Full wwPDB EM Validation Report (i)

Mar 19, 2024 – 03:14 PM JST

PDB ID	:	5X8R
EMDB ID	:	EMD-6710
Title	:	Structure of the 30S small subunit of chloroplast ribosome from spinach
Authors	:	Ahmed, T.; Shi, J.; Bhushan, S.
Deposited on	:	2017-03-03
Resolution	:	3.70 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 (i) 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 (i)) were used in the production of this report:

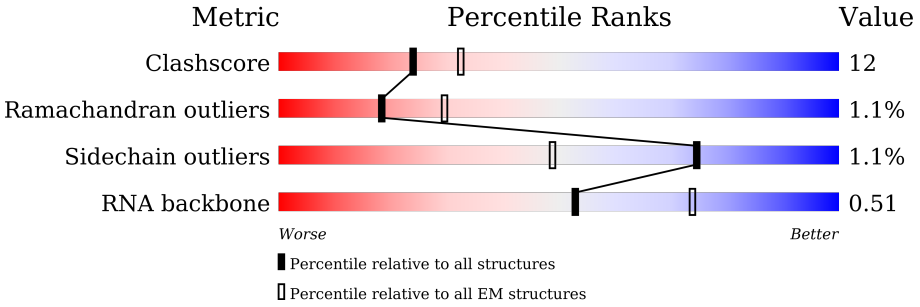
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	b	236	63% 91%
2	c	218	13% 95%
3	e	253	6% 65% 32%
4	f	146	21% 75% 24%
5	g	155	26% 95%
6	h	134	10% 99%
7	i	157	82% 15%

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Mol	Chain	Length	Quality of chain
8	j	122	15% 80% 20%
9	k	138	14% 86% 14%
10	l	123	7% 96%
11	m	126	17% 84% 13%
12	o	90	17% 69% 31%
13	p	88	90% 9%
14	q	108	6% 72% 28%
15	r	101	10% 61% 37%
16	s	92	9% 85% 15%
17	t	108	12% 95%
18	u	137	13% 31% 68%
19	y	236	7% 44% 54%
20	a	1491	67% 29%
21	w	121	67% 56% 10% 31%
22	d	201	13% 95%
23	v	198	89% 81% 12%
24	n	100	11% 99%
25	x	47	11% 74% 21%
26	8	370	41% 23% 11% 58%

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 55412 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 30S ribosomal protein S2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	b	227	1787	1127	326	321	13	0	0

- Molecule 2 is a protein called 30S ribosomal protein S3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	c	213	1719	1099	310	304	6	0	0

- Molecule 3 is a protein called 30S ribosomal protein S5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	e	171	1292	806	250	230	6	0	0

- Molecule 4 is a protein called 30S ribosomal protein S6 alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	f	111	886	566	145	171	4	0	0

- Molecule 5 is a protein called 30S ribosomal protein S7, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	g	149	1161	723	231	204	3	0	0

- Molecule 6 is a protein called 30S ribosomal protein S8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	h	134	1088	684	211	187	6	0	0

- Molecule 7 is a protein called 30S ribosomal protein S9, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	i	133	1020	650	191	178	1	0	0

- Molecule 8 is a protein called protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	j	98	796	512	142	137	5	0	0

- Molecule 9 is a protein called 30S ribosomal protein S11, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	k	118	887	549	182	151	5	0	0

- Molecule 10 is a protein called 30S ribosomal protein S12, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	l	123	967	604	198	162	3	0	0

- Molecule 11 is a protein called 30S ribosomal protein S13, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	m	110	898	559	183	153	3	0	0

- Molecule 12 is a protein called 30S ribosomal protein S15, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	o	62	525	339	100	85	1	0	0

- Molecule 13 is a protein called 30S ribosomal protein S16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	p	80	664	425	123	114	2	0	0

- Molecule 14 is a protein called protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	q	78	635	399	124	108	4	0	0

- Molecule 15 is a protein called 30S ribosomal protein S18, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	r	64	518	326	101	90	1	0	0

- Molecule 16 is a protein called 30S ribosomal protein S19 alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	s	78	627	403	118	104	2	0	0

- Molecule 17 is a protein called protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	t	105	832	514	169	148	1	0	0

- Molecule 18 is a protein called protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	u	44	393	238	87	66	2	0	0

- Molecule 19 is a protein called protein plastid pY.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	y	108	845	521	164	159	1	0	0

- Molecule 20 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
20	a	1480	31777	14168	5863	10266	1480	0	0

- Molecule 21 is a protein called protein cS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	w	84	689	454	115	118	2	0	0

- Molecule 22 is a protein called 30S ribosomal protein S4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	d	199	1633	1032	319	278	4	0	0

- Molecule 23 is a protein called protein cS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	v	190	1464	908	255	298	3	0	0

- Molecule 24 is a protein called 30S ribosomal protein S14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	n	99	819	507	174	135	3	0	0

- Molecule 25 is a protein called protein bTHXc.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	x	37	289	179	65	45	0	0

- Molecule 26 is a protein called 30S ribosomal protein S1, chloroplastic.

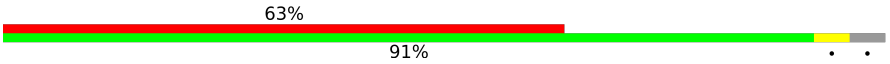
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	8	154	1201	744	222	227	8	0	0

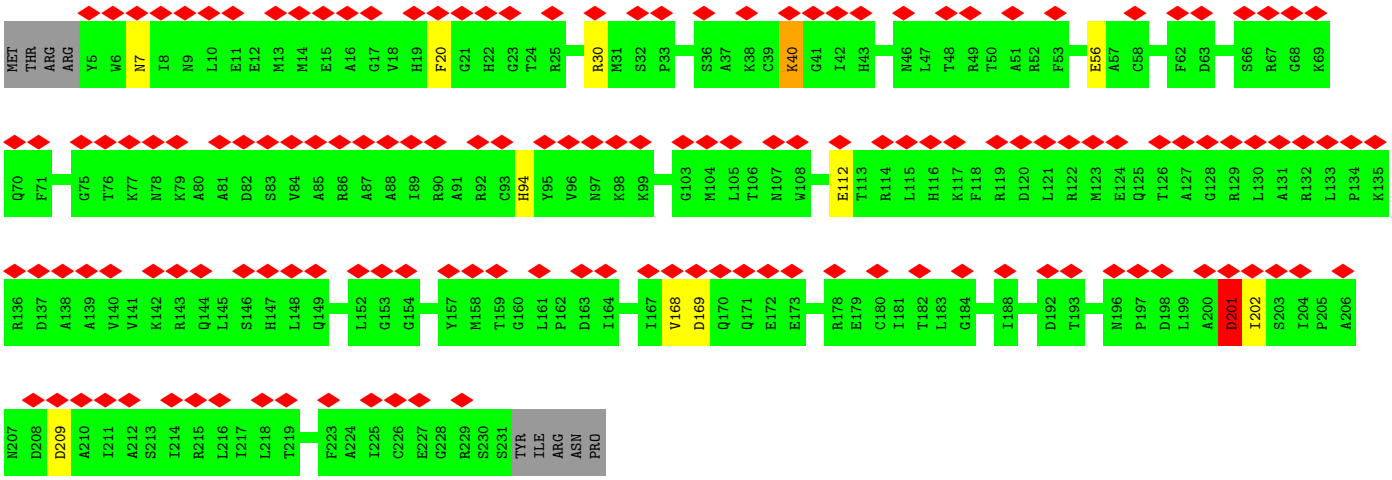
3 Residue-property plots (i)

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: 30S ribosomal protein S2, chloroplastic

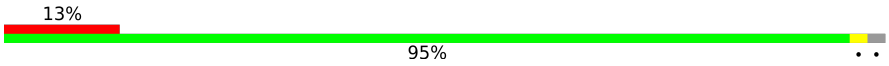
Chain b:

