



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 02:25 AM UTC

PDB ID : 7KWG / pdb_00007kwg
EMDB ID : EMD-23052
Title : Staphylococcus aureus 30S ribosomal subunit in presence of spermidine
Authors : Belinite, M.; Khusainov, I.; Marzi, S.; Romby, P.; Yusupov, M.; Hashem, Y.
Deposited on : 2020-11-30
Resolution : 3.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

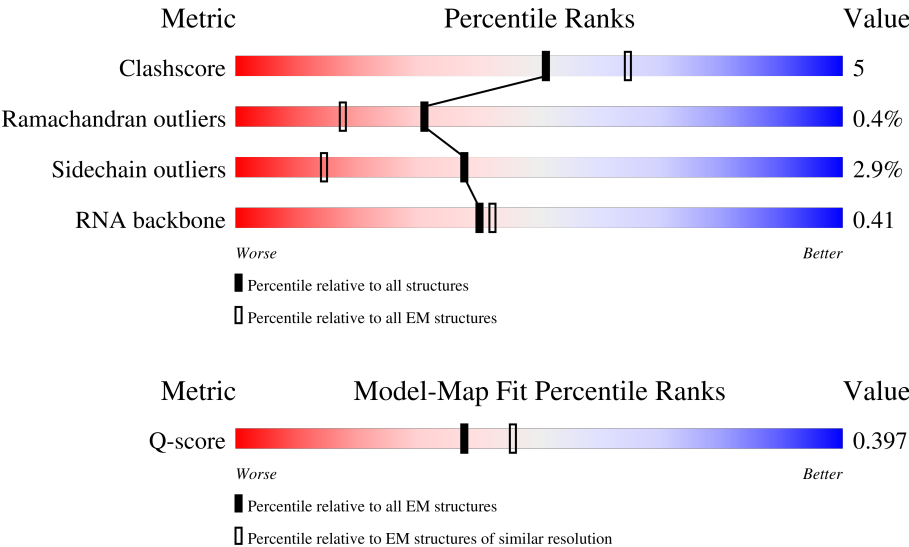
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.75 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	10301 (3.25 - 4.25)

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	32	59% 41% 50% 9%
2	a	1556	5% 63% 31% 6%
3	b	255	36% 68% 17% 12%

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Mol	Chain	Length	Quality of chain
4	c	217	
5	d	200	
6	e	166	
7	f	98	
8	g	156	
9	h	132	
10	i	132	
11	j	102	
12	k	129	
13	l	137	
14	m	121	
15	n	61	
16	o	89	
17	p	91	
18	q	87	
19	r	80	
20	s	92	
21	t	83	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 51870 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 mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	32	Total	C	N	O	P	0	0
			693	311	135	215	32		

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	1552	Total	C	N	O	P	0	0
			33226	14835	6048	10791	1552		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	5	C	A	conflict	GB 87201381

- Molecule 3 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	224	Total	C	N	O	S	0	0
			1802	1147	315	333	7		

- Molecule 4 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	c	202	Total	C	N	O	S	0	0
			1596	1005	300	289	2		

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	196	Total	C	N	O	S	0	0
			1595	1006	299	288	2		

- Molecule 6 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	e	165	Total	C	N	O	S	0	0
			1239	775	229	233	2		

- Molecule 7 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f	96	Total	C	N	O	S	0	0
			798	503	139	153	3		

- Molecule 8 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	g	145	Total	C	N	O	S	0	0
			1177	737	224	212	4		

- Molecule 9 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	h	131	Total	C	N	O	S	0	0
			1032	652	183	193	4		

- Molecule 10 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	i	125	Total	C	N	O	S	0	0
			987	612	195	179	1		

- Molecule 11 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	j	97	Total	C	N	O	S	0	0
			773	487	141	143	2		

- Molecule 12 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	k	118	Total	C	N	O	S	0	0
			880	543	169	165	3		

- Molecule 13 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	l	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 14 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	m	72	Total	C	N	O	S	0	0
			584	361	122	100	1		

- Molecule 15 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	n	59	Total	C	N	O	S	0	0
			497	314	99	79	5		

- Molecule 16 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	o	88	Total	C	N	O	S	0	0
			738	454	153	130	1		

- Molecule 17 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	p	90	Total	C	N	O	S	0	0
			712	448	132	131	1		

- Molecule 18 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	q	86	Total	C	N	O	S	0	0
			707	447	126	133	1		

- Molecule 19 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	r	70	Total	C	N	O	S	0	0
			580	367	114	96	3		

- Molecule 20 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	s	72	Total	C	N	O	S	0	0
			590	381	103	104	2		

- Molecule 21 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	t	80	Total	C	N	O	S	0	0
			606	367	119	118	2		

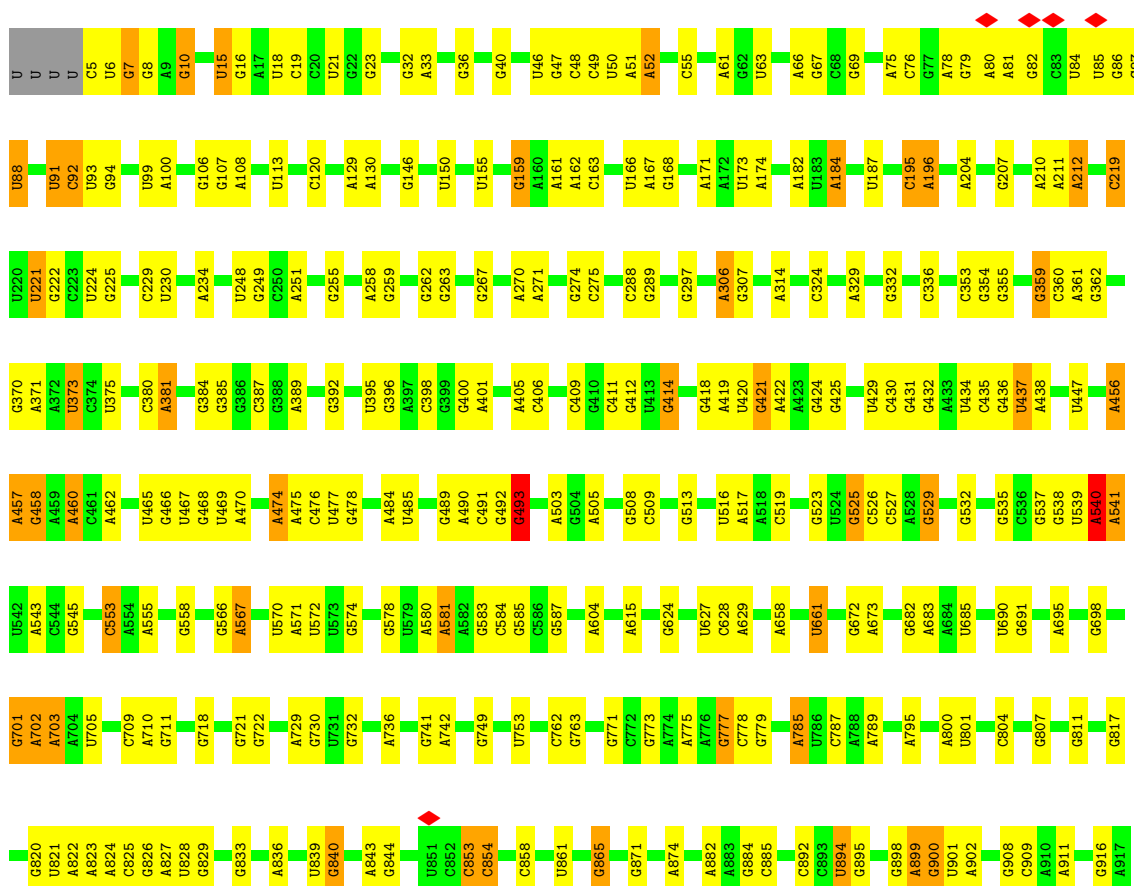
3 Residue-property plots

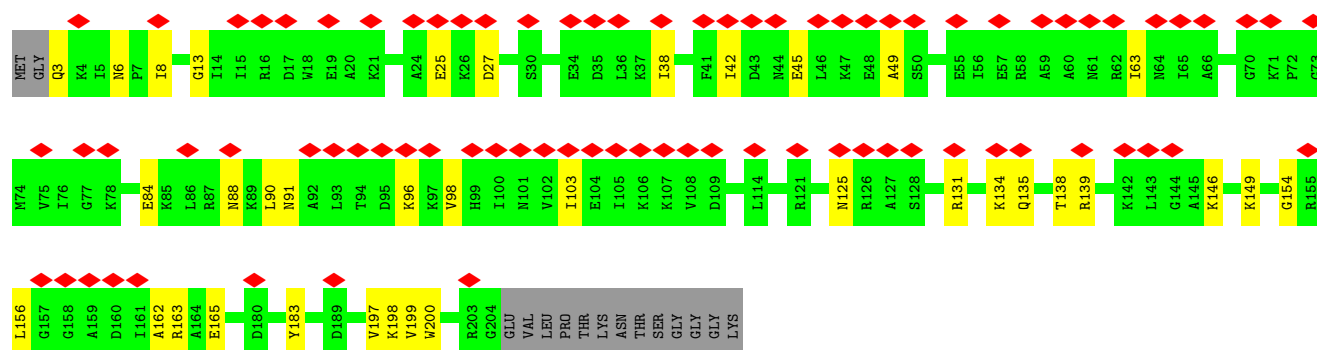
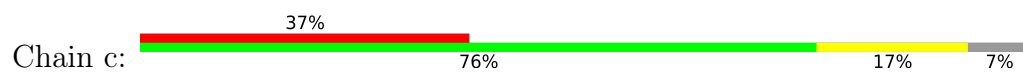
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: mRNA

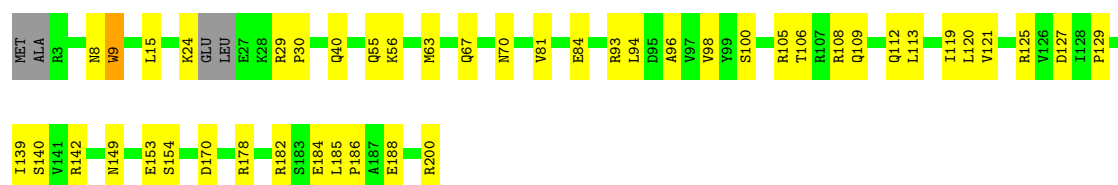
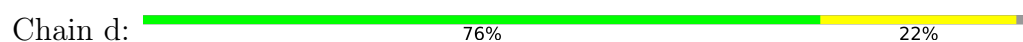


• Molecule 2: 16S ribosomal RNA

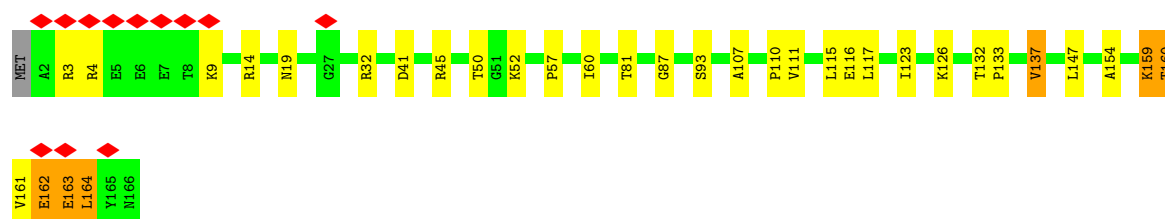
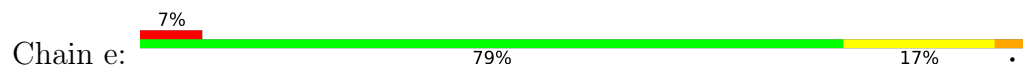




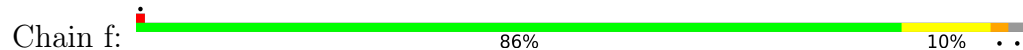
• Molecule 5: 30S ribosomal protein S4



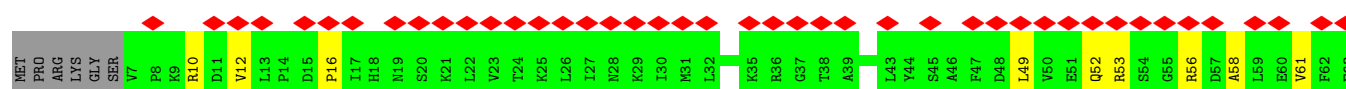
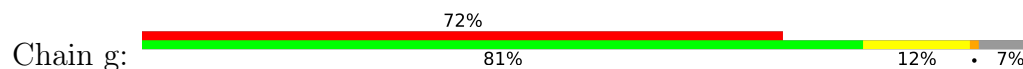
• Molecule 6: 30S ribosomal protein S5

