA:HB3	1.96	0.66
17:S:122:LEU:HD13	17:S:128:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:5:392:ILE:HD12	29:5:398:VAL:HG23	1.78	0.66
1:A:2521:A:H61	3:D:202:ARG:C	2.01	0.66
14:P:118:SER:OG	14:P:121:ASN:ND2	2.28	0.66
1:A:2015:G:N2	1:A:2931:A:C2'	2.48	0.66
1:A:2127:A:H4'	1:A:2251:A:C5	2.30	0.65
15:Q:152:ARG:HG3	15:Q:161:GLU:HG2	1.76	0.65
1:A:1744:A:OP2	28:3:108:LYS:NZ	2.29	0.65
15:Q:250:THR:OG1	15:Q:253:GLN:OE1	2.15	0.65
1:A:1706:C:H1'	19:U:9:LEU:HD11	1.78	0.65
1:A:3220:A:OP1	4:E:260:LYS:NZ	2.30	0.65
19:U:129:MET:SD	19:U:129:MET:N	2.69	0.65
1:A:3158:A:H2'	1:A:3159:A:C8	2.32	0.65
12:N:127:PRO:HA	12:N:152:THR:HG23	1.77	0.65
18:T:123:GLU:O	18:T:127:MET:HG2	1.97	0.65
1:A:2174:G:N2	8:J:102:ARG:O	2.30	0.64
1:A:2528:G:OP2	3:D:208:ARG:NH2	2.29	0.64
5:F:184:GLN:NE2	11:M:21:ARG:HA	2.12	0.64
11:M:247:ILE:HG22	11:M:253:PHE:HD1	1.63	0.64
14:P:85:ARG:NH1	14:P:125:CYS:SG	2.69	0.64
5:F:86:VAL:HG11	5:F:270:GLU:HG2	1.79	0.64
9:K:27:PRO:HG2	9:K:30:LYS:HB2	1.78	0.64
11:M:156:VAL:O	11:M:176:THR:HA	1.98	0.64
18:T:167:MET:HE3	18:T:169:LYS:HD3	1.80	0.64
22:X:110:PHE:HE2	22:X:129:MET:HG2	1.62	0.64
3:D:144:GLY:HA2	29:5:259:ILE:HD13	1.78	0.64
8:J:110:GLY:O	8:J:153:ILE:HA	1.98	0.64
20:V:61:THR:OG1	20:V:75:LYS:NZ	2.30	0.64
1:A:1747:G:N2	1:A:1750:G:O2'	2.30	0.64
1:A:2511:C:H3'	1:A:2512:A:H8	1.63	0.64
4:E:126:ASP:O	4:E:173:LYS:NZ	2.31	0.64
6:H:96:LEU:HD11	6:H:124:LEU:HD21	1.80	0.64
18:T:91:ALA:O	18:T:145:SER:OG	2.15	0.64
29:5:361:THR:OG1	29:5:363:ASP:OD1	2.15	0.64
23:Y:131:ARG:HA	23:Y:134:LYS:HD3	1.80	0.63
7:I:119:HIS:NE2	7:I:158:GLU:O	2.31	0.63
12:N:172:VAL:HG12	12:N:176:LEU:HG	1.80	0.63
1:A:1737:A:N6	1:A:1760:G:H1'	2.13	0.63
1:A:1699:C:O2	23:Y:198:ARG:NH1	2.32	0.63
14:P:63:ARG:NH2	21:W:137:LYS:O	2.32	0.62
15:Q:100:LEU:HD21	15:Q:286:ILE:HD13	1.81	0.62
23:Y:191:ASN:O	23:Y:195:ASN:ND2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:134:GLU:OE2	20:V:136:ARG:NH2	2.32	0.62
1:A:2526:C:OP1	1:A:2533:A:H4'	1.99	0.62
11:M:133:LYS:C	11:M:134:ARG:HD2	2.25	0.62
3:D:124:GLU:HG2	3:D:144:GLY:HA3	1.82	0.62
14:P:72:PHE:HB2	21:W:107:HIS:HA	1.80	0.62
1:A:2529:U:OP2	3:D:208:ARG:HG2	2.00	0.61
1:A:2521:A:N7	3:D:205:GLN:CG	2.63	0.61
5:F:217:LEU:HD11	5:F:243:ILE:HD12	1.81	0.61
20:V:56:LEU:HD23	20:V:86:VAL:HG21	1.82	0.61
1:A:1916:G:N2	1:A:2003:A:C2	2.58	0.61
20:V:121:LYS:HD3	20:V:130:PRO:HB2	1.82	0.61
20:V:190:CYS:SG	20:V:191:LEU:N	2.70	0.61
3:D:194:ASN:OD1	3:D:243:THR:OG1	2.19	0.61
7:I:47:LEU:HD12	12:N:226:ILE:HG12	1.82	0.61
12:N:113:MET:HE2	12:N:113:MET:HA	1.83	0.61
22:X:72:PRO:O	22:X:75:SER:OG	2.18	0.61
3:D:144:GLY:CA	29:5:259:ILE:CD1	2.78	0.61
7:I:124:LYS:HB2	7:I:153:LEU:HB2	1.83	0.61
19:U:11:ARG:NH1	20:V:212:LYS:O	2.34	0.61
2:B:1640:A:OP1	14:P:157:SER:OG	2.10	0.60
4:E:123:GLN:OE1	4:E:125:GLN:NE2	2.26	0.60
15:Q:76:LEU:HD21	15:Q:80:PHE:HB2	1.83	0.60
1:A:2927:C:H2'	1:A:2928:C:H4'	1.83	0.60
1:A:1839:C:H2'	1:A:1840:C:C6	2.36	0.60
1:A:2668:A:H2'	1:A:2669:A:C8	2.36	0.60
29:5:333:ALA:HB1	29:5:363:ASP:HA	1.83	0.60
1:A:2058:C:O2	24:Z:109:LYS:NZ	2.34	0.60
3:D:228:LEU:HD11	3:D:234:MET:HE3	1.83	0.60
23:Y:65:GLU:OE1	23:Y:65:GLU:N	2.19	0.60
15:Q:119:VAL:HG22	15:Q:174:ILE:HG12	1.82	0.60
21:W:128:LYS:HB2	21:W:130:PHE:HE1	1.66	0.60
24:Z:107:ASN:O	24:Z:111:LYS:HG3	2.01	0.60
29:5:409:GLU:HA	29:5:412:ARG:NH1	2.16	0.60
1:A:3174:U:P	1:A:3174:U:O4'	2.59	0.60
15:Q:170:ARG:O	15:Q:170:ARG:HG2	2.01	0.60
1:A:1871:A:H61	1:A:1901:C:H5'	1.67	0.60
29:5:118:LYS:HZ1	29:5:256:PHE:H	1.50	0.60
1:A:2528:G:C5'	3:D:135:ARG:HH21	2.15	0.59
1:A:1916:G:H1	1:A:2003:A:N6	1.99	0.59
15:Q:111:PHE:O	15:Q:140:ARG:NH1	2.35	0.59
20:V:69:ASP:HA	20:V:72:LYS:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:135:ILE:HD11	22:X:141:LEU:HD13	1.83	0.59
19:U:21:ARG:HG2	23:Y:102:TRP:CG	2.38	0.59
1:A:2015:G:H22	1:A:2931:A:H4'	1.67	0.59
22:X:216:ARG:NH2	22:X:220:GLU:OE2	2.36	0.59
1:A:1778:U:C6	5:F:121:ARG:HD2	2.37	0.59
1:A:1901:C:H2'	1:A:1902:C:C6	2.38	0.59
1:A:2531:U:O4	3:D:246:ARG:NH2	2.36	0.59
8:J:111:LEU:HG	8:J:154:ARG:HB3	1.85	0.59
15:Q:225:LYS:HB2	15:Q:226:PRO:HD2	1.85	0.59
22:X:86:ILE:HB	22:X:105:TRP:HB2	1.84	0.59
15:Q:102:ARG:NH2	15:Q:169:PRO:HA	2.18	0.59
14:P:102:VAL:HG12	14:P:103:VAL:HG23	1.84	0.58
22:X:226:LEU:HD23	22:X:229:ILE:HD13	1.85	0.58
23:Y:187:PRO:HG2	23:Y:190:LEU:HD21	1.85	0.58
11:M:102:GLN:O	11:M:106:ASP:HB2	2.02	0.58
12:N:231:SER:N	12:N:234:ASP:OD2	2.36	0.58
14:P:92:ALA:HB1	14:P:132:LEU:HD22	1.85	0.58
11:M:103:TYR:CE1	11:M:107:LEU:HD11	2.38	0.58
15:Q:249:LEU:HD12	15:Q:254:MET:SD	2.43	0.58
1:A:3174:U:OP1	1:A:3174:U:C5	2.57	0.58
13:O:50:ASP:HA	13:O:107:MET:HE1	1.85	0.58
10:L:121:THR:HA	15:Q:156:GLU:OE2	2.03	0.58
1:A:2064:A:OP1	21:W:101:LYS:HE3	2.02	0.58
1:A:1672:C:O2'	18:T:149:ARG:O	2.20	0.58
1:A:2093:U:O2	1:A:2266:U:O2'	2.22	0.58
25:O:90:ASN:O	25:O:94:ARG:HG2	2.03	0.58
12:N:180:ALA:HA	12:N:183:LEU:HD12	1.84	0.58
15:Q:234:GLU:N	15:Q:234:GLU:OE1	2.36	0.58
8:J:32:GLY:O	8:J:36:GLY:N	2.33	0.57
1:A:1800:G:N1	1:A:1803:A:OP2	2.34	0.57
1:A:1908:A:C2	1:A:2733:G:O4'	2.50	0.57
12:N:240:LYS:NZ	12:N:251:VAL:O	2.37	0.57
1:A:2055:U:H2'	1:A:2056:G:H8	1.69	0.57
1:A:1739:A:O2'	1:A:1888:G:H1'	2.04	0.57
1:A:2405:C:N4	29:5:299:LEU:HD11	2.20	0.57
1:A:3139:G:H2'	1:A:3140:A:C8	2.39	0.57
3:D:199:GLU:HB2	3:D:202:ARG:HB2	1.87	0.57
6:H:89:ARG:HG2	6:H:90:PRO:HD2	1.87	0.57
10:L:123:ILE:HD12	10:L:141:ALA:HB2	1.86	0.57
18:T:52:GLU:OE1	18:T:52:GLU:N	2.35	0.57
22:X:79:LEU:HD21	22:X:145:ILE:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1916:G:H1	1:A:2003:A:H61	1.52	0.57
3:D:194:ASN:HA	3:D:207:ILE:CG2	2.33	0.57
29:5:211:ALA:HB1	29:5:322:LEU:HD23	1.86	0.57
11:M:222:TYR:HA	11:M:259:ARG:HH21	1.68	0.57
29:5:307:ASP:OD1	29:5:310:ARG:NH2	2.37	0.57
30:6:51:TYR:HD1	30:6:56:ARG:HG3	1.69	0.57
1:A:1814:A:N3	1:A:1862:U:O2'	2.34	0.57
1:A:2752:C:H2'	1:A:2753:A:H8	1.69	0.57
4:E:221:ARG:HG3	4:E:261:MET:HB2	1.87	0.57
19:U:37:GLU:OE1	19:U:104:THR:HG23	2.04	0.57
5:F:113:LYS:HD2	5:F:157:GLY:HA2	1.87	0.56
29:5:290:THR:HA	29:5:343:GLN:O	2.05	0.56
29:5:340:VAL:HG23	29:5:359:LEU:HB3	1.87	0.56
1:A:2310:G:OP2	25:0:93:ARG:NH2	2.35	0.56
15:Q:96:ARG:HA	15:Q:99:MET:HG3	1.87	0.56
1:A:1908:A:C2	1:A:2733:G:O2'	2.47	0.56
1:A:2521:A:N6	3:D:202:ARG:C	2.57	0.56
6:H:64:LEU:HD23	6:H:64:LEU:H	1.69	0.56
6:H:136:ASN:HA	6:H:139:LEU:HD23	1.87	0.56
11:M:146:ASP:N	11:M:146:ASP:OD1	2.28	0.56
15:Q:145:LEU:HD12	15:Q:167:TYR:HD2	1.69	0.56
19:U:132:GLU:O	19:U:135:GLN:NE2	2.32	0.56
22:X:143:PHE:O	22:X:147:LYS:HB2	2.05	0.56
29:5:200:ARG:NH2	29:5:234:ASP:OD1	2.29	0.56
1:A:2191:A:N6	1:A:2198:A:OP2	2.39	0.56
24:Z:36:PHE:HE2	24:Z:79:PRO:HG3	1.71	0.56
15:Q:120:THR:HG23	15:Q:132:GLN:NE2	2.21	0.56
19:U:25:PHE:CE1	23:Y:139:MET:HE1	2.40	0.56
19:U:44:ILE:HD12	19:U:48:MET:SD	2.46	0.56
1:A:2754:A:H5''	6:H:91:LYS:HE3	1.88	0.56
3:D:194:ASN:HA	3:D:207:ILE:HG21	1.87	0.56
5:F:67:GLU:HG2	5:F:75:GLU:HB3	1.87	0.56
11:M:231:GLU:O	11:M:235:GLU:HG2	2.05	0.56
15:Q:193:ALA:O	15:Q:225:LYS:NZ	2.39	0.56
1:A:2755:A:H2'	1:A:2756:C:C6	2.41	0.56
3:D:130:ARG:NH1	3:D:131:TYR:O	2.39	0.56
12:N:209:ASN:OD1	12:N:211:ASN:N	2.26	0.56
15:Q:176:VAL:HG11	15:Q:179:LEU:HB2	1.87	0.56
21:W:123:GLY:C	30:6:60:ARG:NH2	2.64	0.56
5:F:65:TRP:CE3	5:F:76:ARG:HG2	2.40	0.56
15:Q:123:ASP:OD2	15:Q:126:ALA:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1680:A:H5'	1:A:1681:G:OP2	2.06	0.55
1:A:1789:A:N3	1:A:1915:C:O2'	2.38	0.55
1:A:2142:A:O2'	1:A:2262:C:OP1	2.24	0.55
3:D:187:LEU:HD21	3:D:244:VAL:HG12	1.89	0.55
5:F:61:PRO:HB2	5:F:81:ASP:HB2	1.88	0.55
15:Q:227:LYS:O	15:Q:229:TRP:N	2.39	0.55
29:5:201:ARG:NH1	29:5:418:TYR:O	2.32	0.55
1:A:2015:G:N2	1:A:2931:A:C4'	2.69	0.55
1:A:2364:C:P	1:A:2364:C:H6	2.29	0.55
3:D:180:ASP:OD1	3:D:180:ASP:N	2.40	0.55
29:5:355:LEU:HD21	29:5:374:ALA:HB1	1.87	0.55
1:A:1822:U:O2	1:A:2707:A:O2'	2.24	0.55
1:A:3102:U:O4	25:0:79:ALA:HB3	2.06	0.55
8:J:138:SER:HA	8:J:141:VAL:HG12	1.88	0.55
20:V:134:GLU:OE1	20:V:134:GLU:N	2.36	0.55
1:A:2655:G:N2	1:A:2659:C:O2'	2.39	0.55
1:A:2795:U:H1'	22:X:108:GLN:OE1	2.06	0.55
7:I:40:MET:HE1	7:I:48:MET:HE2	1.88	0.55
4:E:196:ALA:HB1	4:E:199:ARG:HH21	1.71	0.55
11:M:118:LEU:HD12	11:M:157:GLN:HE22	1.72	0.55
18:T:108:PHE:HE2	25:0:116:LEU:HD12	1.72	0.55
1:A:1839:C:H5''	9:K:115:ASN:HB2	1.88	0.55
1:A:2519:G:C4	3:D:228:LEU:HD13	2.42	0.55
6:H:71:PRO:HG3	22:X:65:VAL:HG22	1.89	0.55
11:M:164:ILE:O	11:M:168:GLU:HG3	2.06	0.55
14:P:66:ARG:HD2	14:P:76:GLU:OE2	2.06	0.55
1:A:2194:U:O2'	1:A:2195:A:O4'	2.25	0.55
1:A:2677:A:H2'	1:A:2678:A:C8	2.42	0.55
23:Y:204:TYR:CE2	27:2:73:PRO:HB3	2.42	0.55
1:A:2138:U:H5''	24:Z:73:LYS:HE2	1.89	0.54
12:N:114:ASP:HB2	12:N:118:MET:HE2	1.88	0.54
18:T:107:GLU:HB2	18:T:118:LYS:HE3	1.88	0.54
27:2:82:ARG:CZ	27:2:87:ARG:HD3	2.37	0.54
1:A:2529:U:P	3:D:208:ARG:HE	2.30	0.54
18:T:125:GLN:NE2	18:T:137:ARG:HB3	2.21	0.54
1:A:2065:A:H5'	21:W:74:ARG:HE	1.72	0.54
22:X:7:PRO:HD2	22:X:10:LEU:HD12	1.89	0.54
24:Z:71:ARG:NH2	24:Z:92:GLU:O	2.39	0.54
28:3:116:ARG:NH1	28:3:159:ASP:OD1	2.41	0.54
1:A:2740:A:H5'	1:A:2740:A:H8	1.70	0.54
4:E:347:PHE:CD2	15:Q:124:PRO:HA	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2529:U:C4	3:D:205:GLN:HB3	2.42	0.54
11:M:179:TYR:CE1	11:M:187:VAL:HG21	2.43	0.54
15:Q:120:THR:HG23	15:Q:132:GLN:HE22	1.72	0.54
29:5:382:LEU:HD23	29:5:383:TYR:HD2	1.71	0.54
29:5:409:GLU:H	29:5:409:GLU:CD	2.16	0.54
1:A:2521:A:C8	3:D:205:GLN:CG	2.90	0.54
3:D:127:ILE:HD12	29:5:114:LEU:HD11	1.90	0.54
1:A:2015:G:C2	1:A:2931:A:O2'	2.58	0.54
7:I:87:ALA:HA	7:I:90:PHE:HD2	1.73	0.54
10:L:98:PRO:HG3	10:L:145:VAL:HG12	1.89	0.54
1:A:2745:A:O4'	22:X:101:LEU:HD12	2.07	0.54
10:L:60:VAL:HA	10:L:73:ILE:HG22	1.89	0.54
12:N:218:ILE:HG23	12:N:223:MET:HB2	1.90	0.54
1:A:2015:G:N2	1:A:2931:A:H4'	2.23	0.54
1:A:2072:A:H2'	1:A:2073:A:C8	2.43	0.54
8:J:29:ALA:HB1	8:J:50:CYS:HB2	1.88	0.54
20:V:126:MET:SD	20:V:127:ASP:N	2.81	0.54
7:I:162:LYS:HD2	7:I:196:LYS:HA	1.90	0.53
22:X:196:ILE:HG13	22:X:197:PRO:HD2	1.91	0.53
25:0:184:TRP:H	25:0:184:TRP:CD1	2.26	0.53
2:B:1607:U:O2'	2:B:1608:G:OP1	2.20	0.53
14:P:174:GLU:OE1	14:P:174:GLU:N	2.37	0.53
19:U:3:ARG:H	19:U:23:ASN:HB3	1.73	0.53
1:A:1858:G:H2'	1:A:1859:A:C8	2.44	0.53
2:B:1626:C:N4	14:P:87:GLN:OE1	2.42	0.53
9:K:25:MET:O	9:K:149:ARG:NH1	2.42	0.53
18:T:107:GLU:O	18:T:107:GLU:HG2	2.06	0.53
1:A:2740:A:H2'	1:A:2741:A:C8	2.43	0.53
3:D:207:ILE:HG22	3:D:207:ILE:O	2.06	0.53
11:M:244:LEU:HD22	11:M:245:PRO:HD2	1.89	0.53
12:N:201:ASP:HA	12:N:204:GLU:HG2	1.91	0.53
15:Q:156:GLU:O	15:Q:156:GLU:HG2	2.08	0.53
16:R:47:ILE:O	16:R:51:VAL:HG23	2.08	0.53
22:X:225:PRO:HD2	22:X:228:LYS:HZ3	1.73	0.53
29:5:117:VAL:O	29:5:121:LEU:HD22	2.08	0.53
1:A:2521:A:N1	3:D:202:ARG:CD	2.71	0.53
29:5:220:LEU:HD11	29:5:262:ILE:HD11	1.89	0.53
5:F:69:LEU:HD22	5:F:206:LEU:HD21	1.90	0.53
5:F:94:ASP:N	5:F:94:ASP:OD1	2.41	0.53
21:W:67:ILE:HG21	21:W:131:VAL:HG11	1.90	0.53
26:1:20:MET:HB3	26:1:56:PHE:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2161:A:N3	1:A:3182:A:N1	2.56	0.53
1:A:2403:G:OP1	3:D:133:PRO:HG3	2.08	0.53
5:F:64:ALA:HB3	5:F:189:ILE:HD12	1.90	0.53
5:F:280:TYR:CD1	11:M:125:ARG:HD3	2.44	0.53
15:Q:116:ILE:HG22	15:Q:177:VAL:HB	1.90	0.53
16:R:109:GLU:OE1	17:S:96:PHE:CD1	2.62	0.53
28:3:95:THR:HB	28:3:105:LYS:HB2	1.90	0.53
29:5:118:LYS:HE3	29:5:256:PHE:HB3	1.90	0.53
29:5:146:HIS:O	29:5:194:LYS:NZ	2.41	0.53
29:5:309:LEU:O	29:5:313:MET:HG3	2.08	0.53
