



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 07:07 PM UTC

PDB ID : 6NEQ / pdb_00006neq
EMDB ID : EMD-9358
Title : Structure of human mitochondrial translation initiation factor 3 bound to the small ribosomal subunit-Class-II
Authors : Sharma, M.; Koripella, R.; Agrawal, R.
Deposited on : 2018-12-18
Resolution : 3.32 Å(reported)
Based on initial model : 3JD5

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

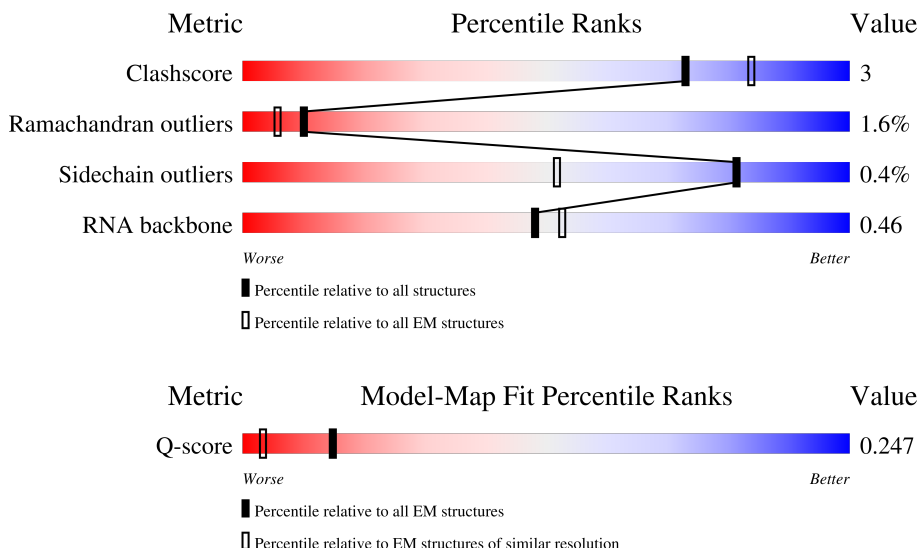
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.32 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.



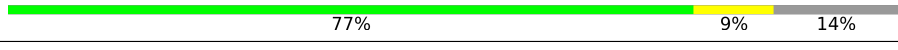
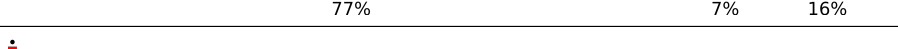
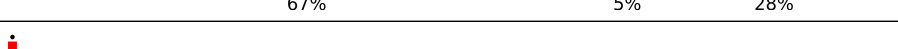
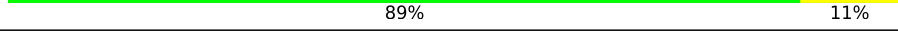
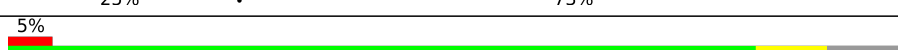
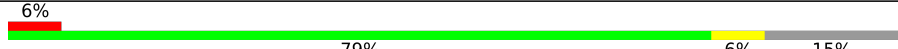
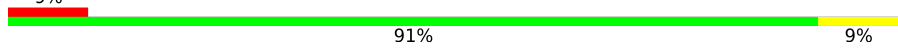
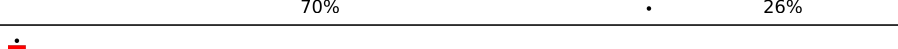
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14518 (2.82 - 3.82)

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	955	
2	C	167	
3	E	430	

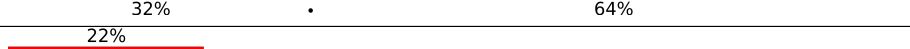
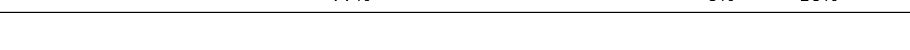
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Mol	Chain	Length	Quality of chain
4	L	139	
5	P	135	
6	Q	130	
7	a	359	
8	c	173	
9	d	205	
10	e	415	
11	j	218	
12	p	258	
13	G	242	
14	I	396	
15	J	201	
16	N	128	
17	g	351	
18	h	386	
19	i	106	
20	k	325	
21	m	118	
22	o	575	
23	B	293	
24	F	124	
25	K	197	
26	O	256	
27	R	143	
28	U	87	

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Mol	Chain	Length	Quality of chain
29	b	190	
30	f	189	
31	n	199	
32	z	247	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 65776 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 28S ribosomal RNA, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	952	Total	C	N	O	P	0	0
			20256	9090	3685	6529	952		

- Molecule 2 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	123	Total	C	N	O	S	0	0
			998	648	177	169	4		

- Molecule 3 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	309	Total	C	N	O	S	0	0
			2464	1535	472	446	11		

- Molecule 4 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	109	Total	C	N	O	S	0	0
			853	534	175	140	4		

- Molecule 5 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	116	Total	C	N	O	S	0	0
			916	580	180	151	5		

- Molecule 6 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	109	Total	C	N	O	S	0	0
			857	555	153	145	4		

- Molecule 7 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	289	Total	C	N	O	S	0	0
			2356	1505	400	443	8		

- Molecule 8 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	c	168	Total	C	N	O	S	0	0
			1374	878	246	241	9		

- Molecule 9 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	d	176	Total	C	N	O	S	0	0
			1463	899	290	272	2		

- Molecule 10 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	e	358	Total	C	N	O	S	0	0
			2950	1886	496	554	14		

- Molecule 11 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	j	213	Total	C	N	O	S	0	0
			1792	1132	346	309	5		

- Molecule 12 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	p	187	Total	C	N	O	S	0	0
			1531	968	288	267	8		

- Molecule 13 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	208	Total	C	N	O	S	0	0
			1721	1093	313	302	13		

- Molecule 14 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	311	Total	C	N	O	S	0	0
			2541	1608	454	467	12		

- Molecule 15 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	128	Total	C	N	O	S	0	0
			1049	676	180	190	3		

- Molecule 16 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	101	Total	C	N	O	S	0	0
			861	538	178	140	5		

- Molecule 17 is a protein called DAP3 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	g	351	Total	C	N	O	S	0	0
			2855	1835	502	508	10		

- Molecule 18 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	h	103	Total	C	N	O	S	0	0
			871	566	141	161	3		

- Molecule 19 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	i	98	Total	C	N	O	S	0	0
			818	519	153	143	3		

- Molecule 20 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	k	275	Total	C	N	O	S	0	0
			2227	1418	377	421	11		

- Molecule 21 is a protein called Coiled-coil-helix-coiled-coil-helix domain containing 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	118	Total	C	N	O	S	0	0
			945	587	185	164	9		

- Molecule 22 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	o	461	Total	C	N	O	S	0	0
			3273	2082	573	605	13		

- Molecule 23 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B	217	Total	C	N	O	S	0	0
			1726	1102	319	298	7		

- Molecule 24 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	F	124	Total	C	N	O	S	0	0
			991	627	179	179	6		

- Molecule 25 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	K	136	Total	C	N	O	S	0	0
			1001	628	193	177	3		

- Molecule 26 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	O	173	Total	C	N	O	S	0	0
			1421	904	258	250	9		

- Molecule 27 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	97	Total	C	N	O	S	0	0
			788	507	136	138	7		

- Molecule 28 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	86	Total	C	N	O	S	0	0
			737	457	148	124	8		

- Molecule 29 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	135	Total	C	N	O	S	0	0
			1108	717	195	194	2		

- Molecule 30 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	98	Total	C	N	O	S	0	0
			775	493	135	143	4		

- Molecule 31 is a protein called Aurora kinase A interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	n	72	Total	C	N	O	S	0	0
			642	409	142	89	2		

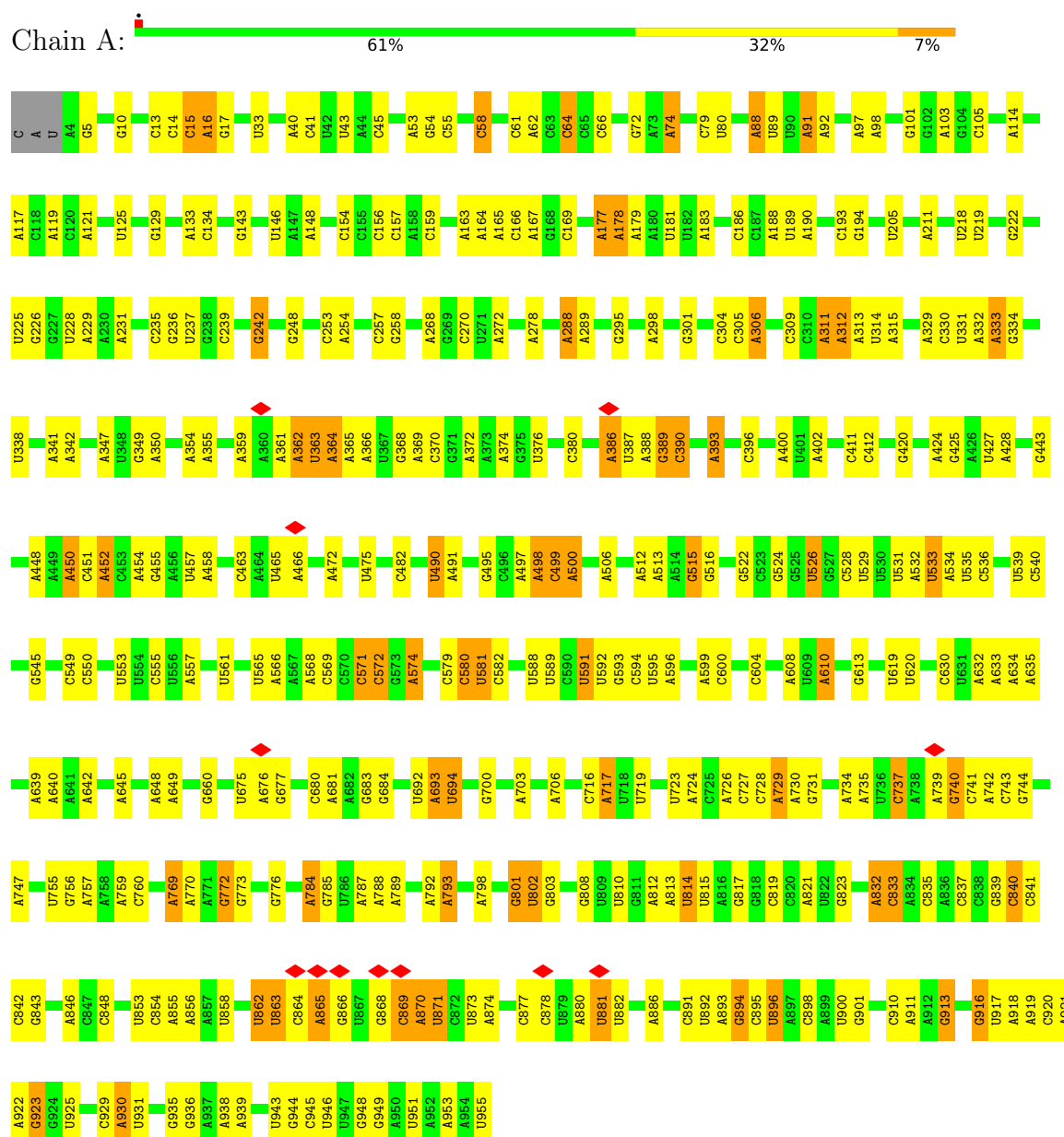
- Molecule 32 is a protein called Translation initiation factor IF-3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	z	207	Total	C	N	O	S	0	0
			1616	998	305	305	8		

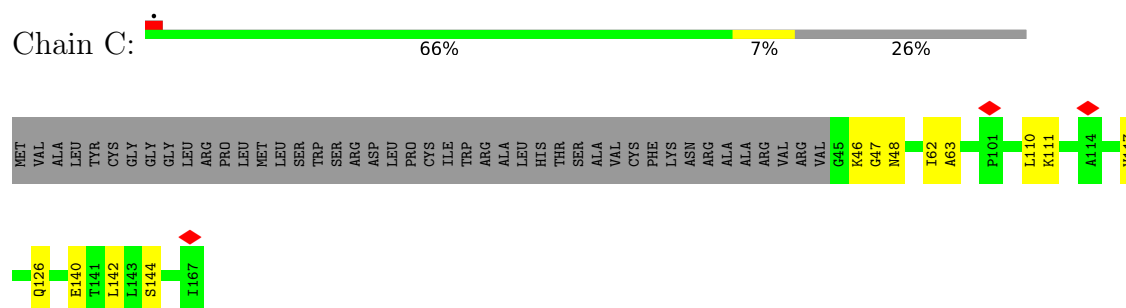
3 Residue-property plots [i](#)