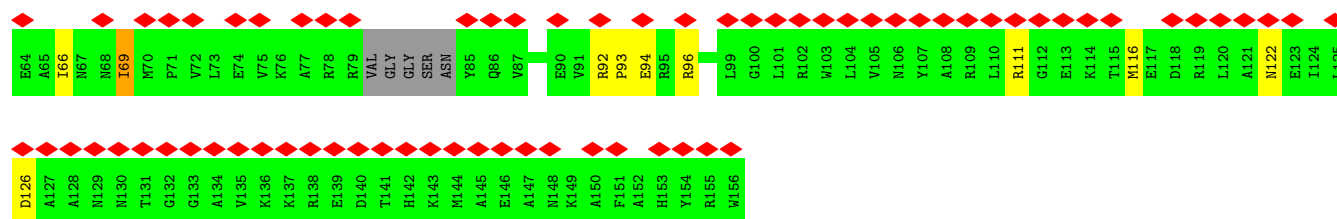


• Molecule 7: 30S ribosomal protein S6

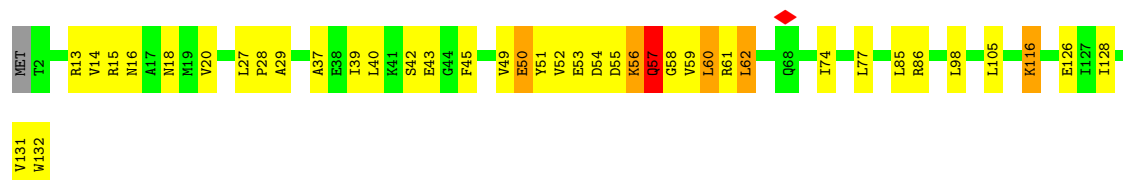


• Molecule 8: 30S ribosomal protein S7

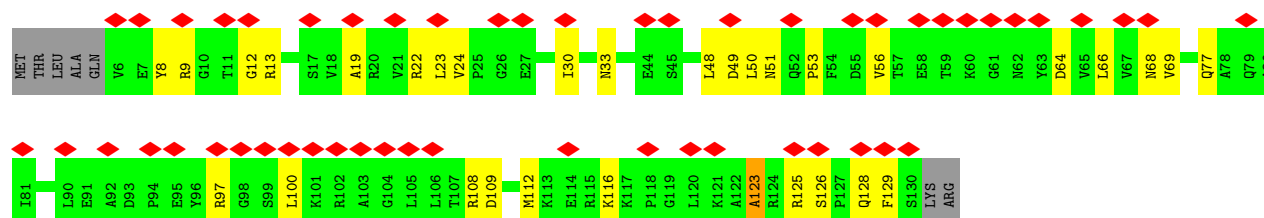




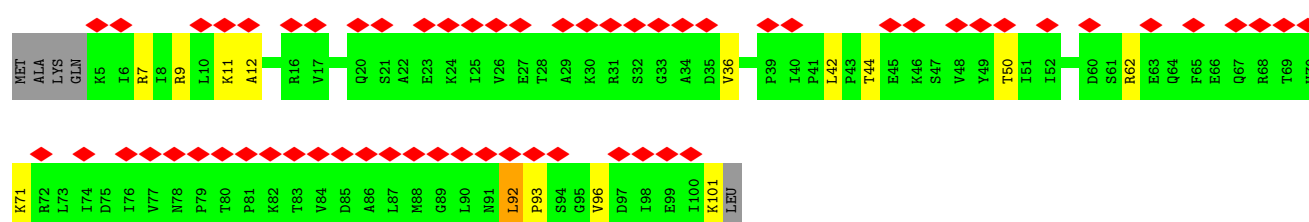
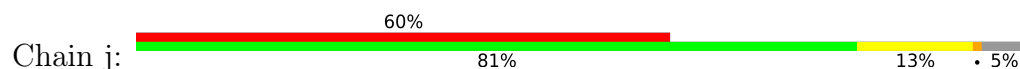
• Molecule 9: 30S ribosomal protein S8



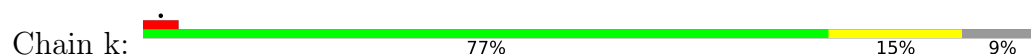
• Molecule 10: 30S ribosomal protein S9



• Molecule 11: 30S ribosomal protein S10

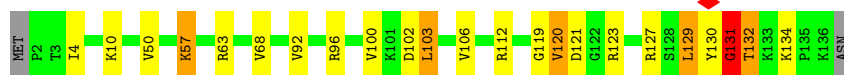


• Molecule 12: 30S ribosomal protein S11

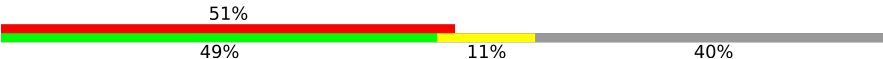


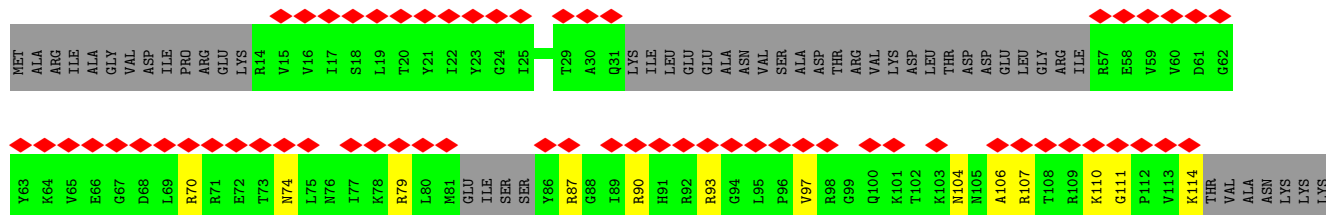
• Molecule 13: 30S ribosomal protein S12

Chain l:  82% 12% ..



- Molecule 14: 30S ribosomal protein S13

Chain m:  51% 49% 11% 40%



- Molecule 15: 30S ribosomal protein S14 type Z

Chain n:  36% 77% 20% .



- Molecule 16: 30S ribosomal protein S15

Chain o:  76% 21% ..



- Molecule 17: 30S ribosomal protein S16

Chain p:  85% 14% .



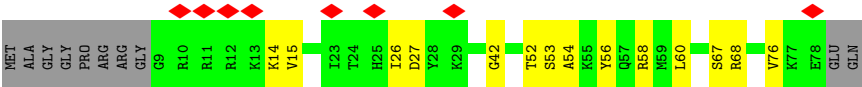
- Molecule 18: 30S ribosomal protein S17

Chain q:  75% 23% ..

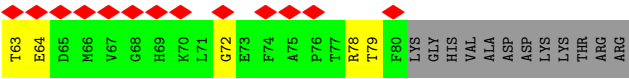
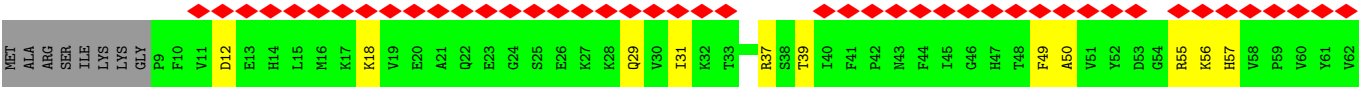


- Molecule 19: 30S ribosomal protein S18

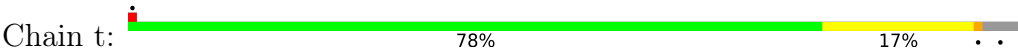
Chain r:  10% 70% 18% 12%



• Molecule 20: 30S ribosomal protein S19



• Molecule 21: 30S ribosomal protein S20



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	529602	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.333	Depositor
Minimum map value	-0.196	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.036	Depositor
Map size (Å)	321.3, 321.3, 321.3	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1899999, 1.1899999, 1.1899999	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.29	0/779	0.60	1/1213 (0.1%)
2	a	0.49	0/37196	0.64	11/58003 (0.0%)
3	b	0.38	0/1829	0.90	3/2454 (0.1%)
4	c	0.35	0/1618	0.76	2/2173 (0.1%)
5	d	0.57	0/1624	0.87	2/2178 (0.1%)
6	e	0.54	0/1253	0.90	0/1687
7	f	0.39	0/809	0.70	0/1085
8	g	0.34	0/1195	0.80	1/1607 (0.1%)
9	h	0.54	0/1044	0.85	0/1401
10	i	0.35	0/1003	0.88	4/1349 (0.3%)
11	j	0.37	0/785	0.86	1/1059 (0.1%)
12	k	0.36	0/895	0.73	0/1207
13	l	0.60	0/1075	0.97	2/1439 (0.1%)
14	m	0.34	0/588	0.82	0/782
15	n	0.32	0/507	0.73	0/671
16	o	0.47	0/747	0.80	0/996
17	p	0.62	0/723	0.90	0/971
18	q	0.51	0/715	0.91	1/955 (0.1%)
19	r	0.49	0/589	0.85	2/785 (0.3%)
20	s	0.36	0/607	0.74	0/817
21	t	0.44	0/606	0.86	3/810 (0.4%)
All	All	0.48	0/56187	0.71	33/83642 (0.0%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	b	194	ASP	N-CA-C	-8.62	104.80	114.62
21	t	39	VAL	N-CA-C	-7.47	106.61	113.71
10	i	51	ASN	CA-C-N	7.16	129.04	120.09
10	i	51	ASN	C-N-CA	7.16	129.04	120.09
2	a	540	A	P-O3'-C3'	7.15	130.92	120.20
21	t	44	ASP	CA-C-N	6.09	130.78	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	t	44	ASP	C-N-CA	6.09	130.78	122.07
2	a	306	A	P-O3'-C3'	5.83	128.95	120.20
10	i	123	ALA	CA-C-N	5.79	130.87	122.36
10	i	123	ALA	C-N-CA	5.79	130.87	122.36
2	a	46	U	C2'-C3'-O3'	5.76	122.34	113.70
2	a	474	A	P-O3'-C3'	5.67	128.70	120.20
2	a	493	G	N9-C1'-C2'	5.59	120.38	112.00
3	b	75	GLN	CA-CB-CG	5.54	125.18	114.10
2	a	1436	A	O4'-C1'-N9	5.50	116.44	108.20
2	a	1542	G	P-O3'-C3'	5.46	128.39	120.20
2	a	306	A	C2'-C3'-O3'	5.46	121.89	113.70
2	a	540	A	C2'-C3'-O3'	5.43	117.65	109.50
2	a	46	U	P-O3'-C3'	5.43	128.34	120.20
4	c	125	ASN	CA-C-N	5.42	129.81	122.07
4	c	125	ASN	C-N-CA	5.42	129.81	122.07
11	j	44	THR	CA-CB-CG2	5.39	119.67	110.50
18	q	72	THR	CA-CB-CG2	5.38	119.65	110.50
13	l	131	GLY	N-CA-C	5.38	125.93	113.18
8	g	69	ILE	N-CA-C	-5.29	107.67	112.96
2	a	474	A	C2'-C3'-O3'	5.19	121.48	113.70
19	r	26	ILE	CA-C-N	5.17	131.42	121.54
19	r	26	ILE	C-N-CA	5.17	131.42	121.54
1	A	17	G	P-O3'-C3'	5.15	127.92	120.20
13	l	103	LEU	CA-CB-CG	5.12	134.21	116.30
5	d	142	ARG	CA-C-N	5.05	131.18	121.54
5	d	142	ARG	C-N-CA	5.05	131.18	121.54
3	b	20	THR	N-CA-C	5.02	118.07	110.64

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	693	0	346	3	0
2	a	33226	0	16731	191	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	b	1802	0	1861	53	0
4	c	1596	0	1659	22	0
5	d	1595	0	1623	29	0
6	e	1239	0	1298	26	0
7	f	798	0	794	6	0
8	g	1177	0	1207	12	0
9	h	1032	0	1082	35	0
10	i	987	0	1005	21	0
11	j	773	0	810	11	0
12	k	880	0	899	11	0
13	l	1058	0	1130	22	0
14	m	584	0	622	11	0
15	n	497	0	522	11	0
16	o	738	0	769	14	0
17	p	712	0	744	7	0
18	q	707	0	749	16	0
19	r	580	0	622	7	0
20	s	590	0	583	12	0
21	t	606	0	650	10	0
All	All	51870	0	35706	445	0