1:A:2868:C:H2'	1:A:2869:A:O4'	2.09	0.53
1:A:3150:U:C2	1:A:3151:A:C8	2.96	0.53
5:F:234:THR:HG21	5:F:242:LEU:HB2	1.91	0.53
7:I:191:PHE:O	7:I:195:SER:CB	2.57	0.53
17:S:173:ARG:HB3	17:S:180:PHE:CE2	2.44	0.53
2:B:1615:A:H2'	2:B:1616:A:C8	2.44	0.53
4:E:54:SER:O	4:E:58:VAL:HG23	2.09	0.53
4:E:316:PHE:HB3	4:E:317:PRO:HD3	1.90	0.53
7:I:83:ARG:HG2	7:I:134:PHE:HE1	1.74	0.53
1:A:2095:U:H2'	1:A:2096:U:C6	2.43	0.53
10:L:82:LYS:HG2	10:L:107:LEU:HD22	1.90	0.53
14:P:80:ARG:NH2	14:P:95:GLU:OE1	2.38	0.53
22:X:208:LEU:O	22:X:212:ILE:HG12	2.08	0.53
29:5:268:CYS:SG	29:5:271:TYR:HB3	2.48	0.53
1:A:1780:U:O2'	1:A:1796:A:N1	2.29	0.52
7:I:128:ASN:HA	7:I:131:LEU:HB3	1.91	0.52
1:A:2212:C:H2'	1:A:2213:A:H8	1.74	0.52
1:A:2519:G:H2'	3:D:232:ARG:HD3	1.91	0.52
13:O:44:ALA:HB3	13:O:49:VAL:HG23	1.91	0.52
29:5:133:PRO:HG2	29:5:136:VAL:HG12	1.92	0.52
29:5:405:GLY:O	29:5:407:LYS:NZ	2.40	0.52
1:A:2521:A:C8	3:D:205:GLN:CD	2.87	0.52
20:V:76:VAL:HG13	20:V:86:VAL:HG13	1.90	0.52
1:A:1828:A:OP1	16:R:52:LYS:NZ	2.41	0.52
1:A:2467:A:O2'	1:A:3154:U:H4'	2.10	0.52
5:F:165:LEU:HB2	5:F:170:ARG:HD3	1.91	0.52
14:P:94:VAL:HG21	14:P:136:CYS:SG	2.49	0.52
18:T:97:MET:HG2	18:T:101:GLN:HG2	1.91	0.52
29:5:242:ARG:HA	29:5:242:ARG:HH11	1.75	0.52
1:A:2275:U:H2'	1:A:2276:C:C6	2.44	0.52
3:D:226:ILE:O	3:D:233:GLN:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:116:SER:O	22:X:120:ASP:N	2.42	0.52
22:X:150:LYS:HA	22:X:159:MET:HE3	1.92	0.52
1:A:1737:A:H61	1:A:1760:G:H1'	1.73	0.52
1:A:2521:A:C8	3:D:205:GLN:OE1	2.63	0.52
1:A:3158:A:H2'	1:A:3159:A:H8	1.74	0.52
16:R:109:GLU:OE1	17:S:96:PHE:CE1	2.62	0.52
22:X:42:HIS:HD2	22:X:69:ILE:HD13	1.75	0.52
26:1:44:LEU:HD11	26:1:53:ARG:HB3	1.92	0.52
4:E:45:SER:OG	4:E:46:GLY:N	2.40	0.52
4:E:86:PRO:HB2	4:E:88:HIS:CE1	2.45	0.52
15:Q:112:TYR:HE2	15:Q:215:VAL:HG21	1.75	0.52
15:Q:118:ARG:HA	15:Q:133:PHE:O	2.10	0.52
1:A:3213:A:H2'	1:A:3214:C:C6	2.45	0.52
5:F:249:ASN:O	5:F:253:MET:HG3	2.10	0.52
12:N:87:PHE:HB2	12:N:163:MET:HB2	1.91	0.52
1:A:2650:C:P	1:A:2650:C:H6	2.33	0.52
13:O:97:TYR:OH	13:O:126:LYS:O	2.23	0.52
29:5:172:LYS:HB3	29:5:172:LYS:HZ2	1.74	0.52
8:J:39:LEU:HB3	8:J:44:VAL:HG11	1.92	0.52
8:J:89:TYR:O	8:J:93:ALA:CB	2.57	0.52
27:2:82:ARG:NH1	27:2:89:SER:O	2.43	0.52
9:K:112:LEU:HD11	9:K:122:MET:HE3	1.92	0.51
22:X:225:PRO:HD2	22:X:228:LYS:HZ1	1.75	0.51
1:A:3102:U:C1'	25:0:81:PRO:HA	2.40	0.51
5:F:108:ARG:HG2	5:F:161:TYR:CD1	2.45	0.51
12:N:228:LYS:HG2	24:Z:36:PHE:CZ	2.45	0.51
14:P:120:ARG:HG2	14:P:120:ARG:O	2.09	0.51
1:A:1707:C:C5	29:5:80:ARG:NH2	2.78	0.51
7:I:83:ARG:O	7:I:87:ALA:CB	2.59	0.51
7:I:191:PHE:O	7:I:195:SER:HB2	2.10	0.51
8:J:128:GLU:HA	8:J:133:GLN:HE21	1.75	0.51
14:P:77:PHE:O	14:P:97:GLN:OE1	2.29	0.51
29:5:208:THR:HA	29:5:224:GLY:O	2.10	0.51
1:A:2086:A:H2'	1:A:2087:U:C6	2.45	0.51
10:L:51:TYR:CE2	10:L:78:LYS:HA	2.45	0.51
17:S:94:ARG:NH2	17:S:111:GLU:OE1	2.39	0.51
29:5:138:SER:HA	29:5:141:ASP:HB2	1.92	0.51
30:6:51:TYR:CD1	30:6:56:ARG:HG3	2.45	0.51
1:A:2094:G:H2'	1:A:2095:U:C6	2.45	0.51
4:E:86:PRO:HB2	4:E:88:HIS:HE1	1.75	0.51
12:N:209:ASN:OD1	12:N:210:GLN:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:107:MET:O	13:O:108:LEU:HD23	2.11	0.51
15:Q:96:ARG:NE	15:Q:285:GLU:OE1	2.28	0.51
17:S:173:ARG:HB3	17:S:180:PHE:HE2	1.75	0.51
25:O:146:GLY:O	25:O:150:LYS:NZ	2.44	0.51
29:5:108:HIS:CE1	29:5:110:ARG:HB3	2.46	0.51
4:E:341:GLY:HA3	15:Q:101:GLU:OE2	2.11	0.51
9:K:119:ARG:O	9:K:123:GLU:HG2	2.10	0.51
10:L:39:ARG:NH2	15:Q:158:GLN:OE1	2.44	0.51
10:L:55:PRO:HB2	10:L:75:LEU:HD11	1.93	0.51
1:A:1756:A:H2'	1:A:1757:A:H8	1.75	0.51
5:F:253:MET:HE3	5:F:259:LEU:HD22	1.93	0.51
22:X:177:HIS:CE1	22:X:183:ARG:HD3	2.46	0.51
1:A:1916:G:C2	1:A:2003:A:N1	2.79	0.51
1:A:2521:A:C2	3:D:202:ARG:NE	2.78	0.51
2:B:1665:C:H2'	2:B:1666:U:C6	2.45	0.51
3:D:154:THR:H	3:D:157:MET:HE3	1.75	0.51
29:5:407:LYS:HB2	29:5:409:GLU:OE1	2.11	0.51
29:5:118:LYS:HZ1	29:5:256:PHE:N	2.08	0.51
15:Q:102:ARG:HH22	15:Q:169:PRO:HA	1.76	0.51
19:U:25:PHE:CE2	23:Y:109:ARG:NH1	2.79	0.51
20:V:25:PRO:HG2	20:V:28:SER:HB3	1.93	0.51
20:V:65:LEU:HD11	20:V:121:LYS:HD2	1.93	0.51
3:D:248:SER:OG	3:D:249:ASN:N	2.43	0.50
4:E:179:PHE:CE1	4:E:298:LYS:HE3	2.46	0.50
5:F:72:PHE:HZ	5:F:205:GLU:HB3	1.76	0.50
16:R:36:ASN:OD1	16:R:37:ARG:HG3	2.11	0.50
29:5:155:LEU:HA	29:5:158:ILE:HD12	1.92	0.50
3:D:145:GLY:O	29:5:259:ILE:HG23	2.11	0.50
5:F:211:ARG:NH1	5:F:211:ARG:HG2	2.26	0.50
6:H:95:GLU:OE1	6:H:132:ALA:HB2	2.11	0.50
8:J:66:LEU:HB3	8:J:82:ILE:HD11	1.92	0.50
26:1:24:ALA:HB3	26:1:54:VAL:HG11	1.93	0.50
3:D:207:ILE:HG12	3:D:229:PRO:HD3	1.94	0.50
13:O:131:PRO:HB3	25:O:184:TRP:HZ3	1.76	0.50
22:X:115:TYR:HD2	22:X:122:LYS:HD3	1.77	0.50
29:5:212:THR:HG21	29:5:273:VAL:HG13	1.92	0.50
1:A:2061:C:H2'	1:A:2062:A:O4'	2.11	0.50
1:A:2180:A:H1'	1:A:2206:C:H4'	1.93	0.50
1:A:2747:U:H2'	1:A:2748:A:H8	1.76	0.50
3:D:166:SER:OG	3:D:182:HIS:ND1	2.40	0.50
4:E:123:GLN:HG3	4:E:282:ILE:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:155:ILE:HD12	15:Q:156:GLU:OE1	2.11	0.50
22:X:77:ARG:HH11	22:X:77:ARG:HB2	1.77	0.50
1:A:3213:A:H2'	1:A:3214:C:H6	1.77	0.50
5:F:211:ARG:HG2	5:F:211:ARG:HH11	1.77	0.50
29:5:116:GLY:N	29:5:119:GLN:OE1	2.43	0.50
1:A:3102:U:H1'	25:0:81:PRO:HA	1.94	0.50
3:D:138:ASP:OD1	3:D:138:ASP:N	2.42	0.50
11:M:103:TYR:O	11:M:107:LEU:HD12	2.12	0.50
28:3:136:LYS:HD3	28:3:140:ARG:HE	1.76	0.50
29:5:49:VAL:HG13	29:5:55:LEU:HD13	1.94	0.50
29:5:127:LYS:HD2	29:5:251:HIS:ND1	2.27	0.50
5:F:49:ARG:HD2	5:F:263:LEU:HD22	1.93	0.50
10:L:40:VAL:HA	10:L:105:VAL:HG12	1.93	0.50
11:M:132:LEU:O	11:M:133:LYS:HB2	2.12	0.50
13:O:116:ASP:OD1	13:O:116:ASP:N	2.36	0.50
1:A:2100:C:H1'	1:A:2135:A:C8	2.46	0.50
1:A:2182:G:H1'	1:A:2199:A:H2'	1.93	0.50
3:D:198:SER:HB2	3:D:206:TYR:OH	2.12	0.50
1:A:2151:A:H2'	1:A:2152:A:C8	2.47	0.50
1:A:2532:U:OP1	3:D:252:HIS:CE1	2.65	0.50
15:Q:278:ILE:O	15:Q:282:ILE:HD12	2.11	0.50
19:U:134:ARG:HA	19:U:137:ARG:NH1	2.27	0.50
3:D:206:TYR:N	3:D:206:TYR:CD1	2.79	0.49
4:E:91:GLU:HG2	4:E:92:PRO:HD2	1.93	0.49
8:J:49:PHE:O	8:J:53:PHE:HB2	2.12	0.49
20:V:122:LEU:HD12	20:V:133:ILE:HG13	1.94	0.49
30:6:46:GLU:H	30:6:46:GLU:CD	2.16	0.49
1:A:2519:G:O6	3:D:230:SER:N	2.44	0.49
15:Q:227:LYS:NZ	15:Q:249:LEU:HD23	2.28	0.49
21:W:62:HIS:HA	21:W:94:GLU:HG3	1.94	0.49
23:Y:194:TYR:OH	29:5:64:MET:O	2.26	0.49
29:5:176:TYR:HA	29:5:179:VAL:HG12	1.94	0.49
1:A:3133:A:N3	1:A:3134:C:H1'	2.28	0.49
5:F:103:GLN:HE22	5:F:249:ASN:HB2	1.77	0.49
12:N:202:GLN:O	12:N:206:GLU:HG3	2.12	0.49
1:A:2691:U:H2'	1:A:2692:G:O4'	2.12	0.49
13:O:130:LEU:HD22	25:0:134:THR:HG23	1.93	0.49
23:Y:237:LYS:HE3	23:Y:237:LYS:HA	1.94	0.49
28:3:162:THR:OG1	28:3:167:LYS:NZ	2.46	0.49
1:A:2275:U:H2'	1:A:2276:C:H6	1.76	0.49
1:A:2318:A:H2'	1:A:2319:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:114:VAL:HG12	6:H:115:LYS:O	2.13	0.49
14:P:153:ALA:O	14:P:159:LYS:NZ	2.46	0.49
15:Q:279:GLU:OE1	15:Q:279:GLU:HA	2.13	0.49
23:Y:144:LYS:O	23:Y:148:GLU:HG3	2.13	0.49
24:Z:78:ARG:HD2	24:Z:116:LEU:HD21	1.93	0.49
1:A:2191:A:H4'	8:J:142:ARG:HG3	1.95	0.49
2:B:1659:U:H2'	2:B:1660:G:H8	1.78	0.49
10:L:119:ILE:HB	10:L:141:ALA:HA	1.93	0.49
15:Q:90:LEU:O	15:Q:94:ILE:HG13	2.13	0.49
3:D:220:VAL:HG12	3:D:221:ASN:H	1.78	0.49
1:A:2710:C:O2'	1:A:3220:A:N1	2.39	0.49
1:A:3217:A:H2'	4:E:292:HIS:CD2	2.48	0.49
3:D:66:TRP:HA	3:D:80:ARG:HH21	1.78	0.49
4:E:82:ASP:O	4:E:84:PRO:HD3	2.13	0.49
10:L:59:HIS:HB3	10:L:74:LEU:HD23	1.95	0.49
14:P:86:THR:HG23	14:P:89:HIS:H	1.78	0.49
20:V:81:ARG:HH11	20:V:81:ARG:HG2	1.78	0.49
26:1:20:MET:HA	26:1:58:GLU:HA	1.95	0.49
3:D:184:LEU:HD13	3:D:226:ILE:HD11	1.95	0.48
4:E:51:GLU:HG2	4:E:52:HIS:CE1	2.49	0.48
13:O:110:ILE:HG22	13:O:111:PRO:O	2.13	0.48
1:A:2285:U:H2'	1:A:2286:A:H8	1.78	0.48
1:A:2379:C:H2'	1:A:2380:C:O4'	2.12	0.48
18:T:55:ASN:ND2	18:T:74:TYR:O	2.45	0.48
18:T:108:PHE:CE2	25:0:116:LEU:HD12	2.47	0.48
23:Y:172:ILE:HD11	27:2:70:LEU:HD13	1.94	0.48
4:E:107:MET:HE3	4:E:121:LEU:HD21	1.95	0.48
4:E:331:ASP:N	4:E:331:ASP:OD1	2.45	0.48
15:Q:150:ILE:HD11	15:Q:161:GLU:HB3	1.95	0.48
1:A:2204:U:O2'	1:A:2207:A:N7	2.42	0.48
2:B:1664:G:H2'	2:B:1665:C:C6	2.48	0.48
1:A:3108:U:C2	4:E:264:ILE:HD13	2.48	0.48
2:B:1659:U:H2'	2:B:1660:G:C8	2.49	0.48
4:E:110:TRP:NE1	4:E:116:LYS:HG3	2.29	0.48
13:O:32:LEU:HB3	13:O:52:MET:HE2	1.96	0.48
13:O:120:MET:HA	13:O:120:MET:HE2	1.95	0.48
29:5:336:LEU:HD21	29:5:362:THR:HG23	1.95	0.48
1:A:1707:C:H5	29:5:80:ARG:NH2	2.11	0.48
1:A:3181:U:OP2	1:A:3182:A:O2'	2.26	0.48
13:O:62:TYR:CZ	13:O:75:MET:HE3	2.48	0.48
19:U:28:LEU:HD23	23:Y:67:PHE:CG	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:5:174:GLU:HG3	29:5:296:LYS:O	2.14	0.48
1:A:2285:U:H2'	1:A:2286:A:C8	2.48	0.48
4:E:187:ILE:HG12	4:E:318:THR:HG23	1.95	0.48
9:K:62:THR:OG1	9:K:100:PRO:O	2.29	0.48
10:L:71:ASP:OD1	10:L:130:ARG:NH1	2.35	0.48
12:N:118:MET:HG2	12:N:167:CYS:HB3	1.96	0.48
20:V:62:VAL:HB	20:V:120:VAL:HG13	1.95	0.48
24:Z:123:LYS:O	24:Z:144:GLU:HA	2.14	0.48
1:A:1690:C:H2'	1:A:1691:C:C6	2.48	0.48
1:A:2173:G:H2'	1:A:2174:G:C8	2.48	0.48
2:B:1648:U:H2'	2:B:1649:C:C6	2.48	0.48
13:O:16:ARG:HD3	13:O:51:GLU:OE1	2.14	0.48
1:A:2405:C:H2'	29:5:302:HIS:NE2	2.27	0.48
1:A:2532:U:OP1	3:D:252:HIS:HE1	1.96	0.48
14:P:81:LEU:HD13	14:P:165:MET:HE2	1.96	0.48
20:V:133:ILE:HD13	20:V:147:SER:HA	1.96	0.48
21:W:83:VAL:HG22	21:W:87:LYS:HA	1.96	0.48
22:X:108:GLN:HG2	22:X:110:PHE:CE1	2.49	0.48
22:X:159:MET:HB3	22:X:205:GLY:HA3	1.95	0.48
22:X:189:ASP:HA	22:X:192:LYS:HG3	1.95	0.48
1:A:2392:U:H2'	1:A:2394:A:H62	1.78	0.48
1:A:2457:A:C2	13:O:17:ARG:NH2	2.82	0.48
21:W:100:THR:OG1	21:W:132:HIS:NE2	2.33	0.48
22:X:180:ASP:OD2	22:X:183:ARG:HD2	2.14	0.48
28:3:169:ARG:NH1	28:3:182:ASP:OD1	2.38	0.48
4:E:154:ARG:HG2	4:E:162:LEU:HD22	1.95	0.47
13:O:38:ARG:NH1	13:O:82:GLU:HG3	2.10	0.47
1:A:2395:A:OP2	29:5:300:ARG:NH1	2.32	0.47
11:M:142:GLU:CD	11:M:142:GLU:H	2.23	0.47
14:P:88:HIS:O	14:P:119:THR:OG1	2.32	0.47
21:W:121:PRO:HA	30:6:50:LYS:HA	1.96	0.47
22:X:148:THR:HG22	22:X:152:ASP:HB2	1.96	0.47
29:5:121:LEU:HD12	29:5:126:THR:HG23	1.95	0.47
1:A:1884:G:N3	1:A:1895:C:O2'	2.48	0.47
10:L:128:ARG:HB2	10:L:129:LYS:HE2	1.95	0.47
14:P:163:SER:O	14:P:167:GLU:HG2	2.14	0.47
19:U:30:ARG:HH12	23:Y:122:GLN:HE22	1.63	0.47
1:A:2056:G:H2'	1:A:2057:C:H6	1.80	0.47
5:F:91:PRO:HG3	11:M:13:LEU:HD23	1.96	0.47
16:R:108:TYR:CE2	18:T:212:LEU:HB2	2.50	0.47
22:X:92:ALA:HB3	22:X:98:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:5:165:GLN:OE1	29:5:175:THR:HG22	2.14	0.47
1:A:2006:C:H2'	1:A:2007:U:C6	2.49	0.47
1:A:2090:A:OP2	28:3:152:LYS:HE2	2.13	0.47
1:A:2403:G:P	3:D:105:ARG:HH12	2.38	0.47
1:A:2666:U:H2'	1:A:2667:U:O4'	2.15	0.47
1:A:2756:C:OP1	6:H:121:ASN:ND2	2.46	0.47
8:J:22:ALA:H	8:J:68:THR:HG22	1.78	0.47
10:L:77:ILE:O	10:L:80:GLN:HG3	2.15	0.47
13:O:60:ILE:HD13	13:O:97:TYR:CD2	2.49	0.47
14:P:102:VAL:HG11	14:P:141:ILE:HD11	1.96	0.47
26:1:20:MET:N	26:1:20:MET:HE2	2.30	0.47
29:5:201:ARG:HB3	29:5:232:THR:HG22	1.94	0.47
1:A:2409:A:O2'	29:5:270:ILE:O	2.31	0.47
1:A:2521:A:C6	3:D:202:ARG:HG3	2.49	0.47
2:B:1603:A:H2'	2:B:1604:G:C8	2.49	0.47
12:N:160:VAL:HG12	12:N:161:VAL:HG23	1.96	0.47
1:A:2015:G:H5'	1:A:2731:U:OP1	2.15	0.47
1:A:3212:C:H3'	1:A:3213:A:H8	1.80	0.47
3:D:123:GLU:HB2	29:5:258:PRO:HB3	1.95	0.47
5:F:76:ARG:HH11	5:F:76:ARG:CG	2.27	0.47
7:I:83:ARG:O	7:I:87:ALA:HB3	2.14	0.47
8:J:113:THR:HA	8:J:156:VAL:HB	1.95	0.47