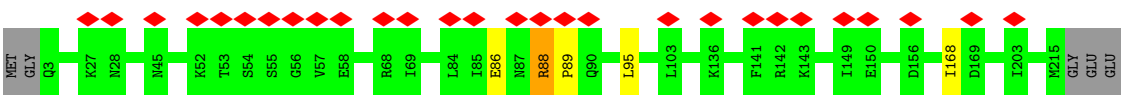




- Molecule 2: 30S ribosomal protein S3, chloroplastic

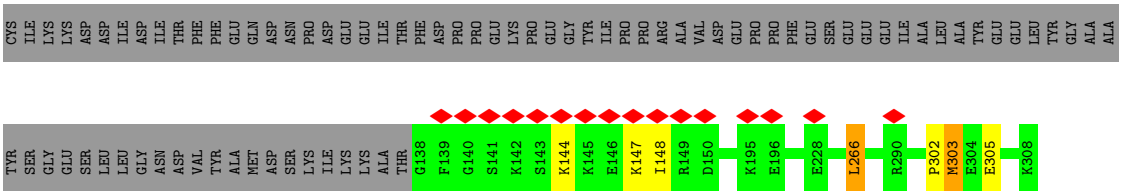
Chain c:





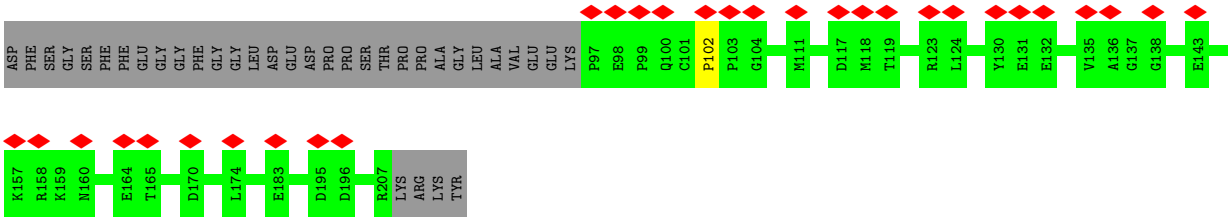
- Molecule 3: 30S ribosomal protein S5, chloroplastic

Chain e:



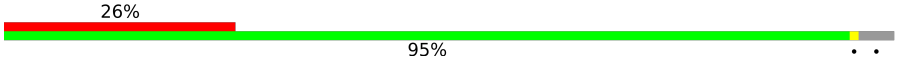
- Molecule 4: 30S ribosomal protein S6 alpha, chloroplastic

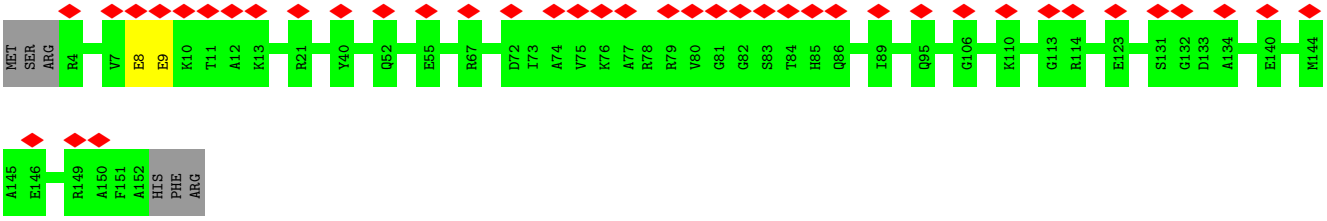
Chain f:



- Molecule 5: 30S ribosomal protein S7, chloroplastic

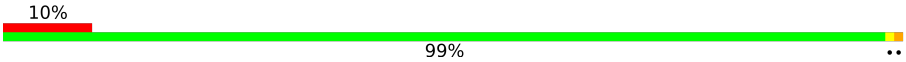
Chain g:

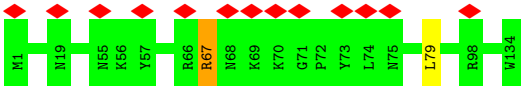




- Molecule 6: 30S ribosomal protein S8, chloroplastic

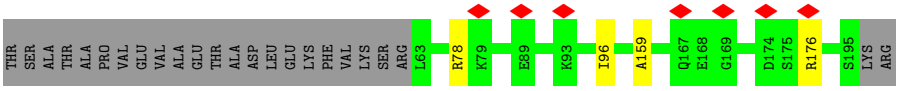
Chain h:





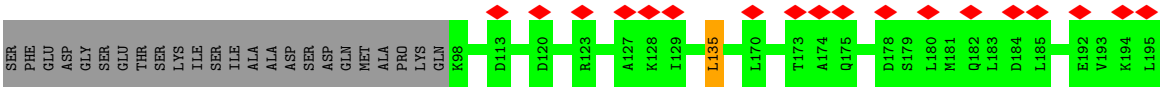
- Molecule 7: 30S ribosomal protein S9, chloroplastic

Chain i:



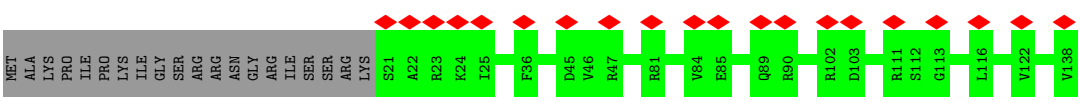
- Molecule 8: protein S10

Chain j:



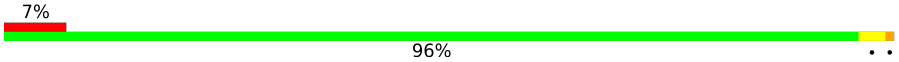
- Molecule 9: 30S ribosomal protein S11, chloroplastic

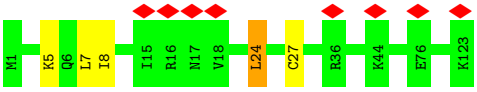
Chain k:



- Molecule 10: 30S ribosomal protein S12, chloroplastic

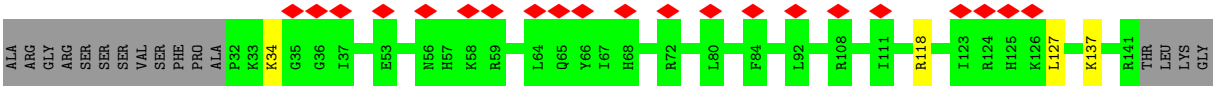
Chain l:





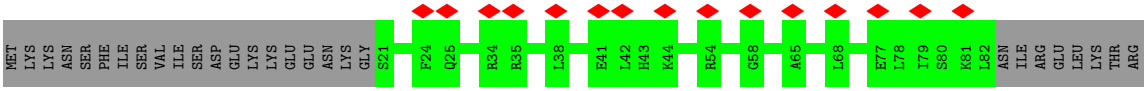
- Molecule 11: 30S ribosomal protein S13, chloroplastic

Chain m:



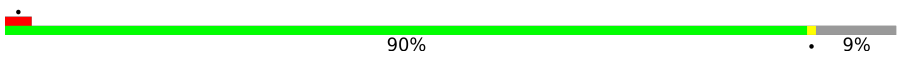
- Molecule 12: 30S ribosomal protein S15, chloroplastic

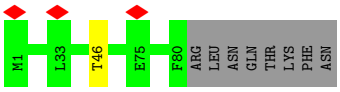
Chain o:



- Molecule 13: 30S ribosomal protein S16, chloroplastic

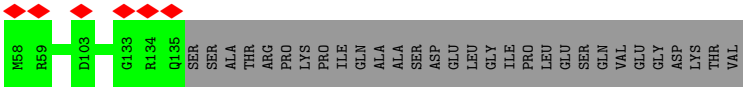
Chain p:





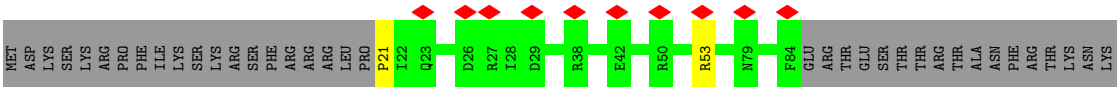
- Molecule 14: protein S17

Chain q:



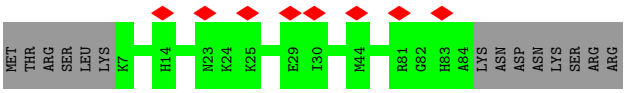
- Molecule 15: 30S ribosomal protein S18, chloroplastic

Chain r:

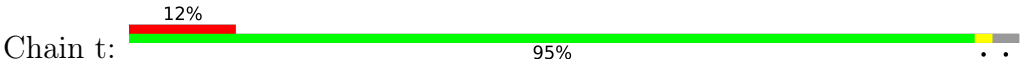


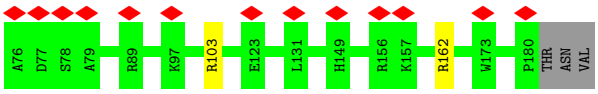
- Molecule 16: 30S ribosomal protein S19 alpha, chloroplastic