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

All (445) 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)
3:b:66:GLN:HG3	3:b:90:PHE:CZ	1.75	1.20
13:l:112:ARG:HG3	13:l:130:TYR:HB3	1.33	1.05
3:b:66:GLN:HG3	3:b:90:PHE:HZ	1.21	1.01
13:l:112:ARG:HB2	13:l:130:TYR:CA	1.94	0.97
3:b:66:GLN:NE2	3:b:90:PHE:CE1	2.33	0.96
3:b:66:GLN:HB3	3:b:90:PHE:HE1	1.30	0.95
3:b:66:GLN:HG3	3:b:90:PHE:CE1	2.02	0.94
2:a:1315:G:H21	2:a:1344:A:H62	0.95	0.94
2:a:1315:G:N2	2:a:1344:A:H62	1.67	0.92
3:b:66:GLN:CG	3:b:90:PHE:CE1	2.53	0.92
2:a:1315:G:H21	2:a:1344:A:N6	1.68	0.91
3:b:66:GLN:CG	3:b:90:PHE:CZ	2.55	0.89
13:l:112:ARG:HB2	13:l:130:TYR:HA	1.54	0.89
13:l:112:ARG:HB2	13:l:130:TYR:C	1.97	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:66:GLN:CB	3:b:90:PHE:HE1	1.89	0.86
9:h:29:ALA:HB3	9:h:58:GLY:HA3	1.59	0.82
2:a:1127:U:H3	2:a:1196:G:H1	1.24	0.82
2:a:773:G:H1	2:a:820:G:HO2'	1.22	0.82
9:h:28:PRO:HB3	9:h:57:GLN:HG3	1.61	0.80
2:a:438:A:OP1	5:d:9:TRP:HB2	1.81	0.80
9:h:52:VAL:HB	9:h:59:VAL:HG21	1.66	0.78
6:e:159:LYS:HD3	6:e:163:GLU:HG2	1.67	0.77
9:h:50:GLU:HG3	9:h:61:ARG:HB3	1.68	0.76
9:h:61:ARG:HG2	9:h:61:ARG:HH11	1.52	0.75
13:l:112:ARG:CG	13:l:130:TYR:HB3	2.13	0.74
2:a:1128:U:H3	2:a:1195:G:H1	1.35	0.73
3:b:221:ILE:HG13	3:b:221:ILE:O	1.91	0.69
9:h:14:VAL:O	9:h:18:ASN:HB2	1.93	0.69
2:a:988:A:C2	2:a:1327:G:N2	2.58	0.69
9:h:43:GLU:OE2	9:h:116:LYS:NZ	2.28	0.67
9:h:57:GLN:HA	9:h:57:GLN:NE2	2.08	0.67
3:b:66:GLN:CG	3:b:90:PHE:HE1	2.00	0.65
2:a:558:G:O2'	13:l:129:LEU:HD21	1.97	0.64
2:a:384:G:H5''	17:p:6:ARG:HB2	1.80	0.64
5:d:96:ALA:O	5:d:100:SER:HB2	1.97	0.64
3:b:24:ASN:HB2	3:b:190:ASN:HA	1.79	0.63
2:a:988:A:H2	2:a:1327:G:H21	1.44	0.63
3:b:81:LYS:HA	3:b:91:TYR:CE2	2.34	0.63
13:l:96:ARG:NH2	13:l:130:TYR:HE1	1.97	0.62
5:d:149:ASN:O	5:d:153:GLU:HB2	1.98	0.62
2:a:1331:C:O5'	2:a:1331:C:H6	1.82	0.61
3:b:66:GLN:HB3	3:b:90:PHE:CE1	2.23	0.61
3:b:216:LYS:O	3:b:220:ALA:HB2	2.00	0.61
3:b:19:GLN:NE2	3:b:188:ASP:OD2	2.33	0.61
3:b:66:GLN:CG	3:b:90:PHE:HZ	2.05	0.61
10:i:8:TYR:HB2	10:i:23:LEU:HB3	1.82	0.60
11:j:92:LEU:N	11:j:93:PRO:HD3	2.16	0.60
2:a:92:C:N4	2:a:94:G:N7	2.49	0.60
21:t:25:LYS:HD3	21:t:29:ARG:HH21	1.67	0.60
3:b:66:GLN:CB	3:b:90:PHE:CE1	2.77	0.60
3:b:66:GLN:CD	3:b:90:PHE:CE1	2.80	0.59
3:b:66:GLN:NE2	3:b:90:PHE:CZ	2.71	0.59
14:m:111:GLY:H	14:m:114:LYS:HD2	1.67	0.58
3:b:207:ILE:O	3:b:211:LYS:HB2	2.03	0.58
2:a:1168:A:H61	2:a:1189:G:N2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:l:112:ARG:CB	13:l:130:TYR:HA	2.32	0.58
1:a:23:A:H2'	2:a:936:G:H22	1.70	0.57
3:b:66:GLN:CD	3:b:90:PHE:CZ	2.82	0.57
11:j:92:LEU:H	11:j:93:PRO:HD3	1.69	0.57
14:m:90:ARG:HH21	14:m:93:ARG:HD3	1.69	0.57
10:i:22:ARG:HB2	10:i:66:LEU:HB2	1.87	0.56
2:a:79:G:N1	2:a:91:U:N3	2.51	0.56
9:h:37:ALA:HB1	9:h:62:LEU:HD11	1.87	0.56
13:l:119:GLY:HA3	13:l:131:GLY:O	2.06	0.56
10:i:12:GLY:O	10:i:19:ALA:HB3	2.07	0.55
13:l:123:ARG:HB2	13:l:132:THR:HG21	1.87	0.55
2:a:722:G:N2	12:k:121:CYS:SG	2.78	0.55
3:b:113:ARG:HA	3:b:116:GLU:HB2	1.89	0.55
6:e:159:LYS:HE2	9:h:42:SER:O	2.06	0.55
2:a:1093:G:N7	6:e:52:LYS:NZ	2.55	0.55
6:e:162:GLU:OE2	6:e:162:GLU:N	2.40	0.55
2:a:1443:G:H21	2:a:1481:A:H62	1.54	0.54
2:a:36:G:O2'	13:l:131:GLY:HA2	2.08	0.54
2:a:421:G:N1	2:a:434:U:OP2	2.39	0.54
2:a:262:G:H5''	18:q:73:LYS:HD2	1.90	0.53
9:h:51:TYR:HD1	9:h:51:TYR:O	1.91	0.53
12:k:34:ILE:HD11	12:k:82:VAL:HG11	1.90	0.53
3:b:157:MET:SD	6:e:4:ARG:NH2	2.81	0.53
4:c:149:LYS:HB3	4:c:200:TRP:HB2	1.91	0.53
18:q:70:SER:O	18:q:74:ARG:NH1	2.41	0.53
2:a:437:U:H5'	5:d:9:TRP:CE3	2.44	0.53
12:k:28:ASN:HA	12:k:58:SER:HB2	1.91	0.53
2:a:1373:C:O5'	2:a:1373:C:H6	1.91	0.53
9:h:105:LEU:O	9:h:128:ILE:HB	2.09	0.53
2:a:1233:G:OP1	20:s:78:ARG:NH2	2.43	0.52
3:b:79:SER:O	3:b:83:GLU:HB2	2.08	0.52
2:a:492:G:H8	2:a:493:G:H1'	1.74	0.52
1:A:36:A:N1	5:d:40:GLN:NE2	2.57	0.52
2:a:1236:A:OP2	20:s:78:ARG:NH1	2.42	0.52
10:i:97:ARG:O	10:i:100:LEU:HB2	2.10	0.52
2:a:948:A:N3	2:a:1387:U:O2'	2.42	0.52
2:a:1058:A:N6	2:a:1222:U:O2'	2.43	0.52
2:a:1244:G:OP2	10:i:128:GLN:NE2	2.43	0.52
2:a:1437:A:N1	2:a:1486:G:O6	2.43	0.52
20:s:50:ALA:HB1	20:s:57:HIS:HB3	1.92	0.52
8:g:53:ARG:HH12	8:g:122:ASN:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:1272:A:N6	2:a:1285:A:O2'	2.43	0.52
2:a:843:A:OP1	19:r:58:ARG:NH2	2.43	0.51
2:a:892:C:OP2	13:l:10:LYS:NZ	2.43	0.51
2:a:958:C:H2'	2:a:959:A:H8	1.75	0.51
3:b:75:GLN:NE2	3:b:205:ASP:O	2.43	0.51
7:f:6:VAL:HG13	7:f:63:VAL:HG13	1.93	0.51
2:a:1216:U:H2'	2:a:1217:G:H8	1.76	0.51
16:o:74:ASP:OD1	16:o:74:ASP:N	2.43	0.51
4:c:45:GLU:O	4:c:49:ALA:HB3	2.11	0.51
3:b:92:ILE:HG22	3:b:92:ILE:O	2.10	0.51
11:j:92:LEU:N	11:j:93:PRO:CD	2.73	0.51
2:a:508:G:H5''	13:l:134:LYS:HE2	1.92	0.51
5:d:8:ASN:HD22	5:d:108:ARG:HD2	1.75	0.51
17:p:6:ARG:NH2	17:p:28:PRO:O	2.44	0.51
2:a:885:C:O2	9:h:16:ASN:ND2	2.41	0.51
2:a:899:A:H2	2:a:918:A:H62	1.58	0.51
20:s:63:THR:OG1	20:s:64:GLU:N	2.43	0.51
2:a:672:G:H22	2:a:749:G:H1	1.58	0.51
3:b:86:ARG:NH2	3:b:219:ASP:OD2	2.44	0.50
9:h:27:LEU:HD11	9:h:60:LEU:HD23	1.93	0.50
2:a:1190:A:OP2	10:i:97:ARG:NH2	2.44	0.50
9:h:61:ARG:HG2	9:h:61:ARG:NH1	2.23	0.50
2:a:955:G:N2	2:a:1345:G:O2'	2.45	0.50
2:a:1015:C:H4'	2:a:1049:C:H1'	1.93	0.50
2:a:424:G:H2'	2:a:425:G:H8	1.76	0.50
2:a:930:U:HO2'	2:a:1093:G:HO2'	1.58	0.50
2:a:571:A:H62	2:a:894:U:H3	1.60	0.50
2:a:833:G:O2'	9:h:13:ARG:NH1	2.44	0.50
10:i:33:ASN:HA	10:i:68:ASN:HA	1.93	0.50
11:j:12:ALA:HB2	11:j:96:VAL:HG23	1.93	0.50
9:h:40:LEU:HD21	9:h:131:VAL:HG21	1.92	0.50
2:a:207:G:N2	21:t:79:MET:SD	2.85	0.50
2:a:865:G:N2	2:a:1552:U:OP1	2.45	0.50
2:a:1025:G:N2	2:a:1229:U:O2	2.45	0.50
7:f:9:ILE:HD12	7:f:88:ARG:HB2	1.94	0.50
9:h:98:LEU:HD22	9:h:132:TRP:HB2	1.94	0.50
18:q:70:SER:OG	18:q:71:ALA:N	2.45	0.50
5:d:121:VAL:HG12	5:d:139:ILE:HG12	1.94	0.50
16:o:5:GLN:OE1	16:o:9:ASN:ND2	2.45	0.50
16:o:47:LYS:O	16:o:53:ARG:NH1	2.45	0.50
2:a:159:G:H21	2:a:162:A:H62	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:224:U:H2'	2:a:225:G:H8	1.77	0.49
4:c:38:ILE:HD11	4:c:90:LEU:HD13	1.93	0.49
2:a:1360:A:N3	2:a:1385:A:N6	2.60	0.49
8:g:16:PRO:HG3	10:i:48:LEU:HB2	1.95	0.49
8:g:49:LEU:HA	8:g:52:GLN:HG2	1.94	0.49
2:a:5:C:O2'	2:a:7:G:N2	2.45	0.49
14:m:107:ARG:HA	14:m:110:LYS:HB2	1.93	0.49
2:a:435:C:OP2	5:d:29:ARG:NH1	2.45	0.49
2:a:698:G:O6	12:k:57:LYS:NZ	2.44	0.49
2:a:1093:G:OP2	6:e:32:ARG:NH2	2.44	0.49
2:a:1357:A:H61	2:a:1385:A:H3'	1.75	0.49
8:g:92:ARG:NH1	8:g:94:GLU:OE2	2.45	0.49
2:a:516:U:OP1	5:d:200:ARG:NH1	2.45	0.49
4:c:198:LYS:HB3	4:c:200:TRP:HE1	1.77	0.49
18:q:13:LYS:HB3	18:q:60:ILE:HD13	1.93	0.49
4:c:27:ASP:OD1	4:c:27:ASP:N	2.46	0.49
4:c:135:GLN:HG3	4:c:139:ARG:HH21	1.78	0.49
5:d:170:ASP:OD1	5:d:170:ASP:N	2.46	0.49
2:a:182:A:O2'	2:a:184:A:N7	2.43	0.49
2:a:1012:U:H3	2:a:1049:C:H42	1.59	0.49
2:a:1150:G:N2	2:a:1154:G:O6	2.46	0.49
2:a:1471:U:H2'	2:a:1472:A:H8	1.77	0.49
2:a:853:C:H1'	2:a:854:C:H2'	1.94	0.49
2:a:898:G:O2'	2:a:919:A:N6	2.45	0.49
2:a:1331:C:H1'	20:s:72:GLY:HA3	1.94	0.49
3:b:75:GLN:HB2	3:b:207:ILE:HG13	1.94	0.49
3:b:104:TYR:HA	3:b:107:ILE:HG22	1.94	0.49
6:e:107:ALA:HB1	6:e:111:VAL:HG13	1.95	0.49
4:c:25:GLU:OE1	11:j:11:LYS:NZ	2.46	0.49
10:i:30:ILE:HG12	10:i:50:LEU:HD11	1.95	0.49
2:a:150:U:H3	2:a:171:A:H62	1.61	0.49
2:a:787:C:O2'	12:k:122:ARG:NH1	2.46	0.49
2:a:1083:C:H2'	2:a:1084:G:H8	1.77	0.49
4:c:163:ARG:NH2	4:c:165:GLU:OE1	2.46	0.49
18:q:56:LYS:NZ	18:q:83:GLU:OE1	2.46	0.49
21:t:17:ALA:O	21:t:21:ASN:HB2	2.12	0.49
6:e:41:ASP:OD2	6:e:45:ARG:NH1	2.46	0.48
17:p:75:LEU:HD22	17:p:80:ILE:HG13	1.95	0.48
18:q:7:ARG:HB3	18:q:65:GLU:HB3	1.95	0.48
2:a:732:G:OP1	2:a:840:G:N2	2.46	0.48
2:a:983:G:O2'	15:n:29:ARG:NH2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:h:27:LEU:CD1	9:h:60:LEU:HD23	2.43	0.48
17:p:6:ARG:NH2	17:p:27:SER:OG	2.46	0.48
2:a:701:G:OP1	12:k:127:ARG:NH2	2.47	0.48
2:a:509:C:OP1	13:l:127:ARG:NH2	2.39	0.48
3:b:80:VAL:HG12	3:b:91:TYR:HD2	1.78	0.48
9:h:51:TYR:CD1	9:h:51:TYR:C	2.91	0.48
2:a:1076:G:O6	2:a:1203:C:N4	2.47	0.48
5:d:178:ARG:NH2	5:d:184:GLU:OE2	2.46	0.48
16:o:16:ARG:NH1	16:o:19:GLU:O	2.46	0.48
16:o:67:LEU:HD11	16:o:87:ILE:HD12	1.95	0.48
2:a:195:C:N4	18:q:2:SER:O	2.46	0.48
2:a:262:G:O2'	18:q:20:ASP:O	2.32	0.48
2:a:1357:A:O2'	8:g:10:ARG:NH1	2.46	0.48
2:a:1381:G:H2'	2:a:1382:G:H8	1.78	0.48
4:c:91:ASN:ND2	4:c:96:LYS:O	2.45	0.48
2:a:553:C:OP2	5:d:55:GLN:NE2	2.46	0.48
4:c:84:GLU:O	4:c:88:ASN:ND2	2.46	0.48
3:b:89:GLN:HE22	3:b:221:ILE:HG12	1.79	0.48
15:n:21:TYR:OH	15:n:23:ARG:NH2	2.47	0.48
2:a:1136:G:N2	2:a:1137:U:O4	2.44	0.48
9:h:29:ALA:CB	9:h:58:GLY:HA3	2.37	0.48
12:k:63:ALA:HB1	12:k:96:ALA:HB2	1.96	0.48
2:a:251:A:N6	2:a:289:G:O2'	2.47	0.48
2:a:1073:G:N7	4:c:3:GLN:NE2	2.62	0.48
12:k:20:VAL:HG23	12:k:83:GLU:HB2	1.96	0.48
2:a:984:A:OP1	15:n:29:ARG:NH2	2.47	0.47
2:a:1005:C:H2'	2:a:1006:A:H8	1.78	0.47
9:h:45:PHE:HB3	9:h:74:ILE:HG12	1.96	0.47
11:j:42:LEU:HD13	11:j:71:LYS:HD2	1.95	0.47
2:a:52:A:N7	2:a:113:U:O2'	2.45	0.47
2:a:682:G:H2'	2:a:683:A:H8	1.79	0.47
3:b:83:GLU:OE2	3:b:86:ARG:NH1	2.47	0.47
6:e:115:LEU:HD13	6:e:123:ILE:HG21	1.96	0.47
2:a:908:G:N2	2:a:911:A:OP2	2.43	0.47
2:a:1331:C:O2'	14:m:87:ARG:NH1	2.47	0.47
3:b:177:ARG:O	6:e:3:ARG:NH1	2.48	0.47
2:a:1505:A:OP2	13:l:57:LYS:NZ	2.47	0.47
2:a:529:G:N7	13:l:63:ARG:NH1	2.63	0.47
1:A:31:A:OP1	2:a:1408:C:N4	2.47	0.47
2:a:263:G:OP1	18:q:73:LYS:NZ	2.46	0.47
2:a:523:G:OP2	2:a:540:A:N6	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:984:A:OP2	15:n:41:ARG:NH1	2.48	0.47
2:a:1251:U:H3'	2:a:1252:G:H8	1.80	0.47
2:a:1321:U:OP1	14:m:79:ARG:NH2	2.47	0.47
2:a:1428:G:O2'	2:a:1495:A:N6	2.44	0.47
5:d:81:VAL:HG23	5:d:84:GLU:HB3	1.96	0.47
2:a:1237:C:H3'	14:m:110:LYS:HZ3	1.79	0.47
4:c:8:ILE:HD12	15:n:50:LYS:HA	1.96	0.47
8:g:93:PRO:HA	8:g:96:ARG:HB2	1.97	0.47
10:i:13:ARG:HG3	10:i:108:ARG:HE	1.80	0.47
10:i:125:ARG:NH1	10:i:126:SER:O	2.47	0.47
5:d:182:ARG:HD3	5:d:185:LEU:HD12	1.97	0.47
6:e:14:ARG:NH1	6:e:116:GLU:OE2	2.44	0.47
2:a:161:A:H2	2:a:355:G:H21	1.64	0.46
2:a:166:U:H2'	2:a:167:A:H8	1.79	0.46