11:M:117:ASP:OD2	11:M:260:LYS:NZ	2.29	0.47
12:N:221:ALA:HB3	12:N:223:MET:HG2	1.96	0.47
15:Q:76:LEU:HD22	15:Q:279:GLU:OE1	2.15	0.47
15:Q:209:GLN:N	15:Q:209:GLN:OE1	2.48	0.47
21:W:122:LYS:HD3	30:6:50:LYS:O	2.15	0.47
23:Y:69:ASP:HB3	23:Y:111:MET:SD	2.55	0.47
26:1:20:MET:HE2	26:1:30:PHE:O	2.15	0.47
28:3:152:LYS:O	28:3:156:LYS:HG2	2.15	0.47
29:5:244:GLU:O	29:5:248:THR:HG23	2.14	0.47
12:N:176:LEU:HB3	12:N:189:ALA:HB2	1.97	0.47
29:5:245:ILE:O	29:5:248:THR:OG1	2.31	0.47
1:A:2407:U:H2'	1:A:2408:U:C6	2.49	0.47
1:A:3124:U:OP2	1:A:3132:G:N1	2.37	0.47
9:K:7:ALA:HB3	9:K:8:PRO:HD3	1.97	0.47
9:K:176:TYR:HD1	9:K:178:LEU:H	1.62	0.47
1:A:1673:U:H5'	18:T:149:ARG:O	2.15	0.47
5:F:187:LEU:HD13	5:F:259:LEU:HD23	1.97	0.47
14:P:66:ARG:HB2	21:W:92:LEU:HD13	1.95	0.47
15:Q:224:MET:HG2	15:Q:229:TRP:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:270:GLU:O	5:F:274:LEU:HB2	2.14	0.46
15:Q:197:TYR:HE2	15:Q:223:LYS:HD2	1.79	0.46
29:5:242:ARG:HH12	29:5:245:ILE:HD12	1.78	0.46
1:A:2065:A:H1'	1:A:2066:C:C2	2.50	0.46
1:A:2124:A:H5'	1:A:2125:C:O5'	2.16	0.46
5:F:116:THR:HG23	5:F:156:ARG:NH1	2.30	0.46
9:K:52:ASP:O	18:T:206:ARG:NH1	2.49	0.46
22:X:225:PRO:O	22:X:229:ILE:HD12	2.16	0.46
26:1:21:VAL:HG22	26:1:29:CYS:SG	2.55	0.46
28:3:172:TYR:HB2	28:3:175:ASP:HB2	1.96	0.46
29:5:84:ASP:OD2	29:5:87:PHE:HD2	1.98	0.46
29:5:293:LEU:O	29:5:346:GLY:HA2	2.15	0.46
1:A:2015:G:C5'	1:A:2731:U:OP1	2.63	0.46
2:B:1615:A:H2'	2:B:1616:A:H8	1.80	0.46
12:N:50:LEU:HD12	12:N:122:TRP:CE2	2.51	0.46
18:T:47:ILE:HG13	18:T:49:ARG:NH1	2.31	0.46
29:5:170:ILE:HD11	29:5:389:LEU:HD21	1.98	0.46
1:A:2405:C:C5	29:5:299:LEU:HG	2.50	0.46
1:A:2661:U:H4'	1:A:3160:A:O2'	2.16	0.46
9:K:32:ALA:HA	9:K:108:ILE:HG12	1.97	0.46
15:Q:192:ASP:O	15:Q:225:LYS:HG2	2.15	0.46
23:Y:172:ILE:HD12	27:2:70:LEU:HD22	1.97	0.46
29:5:142:ASP:C	29:5:142:ASP:OD1	2.57	0.46
29:5:361:THR:HB	29:5:370:VAL:HG23	1.97	0.46
29:5:409:GLU:HA	29:5:412:ARG:HH12	1.80	0.46
1:A:2134:A:O2'	1:A:2135:A:H5'	2.16	0.46
5:F:82:LEU:HB3	5:F:87:PHE:CD2	2.50	0.46
8:J:43:GLY:HA3	8:J:76:ARG:HH12	1.79	0.46
11:M:273:TRP:CE2	11:M:284:LYS:HD3	2.50	0.46
18:T:203:LEU:O	18:T:206:ARG:HG2	2.16	0.46
1:A:2705:U:OP2	9:K:119:ARG:NH2	2.49	0.46
7:I:47:LEU:CD1	12:N:226:ILE:HG12	2.45	0.46
14:P:69:ARG:HD2	14:P:69:ARG:HA	1.76	0.46
29:5:109:HIS:HA	29:5:312:LYS:HE2	1.98	0.46
29:5:210:SER:HA	29:5:222:VAL:O	2.16	0.46
1:A:1788:C:N3	1:A:1916:G:O2'	2.44	0.46
6:H:100:GLN:HE22	6:H:128:LEU:HA	1.80	0.46
9:K:133:ILE:HB	9:K:138:LEU:HG	1.97	0.46
15:Q:75:PHE:CE2	15:Q:110:GLU:HG2	2.51	0.46
18:T:94:ILE:HA	18:T:97:MET:SD	2.56	0.46
18:T:129:VAL:HG21	18:T:137:ARG:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:118:ILE:CG2	22:X:165:MET:HG2	2.43	0.46
1:A:2245:A:H1'	1:A:2246:A:C8	2.51	0.46
1:A:1774:U:H1'	5:F:147:ARG:HG3	1.97	0.46
4:E:81:LYS:O	4:E:81:LYS:HD3	2.16	0.46
15:Q:161:GLU:OE2	15:Q:191:ARG:NH1	2.49	0.46
15:Q:214:LYS:NZ	15:Q:215:VAL:O	2.48	0.46
19:U:30:ARG:NH1	23:Y:122:GLN:HE22	2.12	0.46
22:X:77:ARG:HB2	22:X:77:ARG:NH1	2.31	0.46
23:Y:170:ARG:HG3	23:Y:176:ILE:HD12	1.98	0.46
4:E:152:VAL:HG21	4:E:157:LYS:NZ	2.31	0.46
9:K:122:MET:HE2	9:K:122:MET:HA	1.97	0.46
9:K:168:ARG:HH22	9:K:172:PRO:HD3	1.81	0.46
11:M:141:VAL:HG12	11:M:143:GLU:H	1.81	0.46
17:S:174:PHE:HA	17:S:180:PHE:O	2.16	0.46
28:3:183:ARG:HG2	28:3:186:LEU:HD12	1.97	0.46
29:5:142:ASP:OD1	29:5:145:ASN:N	2.39	0.46
1:A:1908:A:C2	1:A:2733:G:C1'	3.00	0.45
1:A:2181:A:N6	1:A:2206:C:O2'	2.48	0.45
1:A:2529:U:C4	3:D:205:GLN:O	2.69	0.45
2:B:1666:U:H2'	2:B:1667:C:C6	2.51	0.45
4:E:49:TRP:HE1	4:E:156:ARG:HH12	1.64	0.45
5:F:113:LYS:HG3	5:F:157:GLY:H	1.82	0.45
7:I:160:LYS:HG2	7:I:163:GLU:HB3	1.97	0.45
8:J:90:PHE:HE2	8:J:120:ILE:HD13	1.81	0.45
29:5:161:ALA:CB	29:5:180:ILE:HG13	2.46	0.45
1:A:2877:C:H2'	1:A:2878:G:O4'	2.17	0.45
4:E:112:LYS:NZ	4:E:335:GLU:O	2.34	0.45
5:F:241:ASN:OD1	5:F:256:HIS:NE2	2.38	0.45
6:H:126:GLN:N	6:H:126:GLN:OE1	2.49	0.45
7:I:119:HIS:HB3	7:I:121:ILE:HG22	1.98	0.45
11:M:94:LYS:HG3	11:M:129:ILE:HG22	1.98	0.45
15:Q:79:GLU:HB2	15:Q:99:MET:HE1	1.97	0.45
29:5:215:ARG:HG3	29:5:215:ARG:HH11	1.81	0.45
2:B:1603:A:H2'	2:B:1604:G:H8	1.81	0.45
14:P:77:PHE:CE1	14:P:80:ARG:HB2	2.51	0.45
15:Q:150:ILE:HA	15:Q:162:ILE:O	2.16	0.45
17:S:172:MET:HA	17:S:182:LYS:O	2.17	0.45
1:A:2327:U:H2'	1:A:2328:C:O4'	2.16	0.45
1:A:2386:C:H3'	1:A:2387:U:H5''	1.98	0.45
1:A:2668:A:H2'	1:A:2669:A:H8	1.81	0.45
4:E:158:ALA:HB3	4:E:161:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:98:PRO:HA	15:Q:162:ILE:HD11	1.99	0.45
13:O:35:GLY:HA3	13:O:42:ILE:HD11	1.99	0.45
16:R:75:ALA:O	16:R:78:GLU:HB2	2.17	0.45
17:S:107:LYS:HE3	18:T:212:LEU:HD12	1.99	0.45
20:V:36:PRO:O	20:V:39:ILE:HG13	2.16	0.45
3:D:143:ALA:C	29:5:259:ILE:HD12	2.38	0.45
4:E:88:HIS:ND1	4:E:88:HIS:N	2.65	0.45
5:F:289:PRO:HG2	11:M:191:VAL:CG1	2.47	0.45
22:X:172:GLN:HA	22:X:188:TYR:HE2	1.80	0.45
23:Y:148:GLU:HA	23:Y:151:ASP:OD2	2.16	0.45
1:A:2161:A:N1	1:A:3182:A:C4	2.85	0.45
12:N:123:ARG:NH1	12:N:162:GLU:OE2	2.49	0.45
24:Z:84:ASP:O	24:Z:88:MET:HG3	2.16	0.45
29:5:188:CYS:O	29:5:191:GLN:HG2	2.16	0.45
1:A:1679:U:O2'	1:A:1680:A:OP2	2.27	0.45
3:D:127:ILE:CD1	29:5:114:LEU:HD11	2.46	0.45
4:E:143:ALA:HB3	4:E:181:ILE:O	2.16	0.45
9:K:104:VAL:O	9:K:108:ILE:HG13	2.17	0.45
15:Q:75:PHE:CD2	15:Q:110:GLU:HG2	2.51	0.45
15:Q:139:GLN:HB3	15:Q:150:ILE:CG2	2.47	0.45
20:V:123:VAL:HG13	20:V:128:ARG:HA	1.97	0.45
1:A:2455:U:H2'	1:A:2456:U:C6	2.52	0.45
4:E:159:THR:O	4:E:162:LEU:N	2.50	0.45
5:F:60:ARG:HG2	5:F:60:ARG:HH11	1.82	0.45
9:K:5:SER:HB2	9:K:8:PRO:HD2	1.99	0.45
19:U:79:ARG:NH1	19:U:87:ILE:HD12	2.32	0.45
22:X:150:LYS:HB2	22:X:159:MET:HE3	1.99	0.45
29:5:354:PHE:HD2	29:5:417:LEU:HD22	1.82	0.45
1:A:1792:G:O6	27:2:87:ARG:NH2	2.48	0.45
1:A:2369:A:H2'	1:A:2370:A:C8	2.52	0.45
1:A:2508:C:OP2	1:A:2538:C:H3'	2.16	0.45
1:A:2754:A:H5''	6:H:91:LYS:CE	2.47	0.45
10:L:96:MET:HE3	15:Q:165:GLU:H	1.82	0.45
11:M:187:VAL:CG2	11:M:265:ILE:HG23	2.47	0.45
22:X:115:TYR:CE1	22:X:117:GLU:HA	2.50	0.45
29:5:202:ILE:HG22	29:5:285:TYR:CD2	2.52	0.45
29:5:335:VAL:HG13	29:5:370:VAL:HG21	1.99	0.45
1:A:2056:G:H2'	1:A:2057:C:C6	2.52	0.45
1:A:2529:U:O2'	3:D:206:TYR:CA	2.61	0.45
11:M:91:ARG:HH11	11:M:91:ARG:HG2	1.82	0.45
21:W:124:ALA:O	30:6:60:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:174:PRO:O	22:X:184:ARG:NH1	2.50	0.45
1:A:2745:A:C2	1:A:2746:U:H1'	2.52	0.44
1:A:2850:U:H2'	1:A:2851:A:C8	2.52	0.44
12:N:72:ILE:HD11	12:N:96:TYR:CE1	2.52	0.44
15:Q:262:GLN:HA	15:Q:264:TRP:CZ3	2.52	0.44
16:R:81:LEU:HD13	16:R:117:ALA:HB1	2.00	0.44
1:A:2052:A:H2'	1:A:2053:U:O4'	2.17	0.44
1:A:3151:A:O2'	10:L:95:ARG:HD2	2.17	0.44
2:B:1622:A:H2'	2:B:1623:G:C8	2.53	0.44
4:E:307:TYR:HB3	4:E:310:LEU:HD21	1.98	0.44
9:K:99:ASP:OD1	9:K:99:ASP:N	2.49	0.44
10:L:31:ALA:HB1	10:L:66:VAL:HG23	1.99	0.44
29:5:100:LYS:NZ	29:5:271:TYR:O	2.50	0.44
1:A:1689:C:OP2	22:X:5:LYS:NZ	2.50	0.44
1:A:2099:U:H2'	1:A:2100:C:C6	2.52	0.44
3:D:74:ILE:HD13	3:D:148:LYS:HB2	1.98	0.44
4:E:109:LEU:O	4:E:117:HIS:N	2.44	0.44
4:E:130:LEU:O	4:E:189:PRO:HB3	2.18	0.44
5:F:232:GLU:OE1	5:F:236:ARG:NH2	2.51	0.44
11:M:76:ILE:HD13	11:M:76:ILE:HA	1.88	0.44
13:O:108:LEU:CD1	25:0:122:LEU:HD11	2.44	0.44
20:V:54:TRP:NE1	20:V:56:LEU:O	2.50	0.44
21:W:124:ALA:N	30:6:60:ARG:HH22	2.14	0.44
22:X:209:GLU:H	22:X:209:GLU:CD	2.24	0.44
25:0:141:ILE:O	25:0:145:GLU:HB2	2.17	0.44
29:5:350:ARG:HD2	29:5:383:TYR:O	2.18	0.44
1:A:2459:A:N6	1:A:2668:A:O2'	2.48	0.44
2:B:1660:G:H2'	2:B:1661:A:C8	2.51	0.44
5:F:69:LEU:HD21	5:F:212:TRP:HH2	1.83	0.44
10:L:38:VAL:O	10:L:55:PRO:HG2	2.17	0.44
11:M:229:PHE:N	11:M:230:PRO:HD2	2.32	0.44
12:N:71:ASP:OD1	12:N:71:ASP:N	2.37	0.44
22:X:42:HIS:CG	22:X:86:ILE:HD11	2.52	0.44
1:A:2455:U:H2'	1:A:2456:U:H6	1.83	0.44
10:L:102:SER:OG	10:L:104:ASN:OD1	2.33	0.44
23:Y:109:ARG:HH21	23:Y:136:VAL:HA	1.83	0.44
24:Z:133:ASN:OD1	24:Z:133:ASN:N	2.51	0.44
1:A:2087:U:H2'	1:A:2088:U:C6	2.53	0.44
10:L:122:PRO:HA	10:L:143:ASN:O	2.17	0.44
18:T:125:GLN:HE21	18:T:137:ARG:HB3	1.80	0.44
29:5:189:LYS:O	29:5:192:ILE:HG13	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2528:G:OP2	1:A:2528:G:H8	1.94	0.44
5:F:293:PHE:HB3	5:F:294:PRO:HD3	1.99	0.44
9:K:168:ARG:NH2	9:K:172:PRO:HD3	2.33	0.44
13:O:41:ARG:HG3	13:O:124:GLU:HB3	1.98	0.44
17:S:98:VAL:HG23	17:S:135:LEU:HD22	2.00	0.44
22:X:214:LYS:NZ	22:X:214:LYS:HB3	2.33	0.44
22:X:235:ILE:O	22:X:239:GLN:HG2	2.16	0.44
29:5:242:ARG:NH1	29:5:245:ILE:HD12	2.32	0.44
1:A:1750:G:O2'	1:A:1751:A:OP2	2.36	0.44
1:A:1756:A:H2'	1:A:1757:A:C8	2.53	0.44
1:A:2510:U:C2	1:A:2511:C:C5	3.05	0.44
1:A:3113:A:HO2'	1:A:3114:U:P	2.40	0.44
1:A:3201:A:O2'	1:A:3202:U:O5'	2.23	0.44
4:E:61:ILE:O	4:E:65:VAL:HG23	2.18	0.44
5:F:92:ARG:NH1	5:F:94:ASP:OD2	2.51	0.44
8:J:25:ARG:HA	8:J:65:PRO:HA	2.00	0.44
14:P:154:ALA:HA	14:P:159:LYS:HZ1	1.83	0.44
17:S:98:VAL:HG12	17:S:134:LEU:HD11	2.00	0.44
22:X:25:PRO:HG3	22:X:203:TRP:CE2	2.52	0.44
29:5:108:HIS:ND1	29:5:110:ARG:HB3	2.33	0.44
29:5:119:GLN:CD	29:5:119:GLN:H	2.26	0.44
29:5:218:LEU:HG	29:5:262:ILE:HD13	1.99	0.44
1:A:2234:C:O2'	1:A:2688:C:O2'	2.29	0.44
11:M:276:ASN:ND2	11:M:279:ASP:OD1	2.51	0.44
18:T:108:PHE:HE2	25:0:116:LEU:CD1	2.31	0.44
19:U:26:ILE:HD11	19:U:42:PHE:CD2	2.52	0.44
29:5:289:HIS:CE1	29:5:343:GLN:HE21	2.36	0.44
4:E:272:LYS:HD2	4:E:274:TRP:CZ2	2.53	0.43
4:E:347:PHE:CE2	15:Q:124:PRO:HA	2.53	0.43
6:H:97:ILE:HD11	6:H:137:LYS:HD3	1.98	0.43
14:P:86:THR:OG1	14:P:87:GLN:N	2.50	0.43
22:X:36:ARG:H	22:X:36:ARG:HG3	1.65	0.43
25:0:96:ASN:OD1	25:0:99:LYS:HG3	2.18	0.43
1:A:2165:C:O2'	1:A:2166:C:O4'	2.34	0.43
1:A:2410:U:H4'	29:5:98:LEU:HD21	1.99	0.43
2:B:1607:U:HO2'	2:B:1608:G:P	2.37	0.43
5:F:281:ARG:NH2	11:M:128:THR:HG1	2.13	0.43
17:S:81:LYS:HB2	17:S:81:LYS:HE3	1.68	0.43
18:T:141:TYR:CE1	18:T:179:VAL:HB	2.53	0.43
26:1:47:ASP:C	26:1:47:ASP:OD1	2.61	0.43
1:A:1848:U:H2'	1:A:1849:C:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2686:G:H5'	1:A:3104:U:H4'	2.00	0.43
17:S:120:LEU:HB3	17:S:122:LEU:HD12	2.00	0.43
20:V:128:ARG:O	20:V:129:LYS:HD2	2.18	0.43
22:X:36:ARG:HH12	22:X:149:PRO:HB2	1.83	0.43
1:A:1871:A:N6	1:A:1901:C:H5'	2.33	0.43
1:A:2043:C:H2'	1:A:2044:A:O4'	2.18	0.43
2:B:1625:A:OP1	30:6:56:ARG:NH1	2.50	0.43
2:B:1643:A:H2'	2:B:1644:G:O4'	2.18	0.43
4:E:211:ILE:HG12	4:E:292:HIS:HB3	2.01	0.43
4:E:292:HIS:ND1	4:E:293:LYS:O	2.42	0.43
5:F:220:ASP:O	5:F:245:ALA:N	2.51	0.43
7:I:96:ILE:HD11	7:I:153:LEU:HD22	2.00	0.43
13:O:99:ASP:OD1	13:O:99:ASP:N	2.51	0.43
22:X:177:HIS:HB3	22:X:180:ASP:HB3	2.00	0.43
28:3:165:PHE:O	28:3:168:ARG:HG2	2.18	0.43
29:5:69:TRP:HD1	29:5:70:LEU:HD13	1.83	0.43
29:5:95:GLU:CD	29:5:95:GLU:H	2.26	0.43
1:A:1870:A:N6	1:A:1902:C:H2'	2.33	0.43
1:A:2016:C:O2'	1:A:2932:G:H4'	2.18	0.43
3:D:121:PRO:HB3	3:D:166:SER:HA	2.00	0.43
13:O:40:GLU:OE2	13:O:88:LYS:NZ	2.40	0.43
19:U:144:ARG:HD2	19:U:144:ARG:HA	1.70	0.43
29:5:300:ARG:N	29:5:301:PRO:HD2	2.33	0.43
1:A:2161:A:C4	1:A:3182:A:C6	3.06	0.43
1:A:2187:C:H2'	1:A:2188:A:C8	2.54	0.43
14:P:83:VAL:HG11	14:P:158:MET:HE1	2.00	0.43
17:S:161:ILE:HD11	17:S:194:ARG:HB2	2.00	0.43
22:X:103:LYS:HG3	22:X:104:VAL:N	2.34	0.43
22:X:115:TYR:HD2	22:X:122:LYS:CD	2.31	0.43
22:X:130:ARG:HA	22:X:133:ASP:OD2	2.18	0.43
29:5:104:CYS:SG	29:5:105:TYR:N	2.92	0.43
1:A:2740:A:H1'	1:A:2922:A:OP2	2.18	0.43
10:L:49:SER:HB3	10:L:78:LYS:NZ	2.34	0.43
10:L:98:PRO:N	15:Q:162:ILE:HD11	2.33	0.43