Chain s:

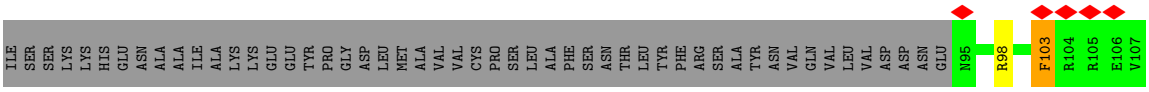


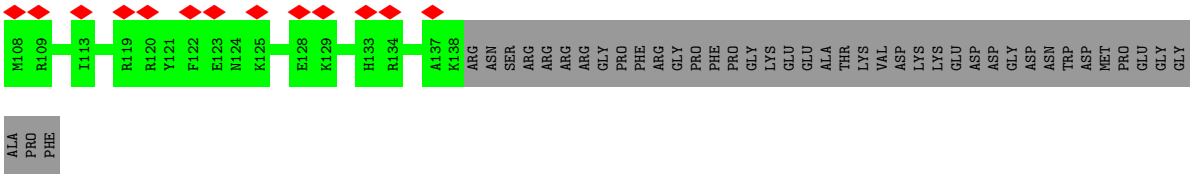
• Molecule 17: protein S20



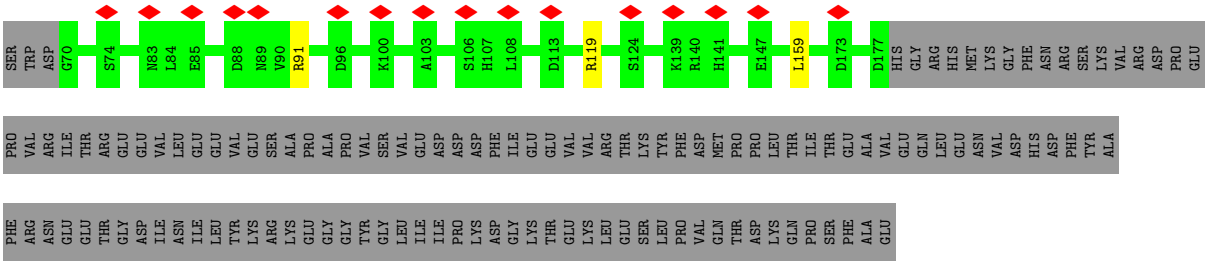


• Molecule 18: protein S21

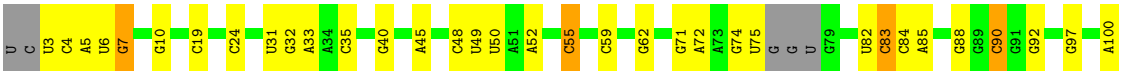


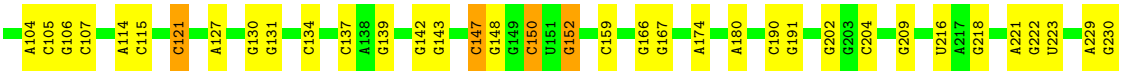


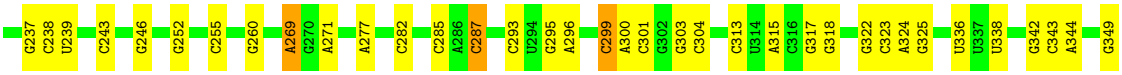
• Molecule 19: protein plastid pY

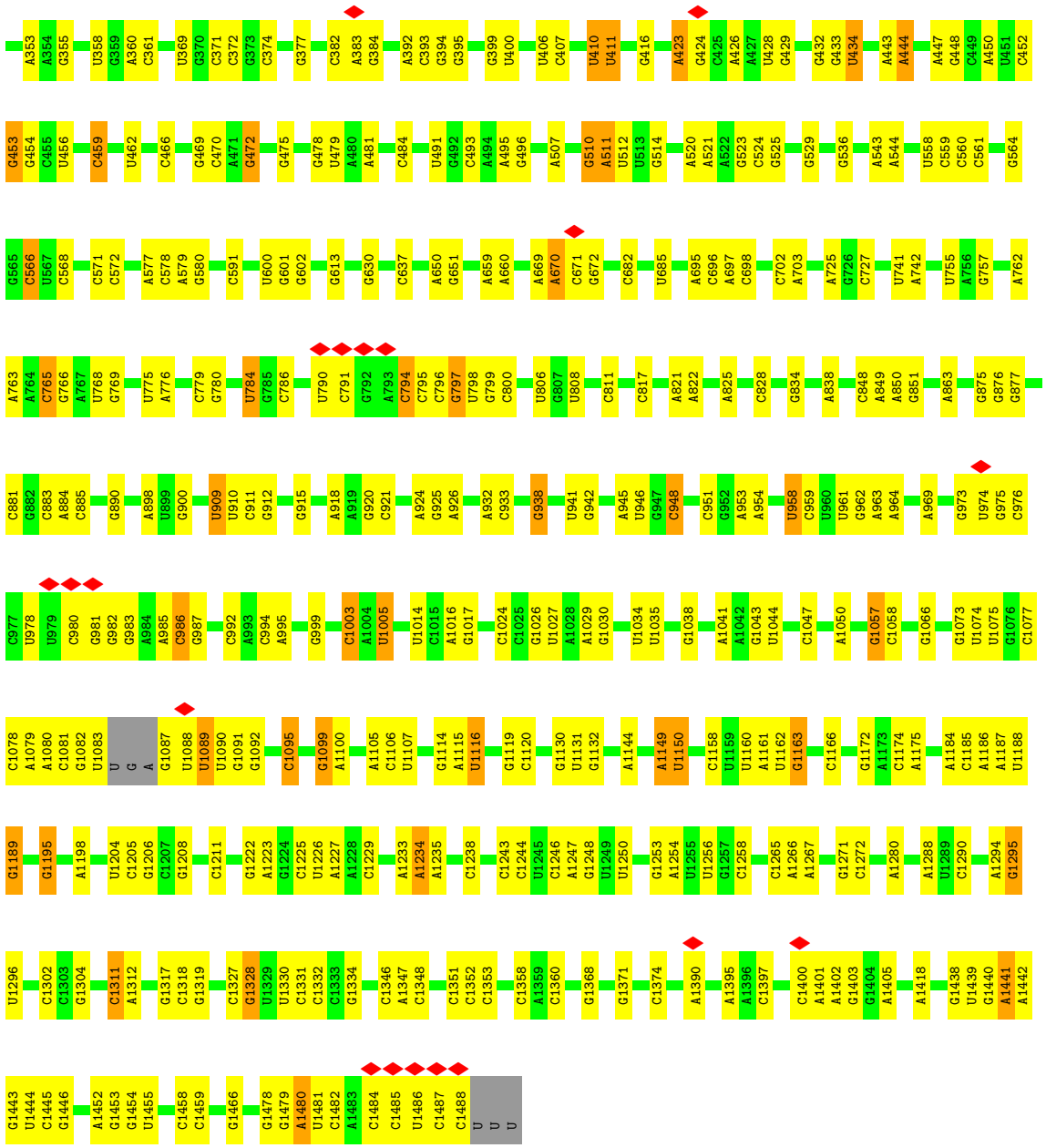


• Molecule 20: 16S rRNA

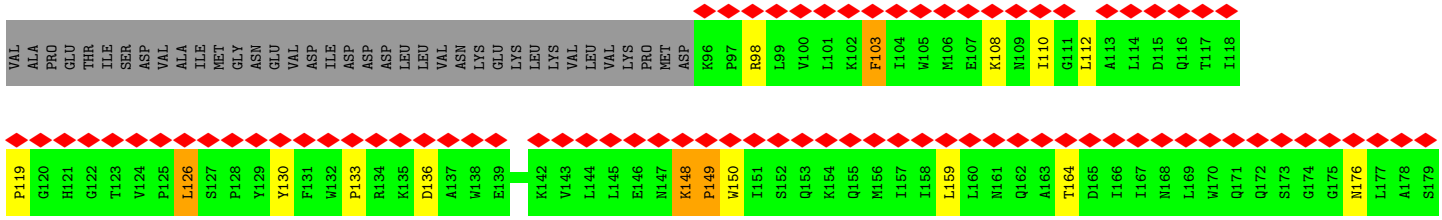






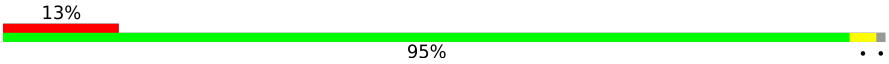


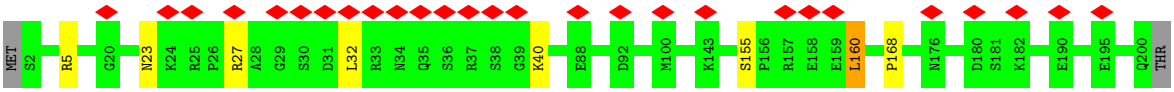
• Molecule 21: protein cS23



• Molecule 22: 30S ribosomal protein S4, chloroplastic

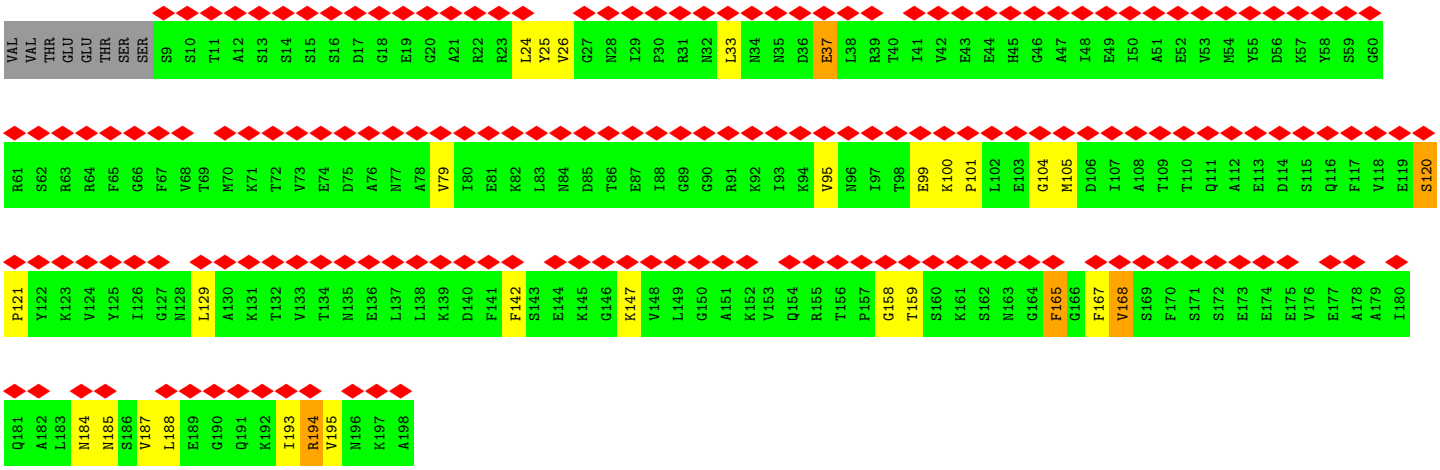
Chain d:





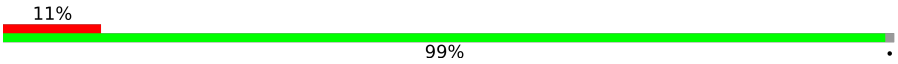
• Molecule 23: protein cS22

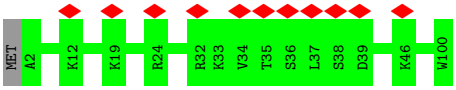
Chain v:



• Molecule 24: 30S ribosomal protein S14, chloroplastic

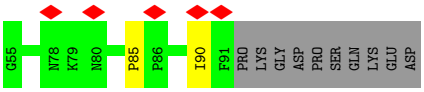
Chain n:





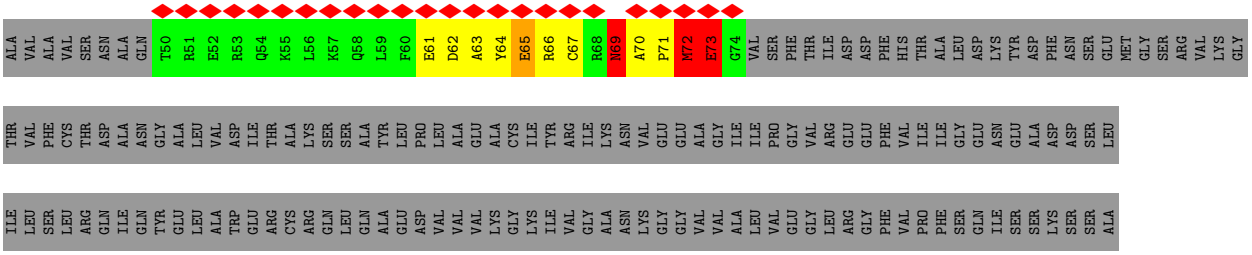
• Molecule 25: protein bTHXc

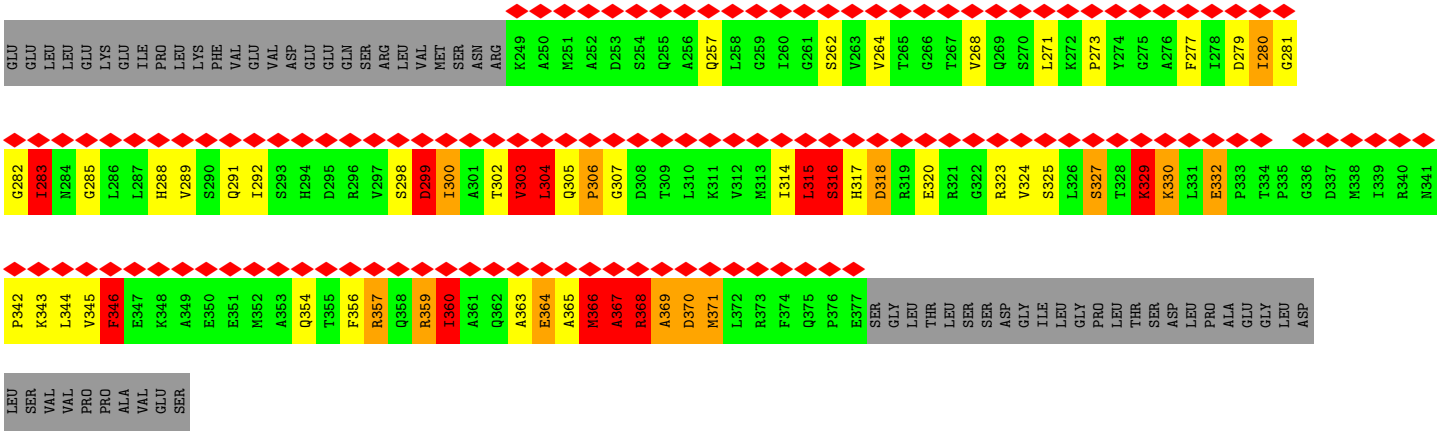
Chain x:



• Molecule 26: 30S ribosomal protein S1, chloroplastic

Chain 8:

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MET
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M251
A252
D253
S254
Q255
A256
Q257
L258
G259
I260
G261
S262
V263
V264
T265
G266
T267
V268
Q269
S270
L271
K272
P273
Y274
G275
A276
F277
I278
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I280
G281
G282
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N284
G285
L286
L287
H288
V289
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Q291