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

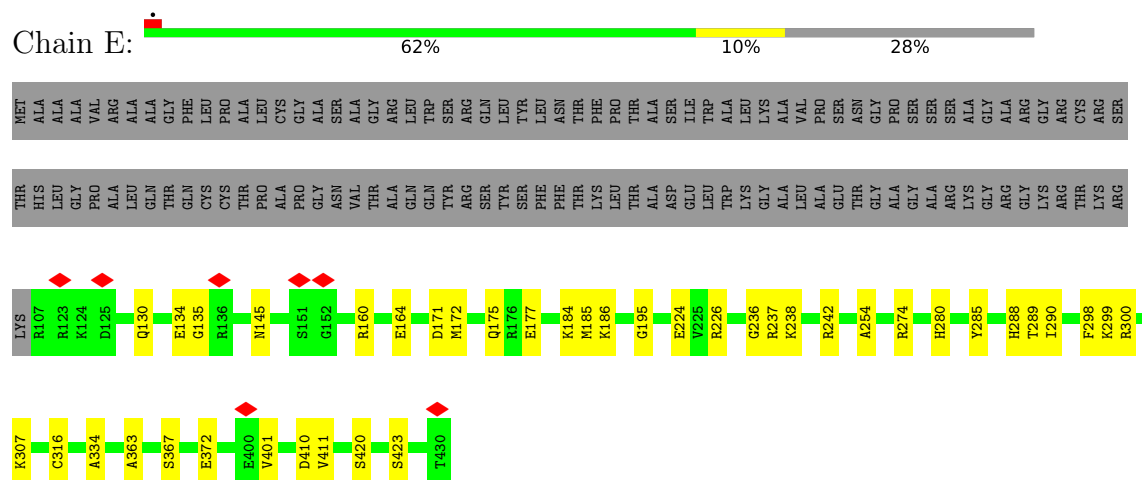
- Molecule 1: 28S ribosomal RNA, mitochondrial



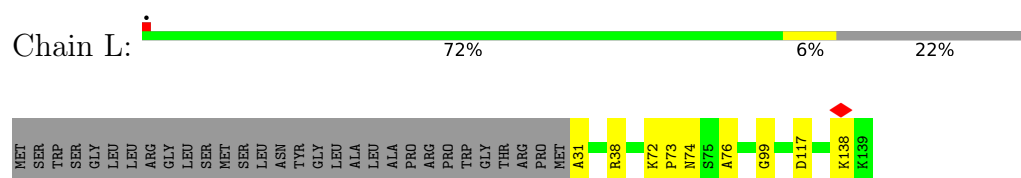
- Molecule 2: 28S ribosomal protein S24, mitochondrial



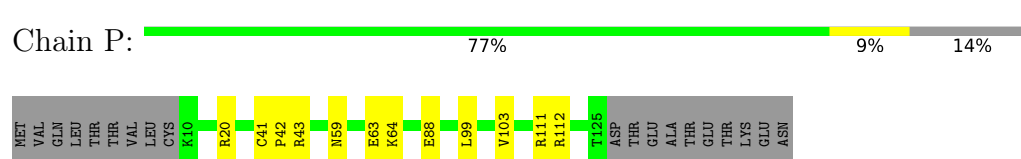
- Molecule 3: 28S ribosomal protein S5, mitochondrial



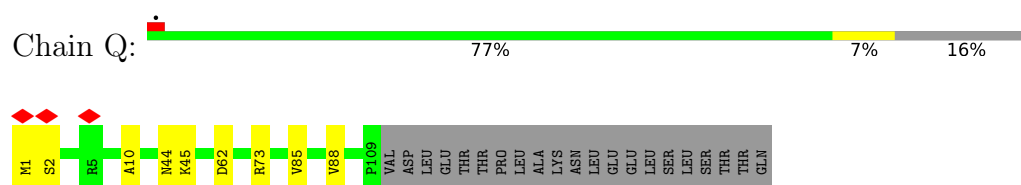
- Molecule 4: 28S ribosomal protein S12, mitochondrial



- Molecule 5: 28S ribosomal protein S16, mitochondrial

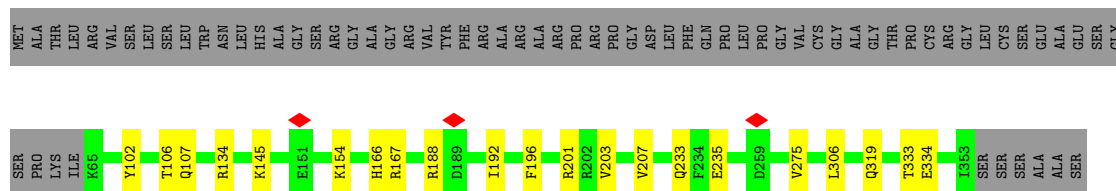


- Molecule 6: 28S ribosomal protein S17, mitochondrial



- Molecule 7: 28S ribosomal protein S22, mitochondrial

Chain a:  75% 6% 19%



- Molecule 8: 28S ribosomal protein S25, mitochondrial

Chain c:  86% 11%



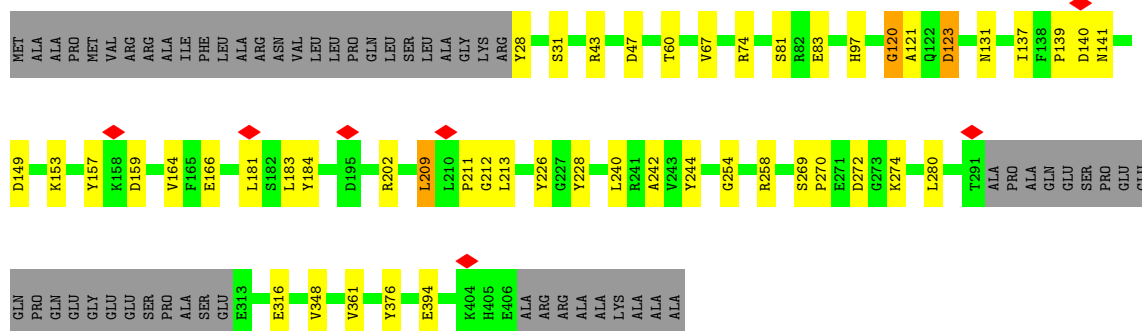
- Molecule 9: 28S ribosomal protein S26, mitochondrial

Chain d:  80% 6% 14%



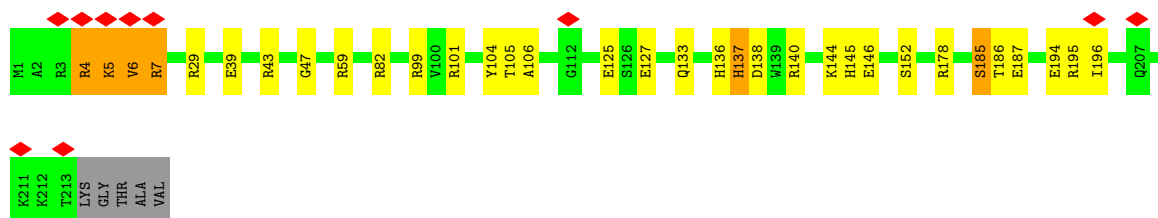
- Molecule 10: 28S ribosomal protein S27, mitochondrial

Chain e:  74% 11% 14%



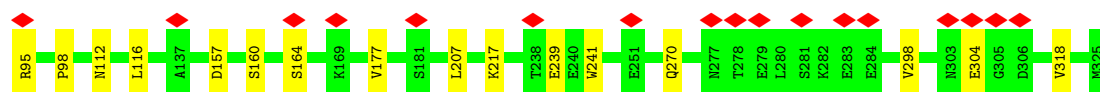
- Molecule 11: 28S ribosomal protein S34, mitochondrial

Chain j:  5% 83% 12%

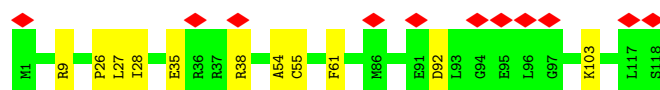


- Molecule 12: 28S ribosomal protein S18b, mitochondrial

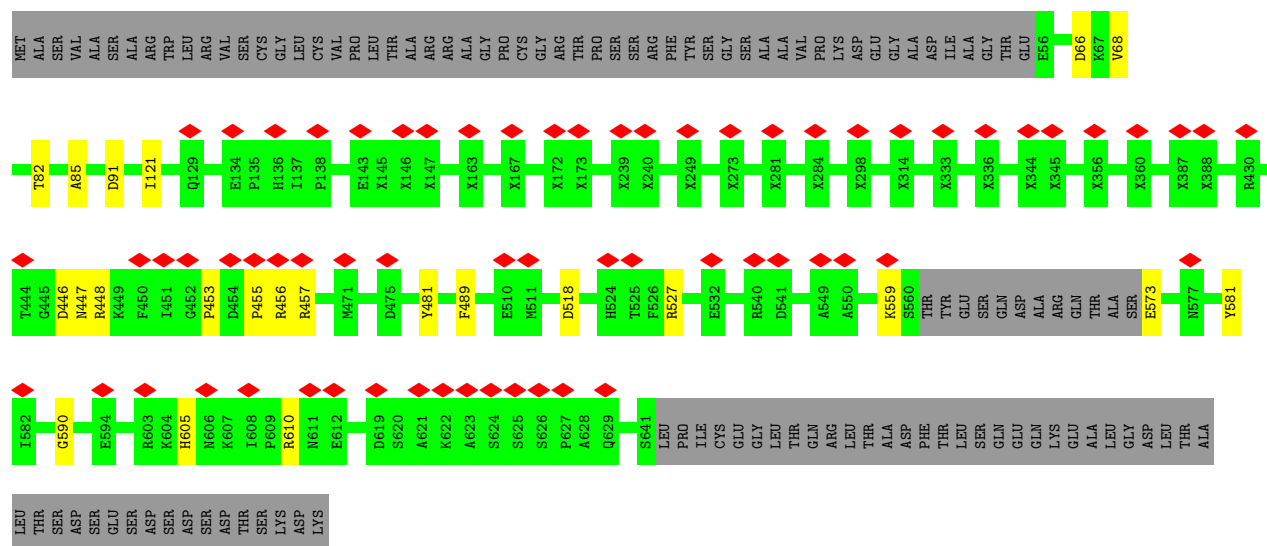
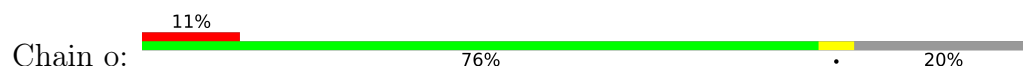




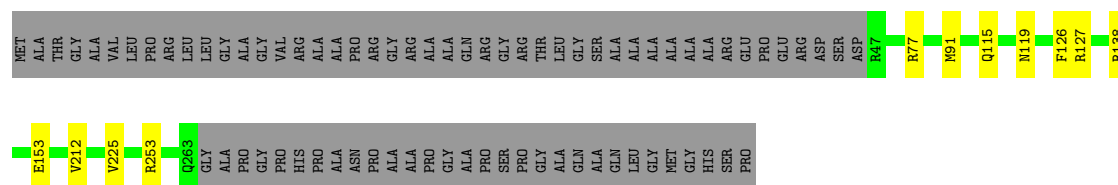
- Molecule 21: Coiled-coil-helix-coiled-coil-helix domain containing 1



- Molecule 22: Pentatricopeptide repeat domain-containing protein 3, mitochondrial



- Molecule 23: 28S ribosomal protein S2, mitochondrial



- Molecule 24: 28S ribosomal protein S6, mitochondrial



- Molecule 25: 28S ribosomal protein S11, mitochondrial



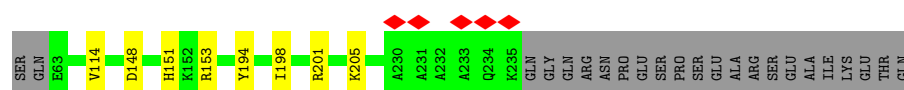
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- Molecule 26: 28S ribosomal protein S15, mitochondrial



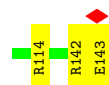
MET LEU ARG ALA TRP ARG ALA LEU SER SER ILE ARG THR GLN ALA VAL THR PRO PRO VAL LEU GLY LEU PRO GLY GLY CYS LYS LEU LEU SER SER SER LEU ILE LEU GLN ALA ALA ARG GLY TYR THR THR LYS PRO VAL GLN



- Molecule 27: 28S ribosomal protein S18c, mitochondrial



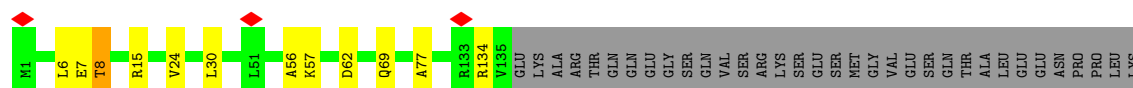
MET ALA VAL LEU LEU CYS GLY GLY LEU LYS ARG LYS PHE THR ARG PHE PRO THR PHE PHE VAL CYS LEU THR ASN SER GLY THR ARG ALA VAL LEU TRP ARG SER CYS SER GLN CYS LYS GLN VAL THR S47 M55 C66 I67 N77 F88 G102 R106



- Molecule 28: 28S ribosomal protein S21, mitochondrial



- Molecule 29: 28S ribosomal protein S23, mitochondrial



GLU VAL PRO GLN ALA HIS LEU GLU SER PRO GLY GLU GLU SER LYS LEU SER PRO PRO

- Molecule 30: 28S ribosomal protein S28, mitochondrial



MET
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E175
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- Molecule 31: Aurora kinase A interacting protein 1