13:O:131:PRO:HD3	25:0:137:ILE:HD12	2.01	0.43
15:Q:224:MET:HE2	15:Q:224:MET:HB2	1.88	0.43
1:A:2528:G:O5'	3:D:208:ARG:NH2	2.52	0.43
1:A:2529:U:O4	3:D:205:GLN:HB3	2.18	0.43
10:L:58:ILE:HD11	10:L:76:ALA:HB2	2.00	0.43
22:X:108:GLN:HG2	22:X:110:PHE:CZ	2.54	0.43
28:3:107:VAL:HG21	28:3:161:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:205:GLN:HB2	3:D:206:TYR:CE1	2.53	0.43
10:L:49:SER:HB3	10:L:78:LYS:HZ2	1.82	0.43
10:L:138:LEU:HD23	10:L:138:LEU:O	2.19	0.43
15:Q:201:ASP:O	15:Q:204:MET:HG2	2.18	0.43
15:Q:221:LYS:HE3	15:Q:244:ARG:HG2	2.01	0.43
16:R:35:LYS:HD2	16:R:45:THR:HG21	2.01	0.43
22:X:109:LEU:HD13	22:X:126:THR:HG21	2.01	0.43
22:X:213:GLU:HA	22:X:216:ARG:HG2	2.00	0.43
24:Z:66:LEU:HD12	24:Z:122:LEU:HD23	2.01	0.43
1:A:1675:A:H3'	1:A:1676:A:H8	1.84	0.43
1:A:2674:U:H2'	1:A:2675:G:O4'	2.19	0.43
1:A:3204:C:H2'	1:A:3205:C:O4'	2.19	0.43
4:E:203:TYR:OH	4:E:272:LYS:NZ	2.50	0.43
15:Q:118:ARG:HB2	15:Q:134:LEU:HD23	2.00	0.43
16:R:100:LYS:O	16:R:104:ASP:OD1	2.37	0.43
24:Z:140:LYS:HE3	24:Z:140:LYS:HB3	1.73	0.43
1:A:2145:G:OP1	17:S:169:ARG:NH2	2.52	0.42
1:A:2870:G:H5'	28:3:140:ARG:HD2	2.01	0.42
4:E:179:PHE:HE1	4:E:300:LYS:HB3	1.83	0.42
4:E:269:TYR:CE1	4:E:303:LYS:HD3	2.54	0.42
11:M:211:VAL:N	11:M:212:PRO:HD2	2.34	0.42
21:W:95:GLY:HA3	21:W:134:VAL:O	2.18	0.42
29:5:295:ASP:OD2	29:5:304:LEU:N	2.51	0.42
1:A:2142:A:C4	1:A:2262:C:H5'	2.54	0.42
1:A:2171:U:C2	1:A:2173:G:H4'	2.54	0.42
5:F:72:PHE:CZ	5:F:205:GLU:HB3	2.54	0.42
10:L:98:PRO:CA	15:Q:162:ILE:HD11	2.48	0.42
20:V:147:SER:OG	20:V:150:SER:O	2.38	0.42
23:Y:162:ARG:CZ	23:Y:162:ARG:HB3	2.49	0.42
29:5:162:ARG:HD3	29:5:176:TYR:CD1	2.54	0.42
1:A:2129:G:O4'	1:A:2152:A:H2	2.01	0.42
1:A:3128:A:O2'	1:A:3129:A:H8	2.01	0.42
1:A:3133:A:H5'	1:A:3134:C:OP2	2.18	0.42
1:A:3226:G:C5'	4:E:174:GLN:HE21	2.33	0.42
4:E:208:ALA:HB2	4:E:297:VAL:HG12	2.00	0.42
5:F:110:SER:O	5:F:158:PRO:HA	2.20	0.42
6:H:133:SER:C	6:H:135:GLU:H	2.27	0.42
17:S:85:GLU:HA	17:S:88:VAL:HG12	2.02	0.42
29:5:221:GLN:NE2	29:5:272:ASP:O	2.52	0.42
1:A:1739:A:HO2'	1:A:1888:G:H1'	1.84	0.42
1:A:1916:G:N2	1:A:2003:A:H2	2.11	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2740:A:H1'	1:A:2922:A:P	2.59	0.42
7:I:121:ILE:HG13	7:I:156:SER:HB2	2.01	0.42
8:J:69:LYS:HD3	8:J:129:ALA:HB1	2.02	0.42
9:K:155:LEU:HD23	9:K:155:LEU:HA	1.86	0.42
13:O:30:ARG:HD2	13:O:78:PHE:O	2.19	0.42
15:Q:162:ILE:HD13	15:Q:162:ILE:HA	1.85	0.42
25:O:136:GLU:OE1	25:O:139:ARG:NE	2.43	0.42
1:A:1834:U:C4	18:T:206:ARG:HA	2.54	0.42
1:A:1837:C:H2'	1:A:1838:C:O4'	2.20	0.42
13:O:110:ILE:HD13	13:O:110:ILE:HG21	1.84	0.42
20:V:118:ARG:HA	20:V:118:ARG:HD3	1.85	0.42
24:Z:87:LYS:HG2	24:Z:92:GLU:OE2	2.20	0.42
1:A:3117:C:H2'	1:A:3118:U:H6	1.85	0.42
10:L:31:ALA:HA	10:L:67:GLY:O	2.20	0.42
10:L:136:LYS:O	10:L:140:ILE:HD13	2.19	0.42
11:M:136:TYR:O	11:M:157:GLN:HG2	2.20	0.42
21:W:53:ILE:HG21	21:W:56:MET:SD	2.60	0.42
28:3:136:LYS:HD3	28:3:140:ARG:NE	2.35	0.42
29:5:384:GLN:HB2	29:5:405:GLY:HA3	1.99	0.42
1:A:3214:C:H2'	1:A:3215:C:H6	1.84	0.42
6:H:84:GLU:OE2	6:H:89:ARG:NH2	2.35	0.42
13:O:33:LEU:HD21	13:O:59:LEU:HD22	2.02	0.42
15:Q:115:SER:HA	15:Q:180:GLU:OE1	2.20	0.42
17:S:132:LYS:HA	17:S:148:LEU:HD22	2.01	0.42
19:U:65:VAL:HG13	19:U:97:VAL:HG13	2.01	0.42
29:5:181:VAL:O	29:5:185:ILE:HD12	2.19	0.42
29:5:351:VAL:HA	29:5:381:LEU:HA	2.02	0.42
1:A:2754:A:H5''	6:H:91:LYS:NZ	2.35	0.42
4:E:179:PHE:CE1	4:E:300:LYS:HB3	2.54	0.42
9:K:100:PRO:HG2	9:K:129:PRO:HB3	2.01	0.42
12:N:209:ASN:OD1	12:N:209:ASN:C	2.63	0.42
15:Q:236:PRO:HG2	15:Q:260:TRP:O	2.20	0.42
26:1:20:MET:HE2	26:1:20:MET:H	1.85	0.42
29:5:52:ILE:HB	29:5:55:LEU:HD11	2.00	0.42
29:5:125:LYS:HG2	29:5:371:LYS:HG2	2.01	0.42
1:A:2515:U:H2'	1:A:2516:C:C6	2.55	0.42
1:A:2521:A:N1	3:D:202:ARG:NE	2.68	0.42
5:F:91:PRO:O	5:F:176:VAL:HG13	2.20	0.42
25:O:119:LYS:O	25:O:120:HIS:CG	2.72	0.42
1:A:2114:C:H2'	1:A:2115:U:H6	1.84	0.42
1:A:2521:A:N9	3:D:205:GLN:OE1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:146:SER:HA	29:5:263:ILE:HD13	2.01	0.42
6:H:123:LEU:HD13	6:H:128:LEU:HB2	2.02	0.42
10:L:98:PRO:HA	15:Q:162:ILE:CD1	2.50	0.42
15:Q:162:ILE:HG21	15:Q:164:PHE:CZ	2.55	0.42
16:R:81:LEU:HD11	16:R:121:SER:OG	2.20	0.42
20:V:66:GLU:HB2	20:V:119:GLN:HG2	2.02	0.42
24:Z:70:THR:HG23	24:Z:95:HIS:HA	2.00	0.42
29:5:68:PRO:HG2	29:5:69:TRP:CE3	2.55	0.42
1:A:2409:A:H2'	1:A:2410:U:C6	2.55	0.41
1:A:2529:U:N1	3:D:205:GLN:O	2.52	0.41
1:A:3127:G:H2'	1:A:3128:A:H2'	2.02	0.41
4:E:248:ILE:HD13	4:E:252:TRP:NE1	2.35	0.41
6:H:53:THR:OG1	6:H:86:THR:OG1	2.27	0.41
6:H:112:VAL:HG23	6:H:114:VAL:HG23	2.02	0.41
7:I:47:LEU:HD12	12:N:226:ILE:CG1	2.50	0.41
12:N:216:GLU:OE2	12:N:238:LYS:HD2	2.20	0.41
23:Y:84:ALA:HB2	23:Y:134:LYS:HB3	2.01	0.41
23:Y:172:ILE:HG23	23:Y:198:ARG:HB2	2.01	0.41
25:0:152:PRO:HG3	25:0:173:ARG:CZ	2.50	0.41
7:I:181:ILE:O	7:I:184:THR:OG1	2.27	0.41
13:O:134:PRO:HD3	25:0:130:VAL:HG21	2.02	0.41
15:Q:184:ASP:OD2	15:Q:189:TYR:OH	2.31	0.41
21:W:125:VAL:HG23	30:6:60:ARG:HE	1.85	0.41
28:3:137:THR:HG23	28:3:140:ARG:H	1.84	0.41
29:5:310:ARG:HA	29:5:313:MET:HE3	2.01	0.41
1:A:2751:G:H2'	1:A:2752:C:C6	2.55	0.41
5:F:107:LYS:HB2	5:F:107:LYS:HE2	1.72	0.41
13:O:38:ARG:NH2	13:O:84:ASP:OD2	2.54	0.41
13:O:46:TRP:CG	13:O:119:LYS:HD2	2.56	0.41
14:P:47:GLU:OE2	21:W:141:THR:HB	2.20	0.41
15:Q:188:LEU:HD22	15:Q:191:ARG:HH21	1.86	0.41
26:1:18:VAL:HG23	26:1:20:MET:SD	2.60	0.41
1:A:2239:A:O3'	9:K:29:GLY:HA3	2.21	0.41
7:I:191:PHE:O	7:I:195:SER:OG	2.36	0.41
8:J:125:ALA:HB2	8:J:140:VAL:HG21	2.01	0.41
10:L:74:LEU:HD12	10:L:81:LYS:HB2	2.03	0.41
18:T:72:GLU:OE2	18:T:177:LYS:NZ	2.29	0.41
18:T:73:ILE:HG23	18:T:132:HIS:ND1	2.35	0.41
22:X:218:LEU:HD23	22:X:218:LEU:HA	1.85	0.41
1:A:3150:U:H2'	1:A:3151:A:H8	1.85	0.41
6:H:94:LEU:HD23	6:H:116:LYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:43:ASN:HB2	10:L:118:ARG:H	1.86	0.41
15:Q:121:THR:HG23	15:Q:131:SER:OG	2.20	0.41
17:S:161:ILE:HD13	17:S:161:ILE:HG21	1.81	0.41
21:W:118:THR:HG23	30:6:51:TYR:O	2.20	0.41
29:5:125:LYS:NZ	29:5:368:GLU:O	2.44	0.41
29:5:355:LEU:HD23	29:5:376:VAL:HG12	2.03	0.41
1:A:2110:A:N6	12:N:96:TYR:HB2	2.36	0.41
5:F:83:HIS:HB3	5:F:86:VAL:CG1	2.47	0.41
8:J:18:GLY:N	8:J:72:VAL:O	2.53	0.41
10:L:126:SER:HA	15:Q:125:TYR:CE2	2.56	0.41
11:M:16:LEU:HD23	11:M:16:LEU:HA	1.93	0.41
18:T:134:VAL:HG13	18:T:180:GLU:HG3	2.02	0.41
22:X:36:ARG:NH1	22:X:149:PRO:HB2	2.35	0.41
24:Z:55:LYS:HB2	24:Z:55:LYS:NZ	2.36	0.41
1:A:2521:A:OP2	3:D:202:ARG:NH2	2.51	0.41
1:A:2687:C:H2'	1:A:2688:C:H6	1.86	0.41
6:H:94:LEU:HD11	6:H:96:LEU:HD13	2.01	0.41
6:H:99:THR:HG23	6:H:100:GLN:HG3	2.01	0.41
8:J:49:PHE:O	8:J:53:PHE:CB	2.68	0.41
12:N:109:ILE:O	12:N:113:MET:HB2	2.20	0.41
30:6:39:ASP:N	30:6:39:ASP:OD1	2.51	0.41
1:A:1677:C:O2	1:A:1798:A:O2'	2.37	0.41
1:A:1857:U:H2'	1:A:1858:G:C8	2.56	0.41
1:A:2081:U:H2'	1:A:2082:G:C8	2.56	0.41
1:A:2519:G:N2	3:D:206:TYR:HB3	2.36	0.41
2:B:1637:C:H2'	2:B:1638:U:O4'	2.21	0.41
12:N:55:ARG:HG2	12:N:99:TRP:CD2	2.55	0.41
19:U:11:ARG:HH21	23:Y:185:VAL:HA	1.85	0.41
20:V:184:GLU:HG2	20:V:186:THR:HG23	2.02	0.41
1:A:1794:A:OP1	5:F:142:ARG:NH2	2.33	0.41
1:A:2664:U:H2'	1:A:2665:U:C6	2.56	0.41
1:A:3108:U:H4'	1:A:3109:U:OP1	2.19	0.41
4:E:52:HIS:HA	13:O:139:ASP:OD2	2.21	0.41
4:E:104:LEU:HD22	15:Q:91:LYS:HB2	2.02	0.41
6:H:95:GLU:OE2	6:H:111:LEU:HB2	2.21	0.41
6:H:132:ALA:HB1	6:H:137:LYS:HZ1	1.86	0.41
15:Q:249:LEU:HD11	15:Q:253:GLN:HB2	2.02	0.41
20:V:63:GLU:OE1	20:V:73:GLN:HG3	2.21	0.41
20:V:93:THR:HA	20:V:111:SER:O	2.21	0.41
21:W:72:HIS:O	21:W:74:ARG:N	2.51	0.41
22:X:35:GLU:N	22:X:35:GLU:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:5:102:GLN:O	29:5:271:TYR:OH	2.29	0.41
29:5:124:THR:HG21	29:5:357:PHE:HZ	1.86	0.41
29:5:224:GLY:HA2	29:5:316:PHE:CZ	2.56	0.41
1:A:1672:C:H2'	1:A:1673:U:O4'	2.21	0.41
1:A:2127:A:H4'	1:A:2251:A:C6	2.56	0.41
1:A:2286:A:H2'	1:A:2287:U:C6	2.55	0.41
2:B:1633:U:H2'	2:B:1634:A:O4'	2.20	0.41
4:E:116:LYS:HB3	4:E:116:LYS:HE2	1.91	0.41
10:L:51:TYR:CG	10:L:78:LYS:HG3	2.55	0.41
12:N:104:MET:HE2	12:N:182:LYS:HB2	2.02	0.41
18:T:54:LYS:HD2	18:T:74:TYR:CE2	2.56	0.41
22:X:238:LEU:HD23	22:X:238:LEU:HA	1.93	0.41
1:A:1750:G:O2'	1:A:1751:A:P	2.78	0.40
1:A:2864:U:OP1	21:W:50:ARG:HG2	2.21	0.40
4:E:252:TRP:HB3	9:K:84:PRO:HD3	2.03	0.40
4:E:300:LYS:HB2	4:E:300:LYS:HE3	1.70	0.40
11:M:78:ILE:HD13	28:3:124:ARG:HD2	2.03	0.40
22:X:224:VAL:HA	22:X:225:PRO:HD3	1.97	0.40
25:0:136:GLU:OE1	25:0:136:GLU:HA	2.22	0.40
11:M:132:LEU:O	11:M:133:LYS:CB	2.69	0.40
12:N:238:LYS:HB3	12:N:240:LYS:HD2	2.02	0.40
15:Q:118:ARG:HB3	15:Q:175:GLN:HG2	2.04	0.40
20:V:39:ILE:HG13	20:V:39:ILE:H	1.74	0.40
1:A:1754:G:N7	28:3:105:LYS:HE2	2.36	0.40
1:A:2400:C:O2'	1:A:2401:A:O5'	2.32	0.40
4:E:222:TRP:CD1	4:E:256:LYS:HB3	2.56	0.40
6:H:100:GLN:NE2	6:H:128:LEU:HA	2.36	0.40
11:M:178:PHE:O	11:M:203:ARG:NH1	2.53	0.40
15:Q:117:LEU:HD12	15:Q:174:ILE:HG23	2.04	0.40
15:Q:154:VAL:HA	15:Q:159:GLY:HA2	2.03	0.40
25:0:137:ILE:HG12	25:0:177:ARG:HD2	2.02	0.40
1:A:1861:U:H2'	1:A:1862:U:C6	2.57	0.40
1:A:2180:A:H4'	1:A:2181:A:C8	2.56	0.40
1:A:2343:G:O5'	19:U:78:LYS:HE3	2.21	0.40
5:F:49:ARG:NH2	5:F:270:GLU:OE1	2.52	0.40
12:N:247:MET:HE2	12:N:247:MET:HB2	1.99	0.40
23:Y:235:LEU:HD12	23:Y:235:LEU:HA	1.74	0.40
1:A:2081:U:H1'	24:Z:105:SER:HB2	2.03	0.40
1:A:2697:G:O2'	1:A:2698:G:H5'	2.22	0.40
3:D:225:ILE:HA	3:D:234:MET:O	2.20	0.40
10:L:141:ALA:HB3	10:L:144:PHE:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:187:VAL:HG22	11:M:265:ILE:HG23	2.03	0.40
11:M:202:LYS:HB2	11:M:263:ARG:HB3	2.02	0.40
12:N:105:MET:HG3	12:N:179:VAL:HG13	2.04	0.40
12:N:249:LYS:HD2	12:N:249:LYS:H	1.86	0.40
22:X:91:TYR:CD2	22:X:96:LYS:HA	2.57	0.40
22:X:168:ARG:HH11	22:X:168:ARG:HG3	1.86	0.40
22:X:177:HIS:ND1	22:X:183:ARG:HD3	2.36	0.40
26:1:17:LEU:HD22	26:1:32:THR:O	2.21	0.40
27:2:59:LYS:O	27:2:63:LYS:HG3	2.22	0.40
29:5:253:LEU:H	29:5:253:LEU:HD23	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	
3	D	171/305 (56%)	162 (95%)	9 (5%)	0	100	100
4	E	281/348 (81%)	270 (96%)	11 (4%)	0	100	100
5	F	236/311 (76%)	224 (95%)	12 (5%)	0	100	100
6	H	81/267 (30%)	76 (94%)	5 (6%)	0	100	100
7	I	154/261 (59%)	142 (92%)	12 (8%)	0	100	100
8	J	138/192 (72%)	122 (88%)	16 (12%)	0	100	100
9	K	175/178 (98%)	170 (97%)	5 (3%)	0	100	100
10	L	113/145 (78%)	104 (92%)	9 (8%)	0	100	100
11	M	252/296 (85%)	245 (97%)	7 (3%)	0	100	100
12	N	167/251 (66%)	164 (98%)	3 (2%)	0	100	100
13	O	150/175 (86%)	146 (97%)	4 (3%)	0	100	100
14	P	139/180 (77%)	135 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	Q	215/292 (74%)	206 (96%)	7 (3%)	2 (1%)	14	26
16	R	138/149 (93%)	135 (98%)	3 (2%)	0	100	100
17	S	154/205 (75%)	149 (97%)	5 (3%)	0	100	100
18	T	155/206 (75%)	153 (99%)	2 (1%)	0	100	100
19	U	135/153 (88%)	130 (96%)	5 (4%)	0	100	100
20	V	188/216 (87%)	179 (95%)	9 (5%)	0	100	100
21	W	99/148 (67%)	96 (97%)	3 (3%)	0	100	100
22	X	241/256 (94%)	234 (97%)	7 (3%)	0	100	100
23	Y	174/250 (70%)	169 (97%)	5 (3%)	0	100	100
24	Z	118/161 (73%)	113 (96%)	5 (4%)	0	100	100
25	0	106/188 (56%)	105 (99%)	1 (1%)	0	100	100
26	1	46/65 (71%)	45 (98%)	1 (2%)	0	100	100
27	2	36/92 (39%)	36 (100%)	0	0	100	100
28	3	93/188 (50%)	91 (98%)	2 (2%)	0	100	100
29	5	367/423 (87%)	348 (95%)	19 (5%)	0	100	100
30	6	33/380 (9%)	31 (94%)	2 (6%)	0	100	100
All	All	4355/6281 (69%)	4180 (96%)	173 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	Q	156	GLU
15	Q	228	PRO