2:a:1291:A:OP1	11:j:9:ARG:NH2	2.46	0.46
9:h:86:ARG:NH1	9:h:126:GLU:OE2	2.47	0.46
19:r:53:SER:OG	19:r:54:ALA:N	2.48	0.46
2:a:1157:A:H2	10:i:9:ARG:HE	1.63	0.46
11:j:50:THR:HG22	11:j:62:ARG:HE	1.79	0.46
14:m:70:ARG:O	14:m:74:ASN:ND2	2.49	0.46
16:o:52:SER:O	16:o:56:LEU:HB3	2.15	0.46
2:a:55:C:OP1	2:a:359:G:N2	2.48	0.46
8:g:66:ILE:HD12	8:g:69:ILE:HD12	1.97	0.46
19:r:56:TYR:O	19:r:60:LEU:HB2	2.15	0.46
2:a:871:G:HO2'	2:a:884:G:HO2'	1.63	0.46
2:a:1372:G:O5'	2:a:1372:G:H8	1.99	0.46
2:a:457:A:H3'	2:a:458:G:H8	1.81	0.46
2:a:1397:G:H2'	2:a:1398:G:H8	1.80	0.46
3:b:90:PHE:HB2	3:b:151:ILE:HG22	1.98	0.46
2:a:21:U:O2'	2:a:581:A:N6	2.49	0.46
2:a:61:A:H2	2:a:385:G:H21	1.64	0.46
2:a:130:A:OP1	18:q:7:ARG:NH2	2.49	0.46
2:a:1253:G:H1	2:a:1306:U:H3	1.61	0.46
18:q:6:ASP:N	18:q:6:ASP:OD1	2.46	0.46
2:a:196:A:N6	18:q:66:THR:OG1	2.48	0.46
13:l:121:ASP:OD1	13:l:121:ASP:N	2.47	0.46
2:a:381:A:O2'	2:a:460:A:N7	2.48	0.46
2:a:1416:G:O2'	2:a:1530:A:O2'	2.34	0.46
6:e:154:ALA:HB1	6:e:160:THR:HA	1.98	0.46
2:a:567:A:OP2	6:e:126:LYS:NZ	2.48	0.46
2:a:778:C:H2'	2:a:779:G:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:1452:G:O2'	2:a:1472:A:N6	2.48	0.46
4:c:154:GLY:O	4:c:162:ALA:HA	2.16	0.46
2:a:736:A:OP1	16:o:54:ARG:NH2	2.48	0.45
2:a:1058:A:H61	2:a:1224:A:H62	1.64	0.45
2:a:1138:U:OP1	11:j:7:ARG:NH1	2.49	0.45
5:d:105:ARG:HG2	5:d:154:SER:HB2	1.97	0.45
6:e:159:LYS:HB3	6:e:163:GLU:HG2	1.97	0.45
2:a:685:U:H3	2:a:721:G:H22	1.64	0.45
6:e:9:LYS:HD3	6:e:41:ASP:HB2	1.99	0.45
6:e:87:GLY:O	6:e:93:SER:HA	2.16	0.45
21:t:82:ASN:N	21:t:82:ASN:OD1	2.49	0.45
2:a:900:G:O2'	2:a:916:G:O6	2.35	0.45
2:a:961:G:O6	14:m:104:ASN:ND2	2.44	0.45
4:c:13:GLY:HA3	15:n:56:VAL:HG23	1.97	0.45
2:a:489:G:OP2	2:a:489:G:N2	2.42	0.45
2:a:990:C:O3'	15:n:9:LYS:NZ	2.50	0.45
2:a:1438:C:H2'	2:a:1439:A:H8	1.81	0.45
12:k:33:THR:HA	12:k:44:TRP:HA	1.98	0.45
16:o:75:ILE:HD11	18:q:87:ILE:HG12	1.98	0.45
2:a:458:G:N2	17:p:14:ARG:O	2.41	0.45
2:a:1068:U:H2'	2:a:1069:G:H8	1.81	0.45
7:f:67:SER:OG	7:f:68:ASP:N	2.50	0.45
10:i:125:ARG:HA	10:i:125:ARG:HD2	1.79	0.45
10:i:24:VAL:HG23	10:i:64:ASP:HB3	1.99	0.45
2:a:79:G:O6	2:a:91:U:O4	2.35	0.45
2:a:1128:U:O2'	10:i:112:MET:SD	2.74	0.45
2:a:1267:C:OP2	2:a:1290:A:N6	2.42	0.45
2:a:795:A:N6	2:a:801:U:OP2	2.49	0.45
6:e:57:PRO:HA	6:e:60:ILE:HG12	1.99	0.45
9:h:51:TYR:O	9:h:51:TYR:CD1	2.70	0.45
10:i:116:LYS:HA	10:i:123:ALA:HB2	1.98	0.45
3:b:115:SER:OG	3:b:152:ARG:NH2	2.50	0.44
13:l:63:ARG:NH2	13:l:102:ASP:OD2	2.45	0.44
2:a:10:G:N7	2:a:566:G:O2'	2.49	0.44
2:a:87:C:H2'	2:a:88:U:H4'	1.99	0.44
2:a:370:G:N2	2:a:373:U:OP2	2.45	0.44
10:i:49:ASP:OD1	10:i:49:ASP:N	2.49	0.44
18:q:56:LYS:N	18:q:59:ASP:OD2	2.50	0.44
21:t:4:ILE:HD12	21:t:8:ILE:HG21	1.99	0.44
2:a:702:A:N7	2:a:703:A:N6	2.66	0.44
2:a:989:C:O2	15:n:19:ARG:NE	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:e:81:THR:HG23	6:e:147:LEU:HD21	1.99	0.44
9:h:60:LEU:HD12	9:h:60:LEU:HA	1.78	0.44
14:m:106:ALA:HB3	14:m:110:LYS:HZ1	1.81	0.44
2:a:108:A:H2	2:a:332:G:H21	1.66	0.44
3:b:123:ASP:OD1	3:b:123:ASP:N	2.49	0.44
5:d:67:GLN:HE22	5:d:93:ARG:HH21	1.66	0.44
8:g:111:ARG:NH2	8:g:126:ASP:OD2	2.50	0.44
9:h:15:ARG:NH2	9:h:77:LEU:O	2.50	0.44
17:p:42:PRO:HA	17:p:48:PRO:HB3	2.00	0.44
20:s:31:ILE:O	20:s:49:PHE:HA	2.17	0.44
19:r:27:ASP:O	19:r:67:SER:OG	2.35	0.44
21:t:79:MET:HE2	21:t:79:MET:HB3	1.87	0.44
4:c:131:ARG:HH22	6:e:57:PRO:HG2	1.81	0.44
7:f:83:SER:OG	7:f:85:ASP:OD1	2.36	0.44
3:b:204:ASP:OD1	3:b:204:ASP:N	2.50	0.44
20:s:56:LYS:HD2	20:s:56:LYS:HA	1.84	0.44
2:a:937:G:O2'	2:a:1515:A:N7	2.49	0.44
10:i:53:PRO:HA	10:i:56:VAL:HG12	2.00	0.44
2:a:225:G:H1'	2:a:478:G:H1	1.83	0.43
2:a:1378:U:H4'	11:j:50:THR:HG21	2.01	0.43
3:b:80:VAL:HG12	3:b:91:TYR:CD2	2.52	0.43
3:b:89:GLN:NE2	3:b:221:ILE:HG12	2.33	0.43
17:p:7:LEU:HG	17:p:71:VAL:HG22	1.99	0.43
3:b:73:LYS:HB3	3:b:76:ALA:HB3	2.00	0.43
5:d:185:LEU:HB3	5:d:186:PRO:HD2	2.00	0.43
2:a:1109:C:O3'	3:b:143:ARG:NH2	2.51	0.43
2:a:212:A:OP1	2:a:229:C:O2'	2.33	0.43
2:a:749:G:H4'	16:o:55:GLY:HA3	2.00	0.43
2:a:773:G:N1	2:a:820:G:O2'	2.37	0.43
10:i:69:VAL:HG23	10:i:77:GLN:HE21	1.82	0.43
11:j:7:ARG:HB2	11:j:101:LYS:HE3	2.00	0.43
2:a:773:G:N2	2:a:821:U:OP2	2.48	0.43
2:a:1534:U:H2'	2:a:1535:G:H8	1.83	0.43
10:i:108:ARG:NH1	10:i:109:ASP:O	2.48	0.43
19:r:14:LYS:HG3	19:r:15:VAL:HG12	2.00	0.43
2:a:18:U:OP1	6:e:19:ASN:ND2	2.46	0.43
3:b:21:ARG:O	3:b:21:ARG:HD3	2.19	0.43
3:b:90:PHE:CB	3:b:151:ILE:HG22	2.48	0.43
2:a:1430:G:O6	2:a:1493:U:O2	2.37	0.42
16:o:48:LYS:HD2	16:o:48:LYS:HA	1.86	0.42
2:a:409:C:OP1	5:d:70:ASN:ND2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:894:U:H4'	2:a:895:G:H5''	2.01	0.42
14:m:104:ASN:OD1	14:m:104:ASN:N	2.51	0.42
2:a:411:C:H5''	5:d:129:PRO:HD2	2.01	0.42
2:a:777:G:OP2	2:a:811:G:O2'	2.36	0.42
2:a:1108:C:O2	2:a:1181:A:O2'	2.34	0.42
21:t:28:MET:HE3	21:t:28:MET:HB3	1.85	0.42
2:a:409:C:O2'	2:a:629:A:N3	2.44	0.42
3:b:91:TYR:N	3:b:91:TYR:CD1	2.88	0.42
15:n:26:ARG:NH2	15:n:43:CYS:SG	2.92	0.42
2:a:1024:A:OP2	20:s:18:LYS:NZ	2.48	0.42
3:b:21:ARG:HD3	3:b:21:ARG:HA	1.57	0.42
5:d:94:LEU:O	5:d:98:VAL:HB	2.19	0.42
9:h:29:ALA:CB	9:h:60:LEU:HD22	2.49	0.42
3:b:68:LEU:HD11	3:b:92:ILE:CD1	2.50	0.42
19:r:52:THR:OG1	19:r:53:SER:N	2.51	0.42
6:e:110:PRO:HB3	6:e:137:VAL:HG23	2.01	0.42
12:k:87:LYS:HG3	12:k:115:PRO:HD3	2.02	0.42
2:a:219:C:H2'	2:a:221:U:H3	1.84	0.42
2:a:967:U:O2'	20:s:55:ARG:NH1	2.52	0.42
5:d:109:GLN:O	5:d:113:LEU:HB2	2.20	0.42
7:f:10:VAL:HB	7:f:59:PHE:HB2	2.02	0.42
15:n:16:TYR:OH	20:s:37:ARG:NH2	2.45	0.42
19:r:42:GLY:O	19:r:68:ARG:NH2	2.50	0.42
2:a:15:U:N3	2:a:18:U:OP2	2.51	0.42
2:a:414:G:N3	5:d:112:GLN:NE2	2.68	0.41
2:a:721:G:H2'	2:a:722:G:C8	2.55	0.41
5:d:120:LEU:HB2	5:d:140:SER:HB2	2.02	0.41
7:f:85:ASP:OD1	7:f:85:ASP:N	2.50	0.41
9:h:39:ILE:HD13	9:h:39:ILE:HA	1.94	0.41
2:a:1330:A:C8	2:a:1334:G:C5	3.07	0.41
5:d:63:MET:HE3	5:d:63:MET:HB2	1.79	0.41
9:h:28:PRO:HA	9:h:58:GLY:O	2.19	0.41
4:c:63:ILE:HB	4:c:98:VAL:HG12	2.02	0.41
16:o:43:LEU:HD13	16:o:53:ARG:HE	1.85	0.41
2:a:19:C:H5''	6:e:132:THR:HG21	2.01	0.41
2:a:525:G:N2	2:a:538:G:OP1	2.46	0.41
2:a:839:U:H3	2:a:865:G:H1	1.68	0.41
2:a:977:C:H4'	10:i:129:PHE:HE1	1.85	0.41
3:b:222:LEU:HD23	3:b:222:LEU:HA	1.90	0.41
4:c:134:LYS:HE3	4:c:134:LYS:HB3	1.90	0.41
13:l:112:ARG:HH21	13:l:120:VAL:HB	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:1001:U:O4	2:a:1223:U:O2'	2.37	0.41
3:b:18:HIS:NE2	3:b:188:ASP:O	2.52	0.41
9:h:18:ASN:ND2	9:h:74:ILE:O	2.53	0.41
9:h:85:LEU:HD13	13:l:4:ILE:HG21	2.02	0.41
2:a:456:A:O2'	2:a:493:G:O6	2.38	0.41
2:a:690:U:H2'	2:a:691:G:H8	1.85	0.41
2:a:1050:A:H2'	2:a:1051:A:H8	1.86	0.41
4:c:6:ASN:HD21	15:n:49:TYR:HB3	1.86	0.41
5:d:125:ARG:NH1	5:d:127:ASP:OD2	2.54	0.41
8:g:58:ALA:HA	8:g:61:VAL:HG12	2.03	0.41
20:s:37:ARG:H	20:s:37:ARG:HG2	1.74	0.41
2:a:1359:U:H2'	2:a:1360:A:H8	1.85	0.41
3:b:161:LEU:HD13	3:b:176:ALA:HB2	2.01	0.41
4:c:183:TYR:HA	4:c:199:VAL:O	2.20	0.41
5:d:106:THR:HG23	5:d:109:GLN:H	1.85	0.41
21:t:43:ALA:O	21:t:46:LYS:NZ	2.47	0.41
2:a:63:U:O2'	2:a:387:C:O2	2.39	0.41
2:a:901:U:H2'	2:a:902:A:H8	1.85	0.41
2:a:960:U:H3	2:a:1242:G:H1	1.68	0.41
3:b:45:LYS:HA	3:b:45:LYS:HD3	1.87	0.41
3:b:96:TRP:HH2	3:b:101:LEU:HD23	1.86	0.41
4:c:156:LEU:HD12	4:c:163:ARG:HB2	2.02	0.41
6:e:132:THR:HA	6:e:133:PRO:HD3	1.93	0.41
2:a:210:A:N3	2:a:230:U:O2'	2.48	0.41
2:a:956:A:H2'	2:a:957:G:H8	1.86	0.41
2:a:1366:A:H2'	2:a:1367:G:H8	1.86	0.41
6:e:164:LEU:H	6:e:164:LEU:HG	1.63	0.41
9:h:29:ALA:HB2	9:h:60:LEU:HD22	2.02	0.41
18:q:19:MET:HE3	18:q:19:MET:HB2	1.84	0.41
2:a:401:A:O2'	2:a:493:G:OP1	2.32	0.41
2:a:685:U:O2	2:a:785:A:O2'	2.36	0.41
2:a:1246:U:O2'	2:a:1316:G:OP1	2.36	0.41
4:c:146:LYS:HB3	4:c:146:LYS:HE3	1.91	0.41
2:a:106:G:O6	21:t:10:ARG:NE	2.51	0.40
2:a:661:U:H5	9:h:56:LYS:HE3	1.86	0.40
2:a:1331:C:H5''	14:m:97:VAL:O	2.22	0.40
3:b:177:ARG:HH21	6:e:3:ARG:HH12	1.69	0.40
5:d:98:VAL:HG21	5:d:119:ILE:HD13	2.03	0.40
9:h:52:VAL:HB	9:h:59:VAL:CG2	2.45	0.40
2:a:1251:U:OP2	8:g:116:MET:N	2.49	0.40
16:o:23:GLY:O	16:o:28:GLN:NE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:263:G:H4'	18:q:21:LYS:HD2	2.02	0.40
2:a:541:A:O2'	2:a:543:A:OP2	2.38	0.40
2:a:1171:G:O6	2:a:1193:G:O6	2.38	0.40
8:g:56:ARG:HD2	8:g:56:ARG:HA	1.92	0.40
8:g:122:ASN:OD1	8:g:122:ASN:N	2.51	0.40
9:h:56:LYS:HB2	9:h:56:LYS:HE2	1.28	0.40
13:l:63:ARG:HB2	13:l:103:LEU:HD11	2.04	0.40
16:o:73:LYS:HD2	16:o:73:LYS:HA	1.87	0.40
21:t:36:LYS:HA	21:t:39:VAL:HG12	2.01	0.40
2:a:777:G:H4'	2:a:1525:A:H4'	2.02	0.40
2:a:1503:G:H2'	2:a:1504:A:H8	1.87	0.40
3:b:26:LYS:NZ	3:b:192:ASP:OD1	2.46	0.40
4:c:135:GLN:HA	4:c:138:THR:HG22	2.03	0.40
6:e:41:ASP:OD1	6:e:41:ASP:N	2.46	0.40
20:s:12:ASP:OD1	20:s:39:THR:OG1	2.35	0.40
2:a:545:G:OP1	13:l:123:ARG:NH1	2.45	0.40
2:a:753:U:OP1	2:a:861:U:O2'	2.37	0.40
5:d:15:LEU:HB3	5:d:56:LYS:HG3	2.03	0.40
5:d:24:LYS:HZ1	5:d:30:PRO:HA	1.87	0.40
12:k:18:ASN:HA	12:k:81:THR:O	2.21	0.40
16:o:3:ILE:HD13	16:o:3:ILE:HA	1.94	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	b	222/255 (87%)	185 (83%)	36 (16%)	1 (0%)	24	56
4	c	200/217 (92%)	182 (91%)	18 (9%)	0	100	100
5	d	192/200 (96%)	172 (90%)	19 (10%)	1 (0%)	24	56
6	e	163/166 (98%)	142 (87%)	20 (12%)	1 (1%)	21	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	f	94/98 (96%)	85 (90%)	9 (10%)	0	100	100
8	g	141/156 (90%)	133 (94%)	8 (6%)	0	100	100
9	h	129/132 (98%)	120 (93%)	8 (6%)	1 (1%)	16	47
10	i	123/132 (93%)	109 (89%)	14 (11%)	0	100	100
11	j	95/102 (93%)	84 (88%)	10 (10%)	1 (1%)	11	40
12	k	116/129 (90%)	108 (93%)	8 (7%)	0	100	100
13	l	133/137 (97%)	112 (84%)	19 (14%)	2 (2%)	8	35
14	m	66/121 (54%)	53 (80%)	13 (20%)	0	100	100
15	n	57/61 (93%)	49 (86%)	8 (14%)	0	100	100
16	o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
17	p	88/91 (97%)	79 (90%)	9 (10%)	0	100	100
18	q	84/87 (97%)	75 (89%)	9 (11%)	0	100	100
19	r	68/80 (85%)	59 (87%)	9 (13%)	0	100	100
20	s	70/92 (76%)	53 (76%)	15 (21%)	2 (3%)	3	25
21	t	78/83 (94%)	76 (97%)	2 (3%)	0	100	100
All	All	2205/2428 (91%)	1959 (89%)	237 (11%)	9 (0%)	31	61