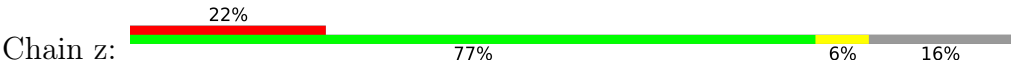


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K199

- Molecule 32: Translation initiation factor IF-3, mitochondrial



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K70
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L89
D96
L97
G98
N99
M100
H101
R102

A103
N104
V105
I106
R107
D110
E111
R112
D113
N120
T121
S122
T123
E124
P125
A126
E127
N150
P151
K152
E160
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K177
N198
V199
D200
V201
M217
P218
A242
F243
S244
K245
N246
E259
R260
D261
T262
L263
N264
LYS
ASP
HIS
GLY
ASN
ASP
LYS
GLU
SER
ASN

VAL
LEU
HIS
GLN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	198355	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.475	Depositor
Minimum map value	-0.896	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	429.30002, 429.30002, 429.30002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07325, 1.07325, 1.07325	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	0.06	0/22681	0.17	0/35318
2	C	0.07	0/1026	0.21	0/1389
3	E	0.09	0/2511	0.23	0/3369
4	L	0.12	0/872	0.26	0/1171
5	P	0.09	0/937	0.23	0/1262
6	Q	0.09	0/874	0.18	0/1183
7	a	0.07	0/2403	0.20	0/3246
8	c	0.08	0/1406	0.21	0/1894
9	d	0.10	0/1489	0.21	0/2008
10	e	0.10	0/3011	0.26	0/4066
11	j	0.12	0/1841	0.28	0/2493
12	p	0.09	0/1583	0.23	0/2149
13	G	0.12	0/1761	0.27	0/2366
14	I	0.10	0/2597	0.24	0/3487
15	J	0.07	0/1071	0.19	0/1447
16	N	0.10	0/878	0.25	0/1179
17	g	0.11	0/2923	0.26	0/3956
18	h	0.07	0/899	0.18	0/1209
19	i	0.09	0/834	0.22	0/1112
20	k	0.08	0/2275	0.22	0/3075
21	m	0.11	0/961	0.25	0/1284
22	o	0.07	0/2605	0.19	0/3526
23	B	0.10	0/1766	0.23	0/2392
24	F	0.11	0/1009	0.22	0/1362
25	K	0.10	0/1021	0.24	0/1380
26	O	0.08	0/1443	0.20	0/1927
27	R	0.08	0/805	0.25	0/1082
28	U	0.12	0/748	0.24	0/995
29	b	0.10	0/1135	0.21	0/1528
30	f	0.07	0/787	0.20	0/1059
31	n	0.10	0/654	0.24	0/862
32	z	0.09	0/1633	0.22	0/2191
All	All	0.08	0/68439	0.21	0/96967

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20256	0	10258	165	0
2	C	998	0	1005	5	0
3	E	2464	0	2489	22	0
4	L	853	0	904	5	0
5	P	916	0	944	9	0
6	Q	857	0	920	6	0
7	a	2356	0	2371	11	0
8	c	1374	0	1395	13	0
9	d	1463	0	1438	10	0
10	e	2950	0	2940	23	0
11	j	1792	0	1810	20	0
12	p	1531	0	1495	7	0
13	G	1721	0	1751	24	0
14	I	2541	0	2498	20	0
15	J	1049	0	1088	7	0
16	N	861	0	890	14	0
17	g	2855	0	2894	22	0
18	h	871	0	814	3	0
19	i	818	0	845	5	0
20	k	2227	0	2267	11	0
21	m	945	0	984	4	0
22	o	3273	0	2695	9	0
23	B	1726	0	1747	8	0
24	F	991	0	1034	5	0
25	K	1001	0	1041	12	0
26	O	1421	0	1526	5	0
27	R	788	0	823	9	0
28	U	737	0	759	8	0
29	b	1108	0	1124	6	0
30	f	775	0	793	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	n	642	0	718	11	0
32	z	1616	0	1600	7	0
All	All	65776	0	55860	387	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 3.