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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81305	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.5	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3700	Depositor
Magnification	133333	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.316	Depositor
Minimum map value	-0.172	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	403.19998, 403.19998, 403.19998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	b	0.75	8/1819 (0.4%)	0.96	8/2458 (0.3%)
2	c	0.48	0/1746	0.72	1/2348 (0.0%)
3	e	0.61	0/1307	0.77	2/1754 (0.1%)
4	f	0.44	0/904	0.69	0/1225
5	g	0.36	0/1175	0.62	0/1574
6	h	0.88	5/1103 (0.5%)	1.69	6/1477 (0.4%)
7	i	0.43	0/1038	0.70	0/1397
8	j	0.51	0/813	0.70	1/1099 (0.1%)
9	k	0.40	0/901	0.63	0/1214
10	l	0.62	0/983	0.80	4/1323 (0.3%)
11	m	0.45	0/909	0.75	2/1209 (0.2%)
12	o	0.42	0/532	0.65	0/707
13	p	0.52	0/674	0.71	0/902
14	q	0.50	0/647	0.64	0/867
15	r	0.49	0/522	0.76	2/697 (0.3%)
16	s	0.40	0/642	0.67	0/866
17	t	0.46	0/842	0.68	0/1127
18	u	1.10	3/396 (0.8%)	0.94	3/518 (0.6%)
19	y	0.45	0/852	0.70	0/1139
20	a	1.13	32/35582 (0.1%)	1.39	473/55510 (0.9%)
21	w	0.80	2/709 (0.3%)	1.23	11/965 (1.1%)
22	d	0.40	0/1661	0.72	2/2230 (0.1%)
23	v	1.49	16/1481 (1.1%)	1.24	13/1991 (0.7%)
24	n	0.37	0/835	0.62	0/1116
25	x	0.55	0/296	0.74	1/390 (0.3%)
26	8	0.87	5/1216 (0.4%)	1.61	28/1631 (1.7%)
All	All	0.97	71/59585 (0.1%)	1.24	557/87734 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	b	0	2
2	c	0	3
3	e	0	1
4	f	0	1
5	g	0	1
7	i	0	2
8	j	0	1
10	l	0	3
11	m	0	2
18	u	0	1
21	w	0	7
22	d	0	2
23	v	0	15
26	8	0	17
All	All	0	58