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	b	21	ARG
9	h	57	GLN
13	l	131	GLY
20	s	29	GLN
20	s	79	THR
5	d	188	GLU
6	e	160	THR
11	j	92	LEU
13	l	57	LYS

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	b	194/221 (88%)	185 (95%)	9 (5%)	24	47
4	c	164/175 (94%)	161 (98%)	3 (2%)	51	66
5	d	172/175 (98%)	171 (99%)	1 (1%)	78	79
6	e	130/131 (99%)	122 (94%)	8 (6%)	16	42
7	f	84/86 (98%)	80 (95%)	4 (5%)	23	47
8	g	124/132 (94%)	123 (99%)	1 (1%)	73	75
9	h	112/113 (99%)	101 (90%)	11 (10%)	7	29
10	i	103/109 (94%)	103 (100%)	0	100	100
11	j	87/91 (96%)	86 (99%)	1 (1%)	65	72
12	k	94/104 (90%)	93 (99%)	1 (1%)	65	72
13	l	117/119 (98%)	109 (93%)	8 (7%)	14	40
14	m	62/104 (60%)	62 (100%)	0	100	100
15	n	52/53 (98%)	52 (100%)	0	100	100
16	o	80/81 (99%)	79 (99%)	1 (1%)	61	71
17	p	76/77 (99%)	73 (96%)	3 (4%)	28	51
18	q	81/82 (99%)	78 (96%)	3 (4%)	30	52
19	r	62/68 (91%)	61 (98%)	1 (2%)	55	68
20	s	64/80 (80%)	64 (100%)	0	100	100
21	t	67/69 (97%)	67 (100%)	0	100	100
All	All	1925/2070 (93%)	1870 (97%)	55 (3%)	38	56

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	b	14	VAL
3	b	21	ARG
3	b	83	GLU
3	b	89	GLN
3	b	90	PHE
3	b	92	ILE
3	b	116	GLU
3	b	117	ILE
3	b	221	ILE
4	c	42	ILE
4	c	103	ILE

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Mol	Chain	Res	Type
4	c	197	VAL
5	d	9	TRP
6	e	50	THR
6	e	117	LEU
6	e	137	VAL
6	e	159	LYS
6	e	161	VAL
6	e	162	GLU
6	e	163	GLU
6	e	164	LEU
7	f	6	VAL
7	f	48	LEU
7	f	63	VAL
7	f	86	ILE
8	g	12	VAL
9	h	20	VAL
9	h	49	VAL
9	h	50	GLU
9	h	53	GLU
9	h	54	ASP
9	h	55	ASP
9	h	56	LYS
9	h	57	GLN
9	h	60	LEU
9	h	62	LEU
9	h	116	LYS
11	j	36	VAL
12	k	116	VAL
13	l	50	VAL
13	l	68	VAL
13	l	92	VAL
13	l	100	VAL
13	l	106	VAL
13	l	120	VAL
13	l	129	LEU
13	l	132	THR
16	o	52	SER
17	p	3	VAL
17	p	22	VAL
17	p	50	ILE
18	q	40	VAL
18	q	61	VAL