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	
3	D	145/245 (59%)	143 (99%)	2 (1%)	59	74
4	E	246/290 (85%)	237 (96%)	9 (4%)	30	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	210/262 (80%)	202 (96%)	8 (4%)	29	51
6	H	78/228 (34%)	72 (92%)	6 (8%)	12	21
7	I	145/232 (62%)	144 (99%)	1 (1%)	76	85
8	J	113/150 (75%)	113 (100%)	0	100	100
9	K	155/156 (99%)	151 (97%)	4 (3%)	40	62
10	L	98/124 (79%)	93 (95%)	5 (5%)	21	39
11	M	223/249 (90%)	212 (95%)	11 (5%)	22	41
12	N	147/211 (70%)	140 (95%)	7 (5%)	23	42
13	O	133/150 (89%)	125 (94%)	8 (6%)	17	31
14	P	123/155 (79%)	117 (95%)	6 (5%)	22	41
15	Q	199/256 (78%)	189 (95%)	10 (5%)	22	40
16	R	118/126 (94%)	116 (98%)	2 (2%)	53	71
17	S	141/180 (78%)	135 (96%)	6 (4%)	26	46
18	T	141/176 (80%)	139 (99%)	2 (1%)	59	74
19	U	124/135 (92%)	116 (94%)	8 (6%)	15	28
20	V	172/191 (90%)	167 (97%)	5 (3%)	37	59
21	W	83/119 (70%)	79 (95%)	4 (5%)	23	42
22	X	219/229 (96%)	215 (98%)	4 (2%)	51	69
23	Y	159/223 (71%)	154 (97%)	5 (3%)	35	57
24	Z	111/147 (76%)	107 (96%)	4 (4%)	31	53
25	0	97/164 (59%)	95 (98%)	2 (2%)	47	66
26	1	45/60 (75%)	44 (98%)	1 (2%)	45	65
27	2	34/72 (47%)	34 (100%)	0	100	100
28	3	88/166 (53%)	85 (97%)	3 (3%)	32	55
29	5	333/368 (90%)	315 (95%)	18 (5%)	20	36
30	6	33/332 (10%)	33 (100%)	0	100	100
All	All	3913/5396 (72%)	3772 (96%)	141 (4%)	32	53