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	v	142	PHE	CE1-CZ	-18.97	1.01	1.37
23	v	142	PHE	CE2-CZ	-17.85	1.03	1.37
23	v	142	PHE	CG-CD2	-15.89	1.15	1.38
6	h	67	ARG	CZ-NH2	-15.34	1.13	1.33
23	v	165	PHE	CE2-CZ	-14.94	1.08	1.37
23	v	142	PHE	CG-CD1	-14.77	1.16	1.38
6	h	67	ARG	CB-CG	-14.59	1.13	1.52
23	v	168	VAL	CB-CG1	-14.33	1.22	1.52
23	v	195	VAL	CB-CG2	-13.41	1.24	1.52
23	v	194	ARG	CG-CD	-12.82	1.19	1.51
18	u	103	PHE	CD1-CE1	-11.76	1.15	1.39
23	v	165	PHE	CG-CD2	-10.85	1.22	1.38
18	u	103	PHE	CD2-CE2	-10.60	1.18	1.39
23	v	26	VAL	CB-CG1	-9.95	1.31	1.52
1	b	7	ASN	CG-ND2	-9.61	1.08	1.32
18	u	103	PHE	CB-CG	-9.12	1.35	1.51
1	b	201	ASP	CB-CG	9.03	1.70	1.51
23	v	142	PHE	CD2-CE2	7.99	1.55	1.39
23	v	142	PHE	CD1-CE1	7.72	1.54	1.39
21	w	149	PRO	CG-CD	-7.71	1.25	1.50
20	a	7	G	C2-N3	-7.63	1.26	1.32
6	h	67	ARG	CZ-NH1	-7.51	1.23	1.33
1	b	209	ASP	CG-OD2	-7.19	1.08	1.25
20	a	4	C	C4-C5	-6.92	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	w	164	THR	CB-CG2	-6.82	1.29	1.52
20	a	1081	C	N3-C4	6.76	1.38	1.33
20	a	1087	G	C6-N1	-6.71	1.34	1.39
20	a	900	G	C6-N1	-6.71	1.34	1.39
23	v	193	ILE	CB-CG2	-6.67	1.32	1.52
20	a	1480	A	N9-C8	-6.61	1.32	1.37
20	a	147	C	N3-C4	-6.49	1.29	1.33
23	v	79	VAL	CB-CG1	-6.48	1.39	1.52
20	a	4	C	C5-C6	-6.41	1.29	1.34
20	a	786	C	N3-C4	-6.40	1.29	1.33
20	a	107	C	N3-C4	-6.37	1.29	1.33
20	a	150	C	N3-C4	-6.30	1.29	1.33
20	a	881	C	N3-C4	-6.28	1.29	1.33
6	h	67	ARG	CG-CD	-6.17	1.36	1.51
20	a	1441	A	N1-C2	-6.03	1.28	1.34
6	h	67	ARG	CA-CB	-6.02	1.40	1.53
20	a	1482	C	C5-C6	-5.97	1.29	1.34
20	a	7	G	C5-C4	-5.94	1.34	1.38
1	b	20	PHE	CE2-CZ	-5.88	1.26	1.37
26	8	289	VAL	CB-CG1	-5.88	1.40	1.52
20	a	951	C	N3-C4	-5.75	1.29	1.33
20	a	448	G	C6-N1	-5.69	1.35	1.39
20	a	1440	G	N3-C4	-5.68	1.31	1.35
1	b	56	GLU	CD-OE2	-5.66	1.19	1.25
20	a	1029	A	N7-C5	-5.61	1.35	1.39
20	a	450	A	C6-N1	-5.58	1.31	1.35
20	a	1016	A	N9-C4	-5.53	1.34	1.37
26	8	327	SER	CB-OG	-5.53	1.35	1.42
23	v	95	VAL	CB-CG2	-5.50	1.41	1.52
26	8	368	ARG	CB-CG	5.45	1.67	1.52
20	a	74	G	O3'-P	-5.41	1.54	1.61
1	b	40	LYS	CD-CE	-5.40	1.37	1.51
20	a	269	A	N9-C4	-5.40	1.34	1.37
20	a	361	C	N3-C4	-5.38	1.30	1.33
26	8	65	GLU	CB-CG	-5.28	1.42	1.52
20	a	7	G	N3-C4	-5.28	1.31	1.35
20	a	898	A	N7-C5	-5.19	1.36	1.39
1	b	112	GLU	CD-OE2	-5.19	1.20	1.25
20	a	1358	C	C2-O2	-5.14	1.19	1.24
20	a	885	C	N3-C4	-5.13	1.30	1.33
20	a	371	C	N3-C4	-5.12	1.30	1.33
1	b	7	ASN	CB-CG	-5.10	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	a	271	A	N7-C5	-5.10	1.36	1.39
23	v	195	VAL	CB-CG1	-5.08	1.42	1.52
20	a	510	G	N9-C4	-5.07	1.33	1.38
26	8	332	GLU	CB-CG	-5.04	1.42	1.52
20	a	428	U	C2-N3	-5.03	1.34	1.37