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Mol	Chain	Res	Type
18	q	66	THR
19	r	76	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	b	8	GLN
3	b	36	ASN
3	b	66	GLN
3	b	75	GLN
3	b	89	GLN
3	b	225	GLN
4	c	88	ASN
4	c	91	ASN
4	c	99	HIS
5	d	8	ASN
5	d	36	HIS
5	d	112	GLN
5	d	115	ASN
5	d	137	GLN
5	d	158	ASN
5	d	159	ASN
5	d	192	GLN
6	e	146	ASN
7	f	53	ASN
8	g	28	ASN
8	g	67	ASN
8	g	129	ASN
9	h	18	ASN
10	i	68	ASN
10	i	77	GLN
10	i	79	GLN
10	i	128	GLN
11	j	15	HIS
11	j	78	ASN
11	j	91	ASN
12	k	18	ASN
13	l	39	ASN
14	m	74	ASN
14	m	76	ASN
15	n	52	GLN
16	o	9	ASN

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Mol	Chain	Res	Type
16	o	37	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	31/32 (96%)	17 (54%)	2 (6%)
2	a	1551/1556 (99%)	387 (24%)	0
All	All	1582/1588 (99%)	404 (25%)	2 (0%)

All (404) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	A
1	A	10	U
1	A	11	A
1	A	12	C
1	A	13	A
1	A	14	G
1	A	16	G
1	A	17	G
1	A	18	G
1	A	19	U
1	A	20	A
1	A	21	U
1	A	23	A
1	A	29	A
1	A	34	G
1	A	35	A
1	A	36	A
2	a	6	U
2	a	7	G
2	a	8	G
2	a	10	G
2	a	15	U
2	a	16	G
2	a	23	G
2	a	32	G
2	a	33	A
2	a	40	G
2	a	47	G
2	a	48	C

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Mol	Chain	Res	Type
2	a	49	C
2	a	50	U
2	a	51	A
2	a	52	A
2	a	66	A
2	a	67	G
2	a	69	G
2	a	75	A
2	a	76	C
2	a	78	A
2	a	80	A
2	a	81	A
2	a	82	G
2	a	84	U
2	a	85	U
2	a	86	G
2	a	88	U
2	a	91	U
2	a	92	C
2	a	93	U
2	a	99	U
2	a	100	A
2	a	107	G
2	a	120	C
2	a	129	A
2	a	146	G
2	a	155	U
2	a	159	G
2	a	163	C
2	a	168	G
2	a	173	U
2	a	174	A
2	a	184	A
2	a	187	U
2	a	195	C
2	a	196	A
2	a	204	A
2	a	211	A
2	a	212	A
2	a	219	C
2	a	221	U
2	a	222	G

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Mol	Chain	Res	Type
2	a	234	A
2	a	248	U
2	a	249	G
2	a	255	G
2	a	258	A
2	a	259	G
2	a	267	G
2	a	270	A
2	a	271	A
2	a	274	G
2	a	275	C
2	a	288	C
2	a	297	G
2	a	306	A
2	a	307	G
2	a	314	A
2	a	324	C
2	a	329	A
2	a	336	C
2	a	353	C
2	a	354	G
2	a	359	G
2	a	360	C
2	a	361	A
2	a	362	G
2	a	371	A
2	a	373	U
2	a	375	U
2	a	380	C
2	a	381	A
2	a	389	A
2	a	392	G
2	a	395	U
2	a	396	G
2	a	398	C
2	a	400	G
2	a	405	A
2	a	406	C
2	a	412	G
2	a	414	G
2	a	418	G
2	a	419	A

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Mol	Chain	Res	Type
2	a	420	U
2	a	421	G
2	a	422	A
2	a	429	U
2	a	430	C
2	a	431	G
2	a	432	G
2	a	436	G
2	a	437	U
2	a	447	U
2	a	456	A
2	a	457	A
2	a	458	G
2	a	460	A
2	a	462	A
2	a	465	U
2	a	466	G
2	a	467	U
2	a	468	G
2	a	469	U
2	a	470	A
2	a	474	A
2	a	475	A
2	a	476	C
2	a	477	U
2	a	484	A
2	a	485	U
2	a	490	A
2	a	491	C
2	a	493	G
2	a	503	A
2	a	505	A
2	a	513	G
2	a	517	A
2	a	519	C
2	a	525	G
2	a	526	C
2	a	527	C
2	a	529	G
2	a	532	G
2	a	535	G
2	a	537	G

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Mol	Chain	Res	Type
2	a	539	U
2	a	540	A
2	a	541	A
2	a	553	C
2	a	555	A
2	a	567	A
2	a	570	U
2	a	572	U
2	a	574	G
2	a	578	G
2	a	580	A
2	a	581	A
2	a	583	G
2	a	584	C
2	a	585	G
2	a	587	G
2	a	604	A
2	a	615	A
2	a	624	G
2	a	627	U
2	a	628	C
2	a	658	A
2	a	661	U
2	a	673	A
2	a	695	A
2	a	701	G
2	a	702	A
2	a	703	A
2	a	705	U
2	a	709	C
2	a	710	A
2	a	711	G
2	a	718	G
2	a	729	A
2	a	730	G
2	a	741	G
2	a	742	A
2	a	762	C
2	a	763	G
2	a	771	G
2	a	775	A
2	a	777	G

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Mol	Chain	Res	Type
2	a	785	A
2	a	789	A
2	a	800	A
2	a	804	C
2	a	807	G
2	a	817	G
2	a	822	A
2	a	823	A
2	a	824	A
2	a	825	C
2	a	826	G
2	a	827	A
2	a	828	U
2	a	829	G
2	a	836	A
2	a	840	G
2	a	844	G
2	a	853	C
2	a	854	C
2	a	858	C
2	a	865	G
2	a	874	A
2	a	882	A
2	a	894	U
2	a	899	A
2	a	900	G
2	a	909	C
2	a	924	A
2	a	926	G
2	a	927	G
2	a	932	G
2	a	936	G
2	a	941	C
2	a	943	G
2	a	944	C
2	a	945	A
2	a	950	C
2	a	955	G
2	a	970	U
2	a	978	A
2	a	979	A
2	a	981	G

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Mol	Chain	Res	Type
2	a	982	C
2	a	983	G
2	a	984	A
2	a	985	A
2	a	992	U
2	a	993	A
2	a	994	C
2	a	999	U
2	a	1002	U
2	a	1003	G
2	a	1007	U
2	a	1014	A
2	a	1016	A
2	a	1019	U
2	a	1025	G
2	a	1028	A
2	a	1033	C
2	a	1034	U
2	a	1035	U
2	a	1036	C
2	a	1038	C
2	a	1039	C
2	a	1040	U
2	a	1044	G
2	a	1054	U
2	a	1055	G
2	a	1056	A
2	a	1057	C
2	a	1058	A
2	a	1066	C
2	a	1067	A
2	a	1068	U
2	a	1076	G
2	a	1077	U
2	a	1090	U
2	a	1097	U
2	a	1106	G
2	a	1107	U
2	a	1108	C
2	a	1113	A
2	a	1116	G
2	a	1123	A

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Mol	Chain	Res	Type
2	a	1124	C
2	a	1130	A
2	a	1131	G
2	a	1135	A
2	a	1136	G
2	a	1138	U
2	a	1139	G
2	a	1141	C
2	a	1142	A
2	a	1144	C
2	a	1150	G
2	a	1151	U
2	a	1152	U
2	a	1153	G
2	a	1157	A
2	a	1163	A
2	a	1168	A
2	a	1170	U
2	a	1171	G
2	a	1172	C
2	a	1177	G
2	a	1178	A
2	a	1179	C
2	a	1182	A
2	a	1192	G
2	a	1195	G
2	a	1207	A
2	a	1208	A
2	a	1212	A
2	a	1216	U
2	a	1217	G
2	a	1223	U
2	a	1224	A
2	a	1225	U
2	a	1233	G
2	a	1235	U
2	a	1236	A
2	a	1237	C
2	a	1238	A
2	a	1239	C
2	a	1247	A
2	a	1249	A

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Mol	Chain	Res	Type
2	a	1251	U
2	a	1261	A
2	a	1267	C
2	a	1268	A
2	a	1269	G
2	a	1271	G
2	a	1272	A
2	a	1277	G
2	a	1280	A
2	a	1281	G
2	a	1291	A
2	a	1296	A
2	a	1297	U
2	a	1298	A
2	a	1304	G
2	a	1308	U
2	a	1310	A
2	a	1316	G
2	a	1323	G
2	a	1324	U
2	a	1326	U
2	a	1327	G
2	a	1328	C
2	a	1329	A
2	a	1330	A
2	a	1333	C
2	a	1339	C
2	a	1342	G
2	a	1343	A
2	a	1344	A
2	a	1346	C
2	a	1347	U
2	a	1351	A
2	a	1357	A
2	a	1359	U
2	a	1364	G
2	a	1372	G
2	a	1374	A
2	a	1375	U
2	a	1390	G
2	a	1392	U
2	a	1393	C

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Mol	Chain	Res	Type
2	a	1395	C
2	a	1408	C
2	a	1409	A
2	a	1411	C
2	a	1412	G
2	a	1429	A
2	a	1436	A
2	a	1437	A
2	a	1443	G
2	a	1453	G
2	a	1457	A
2	a	1462	U
2	a	1463	U
2	a	1464	U
2	a	1465	A
2	a	1487	G
2	a	1504	A
2	a	1506	G
2	a	1509	G
2	a	1511	A
2	a	1512	A
2	a	1515	A
2	a	1518	U
2	a	1519	A
2	a	1520	G
2	a	1531	A
2	a	1541	G
2	a	1542	G
2	a	1543	A
2	a	1544	U
2	a	1545	C
2	a	1546	A
2	a	1547	C
2	a	1549	U
2	a	1550	C
2	a	1551	C
2	a	1552	U
2	a	1553	U
2	a	1554	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	17	G
1	A	22	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.

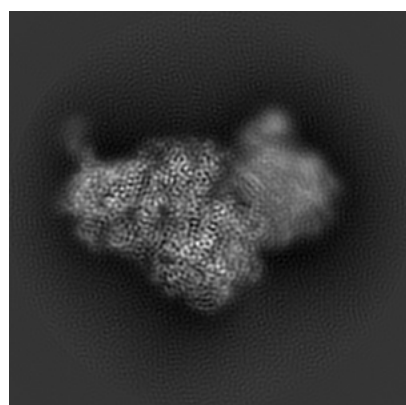
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23052. These allow visual inspection of the internal detail of the map and identification of artifacts.

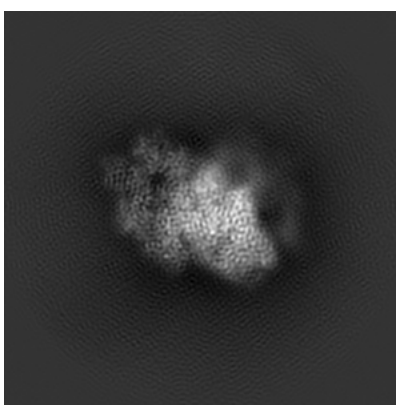
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

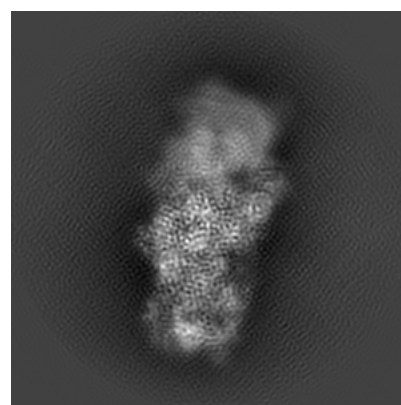
6.1.1 Primary map



X



Y

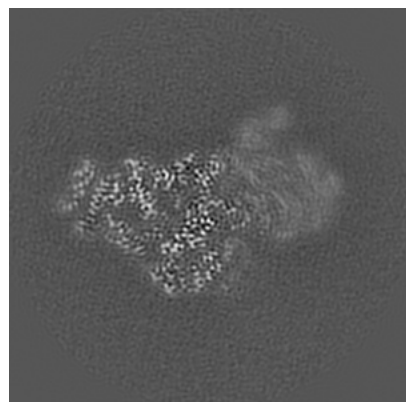


Z

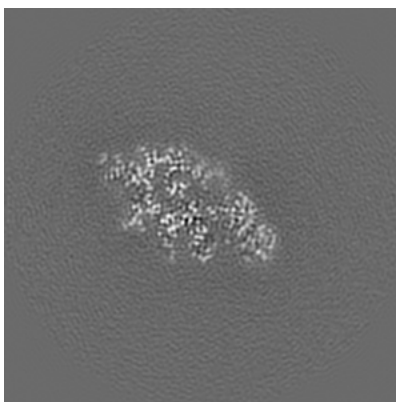
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