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	206	TYR
3	D	236	VAL

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Mol	Chain	Res	Type
4	E	88	HIS
4	E	91	GLU
4	E	107	MET
4	E	119	VAL
4	E	168	LEU
4	E	181	ILE
4	E	204	VAL
4	E	289	VAL
4	E	345	ILE
5	F	107	LYS
5	F	125	ARG
5	F	194	GLU
5	F	218	LEU
5	F	234	THR
5	F	242	LEU
5	F	243	ILE
5	F	258	THR
6	H	54	VAL
6	H	94	LEU
6	H	100	GLN
6	H	123	LEU
6	H	124	LEU
6	H	139	LEU
7	I	146	LEU
9	K	46	VAL
9	K	73	GLU
9	K	101	VAL
9	K	156	ASP
10	L	38	VAL
10	L	66	VAL
10	L	81	LYS
10	L	90	CYS
10	L	105	VAL
11	M	76	ILE
11	M	118	LEU
11	M	127	VAL
11	M	132	LEU
11	M	141	VAL
11	M	146	ASP
11	M	162	LEU
11	M	174	VAL
11	M	175	THR

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Mol	Chain	Res	Type
11	M	219	ASN
11	M	248	THR
12	N	104	MET
12	N	105	MET
12	N	172	VAL
12	N	198	MET
12	N	202	GLN
12	N	204	GLU
12	N	224	LEU
13	O	13	ARG
13	O	18	MET
13	O	20	LEU
13	O	33	LEU
13	O	40	GLU
13	O	42	ILE
13	O	49	VAL
13	O	52	MET
14	P	74	SER
14	P	123	VAL
14	P	134	GLN
14	P	144	MET
14	P	147	GLN
14	P	172	LEU
15	Q	79	GLU
15	Q	150	ILE
15	Q	151	LEU
15	Q	156	GLU
15	Q	204	MET
15	Q	207	VAL
15	Q	222	VAL
15	Q	249	LEU
15	Q	284	LYS
15	Q	289	SER
16	R	10	LEU
16	R	59	LEU
17	S	51	VAL
17	S	104	ARG
17	S	119	GLU
17	S	154	VAL
17	S	181	LYS
17	S	188	THR
18	T	109	ASN

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Mol	Chain	Res	Type
18	T	209	VAL
19	U	24	PHE
19	U	26	ILE
19	U	27	GLN
19	U	28	LEU
19	U	70	THR
19	U	78	LYS
19	U	104	THR
19	U	126	LEU
20	V	45	VAL
20	V	98	ILE
20	V	120	VAL
20	V	153	ILE
20	V	185	ARG
21	W	61	VAL
21	W	105	VAL
21	W	114	VAL
21	W	118	THR
22	X	52	ILE
22	X	64	ASP
22	X	135	ILE
22	X	217	LEU
23	Y	142	LEU
23	Y	153	LEU
23	Y	169	ARG
23	Y	172	ILE
23	Y	177	ILE
24	Z	70	THR
24	Z	105	SER
24	Z	110	LEU
24	Z	144	GLU
25	0	108	ASP
25	0	177	ARG
26	1	42	THR
28	3	130	LYS
28	3	153	THR
28	3	186	LEU
29	5	55	LEU
29	5	67	VAL
29	5	98	LEU
29	5	128	LEU
29	5	147	ILE

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Mol	Chain	Res	Type
29	5	172	LYS
29	5	180	ILE
29	5	212	THR
29	5	230	LEU
29	5	234	ASP
29	5	239	ILE
29	5	294	LEU
29	5	340	VAL
29	5	343	GLN
29	5	358	GLN
29	5	372	ASN
29	5	391	VAL
29	5	392	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	252	HIS
4	E	174	GLN
5	F	105	ASN
5	F	251	HIS
7	I	141	GLN
7	I	150	HIS
7	I	189	GLN
8	J	54	ASN
9	K	40	GLN
9	K	74	GLN
9	K	94	GLN
9	K	160	GLN
11	M	84	ASN
11	M	120	GLN
11	M	130	GLN
11	M	170	ASN
12	N	86	ASN
13	O	150	GLN
14	P	55	ASN
14	P	121	ASN
15	Q	252	GLN
16	R	89	ASN
16	R	94	GLN
16	R	125	HIS
19	U	27	GLN

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Mol	Chain	Res	Type
19	U	84	ASN
22	X	4	HIS
22	X	76	GLN
22	X	93	ASN
23	Y	88	GLN
23	Y	99	HIS
25	0	168	GLN
29	5	372	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	917/1559 (58%)	214 (23%)	13 (1%)
2	B	51/69 (73%)	12 (23%)	1 (1%)
All	All	968/1628 (59%)	226 (23%)	14 (1%)

All (226) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1676	A
1	A	1677	C
1	A	1678	C
1	A	1679	U
1	A	1681	G
1	A	1689	C
1	A	1694	U
1	A	1699	C
1	A	1700	U
1	A	1704	U
1	A	1707	C
1	A	1708	A
1	A	1748	G
1	A	1750	G
1	A	1751	A
1	A	1770	G
1	A	1781	A
1	A	1794	A
1	A	1803	A
1	A	1804	A
1	A	1805	A
1	A	1806	U

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Mol	Chain	Res	Type
1	A	1812	C
1	A	1821	A
1	A	1823	A
1	A	1824	U
1	A	1827	C
1	A	1828	A
1	A	1829	A
1	A	1832	A
1	A	1836	A
1	A	1843	U
1	A	1844	A
1	A	1850	U
1	A	1867	A
1	A	1869	A
1	A	1871	A
1	A	1872	U
1	A	1878	U
1	A	1882	A
1	A	1883	G
1	A	1887	A
1	A	1888	G
1	A	1892	A
1	A	1893	A
1	A	1901	C
1	A	1902	C
1	A	1903	C
1	A	2017	U
1	A	2020	U
1	A	2021	U
1	A	2022	G
1	A	2030	U
1	A	2031	A
1	A	2032	G
1	A	2053	U
1	A	2055	U
1	A	2060	A
1	A	2061	C
1	A	2065	A
1	A	2074	A
1	A	2079	C
1	A	2083	U
1	A	2085	A

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Mol	Chain	Res	Type
1	A	2093	U
1	A	2095	U
1	A	2098	G
1	A	2111	C
1	A	2113	G
1	A	2124	A
1	A	2126	U
1	A	2132	A
1	A	2142	A
1	A	2147	G
1	A	2154	A
1	A	2158	U
1	A	2159	U
1	A	2160	A
1	A	2161	A
1	A	2166	C
1	A	2168	U
1	A	2171	U
1	A	2172	A
1	A	2173	G
1	A	2174	G
1	A	2180	A
1	A	2181	A
1	A	2182	G
1	A	2183	C
1	A	2187	C
1	A	2190	C
1	A	2193	U
1	A	2194	U
1	A	2195	A
1	A	2197	G
1	A	2198	A
1	A	2200	A
1	A	2204	U
1	A	2207	A
1	A	2210	C
1	A	2216	A
1	A	2237	A
1	A	2239	A
1	A	2241	A
1	A	2242	U
1	A	2243	A

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Mol	Chain	Res	Type
1	A	2244	U
1	A	2245	A
1	A	2259	C
1	A	2261	C
1	A	2262	C
1	A	2263	C
1	A	2264	A
1	A	2283	C
1	A	2284	C
1	A	2297	A
1	A	2299	U
1	A	2300	G
1	A	2322	C
1	A	2329	C
1	A	2332	C
1	A	2335	A
1	A	2345	G
1	A	2370	A
1	A	2371	U
1	A	2374	A
1	A	2375	C
1	A	2381	A
1	A	2384	A
1	A	2387	U
1	A	2389	C
1	A	2390	A
1	A	2393	C
1	A	2396	C
1	A	2404	U
1	A	2405	C
1	A	2406	A
1	A	2407	U
1	A	2415	C
1	A	2416	U
1	A	2426	C
1	A	2443	C
1	A	2444	A
1	A	2446	A
1	A	2449	G
1	A	2451	A
1	A	2457	A
1	A	2458	A

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Mol	Chain	Res	Type
1	A	2468	A
1	A	2473	A
1	A	2508	C
1	A	2511	C
1	A	2512	A
1	A	2520	C
1	A	2521	A
1	A	2522	U
1	A	2523	C
1	A	2524	A
1	A	2527	A
1	A	2528	G
1	A	2536	G
1	A	2656	U
1	A	2660	U
1	A	2683	C
1	A	2686	G
1	A	2698	G
1	A	2706	A
1	A	2708	C
1	A	2709	A
1	A	2725	A
1	A	2732	G
1	A	2739	U
1	A	2740	A
1	A	2742	U
1	A	2746	U
1	A	2747	U
1	A	2750	U
1	A	2803	A
1	A	2804	A
1	A	2851	A
1	A	2852	C
1	A	2853	A
1	A	2854	U
1	A	2859	A
1	A	2861	A
1	A	2864	U
1	A	2865	C
1	A	2871	U
1	A	2926	A
1	A	2928	C

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Mol	Chain	Res	Type
1	A	3102	U
1	A	3109	U
1	A	3114	U
1	A	3123	G
1	A	3129	A
1	A	3134	C
1	A	3141	A
1	A	3150	U
1	A	3155	C
1	A	3157	C
1	A	3158	A
1	A	3160	A
1	A	3162	C
1	A	3168	C
1	A	3177	A
1	A	3180	A
1	A	3184	C
1	A	3189	C
1	A	3190	A
1	A	3202	U
1	A	3207	A
1	A	3217	A
1	A	3218	A
1	A	3228	U
2	B	1607	U
2	B	1608	G
2	B	1609	U
2	B	1611	G
2	B	1614	U
2	B	1615	A
2	B	1625	A
2	B	1640	A
2	B	1644	G
2	B	1645	A
2	B	1649	C
2	B	1651	A

All (14) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1805	A
1	A	1843	U

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Mol	Chain	Res	Type
1	A	2030	U
1	A	2165	C
1	A	2172	A
1	A	2186	C
1	A	2243	A
1	A	2457	A
1	A	2507	A
1	A	3108	U
1	A	3113	A
1	A	3159	A
1	A	3201	A
2	B	1607	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

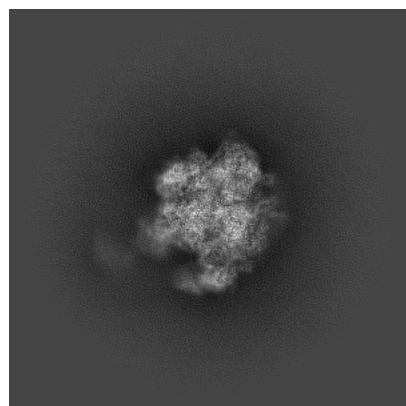
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18460. These allow visual inspection of the internal detail of the map and identification of artifacts.

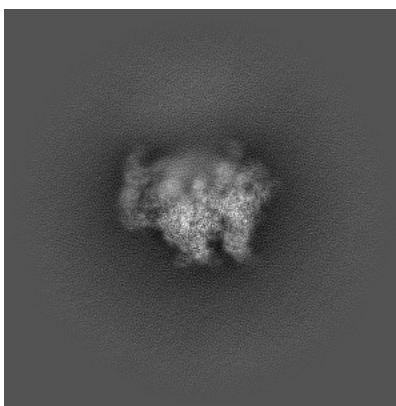
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

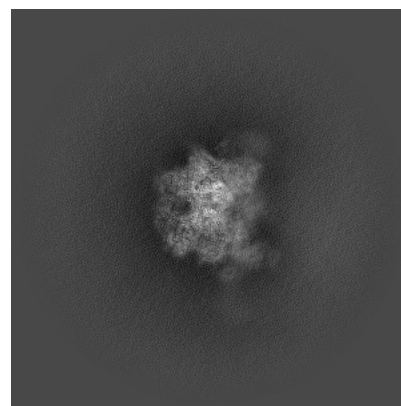
6.1.1 Primary map



X

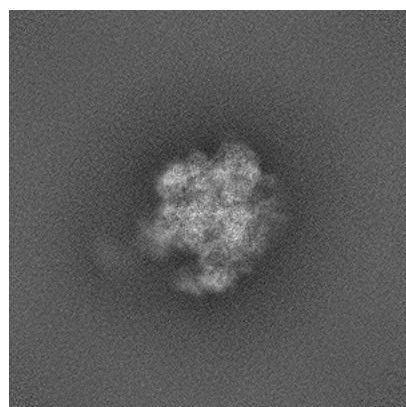


Y

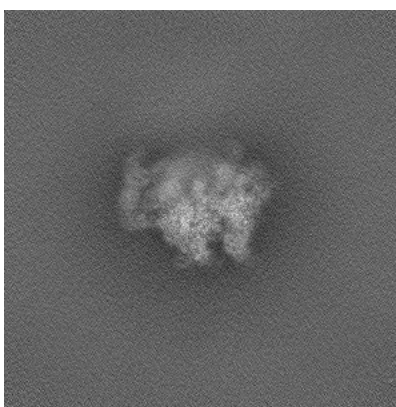


Z

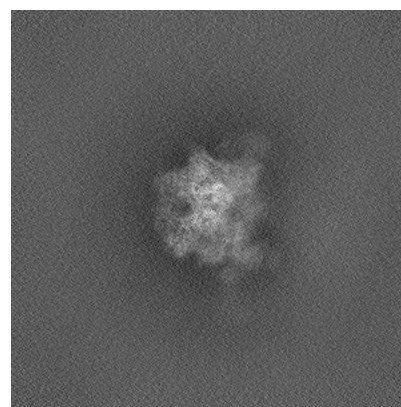
6.1.2 Raw map



X



Y

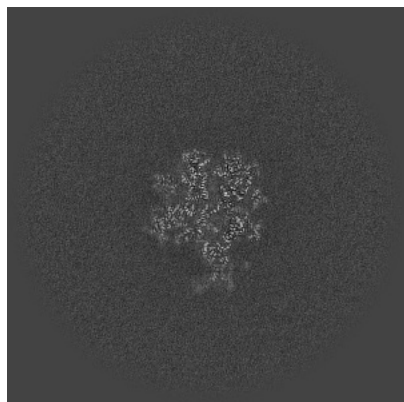


Z

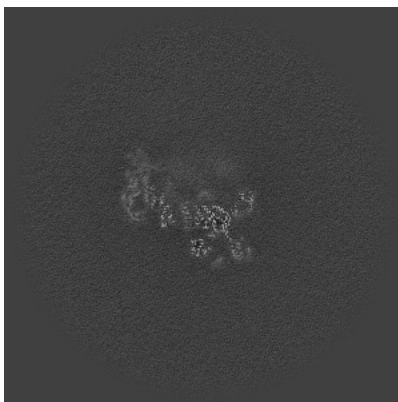
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

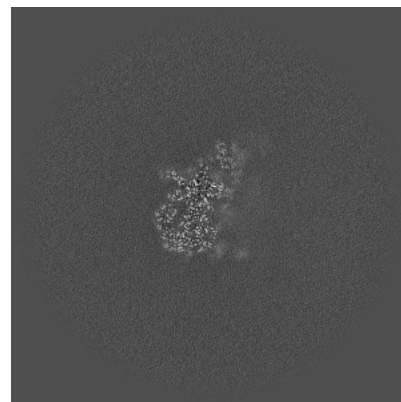
6.2.1 Primary map



X Index: 300

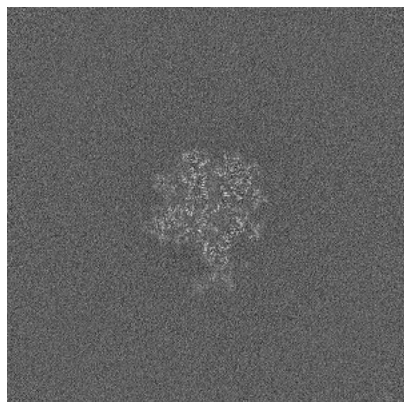


Y Index: 300

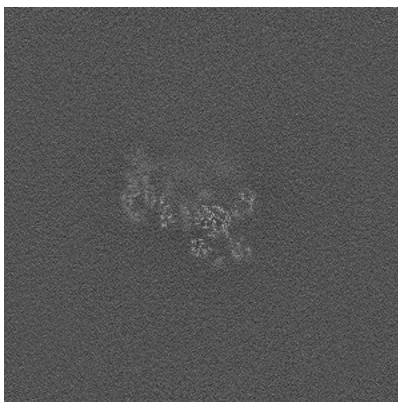


Z Index: 300

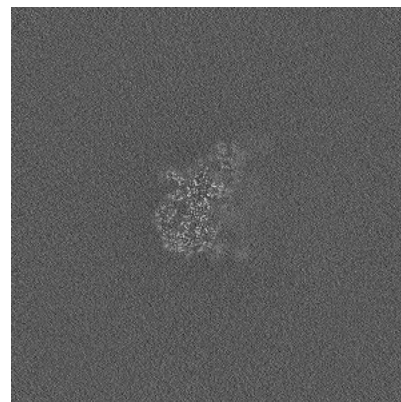
6.2.2 Raw map



X Index: 300



Y Index: 300

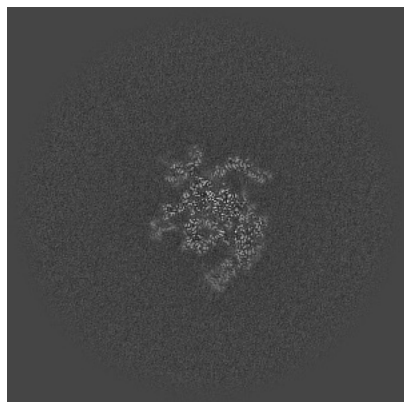


Z Index: 300

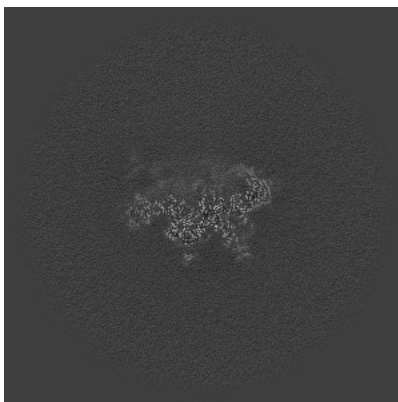
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