All (557) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	h	67	ARG	NE-CZ-NH1	50.54	145.57	120.30
1	b	201	ASP	CB-CG-OD2	20.66	136.90	118.30
20	a	1440	G	N3-C2-N2	-20.49	105.56	119.90
20	a	7	G	C2-N3-C4	20.20	122.00	111.90
20	a	1441	A	N1-C2-N3	20.05	139.32	129.30
20	a	1439	U	C5-C6-N1	18.99	132.19	122.70
6	h	67	ARG	NH1-CZ-NH2	-16.53	101.21	119.40
20	a	147	C	N1-C2-O2	16.52	128.81	118.90
20	a	976	C	N1-C2-O2	16.12	128.57	118.90
20	a	150	C	N1-C2-O2	16.09	128.55	118.90
20	a	1488	C	C5-C6-N1	15.36	128.68	121.00
6	h	67	ARG	NE-CZ-NH2	-15.35	112.62	120.30
20	a	4	C	C6-N1-C2	-15.01	114.30	120.30
20	a	1480	A	N7-C8-N9	14.64	121.12	113.80
20	a	881	C	N1-C2-O2	14.50	127.60	118.90
6	h	67	ARG	CD-NE-CZ	14.42	143.78	123.60
20	a	786	C	N1-C2-O2	14.14	127.38	118.90
20	a	1077	C	N1-C2-O2	13.21	126.83	118.90
20	a	1445	C	C5-C6-N1	13.13	127.56	121.00
20	a	1487	C	C5-C6-N1	12.95	127.48	121.00
20	a	1485	C	C5-C6-N1	12.60	127.30	121.00
6	h	67	ARG	CB-CG-CD	12.09	143.04	111.60
20	a	1195	G	N1-C6-O6	11.53	126.82	119.90
20	a	147	C	N3-C2-O2	-11.49	113.86	121.90
20	a	107	C	N1-C2-O2	11.48	125.79	118.90
20	a	1440	G	N1-C2-N2	11.43	126.49	116.20
20	a	1195	G	C5-C6-O6	-11.39	121.77	128.60
20	a	1486	U	C5-C6-N1	11.28	128.34	122.70
20	a	1488	C	C6-N1-C2	-11.22	115.81	120.30
20	a	976	C	N3-C4-N4	11.18	125.82	118.00
20	a	1238	C	N3-C2-O2	-10.94	114.24	121.90
1	b	209	ASP	CB-CG-OD1	10.94	128.14	118.30
20	a	147	C	C2-N3-C4	10.88	125.34	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	a	976	C	N3-C2-O2	-10.87	114.29	121.90
20	a	951	C	N1-C2-O2	10.85	125.41	118.90
26	8	304	LEU	CA-CB-CG	10.83	140.21	115.30
26	8	344	LEU	CB-CG-CD2	-10.83	92.59	111.00
20	a	1445	C	C6-N1-C2	-10.81	115.97	120.30
23	v	142	PHE	CB-CG-CD1	10.79	128.35	120.80
20	a	1087	G	N3-C2-N2	10.70	127.39	119.90
20	a	4	C	C5-C6-N1	10.68	126.34	121.00
20	a	147	C	N3-C4-N4	10.57	125.40	118.00
20	a	881	C	N3-C2-O2	-10.50	114.55	121.90
20	a	1484	C	C5-C6-N1	10.49	126.25	121.00
20	a	786	C	N3-C4-N4	10.43	125.30	118.00
20	a	1441	A	C2-N3-C4	-10.41	105.39	110.60
20	a	976	C	C2-N3-C4	10.39	125.09	119.90
20	a	786	C	N3-C2-O2	-10.37	114.64	121.90
20	a	150	C	N3-C2-O2	-10.30	114.69	121.90
20	a	1480	A	C5-N7-C8	-10.22	98.79	103.90
20	a	1090	U	N3-C2-O2	-10.22	115.05	122.20
20	a	1256	U	C2-N3-C4	10.16	133.09	127.00
21	w	103	PHE	CB-CG-CD2	-10.12	113.71	120.80
20	a	1441	A	C6-N1-C2	-10.10	112.54	118.60
20	a	1440	G	C6-N1-C2	-10.06	119.06	125.10
20	a	150	C	C2-N3-C4	10.06	124.93	119.90
26	8	318	ASP	CB-CG-OD1	9.99	127.29	118.30
20	a	7	G	N3-C4-C5	-9.96	123.62	128.60
20	a	285	C	N1-C2-O2	9.95	124.87	118.90
20	a	983	G	N1-C6-O6	-9.94	113.93	119.90
20	a	83	C	N1-C2-O2	9.92	124.85	118.90
20	a	448	G	N1-C6-O6	9.90	125.84	119.90
20	a	1116	U	N1-C2-O2	9.88	129.72	122.80
20	a	1081	C	N1-C2-O2	-9.66	113.11	118.90
20	a	1480	A	C8-N9-C4	-9.59	101.96	105.80
20	a	786	C	C2-N3-C4	9.56	124.68	119.90
20	a	1439	U	C6-N1-C2	-9.55	115.27	121.00
26	8	72	MET	N-CA-C	-9.53	85.27	111.00
20	a	147	C	N3-C4-C5	-9.48	118.11	121.90
20	a	786	C	N3-C4-C5	-9.41	118.13	121.90
20	a	1090	U	N1-C2-O2	9.37	129.36	122.80
20	a	794	C	N1-C2-O2	9.37	124.52	118.90
23	v	194	ARG	NE-CZ-NH2	-9.34	115.63	120.30
20	a	881	C	N3-C4-N4	9.29	124.50	118.00
20	a	1487	C	C6-N1-C2	-9.21	116.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	a	572	C	N1-C2-O2	9.21	124.43	118.90
20	a	255	C	N1-C2-O2	9.15	124.39	118.90
21	w	103	PHE	CB-CG-CD1	9.15	127.20	120.80
20	a	107	C	N3-C2-O2	-9.13	115.51	121.90
20	a	976	C	N3-C4-C5	-9.11	118.26	121.90
20	a	1116	U	N3-C2-O2	-9.10	115.83	122.20
20	a	285	C	N3-C2-O2	-9.04	115.58	121.90
20	a	951	C	N3-C2-O2	-9.02	115.58	121.90
20	a	948	C	C5-C6-N1	9.01	125.51	121.00
20	a	885	C	N1-C2-O2	8.95	124.27	118.90
20	a	142	G	N1-C6-O6	-8.94	114.54	119.90
20	a	1374	C	C6-N1-C2	-8.91	116.73	120.30
20	a	1238	C	N1-C2-O2	8.89	124.23	118.90
20	a	1485	C	C6-N1-C2	-8.85	116.76	120.30
20	a	1166	C	O5'-P-OP1	-8.75	97.83	105.70
26	8	73	GLU	N-CA-C	-8.74	87.39	111.00
20	a	1439	U	C4-C5-C6	-8.71	114.48	119.70
1	b	201	ASP	OD1-CG-OD2	-8.70	106.77	123.30
20	a	948	C	C6-N1-C2	-8.69	116.83	120.30
1	b	201	ASP	CB-CG-OD1	-8.68	110.49	118.30
23	v	165	PHE	CB-CG-CD1	8.68	126.88	120.80
20	a	1077	C	C2-N3-C4	8.63	124.22	119.90
3	e	266	LEU	CA-CB-CG	8.60	135.08	115.30
20	a	301	C	N1-C2-O2	8.58	124.05	118.90
20	a	150	C	N3-C4-N4	8.54	123.98	118.00
20	a	786	C	C6-N1-C2	-8.53	116.89	120.30
20	a	1081	C	C5-C4-N4	-8.53	114.23	120.20
20	a	1003	C	N1-C2-O2	8.49	124.00	118.90
20	a	1077	C	N3-C2-O2	-8.49	115.95	121.90
20	a	1003	C	N3-C2-O2	-8.47	115.97	121.90
20	a	1481	U	C5-C6-N1	8.47	126.94	122.70
20	a	797	G	N1-C6-O6	-8.41	114.86	119.90
1	b	40	LYS	CD-CE-NZ	-8.39	92.39	111.70
26	8	304	LEU	CB-CG-CD1	8.38	125.25	111.00
20	a	987	G	N1-C6-O6	-8.38	114.87	119.90
20	a	1081	C	C2-N3-C4	-8.38	115.71	119.90
20	a	159	C	N1-C2-O2	8.26	123.86	118.90
20	a	1358	C	C6-N1-C2	-8.24	117.00	120.30
20	a	1488	C	C4-C5-C6	-8.17	113.32	117.40
23	v	142	PHE	CD1-CG-CD2	-8.14	107.71	118.30
26	8	315	LEU	CB-CG-CD1	8.11	124.79	111.00
20	a	1244	C	N1-C2-O2	8.11	123.76	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	8	299	ASP	N-CA-C	-8.11	89.11	111.00
20	a	1225	C	N1-C2-O2	8.09	123.76	118.90