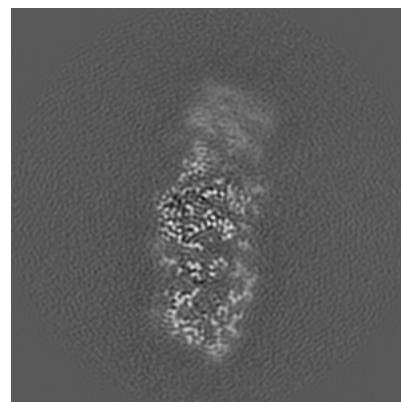
6.2.1 Primary map



X Index: 135



Y Index: 135

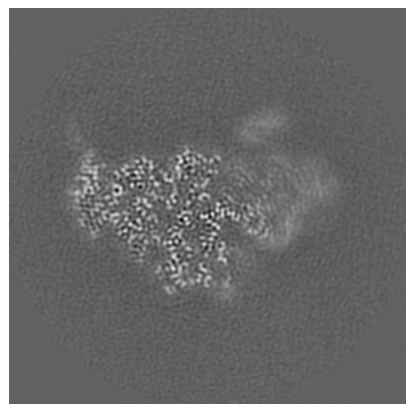


Z Index: 135

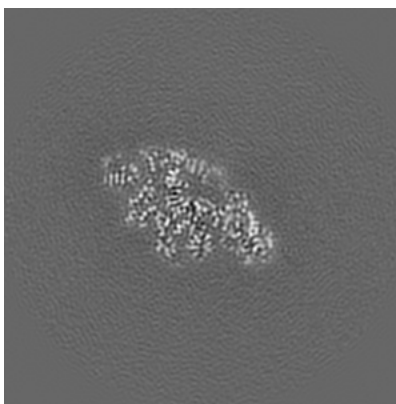
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

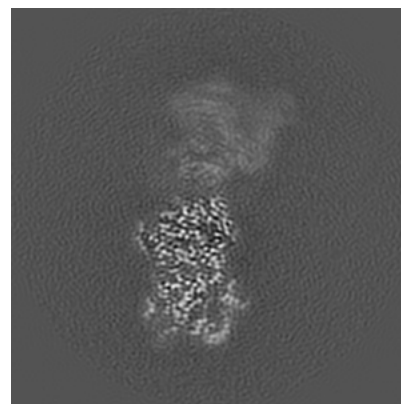
6.3.1 Primary map



X Index: 127



Y Index: 132

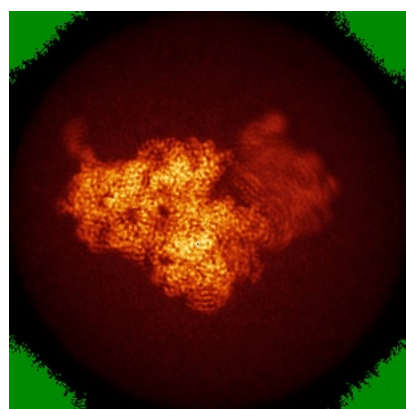


Z Index: 158

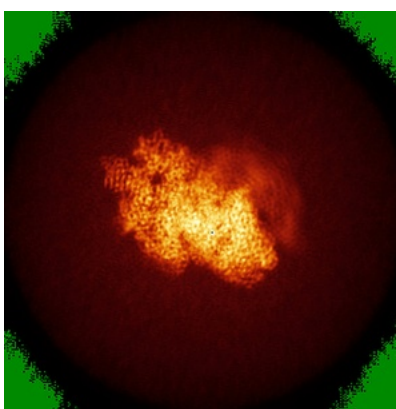
The images above show the largest variance slices of the map in three orthogonal directions.

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

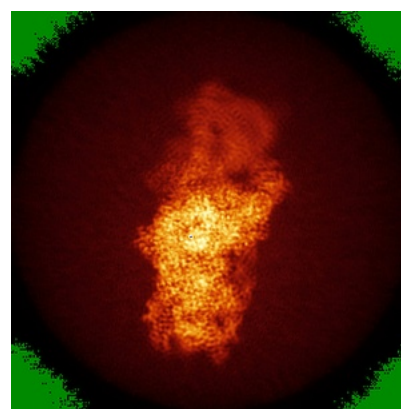
6.4.1 Primary map



X



Y

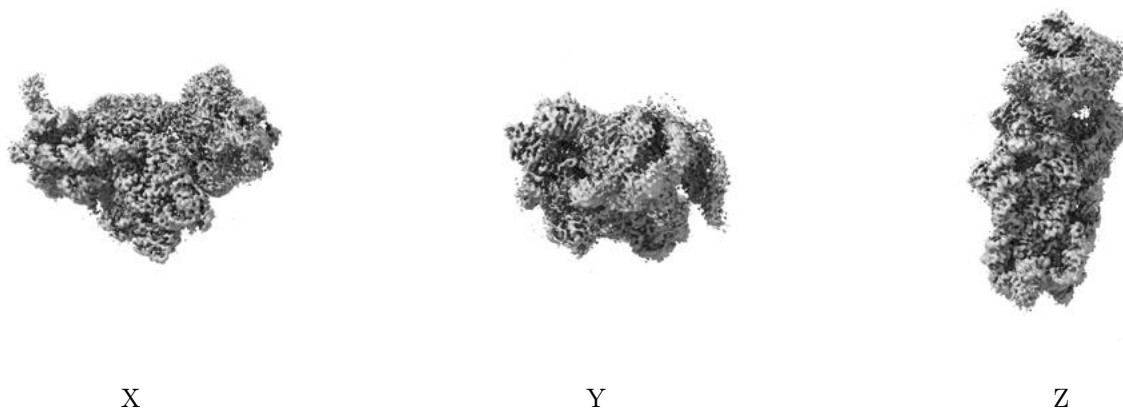


Z

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 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

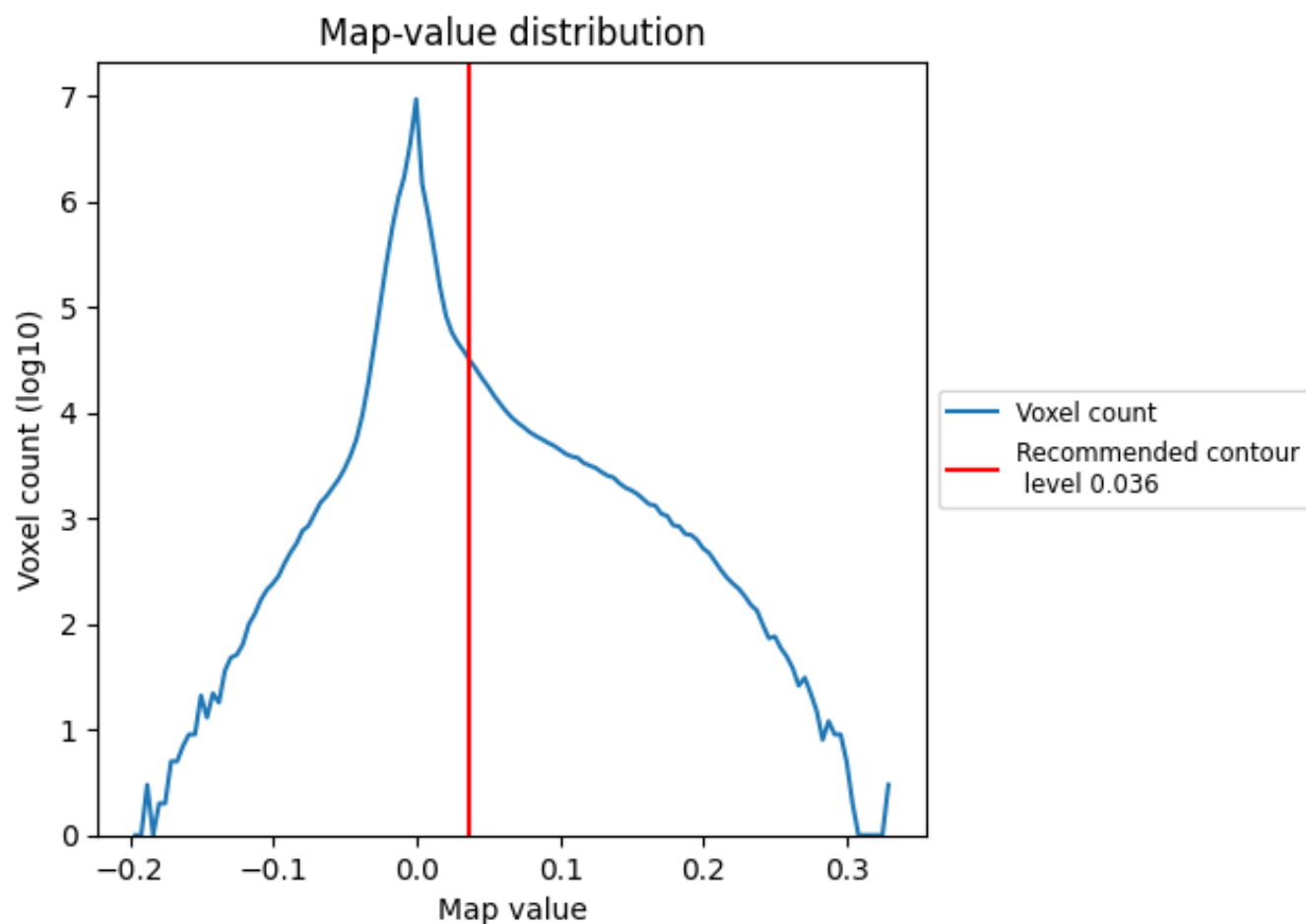
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

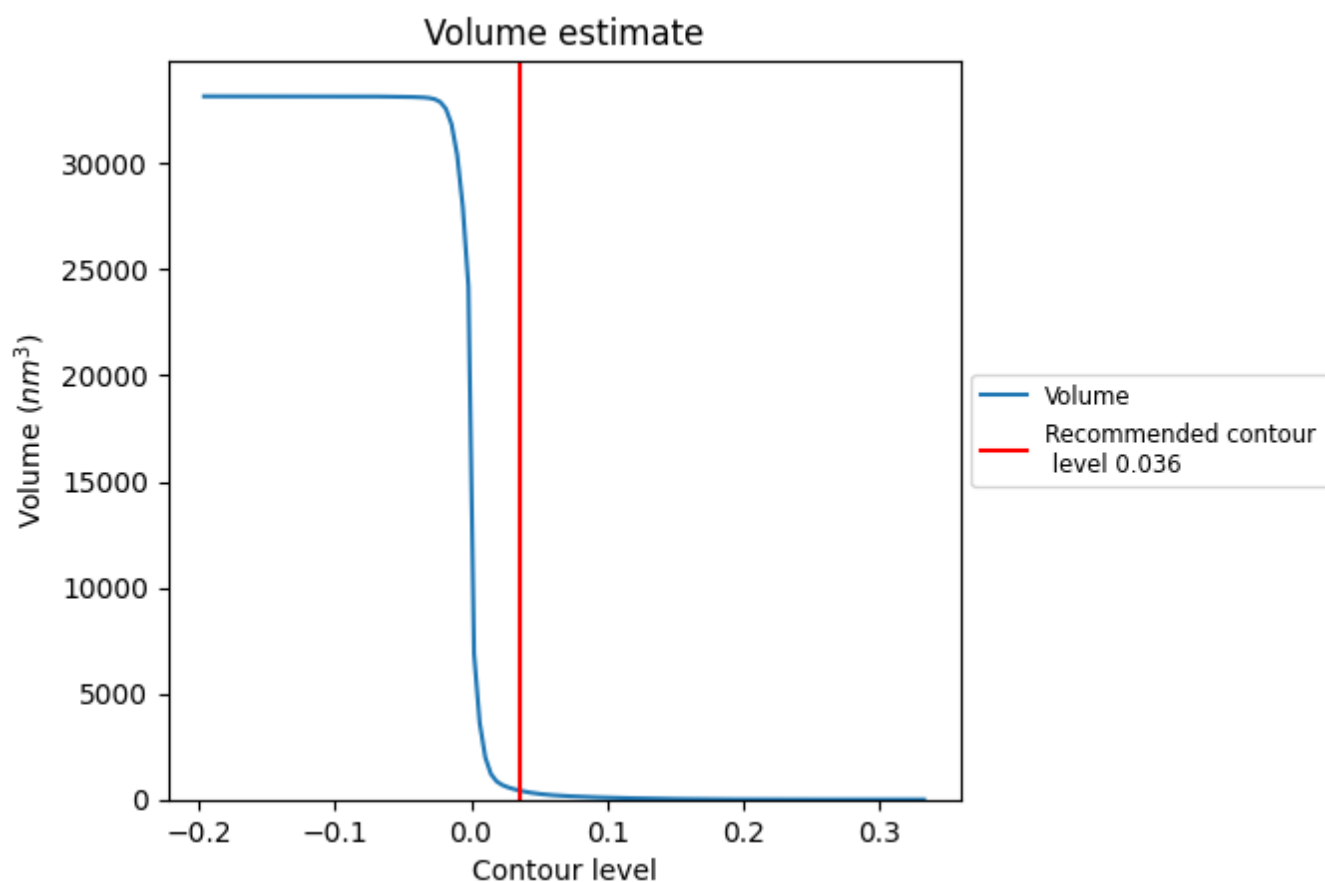
This section contains the results of statistical analysis of the map.

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.