All (387) 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:79:C:O2	1:A:101:G:N2	2.03	0.91
1:A:242:G:HO2'	1:A:257:C:HO2'	1.15	0.87
1:A:580:C:O2'	1:A:581:U:OP1	1.95	0.84
11:j:144:LYS:O	11:j:146:GLU:N	2.12	0.81
10:e:157:TYR:O	10:e:184:TYR:OH	1.98	0.81
1:A:737:C:O2'	1:A:740:G:N2	2.14	0.80
1:A:755:U:O2'	1:A:798:A:N3	2.14	0.80
1:A:515:G:O2'	31:n:128:ARG:NE	2.15	0.79
1:A:88:A:N6	1:A:91:A:N7	2.30	0.79
1:A:863:U:O5'	1:A:865:A:N6	2.14	0.79
10:e:202:ARG:NE	10:e:242:ALA:O	2.15	0.79
1:A:193:C:N4	1:A:194:G:O6	2.17	0.78
32:z:173:ASP:OD2	32:z:177:LYS:NZ	2.18	0.77
13:G:70:LYS:NZ	14:I:195:ILE:O	2.16	0.77
1:A:89:U:OP1	9:d:68:ARG:NE	2.19	0.76
13:G:37:TYR:OH	14:I:373:ASP:OD1	2.03	0.76
1:A:865:A:O2'	1:A:866:G:O4'	2.03	0.76
1:A:295:G:O2'	26:O:153:ARG:NH2	2.20	0.74
1:A:338:U:OP2	25:K:96:ASN:ND2	2.20	0.74
12:p:201:PRO:O	12:p:206:LYS:NZ	2.20	0.74
7:a:201:ARG:NH1	7:a:233:GLN:O	2.20	0.73
1:A:528:C:O2'	21:m:35:GLU:OE2	2.07	0.73
1:A:580:C:HO2'	1:A:581:U:P	2.10	0.73
1:A:368:G:OP2	21:m:9:ARG:NH2	2.21	0.73
1:A:495:G:OP1	26:O:201:ARG:NE	2.21	0.73
1:A:635:A:OP2	3:E:242:ARG:NH1	2.21	0.72
1:A:881:U:OP1	11:j:99:ARG:NH2	2.23	0.72
1:A:938:A:OP1	31:n:141:HIS:NE2	2.23	0.72
7:a:166:HIS:O	7:a:188:ARG:NH2	2.23	0.72
1:A:498:A:O2'	1:A:499:C:O5'	2.07	0.71
1:A:15:C:O2'	1:A:16:A:OP1	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:G:OP1	6:Q:44:ASN:ND2	2.23	0.71
8:c:51:ASN:OD1	8:c:95:ASN:ND2	2.24	0.70
1:A:55:C:O2	1:A:193:C:O2'	2.08	0.70
1:A:374:A:O2'	1:A:400:A:O4'	2.09	0.70
1:A:772:G:O2'	1:A:773:G:O4'	2.09	0.70
14:I:202:LYS:NZ	14:I:215:ASP:OD1	2.23	0.70
1:A:134:C:OP2	4:L:38:ARG:NH1	2.23	0.70
1:A:235:C:N4	1:A:236:G:O6	2.25	0.70
10:e:244:TYR:OH	11:j:140:ARG:NH2	2.25	0.70
27:R:102:GLY:O	27:R:106:ARG:NH1	2.24	0.70
1:A:298:A:N6	1:A:393:A:O4'	2.25	0.69
8:c:89:ASP:O	8:c:93:LYS:NZ	2.26	0.69
4:L:31:ALA:O	8:c:4:LYS:NZ	2.25	0.69
1:A:729:A:O4'	17:g:392:ARG:NH1	2.25	0.69
1:A:723:U:O4	1:A:724:A:N6	2.26	0.69
1:A:842:C:O2	1:A:938:A:O2'	2.08	0.69
29:b:6:LEU:O	29:b:15:ARG:NH1	2.26	0.69
10:e:74:ARG:NH2	10:e:394:GLU:OE1	2.26	0.68
18:h:291:GLU:OE2	18:h:295:TRP:NE1	2.26	0.68
1:A:862:U:O2'	1:A:863:U:OP1	2.11	0.67
1:A:524:G:O2'	1:A:526:U:OP1	2.08	0.67
3:E:172:MET:SD	3:E:175:GLN:NE2	2.68	0.66
1:A:743:C:OP2	1:A:769:A:N6	2.28	0.66
1:A:133:A:OP2	26:O:194:TYR:OH	2.09	0.66
1:A:717:A:N6	1:A:734:A:O2'	2.28	0.66
1:A:719:U:O4	13:G:192:ARG:NE	2.30	0.65
16:N:41:ARG:NH2	16:N:88:ARG:O	2.29	0.65
1:A:314:U:O4	1:A:315:A:N6	2.29	0.65
13:G:71:THR:OG1	14:I:251:GLN:O	2.15	0.65
9:d:187:TYR:O	27:R:77:ASN:ND2	2.29	0.65
1:A:871:U:O2	1:A:873:U:N3	2.30	0.65
23:B:115:GLN:OE1	23:B:119:ASN:ND2	2.30	0.64
1:A:163:A:O2'	1:A:164:A:O4'	2.10	0.64
7:a:167:ARG:NE	12:p:174:ASP:OD2	2.30	0.64
1:A:288:A:O3'	31:n:128:ARG:NH1	2.30	0.64
1:A:539:U:O2	1:A:814:U:O2'	2.08	0.64
1:A:79:C:N3	1:A:101:G:N1	2.45	0.64
13:G:68:LEU:HD21	14:I:366:GLN:HB2	1.80	0.63
1:A:72:G:O2'	11:j:7:ARG:NH2	2.31	0.63
1:A:549:C:O2'	1:A:802:U:O4	2.17	0.63
23:B:127:ARG:NH1	29:b:30:LEU:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:A:O2'	1:A:454:A:OP2	2.16	0.63
1:A:693:A:O2'	1:A:694:U:OP2	2.14	0.63
27:R:143:GLU:O	28:U:28:ARG:NH1	2.32	0.63
1:A:571:C:N3	1:A:801:G:N2	2.46	0.63
1:A:532:A:N6	1:A:819:C:O2'	2.32	0.62
11:j:82:ARG:NH2	11:j:133:GLN:OE1	2.32	0.62
20:k:239:GLU:OE1	20:k:241:TRP:NE1	2.31	0.62
1:A:311:A:OP2	27:R:106:ARG:NH2	2.32	0.62
1:A:363:U:O2'	1:A:364:A:OP1	2.14	0.62
1:A:579:C:O2'	16:N:86:ARG:NH2	2.33	0.62
5:P:20:ARG:NH2	5:P:42:PRO:O	2.32	0.62
10:e:254:GLY:O	10:e:258:ARG:NH1	2.33	0.62
10:e:43:ARG:NH2	10:e:376:TYR:OH	2.32	0.62
1:A:571:C:HO2'	1:A:803:G:HO2'	1.47	0.62
1:A:784:A:N6	1:A:813:A:OP2	2.33	0.62
1:A:288:A:OP1	31:n:128:ARG:N	2.32	0.62
1:A:448:A:OP2	1:A:450:A:N6	2.33	0.62
22:o:581:TYR:OH	22:o:610:ARG:NH1	2.33	0.62
17:g:170:SER:N	17:g:176:ARG:O	2.33	0.61
17:g:227:GLN:OE1	17:g:231:ARG:NH1	2.34	0.61
1:A:402:A:O2'	1:A:931:U:O2'	2.09	0.61
1:A:810:U:O2'	13:G:102:GLY:O	2.18	0.61
1:A:953:A:N3	28:U:61:ARG:NH1	2.48	0.61
1:A:359:A:O2'	25:K:187:ASN:O	2.18	0.61
1:A:877:C:O2'	1:A:880:A:OP2	2.19	0.61
14:I:135:GLN:OE1	14:I:136:ARG:N	2.34	0.61
1:A:846:A:N6	1:A:913:G:O6	2.34	0.61
18:h:352:ASN:ND2	19:i:37:PHE:O	2.34	0.61
1:A:930:A:N6	1:A:944:G:O6	2.34	0.60
1:A:258:G:O2'	4:L:138:LYS:O	2.14	0.60
1:A:833:C:O5'	1:A:839:G:N2	2.34	0.60
14:I:237:GLU:N	14:I:237:GLU:OE1	2.32	0.60
15:J:89:ASP:OD1	15:J:141:ARG:NH2	2.35	0.60
25:K:161:ARG:NH2	25:K:180:ASP:OD1	2.34	0.60
14:I:260:LEU:N	14:I:269:PHE:O	2.34	0.60
17:g:271:THR:HG22	17:g:273:LEU:H	1.67	0.60
1:A:553:U:OP1	1:A:572:C:N4	2.34	0.60
13:G:85:VAL:O	17:g:369:LYS:NZ	2.24	0.60
1:A:54:G:O6	1:A:62:A:N6	2.36	0.59
1:A:74:A:OP1	11:j:4:ARG:NE	2.36	0.59
1:A:188:A:N6	1:A:205:U:O4'	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:917:U:O2	1:A:918:A:N6	2.35	0.59
26:O:205:LYS:HE3	31:n:176:ILE:HD11	1.85	0.59
1:A:228:U:OP2	1:A:229:A:O2'	2.06	0.59
1:A:342:A:O2'	1:A:420:G:O3'	2.21	0.58
1:A:894:G:O4'	31:n:178:GLN:NE2	2.36	0.58
29:b:77:ALA:O	29:b:134:ARG:NH2	2.37	0.58
3:E:410:ASP:OD1	3:E:411:VAL:N	2.36	0.58
1:A:814:U:OP1	13:G:93:LYS:NZ	2.37	0.58
32:z:242:ALA:O	32:z:244:SER:N	2.37	0.58
14:I:231:LEU:O	14:I:233:CYS:N	2.37	0.58
1:A:15:C:HO2'	1:A:16:A:P	2.25	0.58
10:e:123:ASP:OD1	10:e:123:ASP:N	2.37	0.58
1:A:121:A:OP1	6:Q:73:ARG:NH1	2.36	0.57
3:E:316:CYS:SG	3:E:334:ALA:N	2.77	0.57
20:k:177:VAL:O	20:k:207:LEU:N	2.37	0.57
10:e:28:TYR:N	10:e:149:ASP:OD1	2.38	0.57
1:A:540:C:O3'	13:G:185:LYS:NZ	2.30	0.57
1:A:571:C:O2'	1:A:803:G:O2'	2.14	0.57
12:p:60:ASP:OD1	12:p:121:LYS:NZ	2.38	0.56
1:A:425:G:N1	1:A:917:U:OP1	2.32	0.56
13:G:68:LEU:HD22	14:I:362:GLU:HG3	1.86	0.56
17:g:161:VAL:HG12	17:g:271:THR:HG23	1.87	0.56
17:g:202:LYS:O	17:g:249:GLN:NE2	2.38	0.56
4:L:74:ASN:ND2	4:L:117:ASP:OD1	2.39	0.55
10:e:209:LEU:HD11	10:e:228:TYR:CZ	2.41	0.55
3:E:164:GLU:N	3:E:164:GLU:OE1	2.38	0.55
10:e:316:GLU:O	12:p:218:ARG:NH1	2.39	0.55
11:j:178:ARG:NH2	11:j:185:SER:O	2.39	0.55
17:g:122:ARG:NH2	17:g:298:ASN:OD1	2.38	0.55
27:R:88:PHE:O	28:U:10:ARG:N	2.38	0.55
14:I:110:TYR:OH	20:k:116:LEU:O	2.23	0.55
13:G:240:ARG:NE	13:G:242:TRP:O	2.39	0.55
1:A:372:A:OP1	1:A:386:A:N6	2.40	0.55
20:k:157:ASP:OD1	20:k:217:LYS:NZ	2.40	0.55
11:j:29:ARG:NH1	11:j:104:TYR:O	2.40	0.55
25:K:88:ILE:N	25:K:103:VAL:O	2.38	0.55
16:N:96:ARG:NH1	16:N:98:ARG:O	2.40	0.54
23:B:126:PHE:O	23:B:253:ARG:NH1	2.39	0.54
26:O:148:ASP:OD2	26:O:151:HIS:ND1	2.40	0.54
12:p:73:VAL:HG12	12:p:74:TRP:H	1.72	0.54
1:A:425:G:N2	1:A:916:G:O3'	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:C:O2'	1:A:841:C:O4'	2.25	0.54
1:A:103:A:OP1	6:Q:10:ALA:N	2.40	0.54
5:P:112:ARG:NH2	9:d:52:GLU:OE2	2.40	0.54
10:e:183:LEU:HD22	10:e:361:VAL:HG11	1.90	0.54
10:e:139:PRO:O	10:e:141:ASN:N	2.41	0.54
1:A:522:G:O2'	1:A:837:C:OP2	2.23	0.54
11:j:43:ARG:O	11:j:47:GLY:N	2.39	0.53
1:A:288:A:O2'	31:n:128:ARG:NH2	2.41	0.53
6:Q:62:ASP:OD1	6:Q:88:VAL:N	2.40	0.53
20:k:58:ARG:NH2	22:o:91:ASP:OD1	2.41	0.53
14:I:155:LYS:NZ	14:I:217:ASP:OD2	2.42	0.53
1:A:862:U:O2	1:A:894:G:N1	2.41	0.53
3:E:420:SER:OG	3:E:423:SER:OG	2.26	0.53
15:J:104:ILE:O	15:J:105:SER:OG	2.25	0.53
3:E:254:ALA:O	3:E:280:HIS:N	2.41	0.53
14:I:198:ARG:HG2	14:I:248:VAL:HG12	1.90	0.52
15:J:123:SER:OG	15:J:124:VAL:N	2.40	0.52
25:K:83:PHE:O	25:K:151:ARG:NH2	2.43	0.52
22:o:455:PRO:O	22:o:457:ARG:N	2.42	0.52
3:E:135:GLY:O	3:E:160:ARG:NH2	2.42	0.52
16:N:94:THR:O	16:N:95:SER:OG	2.22	0.51
24:F:5:GLU:N	24:F:94:VAL:O	2.43	0.51
1:A:189:U:O2	5:P:43:ARG:NH1	2.42	0.51
17:g:48:SER:OG	17:g:49:ARG:N	2.42	0.51
1:A:457:U:O4	1:A:458:A:N6	2.43	0.51
20:k:66:GLN:OE1	22:o:82:THR:OG1	2.25	0.51
27:R:142:ARG:O	28:U:28:ARG:NH1	2.44	0.51
1:A:354:A:OP2	24:F:57:ARG:NH1	2.42	0.51
16:N:88:ARG:NH1	16:N:97:PRO:O	2.40	0.51
20:k:58:ARG:NH2	22:o:85:ALA:O	2.44	0.51
12:p:81:HIS:NE2	12:p:83:GLY:O	2.44	0.51
1:A:500:A:N3	31:n:151:ARG:NH2	2.59	0.51
18:h:328:TYR:O	18:h:368:ARG:NH2	2.43	0.51
11:j:194:GLU:OE2	11:j:195:ARG:NH1	2.44	0.51
8:c:89:ASP:OD2	9:d:120:ARG:NH2	2.38	0.50
3:E:298:PHE:O	3:E:300:ARG:N	2.44	0.50
1:A:581:U:O2'	16:N:98:ARG:NH1	2.44	0.50
1:A:882:U:OP1	11:j:101:ARG:NH2	2.45	0.50
5:P:88:GLU:OE1	9:d:63:TYR:OH	2.25	0.50
22:o:481:TYR:OH	22:o:518:ASP:OD2	2.30	0.50
17:g:301:GLN:OE1	20:k:270:GLN:NE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:U:OP1	8:c:133:LYS:NZ	2.44	0.50
1:A:332:A:H2'	1:A:333:A:O4'	2.12	0.50
3:E:171:ASP:OD1	3:E:172:MET:N	2.45	0.50
1:A:119:A:N3	1:A:129:G:O2'	2.34	0.50
21:m:26:PRO:O	21:m:28:ILE:N	2.44	0.50
1:A:491:A:O2'	1:A:853:U:O2'	2.30	0.50
2:C:140:GLU:O	2:C:144:SER:OG	2.27	0.50
23:B:138:ARG:NH2	28:U:84:TRP:O	2.44	0.50
1:A:700:G:OP1	16:N:80:ARG:NH1	2.41	0.49
17:g:122:ARG:NH1	17:g:296:VAL:O	2.45	0.49
17:g:178:ASP:OD2	17:g:236:THR:OG1	2.30	0.49
29:b:7:GLU:O	29:b:8:THR:OG1	2.23	0.49
1:A:15:C:O2'	1:A:16:A:P	2.70	0.49
1:A:330:C:H42	1:A:350:A:H61	1.59	0.49
1:A:642:A:N6	28:U:80:ARG:O	2.46	0.49
3:E:285:TYR:OH	3:E:372:GLU:OE1	2.31	0.49
1:A:574:A:OP2	16:N:96:ARG:NH1	2.46	0.49
10:e:31:SER:OG	10:e:153:LYS:NZ	2.41	0.49
13:G:187:MET:HE1	13:G:208:GLU:CB	2.43	0.49
1:A:105:C:OP2	6:Q:45:LYS:NZ	2.43	0.49
10:e:211:PRO:O	10:e:213:LEU:N	2.46	0.49
1:A:166:C:O2	1:A:169:C:N4	2.40	0.48
13:G:203:GLU:OE2	13:G:207:GLN:NE2	2.46	0.48
10:e:120:GLY:O	10:e:121:ALA:HB3	2.13	0.48
30:f:153:ARG:NE	30:f:160:ASP:OD1	2.45	0.48
1:A:855:A:OP1	31:n:164:ARG:NH2	2.46	0.48
1:A:380:C:O2'	24:F:93:VAL:O	2.31	0.48
16:N:56:SER:O	16:N:60:ASN:ND2	2.41	0.48
13:G:114:THR:HG21	13:G:205:LEU:HD22	1.95	0.48
16:N:113:HIS:O	16:N:117:HIS:ND1	2.44	0.48
22:o:527:ARG:NE	22:o:573:GLU:OE2	2.47	0.48
1:A:341:A:OP1	25:K:121:ARG:NH2	2.47	0.48
31:n:173:LEU:HA	31:n:176:ILE:HD12	1.96	0.48
1:A:412:C:HO2'	25:K:189:CYS:HG	1.62	0.47
7:a:106:THR:HG22	7:a:107:GLN:H	1.79	0.47
17:g:332:GLY:O	17:g:336:LEU:HD23	2.14	0.47
20:k:160:SER:OG	20:k:164:SER:O	2.32	0.47
8:c:139:CYS:SG	8:c:140:ILE:N	2.86	0.47
1:A:97:A:H2'	1:A:98:A:C8	2.49	0.47
1:A:896:U:OP2	31:n:171:ARG:NH1	2.48	0.47
5:P:64:LYS:N	7:a:154:LYS:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:g:123:TYR:O	17:g:307:LEU:N	2.48	0.47
1:A:757:A:OP1	16:N:51:ARG:NH1	2.47	0.47
1:A:832:A:N6	1:A:923:G:O2'	2.47	0.47
1:A:880:A:H3'	1:A:881:U:C5'	2.44	0.47
16:N:91:CYS:SG	16:N:92:VAL:N	2.84	0.47
2:C:62:ILE:O	2:C:63:ALA:HB3	2.15	0.47
10:e:159:ASP:OD1	10:e:159:ASP:N	2.47	0.47
29:b:62:ASP:OD1	29:b:62:ASP:N	2.46	0.47
1:A:43:U:O4	1:A:45:C:N4	2.48	0.47
1:A:808:G:OP2	14:I:377:ARG:NH1	2.47	0.47
1:A:58:C:N4	11:j:137:HIS:O	2.46	0.46
3:E:236:GLY:O	3:E:238:LYS:N	2.48	0.46
5:P:20:ARG:NH2	5:P:41:CYS:SG	2.88	0.46
13:G:119:LYS:NZ	17:g:364:TRP:O	2.45	0.46
14:I:72:ASP:OD1	14:I:73:PHE:N	2.48	0.46
1:A:331:U:O2'	25:K:112:ARG:NH2	2.49	0.46
7:a:275:VAL:HG11	7:a:306:LEU:HD12	1.98	0.46
1:A:237:U:O4	1:A:254:A:N7	2.48	0.46
1:A:237:U:H3	1:A:254:A:H62	1.62	0.46
2:C:110:LEU:HD23	2:C:111:LYS:N	2.31	0.46
1:A:531:U:O4	1:A:532:A:N6	2.45	0.46
10:e:60:THR:HG21	10:e:67:VAL:HG12	1.97	0.46
10:e:137:ILE:HD12	10:e:139:PRO:HG3	1.98	0.46
8:c:48:VAL:HA	8:c:52:ILE:HD12	1.98	0.45
1:A:532:A:N6	1:A:823:G:O6	2.49	0.45
13:G:187:MET:HE3	13:G:191:CYS:HB3	1.96	0.45
24:F:111:VAL:HG13	24:F:111:VAL:O	2.16	0.45
10:e:272:ASP:HB2	10:e:348:VAL:HG21	1.97	0.45
1:A:61:C:O2'	1:A:193:C:OP1	2.35	0.45
1:A:744:G:N2	1:A:770:A:N7	2.65	0.45
8:c:91:GLU:OE2	9:d:123:ARG:NH2	2.49	0.45
1:A:380:C:OP1	27:R:114:ARG:NE	2.46	0.45
3:E:224:GLU:OE2	3:E:226:ARG:NH2	2.50	0.45
12:p:73:VAL:HG12	12:p:74:TRP:N	2.31	0.45
1:A:362:A:O5'	25:K:187:ASN:ND2	2.50	0.45
9:d:134:TRP:NE1	9:d:138:GLU:OE2	2.50	0.45
1:A:222:G:O2'	1:A:270:C:O2	2.34	0.44
1:A:574:A:OP1	16:N:98:ARG:NE	2.42	0.44
1:A:683:G:H2'	1:A:684:G:N9	2.32	0.44
1:A:855:A:N6	1:A:901:G:OP2	2.50	0.44
25:K:74:SER:OG	25:K:75:SER:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R:55:MET:SD	29:b:69:GLN:NE2	2.90	0.44
14:I:214:SER:OG	14:I:215:ASP:N	2.51	0.44
19:i:19:PHE:O	19:i:20:SER:OG	2.30	0.44
10:e:164:VAL:HG21	10:e:184:TYR:HD2	1.82	0.44
32:z:100:MET:SD	32:z:104:ASN:ND2	2.90	0.44
11:j:6:VAL:HG12	11:j:7:ARG:H	1.83	0.44
1:A:545:G:N1	1:A:776:G:OP2	2.50	0.44
1:A:719:U:C4	13:G:98:MET:HE1	2.53	0.44
5:P:111:ARG:NH2	7:a:145:LYS:O	2.51	0.44
1:A:402:A:OP1	1:A:943:U:O2'	2.35	0.44
10:e:164:VAL:HG22	10:e:181:LEU:HD13	2.00	0.44
13:G:133:GLU:O	13:G:137:VAL:HG12	2.18	0.44
15:J:85:LYS:NZ	15:J:110:GLU:OE2	2.50	0.44
20:k:112:ASN:OD1	20:k:112:ASN:N	2.51	0.44
1:A:842:C:H2'	1:A:843:G:C8	2.53	0.44
6:Q:1:MET:O	6:Q:2:SER:OG	2.34	0.44
9:d:102:HIS:NE2	9:d:106:MET:HE3	2.32	0.44
1:A:880:A:O2'	11:j:99:ARG:NE	2.50	0.44
10:e:81:SER:OG	10:e:83:GLU:OE1	2.35	0.44
1:A:787:A:C4	1:A:812:A:N6	2.86	0.43
1:A:306:A:O2'	1:A:387:U:OP1	2.19	0.43
11:j:136:HIS:O	11:j:138:ASP:N	2.49	0.43
17:g:344:VAL:O	17:g:344:VAL:HG13	2.19	0.43
8:c:26:SER:O	8:c:81:ASP:N	2.51	0.43
8:c:51:ASN:ND2	8:c:99:MET:SD	2.92	0.43
11:j:5:LYS:HA	11:j:6:VAL:HB	1.99	0.43
32:z:81:LYS:O	32:z:83:SER:N	2.51	0.43
1:A:610:A:N6	1:A:680:C:O2	2.52	0.43
2:C:142:LEU:HA	22:o:121:ILE:HD11	2.00	0.43
22:o:446:ASP:O	22:o:448:ARG:N	2.52	0.43
32:z:96:ASP:OD1	32:z:97:LEU:N	2.52	0.43
1:A:331:U:O2	1:A:349:G:O6	2.36	0.43
13:G:105:ILE:HD12	14:I:337:ARG:CZ	2.48	0.43
15:J:79:LEU:O	15:J:171:GLU:N	2.49	0.43
32:z:217:MET:SD	32:z:217:MET:N	2.86	0.43
5:P:59:ASN:OD1	5:P:63:GLU:N	2.51	0.43
13:G:59:THR:HG23	13:G:60:GLU:N	2.34	0.43
17:g:166:ASP:O	17:g:179:GLN:NE2	2.51	0.43
1:A:591:U:O4	1:A:692:U:O2'	2.30	0.43
1:A:630:C:OP2	3:E:274:ARG:NH1	2.47	0.43
1:A:731:G:O2'	17:g:163:ASN:ND2	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:192:ILE:O	7:a:196:PHE:N	2.46	0.43
14:I:254:LYS:HD2	14:I:361:VAL:HG11	2.01	0.43
16:N:102:ARG:NH2	19:i:47:GLU:OE1	2.52	0.43
25:K:153:VAL:HG23	25:K:153:VAL:O	2.18	0.43
5:P:99:LEU:HD11	5:P:103:VAL:HG11	2.00	0.42
8:c:158:GLU:O	8:c:164:GLN:NE2	2.51	0.42
19:i:73:ASP:OD1	19:i:74:GLU:N	2.49	0.42
8:c:32:VAL:HG11	8:c:48:VAL:HG22	2.01	0.42
23:B:77:ARG:NH1	30:f:119:GLY:O	2.52	0.42
1:A:177:A:O2'	1:A:178:A:O5'	2.26	0.42
1:A:549:C:N3	1:A:550:C:N4	2.67	0.42
1:A:154:C:O3'	1:A:167:A:N6	2.53	0.42
1:A:935:G:N2	1:A:938:A:OP2	2.52	0.42
3:E:184:LYS:O	3:E:186:LYS:N	2.53	0.42
3:E:363:ALA:O	3:E:367:SER:N	2.49	0.42
11:j:178:ARG:NH1	11:j:187:GLU:O	2.52	0.42
13:G:98:MET:HE2	13:G:110:LEU:CD1	2.50	0.42
1:A:490:U:C2	1:A:506:A:N7	2.87	0.42
1:A:532:A:H4'	1:A:533:U:OP2	2.19	0.42
1:A:869:C:HO2'	1:A:870:A:P	2.42	0.42
25:K:187:ASN:OD1	28:U:42:ARG:NH1	2.49	0.42
1:A:593:G:H8	1:A:693:A:H61	1.66	0.42
3:E:134:GLU:OE1	3:E:134:GLU:N	2.53	0.42
17:g:205:ASP:OD1	17:g:248:ARG:NH1	2.53	0.42
9:d:169:THR:HG22	9:d:170:ARG:H	1.83	0.42
1:A:64:C:O2	1:A:66:C:N4	2.53	0.41
1:A:945:C:C2	1:A:946:U:C5	3.08	0.41
17:g:339:PHE:O	20:k:318:VAL:HG11	2.20	0.41
1:A:498:A:O2'	1:A:499:C:O4'	2.38	0.41
1:A:784:A:O5'	13:G:35:SER:OG	2.38	0.41
11:j:105:THR:OG1	11:j:106:ALA:N	2.53	0.41
1:A:929:C:N4	1:A:930:A:H62	2.17	0.41
3:E:130:GLN:O	19:i:72:ARG:NH1	2.53	0.41
1:A:792:A:H2'	1:A:793:A:O4'	2.21	0.41
10:e:226:TYR:CZ	10:e:280:LEU:HD13	2.55	0.41
15:J:166:GLU:N	15:J:166:GLU:OE1	2.53	0.41
21:m:92:ASP:OD1	21:m:103:LYS:NZ	2.51	0.41
27:R:66:CYS:SG	27:R:67:ILE:N	2.93	0.41
1:A:389:G:H1'	1:A:390:C:P	2.60	0.41
1:A:858:U:O4	1:A:898:C:N3	2.54	0.41
1:A:642:A:N3	23:B:138:ARG:NH1	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:A:N6	1:A:789:A:N6	2.69	0.41
1:A:862:U:H4'	1:A:863:U:OP2	2.21	0.41
3:E:307:LYS:NZ	7:a:102:TYR:OH	2.54	0.41
7:a:134:ARG:NH1	7:a:235:GLU:OE1	2.54	0.41
8:c:86:VAL:HG21	9:d:106:MET:HE1	2.03	0.41
13:G:71:THR:CB	14:I:251:GLN:O	2.69	0.41
13:G:73:VAL:O	13:G:73:VAL:HG23	2.21	0.41
24:F:49:TYR:OH	24:F:90:ARG:NH1	2.54	0.41
1:A:17:G:N2	1:A:512:A:O2'	2.53	0.41
1:A:716:C:O3'	1:A:773:G:N2	2.54	0.41
3:E:289:THR:HG22	3:E:290:ILE:N	2.36	0.41
14:I:103:ASP:OD1	14:I:106:ARG:NH2	2.54	0.41
15:J:175:THR:O	15:J:175:THR:HG23	2.21	0.41
23:B:225:VAL:HG13	23:B:225:VAL:O	2.20	0.40
28:U:5:LEU:HB2	28:U:8:ILE:HD11	2.02	0.40
11:j:125:GLU:O	11:j:127:GLU:N	2.54	0.40
17:g:264:VAL:HG13	17:g:267:LEU:HD12	2.03	0.40
1:A:129:G:H2'	1:A:129:G:N3	2.36	0.40
1:A:424:A:O2'	32:z:160:GLU:O	2.37	0.40
2:C:110:LEU:HD21	2:C:117:VAL:HG13	2.03	0.40
3:E:401:VAL:O	3:E:401:VAL:HG22	2.22	0.40
4:L:72:LYS:N	4:L:73:PRO:HD2	2.37	0.40
7:a:207:VAL:HG12	7:a:207:VAL:O	2.21	0.40
3:E:285:TYR:N	3:E:289:THR:O	2.48	0.40
17:g:297:LYS:O	17:g:298:ASN:C	2.65	0.40
1:A:312:A:O2'	1:A:376:U:O2	2.35	0.40
11:j:39:GLU:O	11:j:59:ARG:NH2	2.54	0.40
23:B:91:MET:HE1	23:B:212:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	121/167 (72%)	102 (84%)	15 (12%)	4 (3%)	3	19
3	E	307/430 (71%)	258 (84%)	43 (14%)	6 (2%)	6	28
4	L	107/139 (77%)	97 (91%)	8 (8%)	2 (2%)	6	29
5	P	114/135 (84%)	102 (90%)	12 (10%)	0	100	100
6	Q	107/130 (82%)	92 (86%)	14 (13%)	1 (1%)	14	43
7	a	287/359 (80%)	258 (90%)	25 (9%)	4 (1%)	9	34
8	c	166/173 (96%)	149 (90%)	16 (10%)	1 (1%)	21	52
9	d	174/205 (85%)	169 (97%)	4 (2%)	1 (1%)	21	52
10	e	354/415 (85%)	317 (90%)	30 (8%)	7 (2%)	6	28
11	j	211/218 (97%)	160 (76%)	41 (19%)	10 (5%)	2	13
12	p	185/258 (72%)	161 (87%)	21 (11%)	3 (2%)	7	32
13	G	206/242 (85%)	190 (92%)	15 (7%)	1 (0%)	24	56
14	I	307/396 (78%)	280 (91%)	25 (8%)	2 (1%)	18	49
15	J	126/201 (63%)	108 (86%)	13 (10%)	5 (4%)	2	16
16	N	99/128 (77%)	92 (93%)	6 (6%)	1 (1%)	12	41
17	g	349/351 (99%)	313 (90%)	33 (10%)	3 (1%)	14	43
18	h	101/386 (26%)	87 (86%)	13 (13%)	1 (1%)	12	41
19	i	96/106 (91%)	84 (88%)	10 (10%)	2 (2%)	5	27
20	k	273/325 (84%)	237 (87%)	31 (11%)	5 (2%)	6	30
21	m	116/118 (98%)	95 (82%)	16 (14%)	5 (4%)	2	15
22	o	306/575 (53%)	265 (87%)	32 (10%)	9 (3%)	3	22
23	B	215/293 (73%)	189 (88%)	25 (12%)	1 (0%)	24	56
24	F	122/124 (98%)	114 (93%)	7 (6%)	1 (1%)	16	45
25	K	134/197 (68%)	112 (84%)	22 (16%)	0	100	100
26	O	171/256 (67%)	156 (91%)	13 (8%)	2 (1%)	10	37
27	R	95/143 (66%)	82 (86%)	12 (13%)	1 (1%)	11	40
28	U	84/87 (97%)	78 (93%)	6 (7%)	0	100	100
29	b	133/190 (70%)	116 (87%)	13 (10%)	4 (3%)	3	21
30	f	96/189 (51%)	89 (93%)	7 (7%)	0	100	100
31	n	70/199 (35%)	65 (93%)	5 (7%)	0	100	100
32	z	205/247 (83%)	174 (85%)	26 (13%)	5 (2%)	4	25
All	All	5437/7382 (74%)	4791 (88%)	559 (10%)	87 (2%)	10	32