26	8	367	ALA	N-CA-CB	8.09	121.43	110.10
20	a	881	C	C6-N1-C2	-8.06	117.08	120.30
20	a	1440	G	C8-N9-C4	-8.00	103.20	106.40
20	a	7	G	N1-C2-N3	-8.00	119.10	123.90
20	a	1244	C	N3-C2-O2	-7.99	116.31	121.90
21	w	148	LYS	C-N-CD	-7.95	103.10	120.60
20	a	881	C	C2-N3-C4	7.90	123.85	119.90
26	8	368	ARG	CB-CG-CD	7.89	132.11	111.60
20	a	794	C	C2-N1-C1'	7.82	127.41	118.80
20	a	4	C	N3-C4-C5	-7.80	118.78	121.90
20	a	84	C	N1-C2-O2	7.79	123.58	118.90
20	a	1106	C	C2-N1-C1'	7.70	127.27	118.80
20	a	1484	C	C6-N1-C2	-7.67	117.23	120.30
20	a	987	G	N3-C2-N2	-7.67	114.53	119.90
20	a	139	G	N1-C6-O6	-7.63	115.32	119.90
20	a	1116	U	C2-N1-C1'	7.63	126.86	117.70
26	8	360	ILE	N-CA-C	-7.62	90.42	111.00
20	a	1258	C	N1-C2-O2	7.58	123.45	118.90
20	a	361	C	N1-C2-O2	7.58	123.45	118.90
20	a	1163	G	N1-C6-O6	7.57	124.44	119.90
26	8	279	ASP	CB-CG-OD1	7.57	125.11	118.30
20	a	881	C	C2-N1-C1'	7.55	127.10	118.80
20	a	1077	C	C2-N1-C1'	7.54	127.10	118.80
20	a	1087	G	N1-C2-N2	-7.53	109.43	116.20
20	a	147	C	C6-N1-C2	-7.50	117.30	120.30
26	8	73	GLU	CB-CA-C	7.46	125.33	110.40
20	a	1095	C	N1-C2-O2	7.42	123.35	118.90
20	a	150	C	N3-C4-C5	-7.41	118.94	121.90
22	d	32	LEU	CA-CB-CG	7.41	132.34	115.30
20	a	794	C	N3-C2-O2	-7.40	116.72	121.90
20	a	1089	U	C5-C6-N1	7.40	126.40	122.70
26	8	62	ASP	CB-CG-OD2	-7.37	111.66	118.30
20	a	1453	G	N1-C6-O6	7.37	124.32	119.90
20	a	959	C	N1-C2-O2	7.36	123.31	118.90
20	a	1158	C	N1-C2-O2	7.33	123.30	118.90
20	a	1272	C	N1-C2-O2	7.33	123.30	118.90
20	a	7	G	C5-C6-N1	7.31	115.15	111.50
20	a	295	G	C8-N9-C4	-7.30	103.48	106.40
20	a	881	C	N3-C4-C5	-7.29	118.98	121.90
20	a	572	C	N3-C2-O2	-7.28	116.81	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	a	951	C	C6-N1-C2	-7.27	117.39	120.30
20	a	1003	C	C6-N1-C2	-7.27	117.39	120.30
20	a	139	G	N3-C2-N2	-7.26	114.82	119.90
20	a	951	C	N3-C4-N4	7.26	123.08	118.00
20	a	1003	C	C2-N1-C1'	7.25	126.78	118.80
20	a	1077	C	C6-N1-C2	-7.23	117.41	120.30
20	a	1077	C	N3-C4-N4	7.23	123.06	118.00
20	a	910	U	N3-C2-O2	-7.22	117.15	122.20
20	a	1358	C	N3-C2-O2	-7.22	116.85	121.90
20	a	885	C	N3-C2-O2	-7.21	116.85	121.90
20	a	794	C	C6-N1-C2	-7.21	117.42	120.30
20	a	1083	U	C5-C6-N1	7.21	126.30	122.70
20	a	951	C	N3-C4-C5	-7.20	119.02	121.90
20	a	1120	C	N3-C2-O2	-7.19	116.86	121.90
20	a	951	C	C2-N3-C4	7.19	123.49	119.90
20	a	1290	C	N1-C2-O2	7.15	123.19	118.90
18	u	98	ARG	NE-CZ-NH1	-7.14	116.73	120.30
20	a	361	C	C6-N1-C2	-7.13	117.45	120.30
20	a	428	U	N3-C2-O2	-7.13	117.21	122.20
26	8	357	ARG	NE-CZ-NH1	-7.13	116.74	120.30
20	a	434	U	C2-N1-C1'	7.11	126.24	117.70
20	a	670	A	C2-N3-C4	7.11	114.16	110.60
23	v	165	PHE	CZ-CE2-CD2	7.11	128.63	120.10
20	a	1030	G	N1-C6-O6	7.09	124.15	119.90
20	a	976	C	C6-N1-C2	-7.08	117.47	120.30
20	a	83	C	N3-C2-O2	-7.05	116.96	121.90
26	8	70	ALA	N-CA-CB	7.01	119.92	110.10
20	a	1485	C	C4-C5-C6	-7.00	113.90	117.40
20	a	1087	G	C6-N1-C2	7.00	129.30	125.10
20	a	877	G	C6-C5-N7	-6.99	126.20	130.40
26	8	318	ASP	CB-CG-OD2	-6.99	112.01	118.30
20	a	1445	C	C4-C5-C6	-6.99	113.91	117.40
20	a	84	C	N3-C2-O2	-6.98	117.02	121.90
1	b	201	ASP	N-CA-CB	6.97	123.14	110.60
20	a	1328	G	N1-C6-O6	-6.96	115.73	119.90
20	a	223	U	N1-C2-O2	6.95	127.66	122.80
20	a	1150	U	N3-C2-O2	-6.89	117.38	122.20
20	a	561	C	N1-C2-O2	6.86	123.02	118.90
20	a	938	G	N1-C6-O6	6.86	124.02	119.90
20	a	55	C	N3-C2-O2	-6.85	117.11	121.90
26	8	283	ILE	CG1-CB-CG2	-6.83	96.37	111.40
20	a	491	U	N3-C2-O2	-6.82	117.43	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	a	55	C	N1-C2-O2	6.82	122.99	118.90
20	a	1150	U	N1-C2-O2	6.80	127.56	122.80
20	a	511	A	C2-N3-C4	6.80	114.00	110.60
20	a	301	C	N3-C2-O2	-6.79	117.15	121.90
20	a	1440	G	N7-C8-N9	6.79	116.49	113.10
22	d	160	LEU	CA-CB-CG	6.78	130.89	115.30
26	8	316	SER	C-N-CA	6.78	138.64	121.70
20	a	1120	C	N1-C2-O2	6.78	122.97	118.90
20	a	223	U	C2-N1-C1'	6.77	125.82	117.70
23	v	165	PHE	CB-CG-CD2	-6.75	116.07	120.80
20	a	1092	G	N1-C6-O6	-6.75	115.85	119.90
20	a	1440	G	N1-C2-N3	6.74	127.94	123.90
20	a	1172	G	N3-C4-N9	-6.74	121.96	126.00
20	a	243	C	N1-C2-O2	6.71	122.93	118.90
20	a	784	U	N3-C2-O2	-6.71	117.50	122.20
20	a	890	G	N3-C2-N2	-6.69	115.22	119.90
20	a	150	C	C6-N1-C2	-6.69	117.62	120.30
21	w	133	PRO	CA-N-CD	-6.68	102.15	111.50
20	a	255	C	N3-C4-N4	6.67	122.67	118.00
20	a	558	U	N3-C2-O2	-6.65	117.54	122.20
20	a	1334	G	N1-C6-O6	-6.65	115.91	119.90
20	a	448	G	C5-C6-O6	-6.65	124.61	128.60
20	a	255	C	N3-C2-O2	-6.65	117.25	121.90
20	a	3	U	C5-C6-N1	6.64	126.02	122.70
20	a	1440	G	C5-C6-O6	-6.63	124.62	128.60
20	a	1149	A	C8-N9-C4	6.62	108.45	105.80
20	a	1029	A	C6-C5-N7	-6.58	127.69	132.30
20	a	83	C	C6-N1-C2	-6.58	117.67	120.30
20	a	285	C	C6-N1-C2	-6.56	117.68	120.30
20	a	150	C	C2-N1-C1'	6.56	126.01	118.80
20	a	511	A	N1-C6-N6	-6.55	114.67	118.60
20	a	90	C	C6-N1-C2	-6.54	117.69	120.30
20	a	1087	G	C5-C6-O6	6.51	132.50	128.60
20	a	976	C	C5-C4-N4	-6.50	115.65	120.20
20	a	958	U	N1-C2-O2	6.49	127.34	122.80
20	a	1254	A	N7-C8-N9	6.48	117.04	113.80
20	a	571	C	N1-C2-O2	6.48	122.79	118.90
20	a	1058	C	N3-C2-O2	-6.48	117.37	121.90
2	c	95	LEU	CA-CB-CG	6.46	130.16	115.30
20	a	407	C	C6-N1-C2	-6.46	117.72	120.30
20	a	1487	C	C4-C5-C6	-6.44	114.18	117.40