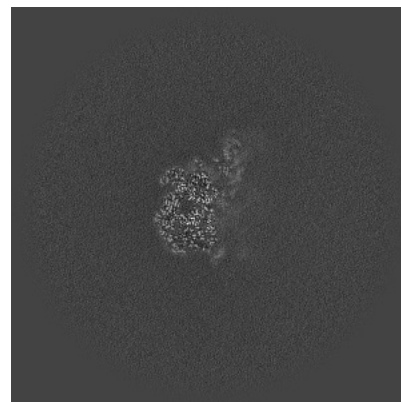
6.3.1 Primary map



X Index: 283

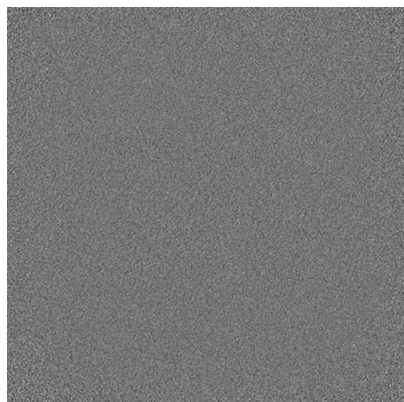


Y Index: 327

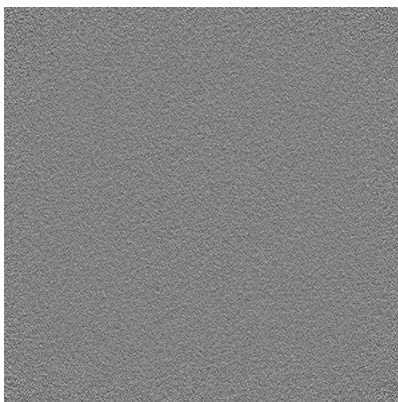


Z Index: 294

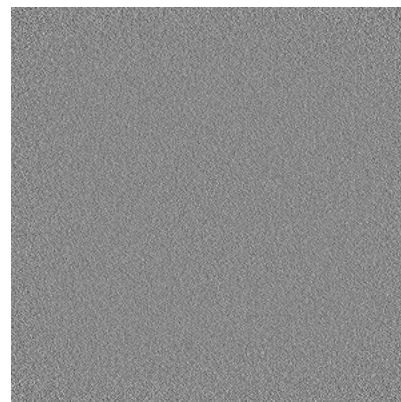
6.3.2 Raw map



X Index: 0



Y Index: 0

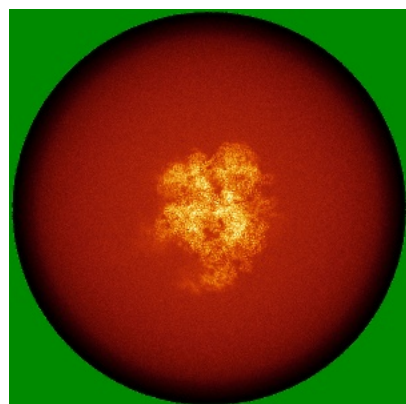


Z Index: 0

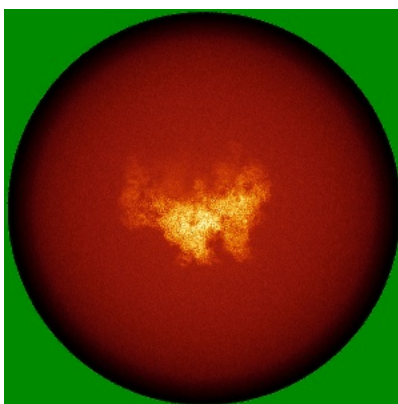
The images above show the largest variance slices of the map in three orthogonal directions.

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

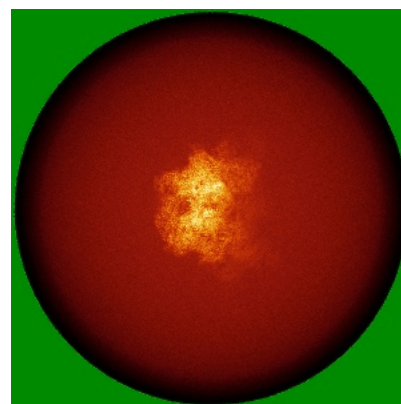
6.4.1 Primary map



X

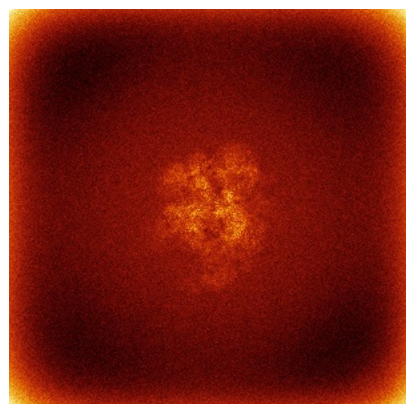


Y

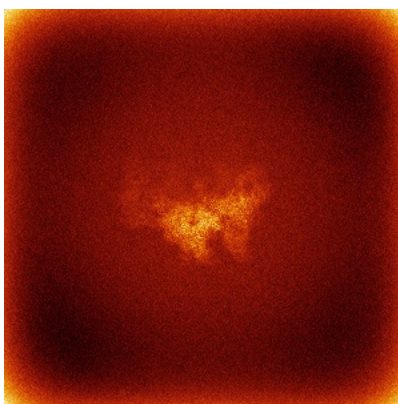


Z

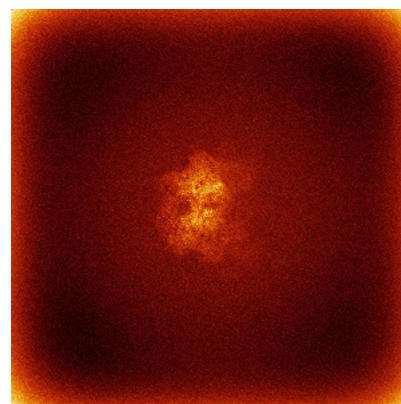
6.4.2 Raw map



X



Y

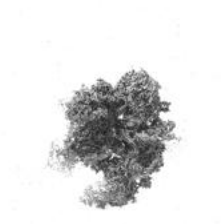


Z

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

6.5 Orthogonal surface views [i](#)

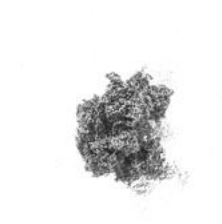
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

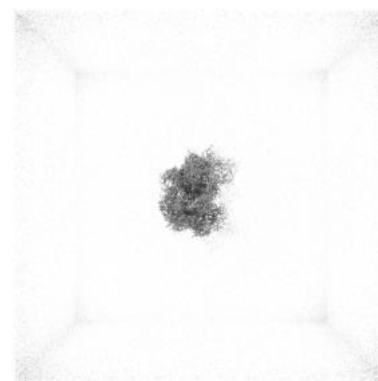
6.5.2 Raw map



X



Y



Z

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.

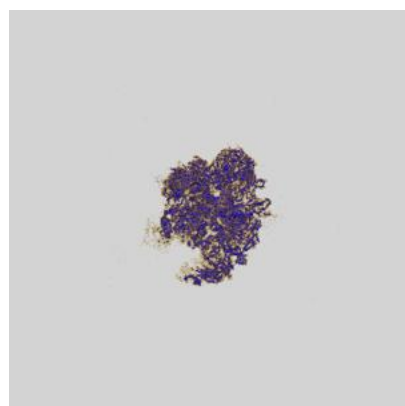
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

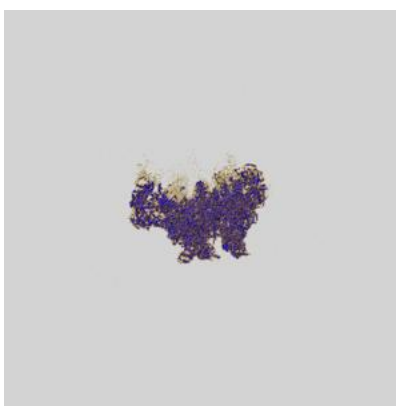
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

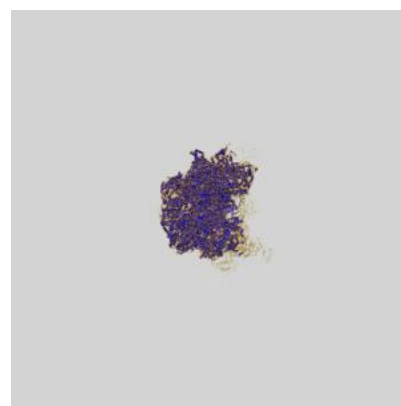
6.6.1 emd_18460_msk_1.map [i](#)



X



Y

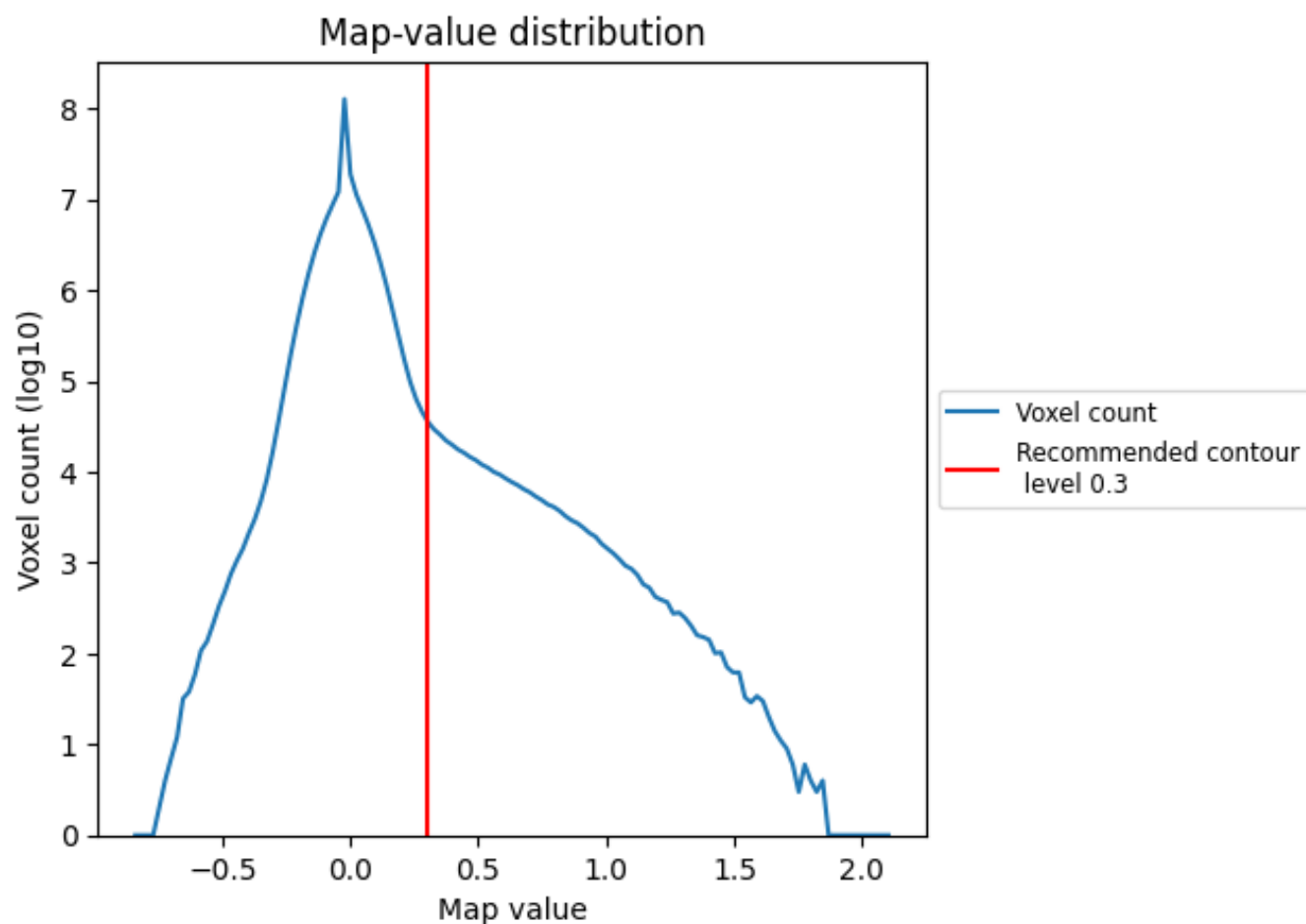


Z

7 Map analysis [i](#)

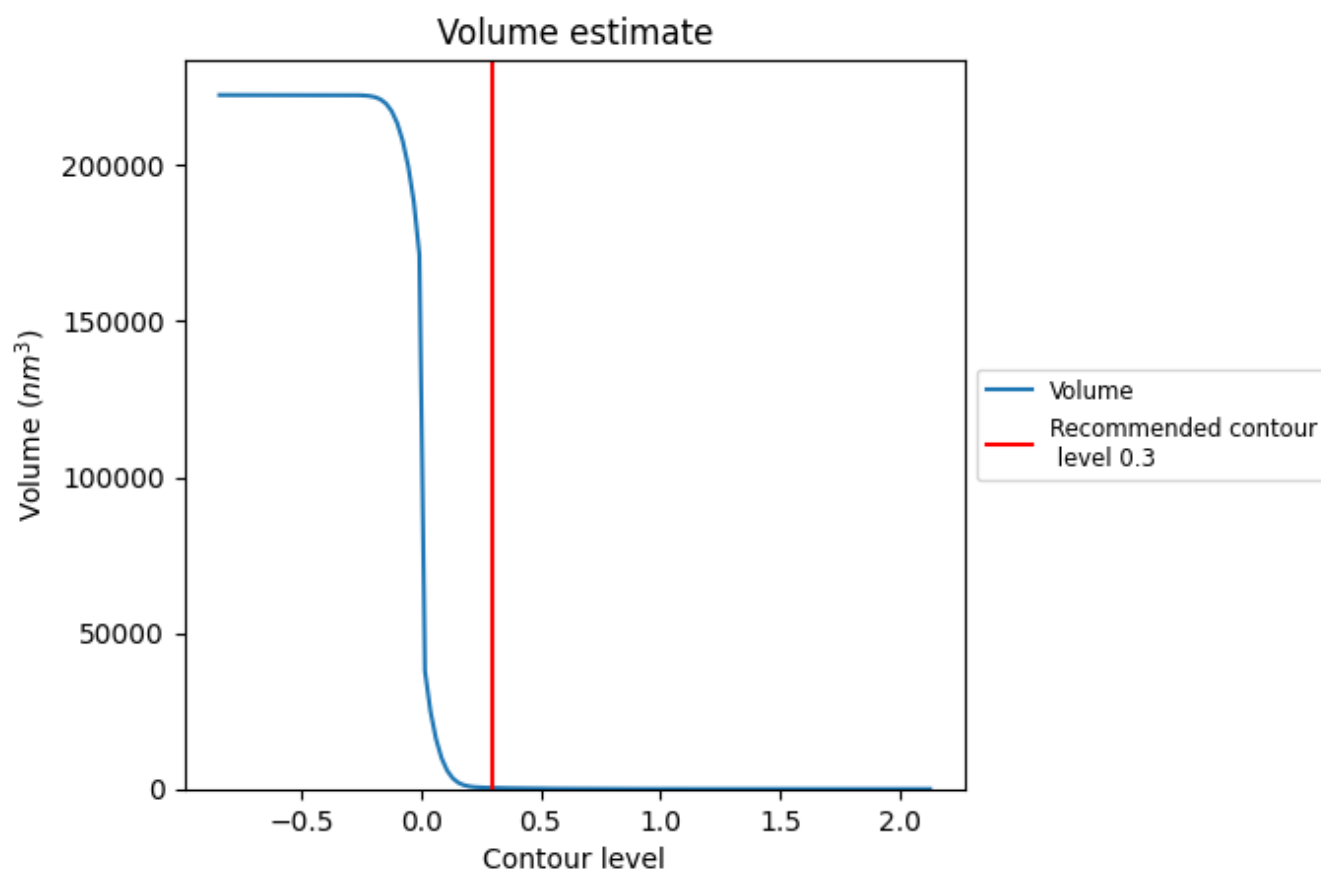
This section contains the results of statistical analysis of the map.

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.