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	145	ASN
11	j	6	VAL
11	j	145	HIS
20	k	98	PRO
32	z	218	PRO
3	E	185	MET
3	E	195	GLY
3	E	288	HIS
3	E	299	LYS
7	a	319	GLN
7	a	333	THR
10	e	140	ASP
10	e	212	GLY
10	e	270	PRO
17	g	298	ASN
21	m	27	LEU
22	o	456	ARG
29	b	8	THR
29	b	57	LYS
32	z	82	ILE
32	z	243	PHE
2	C	48	ASN
3	E	237	ARG
7	a	334	GLU
10	e	120	GLY
11	j	4	ARG
11	j	137	HIS
11	j	152	SER
11	j	185	SER
12	p	199	TRP
13	G	54	PRO
14	I	232	PRO
15	J	123	SER
20	k	95	ARG
20	k	304	GLU
21	m	38	ARG
22	o	447	ASN
22	o	453	PRO
22	o	489	PHE
23	B	153	GLU
24	F	71	PRO
29	b	56	ALA

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Mol	Chain	Res	Type
32	z	244	SER
2	C	46	LYS
4	L	99	GLY
8	c	145	GLY
9	d	86	ARG
10	e	47	ASP
11	j	7	ARG
15	J	105	SER
15	J	127	PHE
17	g	175	GLN
21	m	55	CYS
21	m	61	PHE
22	o	66	ASP
22	o	605	HIS
27	R	66	CYS
2	C	47	GLY
2	C	126	GLN
4	L	76	ALA
10	e	274	LYS
11	j	5	LYS
11	j	186	THR
15	J	147	HIS
15	J	185	LYS
19	i	99	GLY
21	m	54	ALA
22	o	68	VAL
22	o	559	LYS
32	z	67	LYS
6	Q	85	VAL
10	e	131	ASN
14	I	287	GLY
18	h	324	PHE
19	i	54	ASN
29	b	24	VAL
12	p	209	PRO
16	N	97	PRO
26	O	198	ILE
7	a	203	VAL
20	k	93	VAL
12	p	229	GLY
11	j	196	ILE
17	g	254	VAL