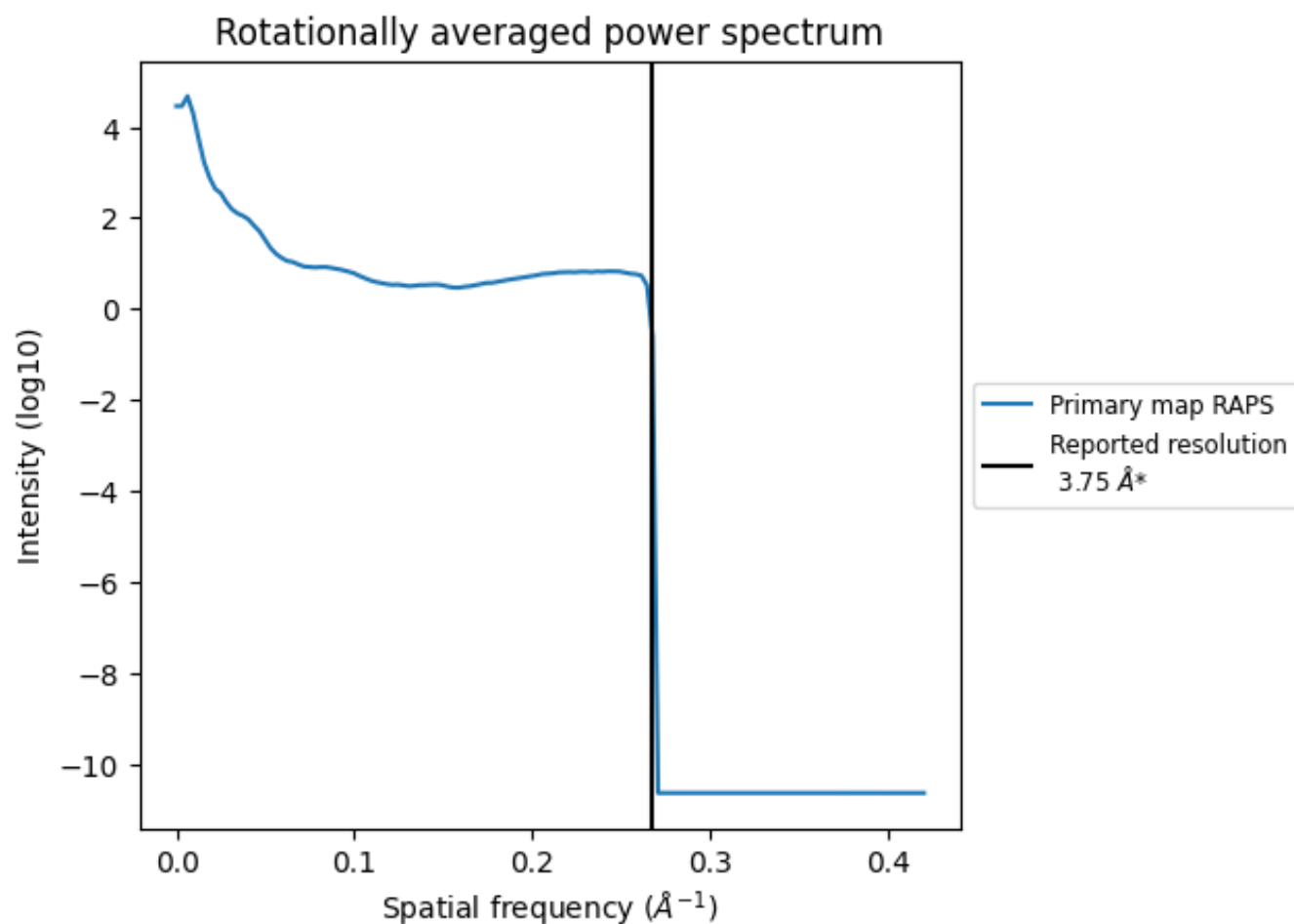
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 421 nm³; this corresponds to an approximate mass of 380 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 0.267 Å⁻¹

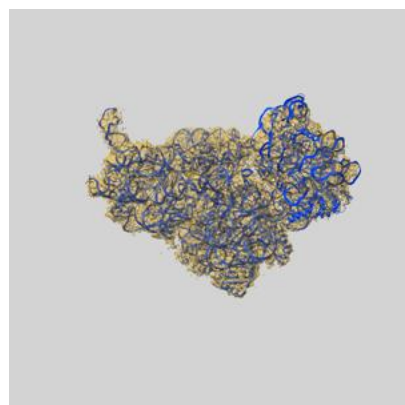
8 Fourier-Shell correlation

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

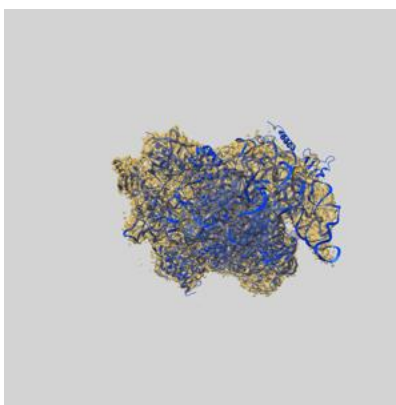
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23052 and PDB model 7KWG. Per-residue inclusion information can be found in section 3 on page 8.

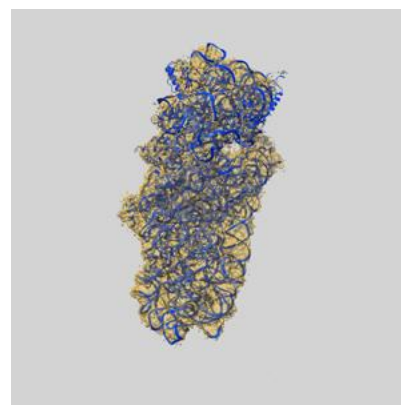
9.1 Map-model overlay [i](#)



X



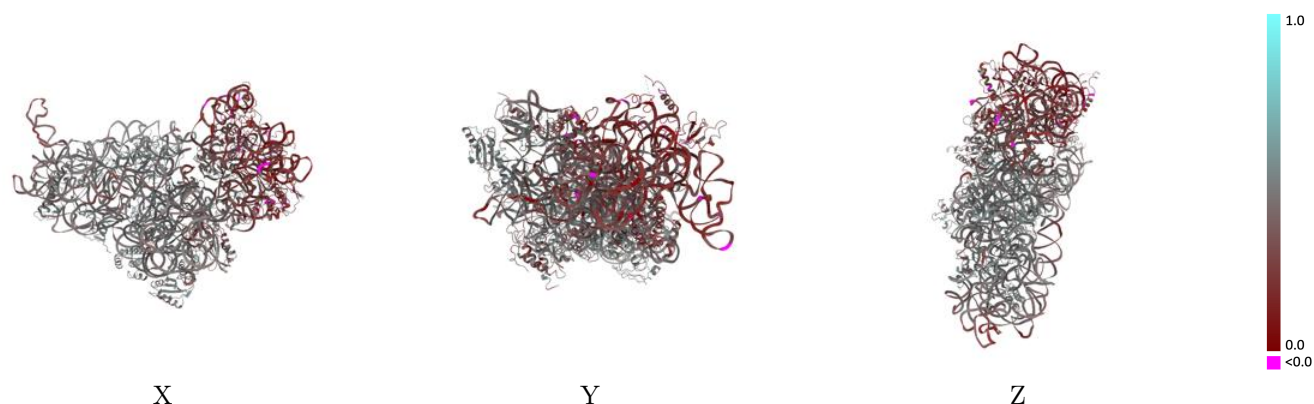
Y



Z

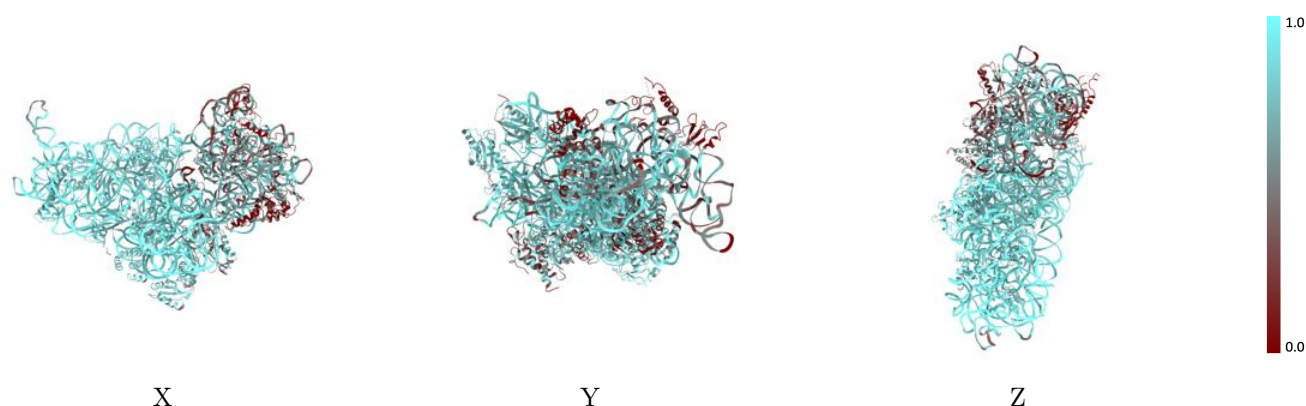
The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



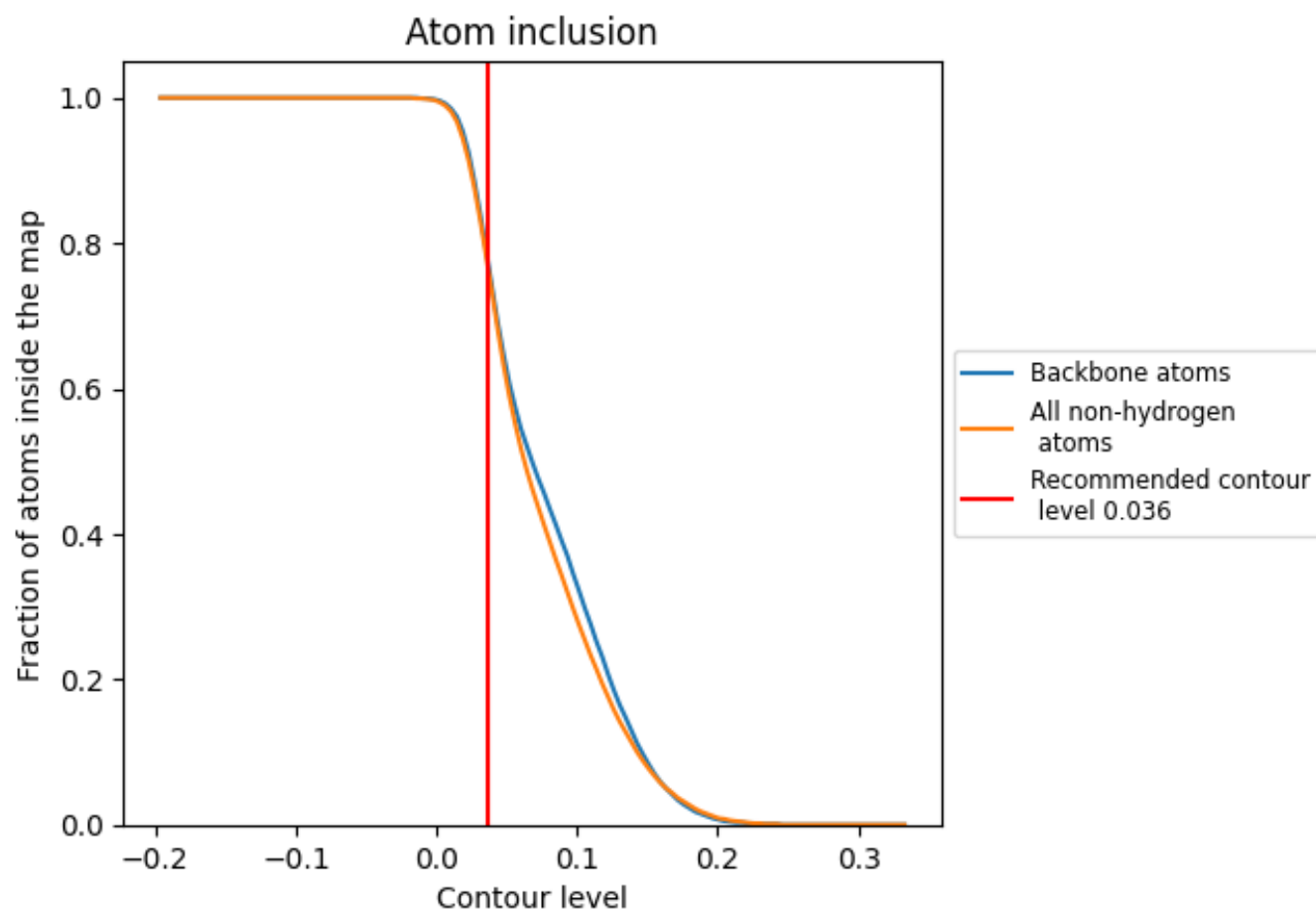
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.036).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 78% 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 (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7760	 0.3970
A	 0.3260	 0.2890
a	 0.8640	 0.3910
b	 0.4640	 0.3900
c	 0.4970	 0.3860
d	 0.8670	 0.4990
e	 0.7770	 0.4780
f	 0.7750	 0.4750
g	 0.2340	 0.2840
h	 0.8460	 0.4960
i	 0.4460	 0.2700
j	 0.3130	 0.2770
k	 0.7270	 0.4490
l	 0.8840	 0.5180
m	 0.1280	 0.1910
n	 0.5130	 0.3360
o	 0.8550	 0.4770
p	 0.8720	 0.5010
q	 0.8280	 0.4910
r	 0.7540	 0.4640
s	 0.2120	 0.2480
t	 0.8460	 0.4910