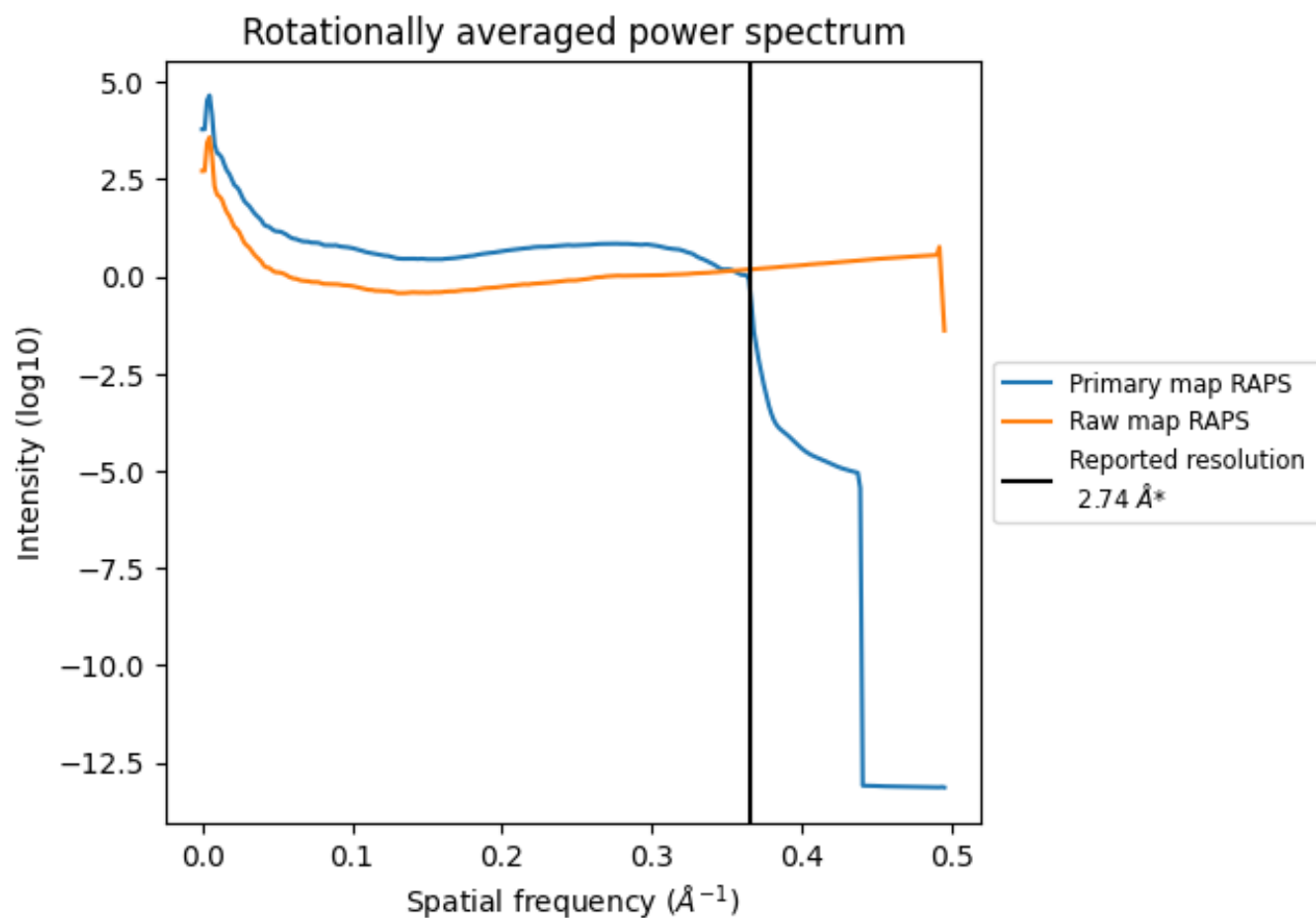
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 342 nm^3 ; this corresponds to an approximate mass of 309 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 ⓘ

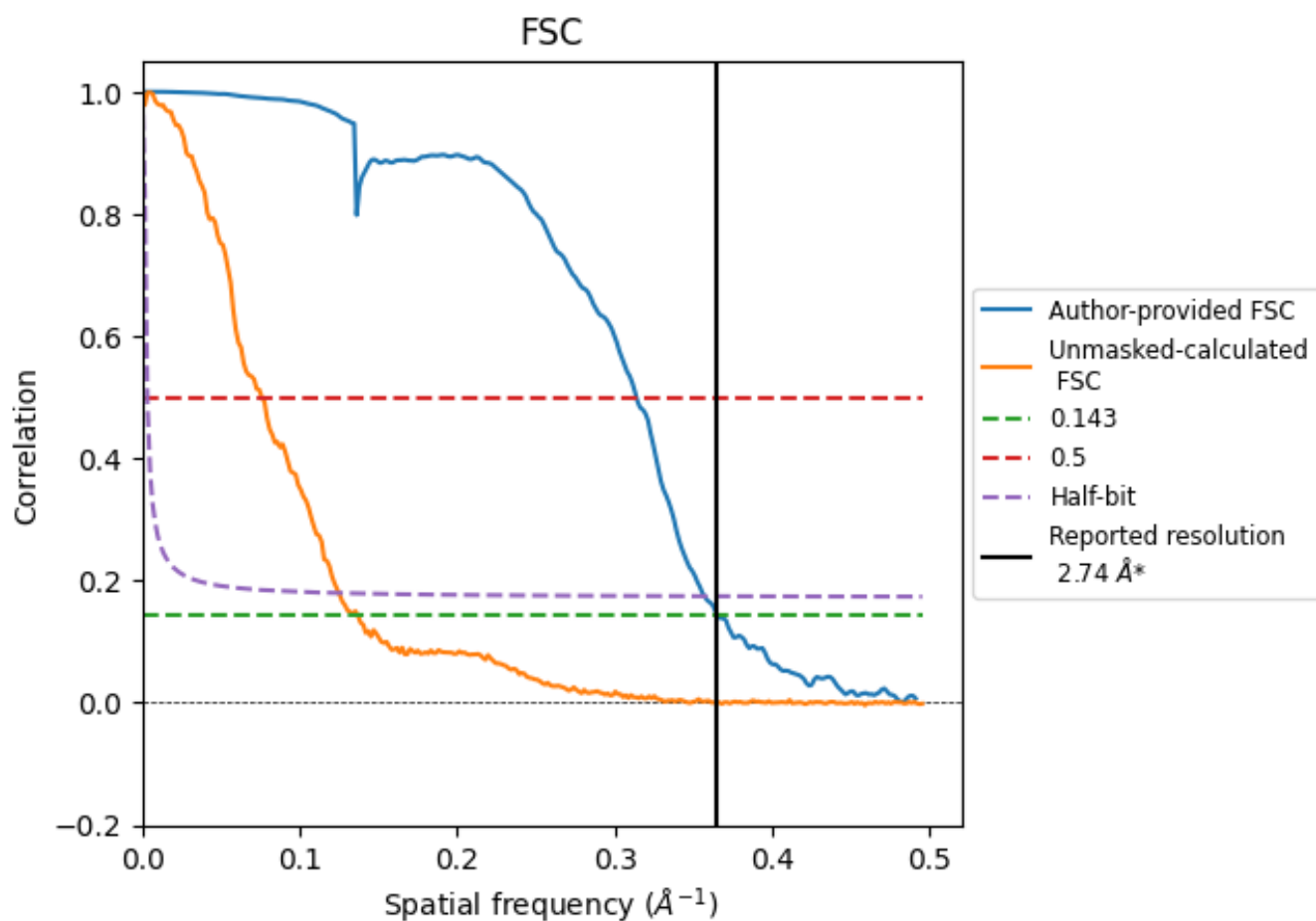


*Reported resolution corresponds to spatial frequency of 0.365 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.365 Å⁻¹

8.2 Resolution estimates [i](#)

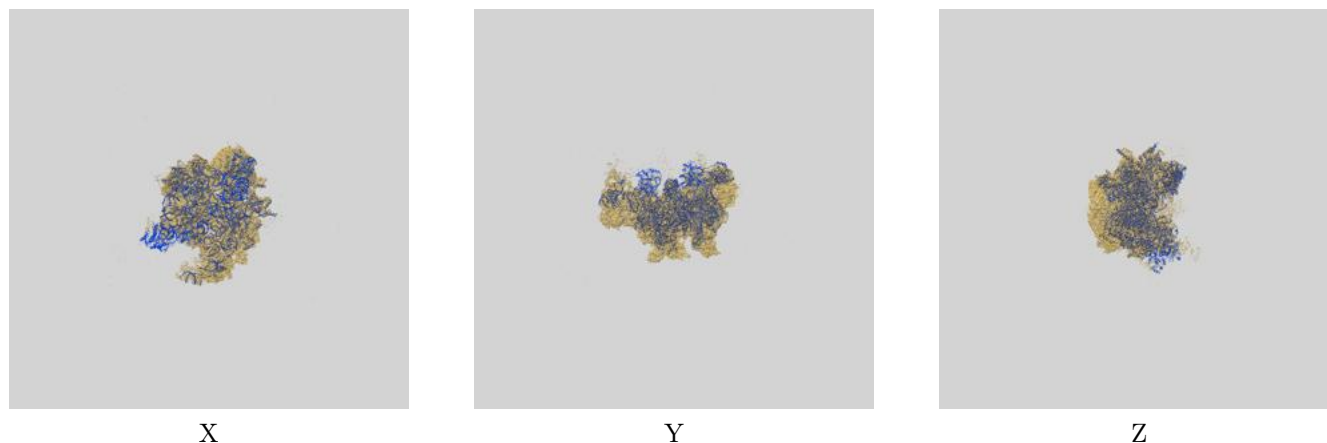
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	2.74	3.19	2.80
Unmasked-calculated*	7.32	13.18	8.01

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.32 differs from the reported value 2.74 by more than 10 %

9 Map-model fit [i](#)

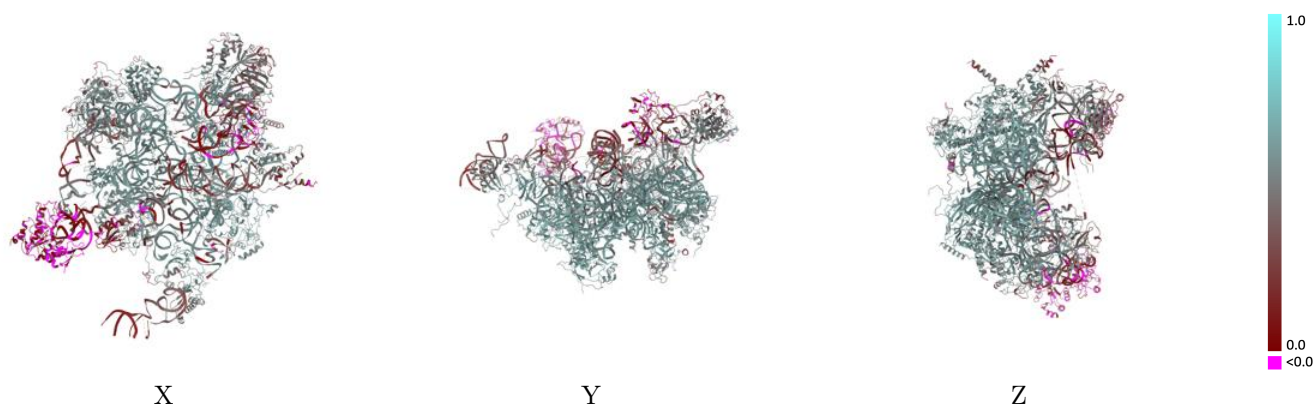
This section contains information regarding the fit between EMDB map EMD-18460 and PDB model 8QU1. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



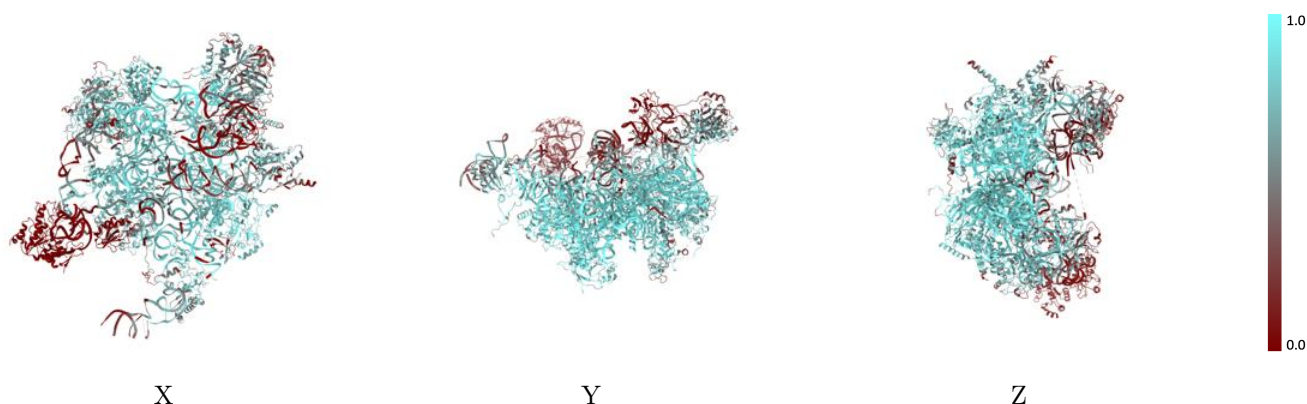
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



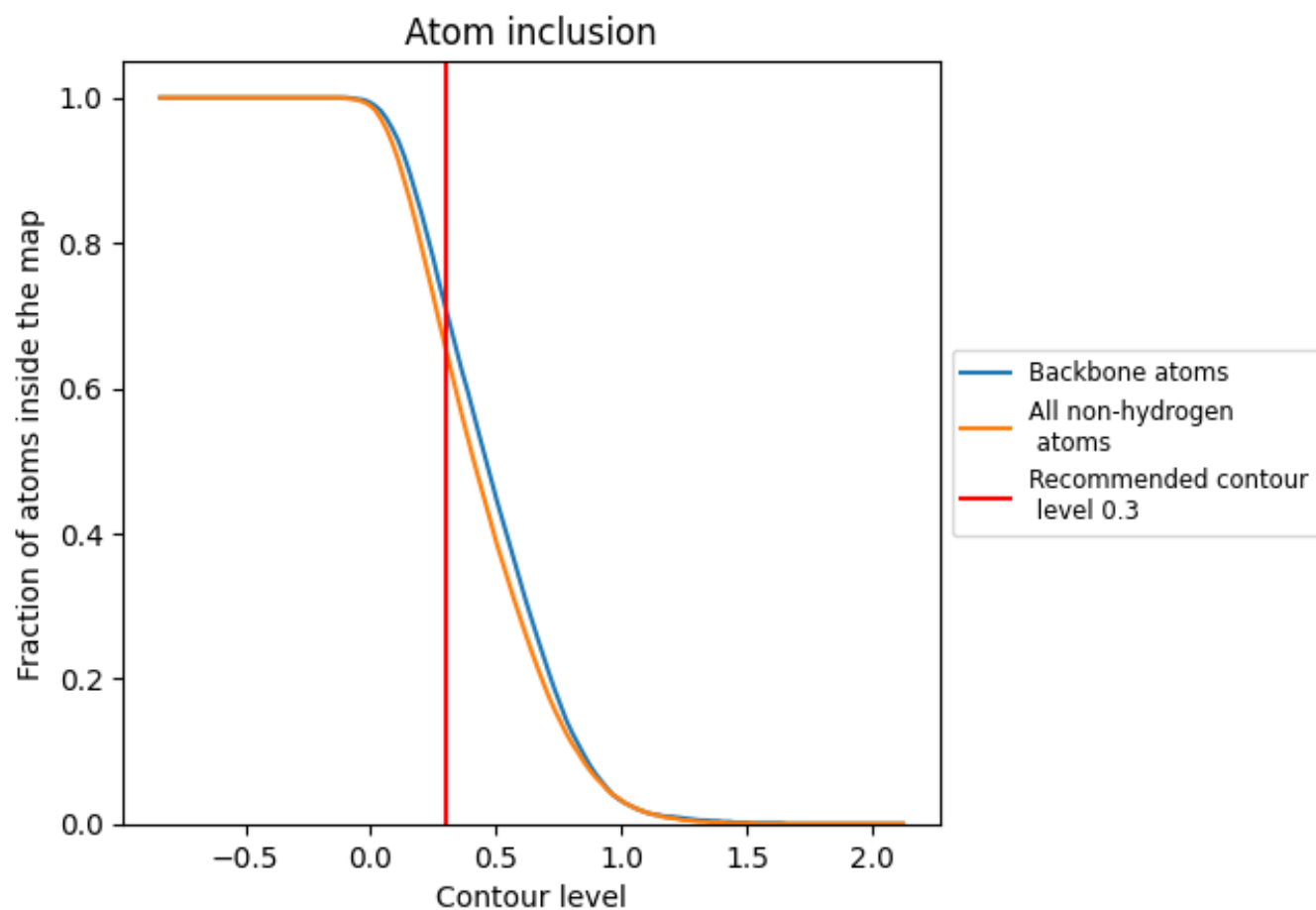
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 65% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6540	 0.4790
0	 0.7840	 0.5710
1	 0.3570	 0.3550
2	 0.8550	 0.6220
3	 0.8670	 0.6100
5	 0.5440	 0.4530
6	 0.3910	 0.4050
A	 0.7090	 0.4820
B	 0.4830	 0.2760
D	 0.0230	 0.1330
E	 0.6900	 0.5340
F	 0.8660	 0.6080
H	 0.4500	 0.3940
I	 0.0920	 0.1150
J	 0.0020	 0.0200
K	 0.8170	 0.5860
L	 0.3230	 0.3590
M	 0.8370	 0.5920
N	 0.2480	 0.3090
O	 0.8220	 0.5870
P	 0.6560	 0.5160
Q	 0.5850	 0.4850
R	 0.8670	 0.6070
S	 0.7910	 0.5730
T	 0.8210	 0.5980
U	 0.7890	 0.5650
V	 0.6770	 0.5280
W	 0.7390	 0.5600
X	 0.6670	 0.5110
Y	 0.8120	 0.5820
Z	 0.8350	 0.5910