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Mol	Chain	Res	Type
26	O	114	VAL
20	k	298	VAL
22	o	590	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	106/142 (75%)	106 (100%)	0	100	100
3	E	258/346 (75%)	257 (100%)	1 (0%)	84	83
4	L	94/118 (80%)	94 (100%)	0	100	100
5	P	95/113 (84%)	95 (100%)	0	100	100
6	Q	95/115 (83%)	95 (100%)	0	100	100
7	a	255/307 (83%)	255 (100%)	0	100	100
8	c	152/155 (98%)	152 (100%)	0	100	100
9	d	147/168 (88%)	146 (99%)	1 (1%)	76	79
10	e	321/362 (89%)	315 (98%)	6 (2%)	50	68
11	j	190/193 (98%)	190 (100%)	0	100	100
12	p	166/226 (74%)	166 (100%)	0	100	100
13	G	183/208 (88%)	181 (99%)	2 (1%)	65	74
14	I	267/333 (80%)	264 (99%)	3 (1%)	65	74
15	J	118/182 (65%)	118 (100%)	0	100	100
16	N	91/113 (80%)	91 (100%)	0	100	100
17	g	312/312 (100%)	310 (99%)	2 (1%)	78	80
18	h	94/341 (28%)	94 (100%)	0	100	100
19	i	88/94 (94%)	88 (100%)	0	100	100
20	k	252/292 (86%)	252 (100%)	0	100	100
21	m	102/102 (100%)	102 (100%)	0	100	100
22	o	277/369 (75%)	277 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	B	186/230 (81%)	186 (100%)	0	100	100
24	F	109/109 (100%)	109 (100%)	0	100	100
25	K	102/151 (68%)	102 (100%)	0	100	100
26	O	159/226 (70%)	159 (100%)	0	100	100
27	R	89/126 (71%)	89 (100%)	0	100	100
28	U	77/78 (99%)	76 (99%)	1 (1%)	61	73
29	b	115/163 (71%)	115 (100%)	0	100	100
30	f	85/160 (53%)	84 (99%)	1 (1%)	63	74
31	n	66/173 (38%)	66 (100%)	0	100	100
32	z	168/219 (77%)	168 (100%)	0	100	100
All	All	4819/6226 (77%)	4802 (100%)	17 (0%)	81	83

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	177	GLU
9	d	169	THR
10	e	97	HIS
10	e	123	ASP
10	e	166	GLU
10	e	209	LEU
10	e	240	LEU
10	e	269	SER
13	G	64	TYR
13	G	205	LEU
14	I	91	MET
14	I	205	LEU
14	I	251	GLN
17	g	98	LEU
17	g	367	HIS
28	U	79	ASN
30	f	109	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	302	HIS

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Mol	Chain	Res	Type
4	L	106	HIS
5	P	28	ASN
7	a	107	GLN
8	c	33	ASN
8	c	51	ASN
8	c	95	ASN
8	c	118	GLN
9	d	126	GLN
10	e	78	ASN
10	e	188	GLN
10	e	217	ASN
10	e	261	GLN
10	e	359	GLN
11	j	89	HIS
12	p	125	GLN
12	p	130	HIS
13	G	42	GLN
13	G	140	ASN
14	I	101	GLN
14	I	163	HIS
14	I	280	ASN
14	I	318	HIS
14	I	366	GLN
17	g	53	ASN
17	g	65	GLN
17	g	163	ASN
17	g	173	ASN
20	k	263	ASN
21	m	59	ASN
23	B	115	GLN
23	B	119	ASN
24	F	81	HIS
25	K	107	HIS
25	K	149	HIS
31	n	166	GLN
31	n	178	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	951/955 (99%)	212 (22%)	8 (0%)

All (212) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	G
1	A	10	G
1	A	13	C
1	A	15	C
1	A	16	A
1	A	33	U
1	A	40	A
1	A	41	C
1	A	53	A
1	A	58	C
1	A	64	C
1	A	74	A
1	A	80	U
1	A	88	A
1	A	91	A
1	A	92	A
1	A	114	A
1	A	117	A
1	A	125	U
1	A	143	G
1	A	148	A
1	A	156	C
1	A	157	C
1	A	159	C
1	A	165	A
1	A	178	A
1	A	179	A
1	A	181	U
1	A	183	A
1	A	186	C
1	A	190	A
1	A	211	A
1	A	218	U
1	A	219	U
1	A	226	G
1	A	231	A
1	A	239	C
1	A	242	G
1	A	248	G
1	A	253	C
1	A	268	A
1	A	272	A

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Mol	Chain	Res	Type
1	A	278	A
1	A	288	A
1	A	289	A
1	A	304	C
1	A	305	C
1	A	306	A
1	A	309	C
1	A	311	A
1	A	312	A
1	A	313	A
1	A	329	A
1	A	333	A
1	A	334	G
1	A	347	A
1	A	355	A
1	A	361	A
1	A	362	A
1	A	363	U
1	A	364	A
1	A	365	A
1	A	366	A
1	A	369	A
1	A	370	C
1	A	386	A
1	A	388	A
1	A	389	G
1	A	390	C
1	A	393	A
1	A	396	C
1	A	411	C
1	A	427	U
1	A	428	A
1	A	443	G
1	A	450	A
1	A	451	C
1	A	452	A
1	A	455	G
1	A	463	C
1	A	465	U
1	A	466	A
1	A	472	A
1	A	475	U

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Mol	Chain	Res	Type
1	A	482	C
1	A	490	U
1	A	497	A
1	A	498	A
1	A	499	C
1	A	500	A
1	A	513	A
1	A	515	G
1	A	516	G
1	A	526	U
1	A	529	U
1	A	533	U
1	A	534	A
1	A	535	U
1	A	536	C
1	A	555	C
1	A	557	A
1	A	561	U
1	A	565	U
1	A	566	A
1	A	568	A
1	A	569	C
1	A	571	C
1	A	572	C
1	A	574	A
1	A	581	U
1	A	582	C
1	A	588	U
1	A	589	U
1	A	591	U
1	A	592	U
1	A	594	C
1	A	595	U
1	A	596	A
1	A	599	A
1	A	600	C
1	A	604	C
1	A	608	A
1	A	610	A
1	A	613	G
1	A	619	U
1	A	620	U

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Mol	Chain	Res	Type
1	A	632	A
1	A	633	A
1	A	634	A
1	A	639	A
1	A	640	A
1	A	645	A
1	A	648	A
1	A	649	A
1	A	660	G
1	A	675	U
1	A	676	A
1	A	677	G
1	A	681	A
1	A	693	A
1	A	694	U
1	A	703	A
1	A	706	A
1	A	717	A
1	A	726	A
1	A	727	C
1	A	728	C
1	A	729	A
1	A	730	A
1	A	735	A
1	A	737	C
1	A	739	A
1	A	740	G
1	A	741	C
1	A	742	A
1	A	747	A
1	A	756	G
1	A	759	A
1	A	760	C
1	A	769	A
1	A	772	G
1	A	784	A
1	A	785	G
1	A	793	A
1	A	801	G
1	A	802	U
1	A	814	U
1	A	815	U

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Mol	Chain	Res	Type
1	A	817	G
1	A	821	A
1	A	832	A
1	A	833	C
1	A	835	C
1	A	840	C
1	A	848	C
1	A	854	C
1	A	856	A
1	A	863	U
1	A	864	C
1	A	865	A
1	A	868	G
1	A	869	C
1	A	870	A
1	A	871	U
1	A	874	A
1	A	878	C
1	A	881	U
1	A	886	A
1	A	891	C
1	A	892	U
1	A	893	A
1	A	894	G
1	A	895	C
1	A	896	U
1	A	900	U
1	A	910	C
1	A	911	A
1	A	913	G
1	A	916	G
1	A	919	A
1	A	920	C
1	A	921	A
1	A	922	A
1	A	923	G
1	A	925	U
1	A	930	A
1	A	936	G
1	A	939	A
1	A	948	G
1	A	949	G

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Mol	Chain	Res	Type
1	A	951	U
1	A	955	U

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	14	C
1	A	15	C
1	A	177	A
1	A	225	U
1	A	363	U
1	A	389	G
1	A	580	C
1	A	862	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	o	13

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	o	383:TYR	C	386:UNK	N	27.56
1	o	143:GLU	C	145:UNK	N	20.71
1	o	399:UNK	C	417:MET	N	20.68
1	o	173:UNK	C	220:UNK	N	13.81
1	o	300:UNK	C	311:UNK	N	13.34
1	o	285:UNK	C	290:UNK	N	12.38
1	o	362:UNK	C	371:SER	N	12.19
1	o	326:UNK	C	331:UNK	N	11.71
1	o	232:UNK	C	237:UNK	N	10.14
1	o	345:UNK	C	353:UNK	N	9.75
1	o	250:UNK	C	255:UNK	N	8.18
1	o	156:UNK	C	161:UNK	N	6.08
1	o	269:UNK	C	272:UNK	N	5.43

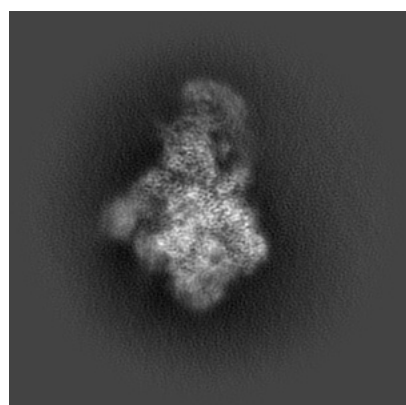
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9358. These allow visual inspection of the internal detail of the map and identification of artifacts.

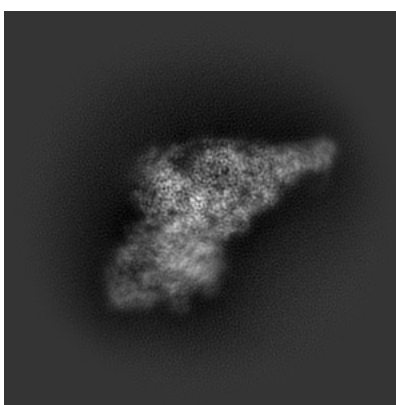
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

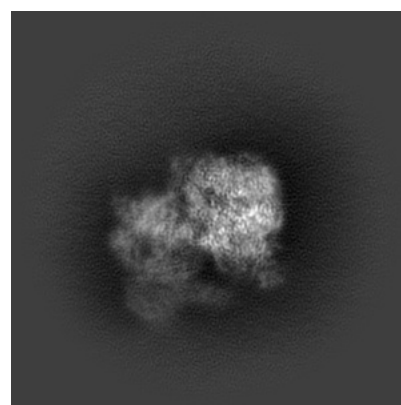
6.1.1 Primary map



X



Y

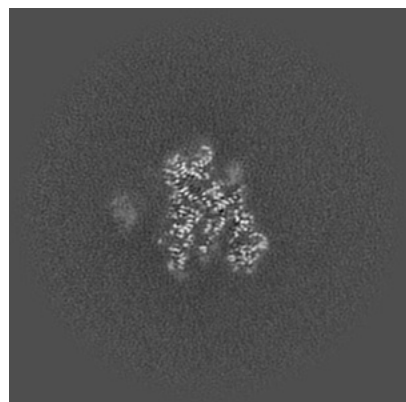


Z

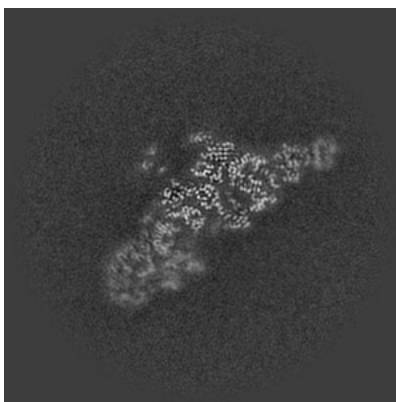
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

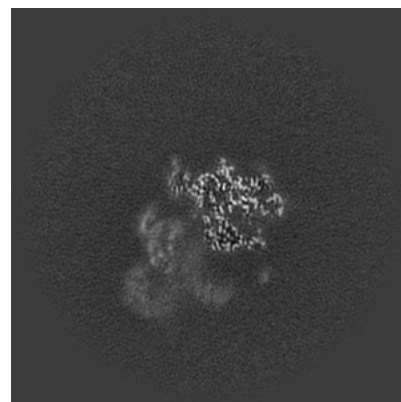
6.2.1 Primary map



X Index: 200



Y Index: 200

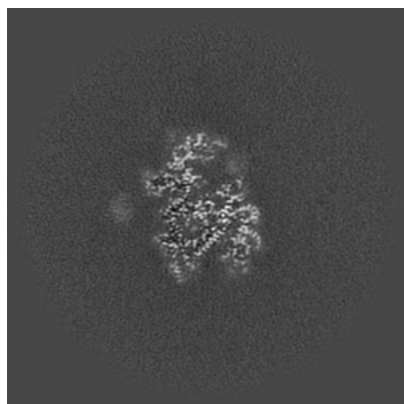


Z Index: 200

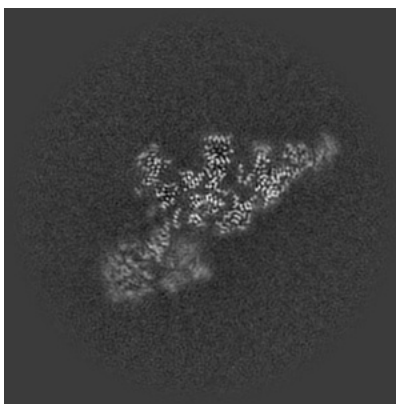
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

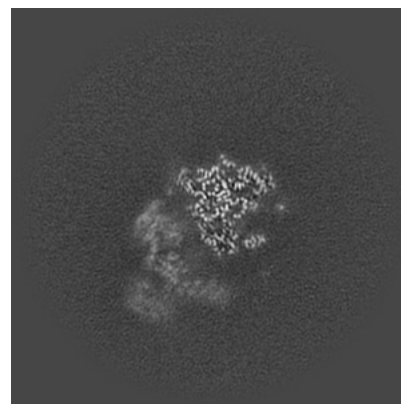
6.3.1 Primary map



X Index: 212



Y Index: 192

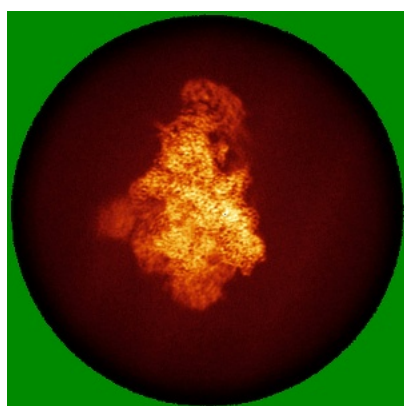


Z Index: 193

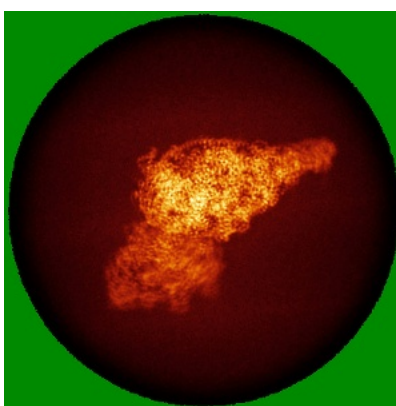
The images above show the largest variance slices of the map in three orthogonal directions.

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

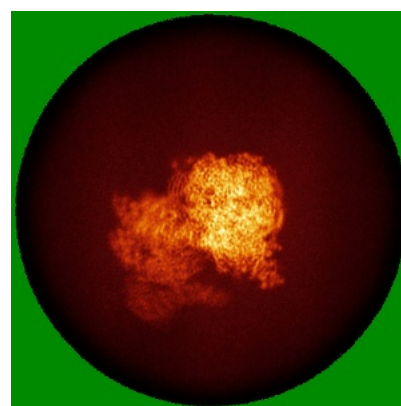
6.4.1 Primary map



X



Y

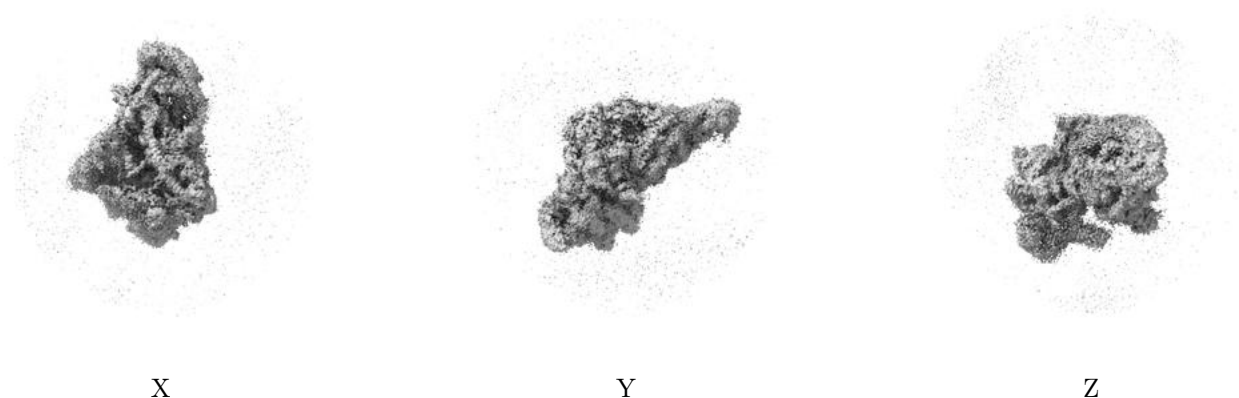


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

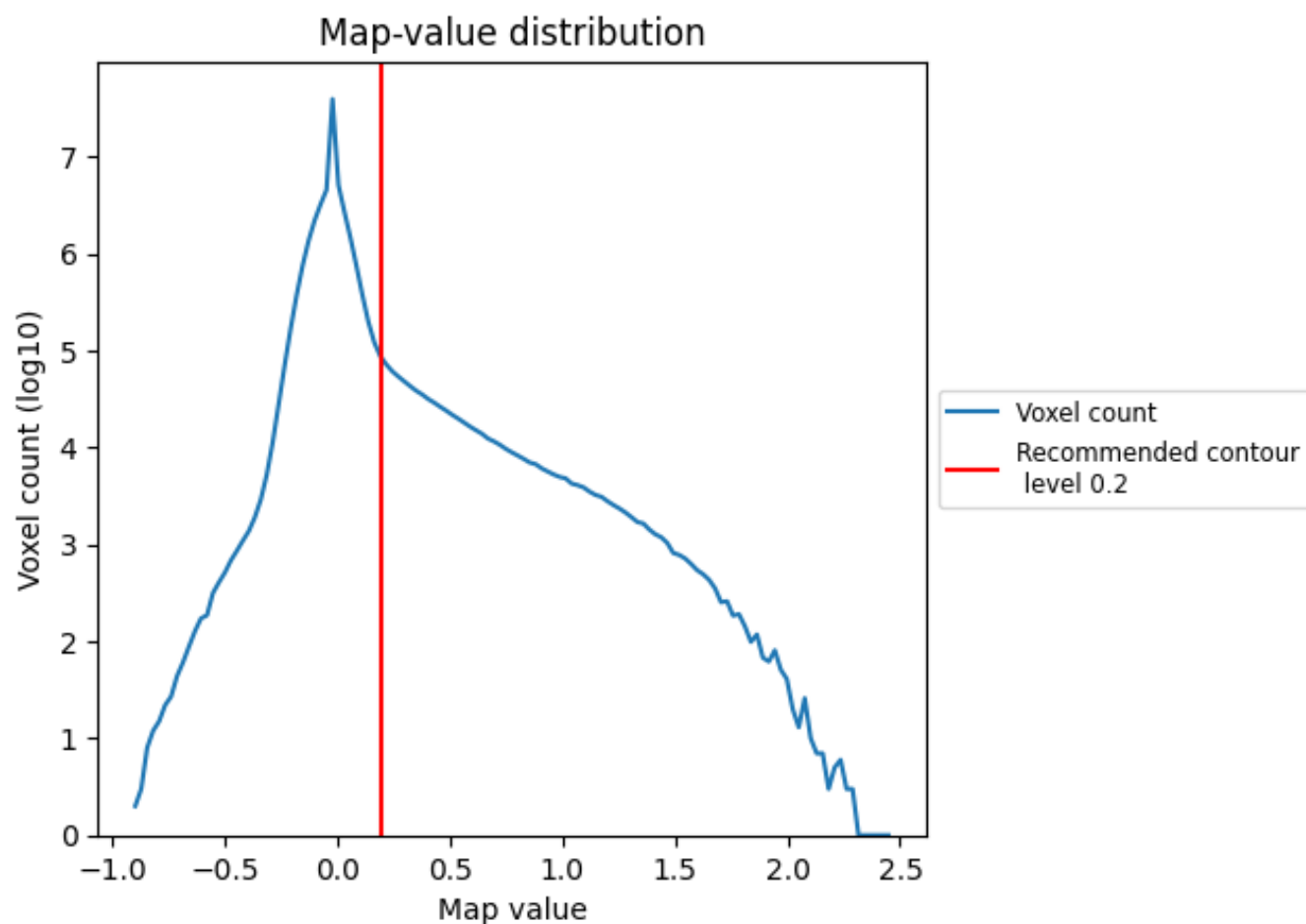
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

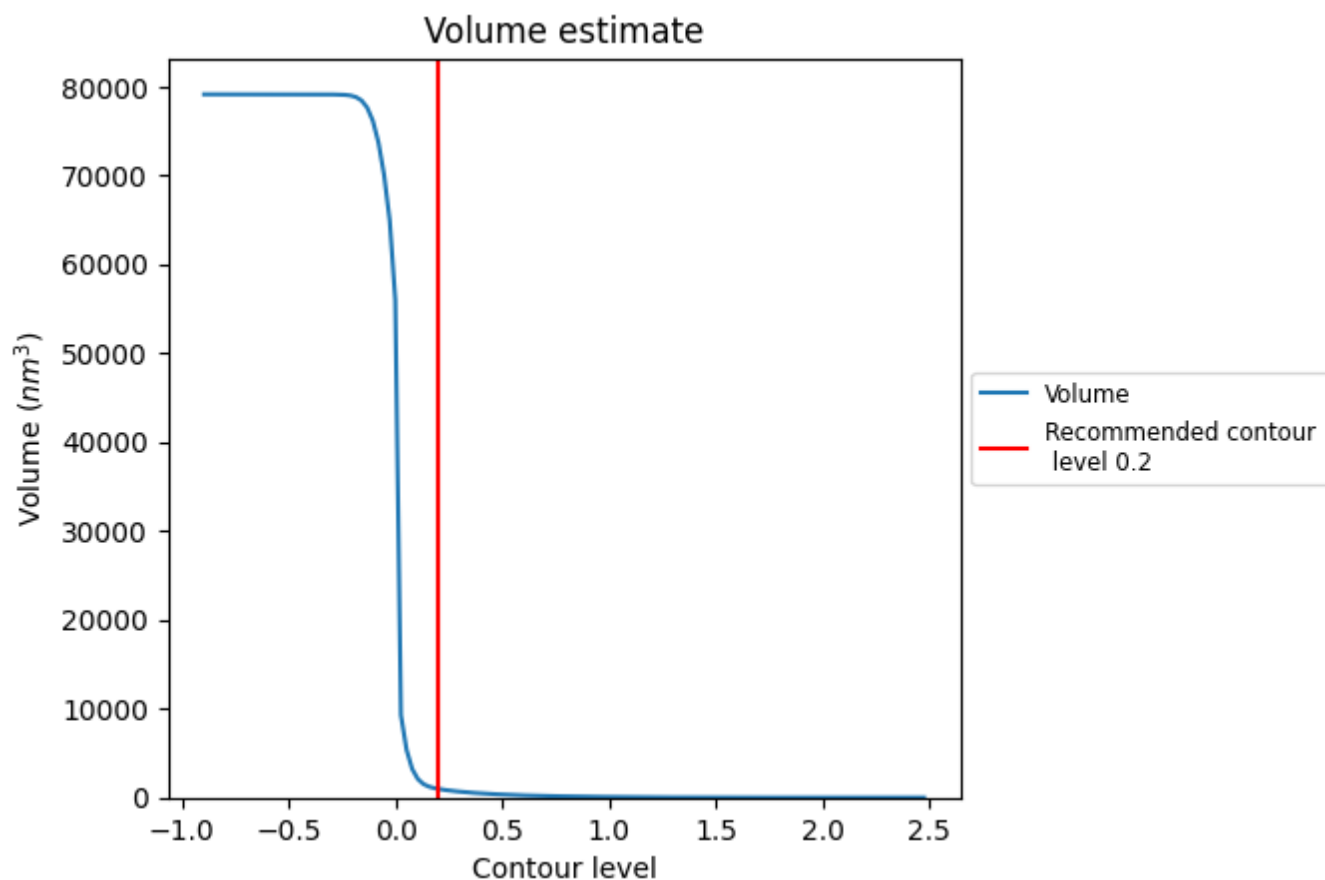
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

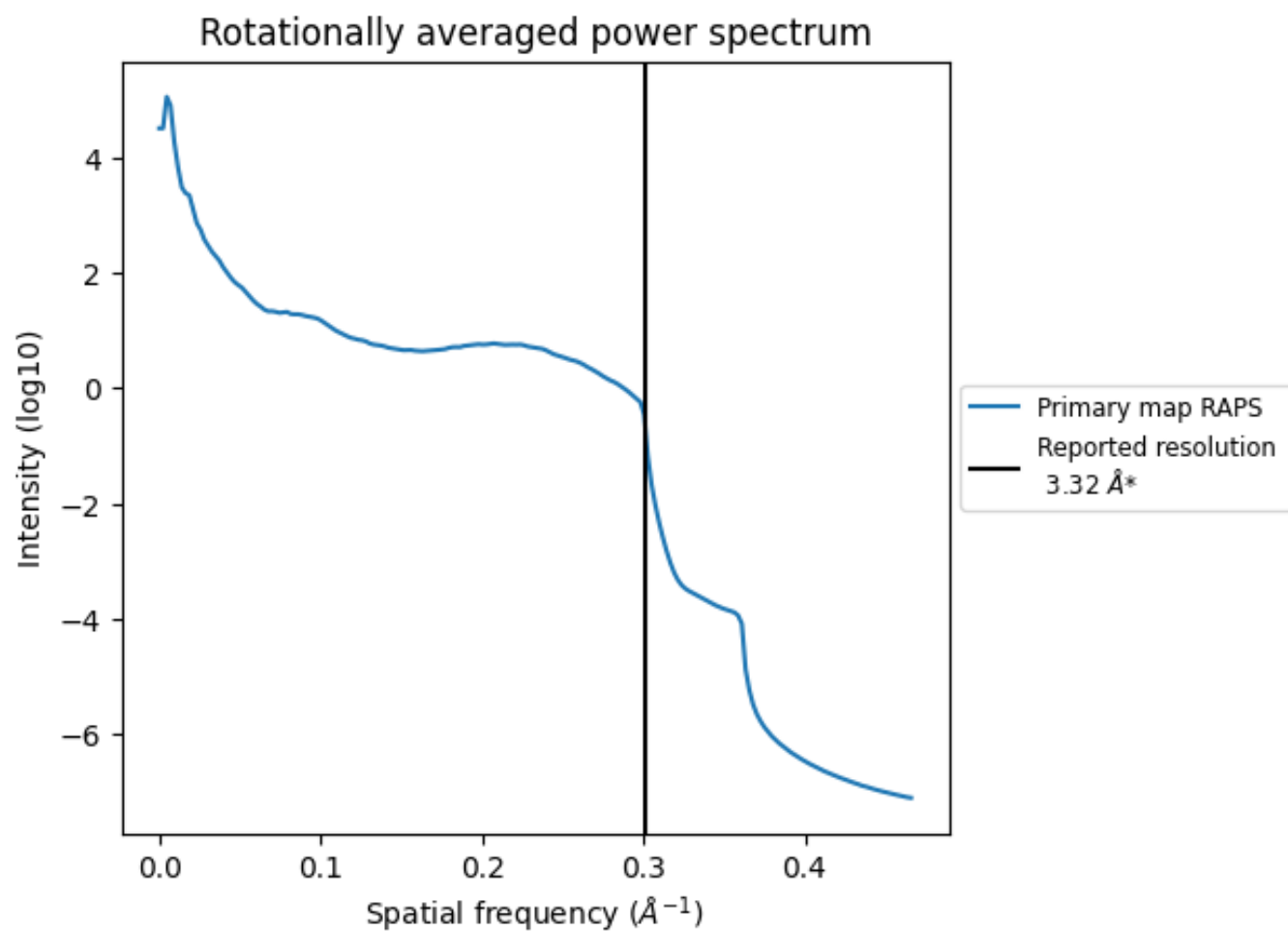
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 980 nm³; this corresponds to an approximate mass of 886 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 0.301 Å⁻¹

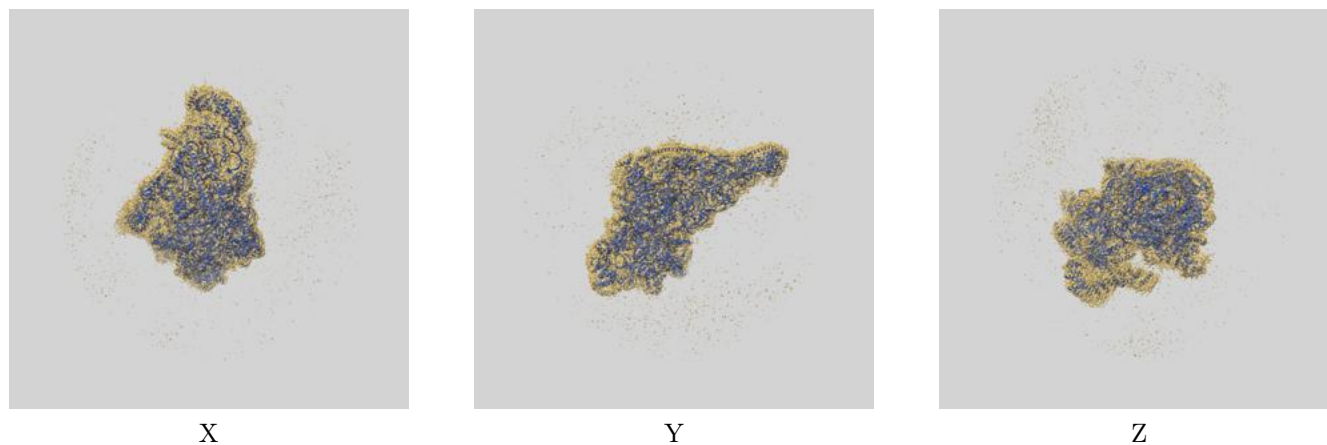
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

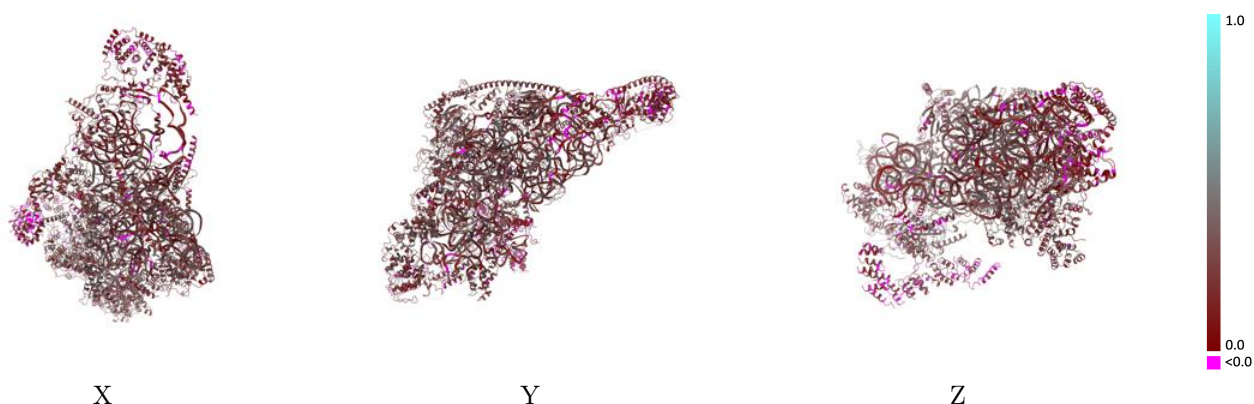
This section contains information regarding the fit between EMDB map EMD-9358 and PDB model 6NEQ. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



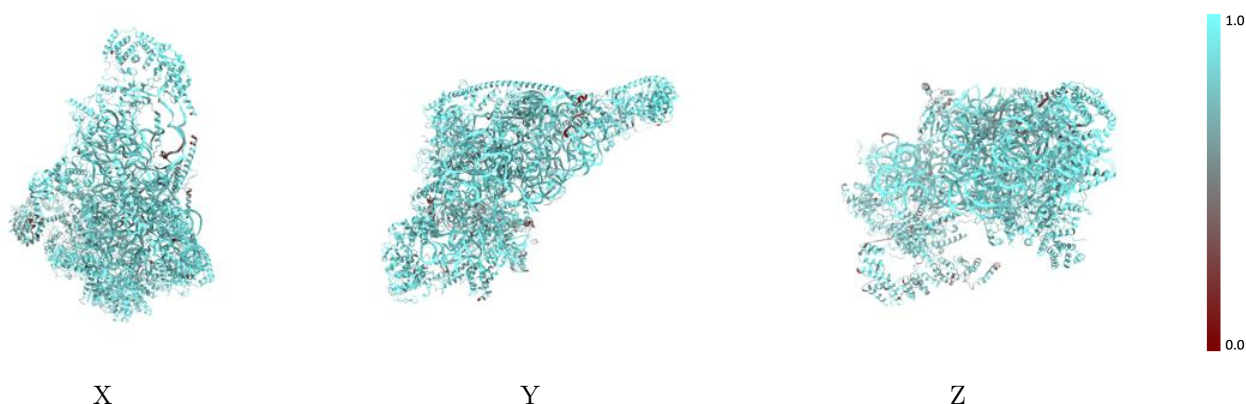
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



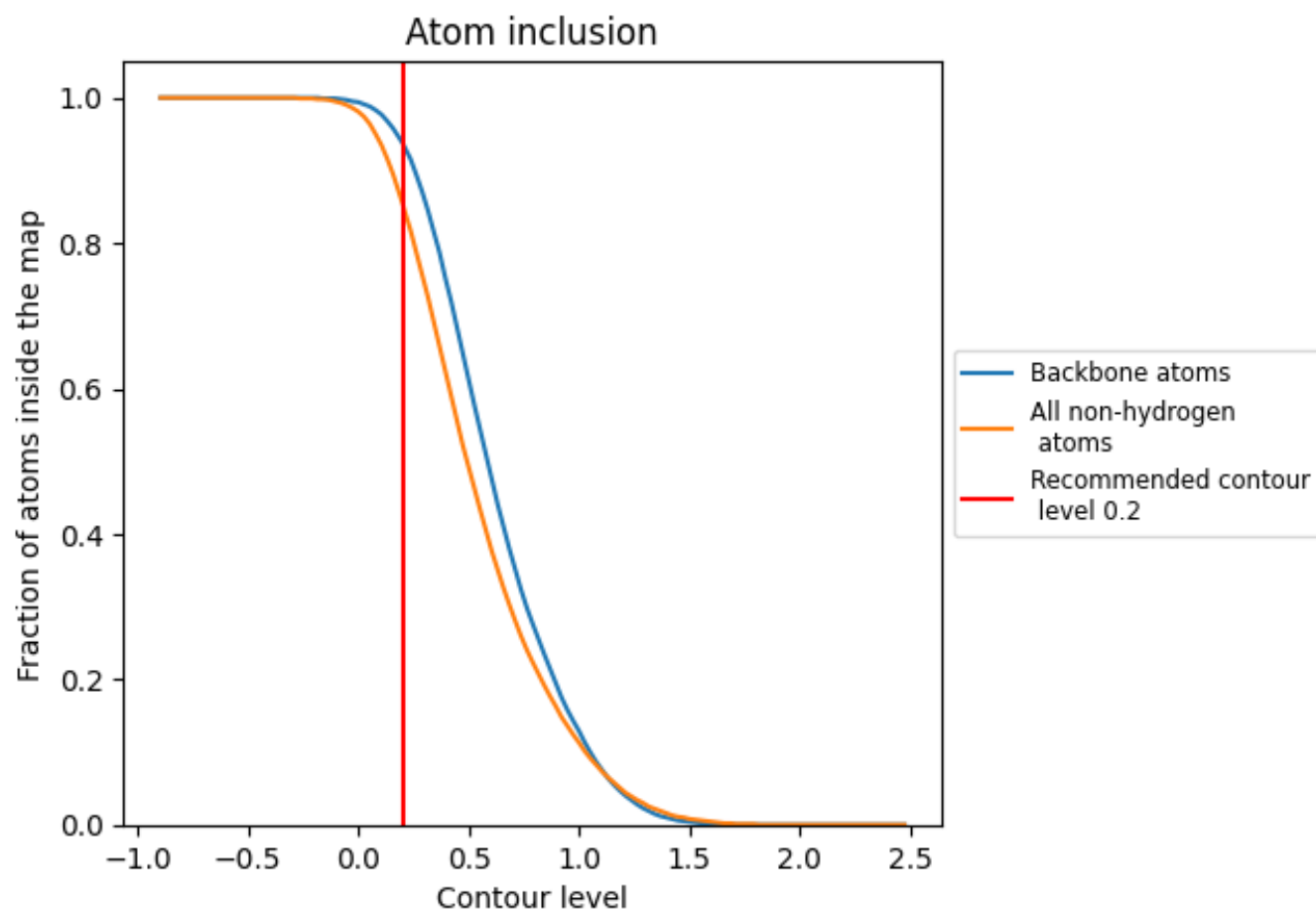
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 86% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8550	 0.2470
A	 0.9150	 0.2470
B	 0.8690	 0.3240
C	 0.8230	 0.2750
E	 0.8210	 0.2840
F	 0.8540	 0.2960
G	 0.8820	 0.2620
I	 0.8590	 0.3220
J	 0.8400	 0.3030
K	 0.8610	 0.2990
L	 0.8470	 0.3080
N	 0.8770	 0.2800
O	 0.8170	 0.2680
P	 0.8380	 0.2560
Q	 0.8210	 0.2880
R	 0.8510	 0.3140
U	 0.8420	 0.2880
a	 0.8350	 0.2550
b	 0.8440	 0.2830
c	 0.8200	 0.2670
d	 0.8590	 0.2530
e	 0.8840	 0.1440
f	 0.8380	 0.3020
g	 0.8980	 0.2730
h	 0.8250	 0.2660
i	 0.7800	 0.1170
j	 0.8180	 0.1760
k	 0.7780	 0.2000
m	 0.7630	 0.2380
n	 0.8220	 0.2480
o	 0.7290	 0.1080
p	 0.8690	 0.2920
z	 0.6200	 0.2160