20	a	1311	C	N3-C2-O2	-6.43	117.40	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	a	1254	A	C8-N9-C4	-6.43	103.23	105.80
20	a	1029	A	C4-C5-N7	6.43	113.91	110.70
20	a	1077	C	N3-C4-C5	-6.43	119.33	121.90
20	a	1348	C	N1-C2-O2	-6.42	115.05	118.90
20	a	784	U	C2-N1-C1'	6.41	125.40	117.70
20	a	411	U	N1-C2-O2	6.41	127.29	122.80
20	a	1081	C	C5-C6-N1	6.41	124.20	121.00
20	a	59	C	C6-N1-C2	-6.39	117.74	120.30
20	a	828	C	O5'-P-OP1	-6.39	99.95	105.70
20	a	407	C	N1-C2-O2	6.38	122.73	118.90
20	a	1120	C	C6-N1-C2	-6.38	117.75	120.30
20	a	560	C	N1-C2-O2	6.38	122.73	118.90
20	a	890	G	N1-C6-O6	-6.38	116.07	119.90
20	a	682	C	C5-C6-N1	6.38	124.19	121.00
20	a	371	C	N1-C2-O2	6.37	122.72	118.90
26	8	329	LYS	CD-CE-NZ	6.36	126.33	111.70
20	a	1078	C	C2-N1-C1'	6.35	125.79	118.80
20	a	361	C	N3-C2-O2	-6.34	117.46	121.90
20	a	959	C	N3-C2-O2	-6.34	117.46	121.90
21	w	112	LEU	CB-CG-CD1	-6.33	100.23	111.00
20	a	1149	A	N9-C4-C5	-6.32	103.27	105.80
20	a	1302	C	C6-N1-C2	-6.30	117.78	120.30
20	a	434	U	N3-C2-O2	-6.30	117.79	122.20
20	a	1374	C	C5-C6-N1	6.30	124.15	121.00
20	a	784	U	N1-C2-O2	6.30	127.21	122.80
6	h	67	ARG	N-CA-CB	-6.30	99.27	110.60
20	a	1353	C	N1-C2-O2	6.29	122.67	118.90
20	a	811	C	N1-C2-O2	6.25	122.65	118.90
20	a	318	G	N1-C6-O6	6.24	123.64	119.90
20	a	794	C	C5-C6-N1	6.23	124.11	121.00
20	a	243	C	N3-C2-O2	-6.22	117.55	121.90
20	a	97	G	N1-C6-O6	-6.22	116.17	119.90
20	a	4	C	N3-C4-N4	6.21	122.35	118.00
20	a	83	C	C2-N3-C4	6.20	123.00	119.90
26	8	69	ASN	N-CA-C	6.20	127.73	111.00
20	a	1360	C	C6-N1-C2	-6.19	117.83	120.30
20	a	755	U	C2-N3-C4	6.18	130.71	127.00
20	a	912	G	N1-C6-O6	-6.17	116.19	119.90
20	a	1077	C	C5-C6-N1	6.17	124.09	121.00
20	a	223	U	N3-C2-O2	-6.17	117.88	122.20
20	a	808	U	N3-C2-O2	-6.17	117.88	122.20
20	a	1029	A	N1-C6-N6	6.16	122.30	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	l	7	LEU	CA-CB-CG	6.16	129.47	115.30
20	a	159	C	N3-C2-O2	-6.15	117.59	121.90
20	a	407	C	C5-C6-N1	6.15	124.08	121.00
23	v	142	PHE	CZ-CE2-CD2	6.14	127.47	120.10
20	a	1459	C	N1-C2-O2	6.12	122.57	118.90
20	a	448	G	C6-C5-N7	-6.12	126.73	130.40
20	a	1258	C	N3-C2-O2	-6.12	117.61	121.90
26	8	367	ALA	C-N-CA	6.11	136.97	121.70
20	a	434	U	N1-C2-O2	6.11	127.08	122.80
20	a	958	U	N3-C2-O2	-6.11	117.92	122.20
20	a	1158	C	N3-C2-O2	-6.10	117.63	121.90
20	a	1195	G	C6-C5-N7	-6.09	126.75	130.40
20	a	1057	G	C4-N9-C1'	6.09	134.41	126.50
1	b	201	ASP	CA-CB-CG	6.08	126.79	113.40
20	a	698	C	C6-N1-C2	-6.08	117.87	120.30
20	a	1058	C	N1-C2-O2	6.08	122.55	118.90
20	a	1024	C	C5-C6-N1	6.08	124.04	121.00
20	a	411	U	N3-C2-O2	-6.07	117.95	122.20
21	w	126	LEU	CB-CG-CD2	-6.07	100.68	111.00
20	a	1482	C	C6-N1-C2	-6.07	117.87	120.30
10	l	7	LEU	CB-CG-CD2	-6.05	100.72	111.00
20	a	1332	C	N1-C2-O2	6.03	122.52	118.90
20	a	571	C	C6-N1-C2	-6.02	117.89	120.30
20	a	1444	U	C5-C6-N1	6.01	125.71	122.70
20	a	910	U	N1-C2-N3	6.01	118.50	114.90
20	a	817	C	N1-C2-O2	6.01	122.50	118.90
20	a	1035	U	N3-C2-O2	-6.01	118.00	122.20
15	r	53	ARG	CA-CB-CG	-6.00	100.19	113.40
20	a	591	C	C6-N1-C2	-5.98	117.91	120.30
20	a	1304	G	N3-C2-N2	5.97	124.08	119.90
20	a	1172	G	C6-C5-N7	5.96	133.97	130.40
20	a	190	C	N1-C2-O2	5.96	122.47	118.90
15	r	21	PRO	N-CA-CB	5.95	110.44	103.30
20	a	921	C	C6-N1-C2	-5.95	117.92	120.30
20	a	1225	C	N3-C2-O2	-5.94	117.74	121.90
20	a	1484	C	C4-C5-C6	-5.92	114.44	117.40
20	a	282	C	C6-N1-C2	-5.92	117.93	120.30
20	a	313	C	N3-C4-C5	5.92	124.27	121.90
20	a	571	C	N3-C4-N4	5.92	122.14	118.00
20	a	682	C	C6-N1-C2	-5.92	117.93	120.30
20	a	698	C	C5-C6-N1	5.91	123.96	121.00
20	a	83	C	C2-N1-C1'	5.91	125.30	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	a	877	G	C4-C5-N7	5.90	113.16	110.80
20	a	564	G	N1-C6-O6	-5.90	116.36	119.90
20	a	932	A	C4-N9-C1'	5.89	136.90	126.30
20	a	1290	C	N3-C2-O2	-5.88	117.78	121.90
18	u	98	ARG	CA-CB-CG	5.88	126.34	113.40
20	a	484	C	N1-C2-O2	5.88	122.43	118.90
20	a	1296	U	N3-C2-O2	-5.88	118.08	122.20
23	v	142	PHE	CD1-CE1-CZ	5.86	127.14	120.10
20	a	107	C	N3-C4-N4	5.85	122.10	118.00
1	b	202	ILE	CG1-CB-CG2	-5.84	98.56	111.40
20	a	452	C	C6-N1-C2	-5.84	117.97	120.30
20	a	450	A	N1-C2-N3	-5.83	126.39	129.30
20	a	848	C	N1-C2-O2	5.83	122.40	118.90
20	a	1172	G	C4-N9-C1'	-5.83	118.92	126.50
10	l	24	LEU	CA-CB-CG	5.81	128.66	115.30
20	a	459	C	N1-C2-O2	-5.80	115.42	118.90
20	a	702	C	C2-N1-C1'	5.80	125.18	118.80
20	a	204	C	C2-N1-C1'	5.79	125.16	118.80
20	a	1441	A	N1-C6-N6	-5.77	115.14	118.60
20	a	304	C	N1-C2-O2	5.76	122.36	118.90
20	a	1030	G	C5-C6-O6	-5.76	125.15	128.60
20	a	371	C	C6-N1-C2	-5.75	118.00	120.30
20	a	293	C	C6-N1-C2	-5.75	118.00	120.30
20	a	137	C	N1-C2-O2	5.74	122.34	118.90
20	a	523	G	N3-C4-N9	-5.74	122.56	126.00
20	a	374	C	N3-C4-C5	5.73	124.19	121.90
20	a	1172	G	C8-N9-C1'	5.73	134.45	127.00
20	a	1026	G	C6-C5-N7	-5.73	126.96	130.40
20	a	1440	G	N9-C4-C5	5.72	107.69	105.40
20	a	558	U	N1-C2-O2	5.72	126.81	122.80
20	a	142	G	C5-C6-O6	5.72	132.03	128.60
20	a	24	C	C5-C6-N1	5.70	123.85	121.00
20	a	797	G	N3-C2-N2	-5.70	115.91	119.90
20	a	71	G	N1-C6-O6	-5.69	116.48	119.90
20	a	1029	A	N9-C4-C5	-5.69	103.53	105.80
20	a	496	G	C6-C5-N7	-5.68	126.99	130.40
20	a	1374	C	N1-C2-O2	5.68	122.31	118.90
20	a	411	U	C2-N1-C1'	5.68	124.51	117.70
20	a	685	U	C5-C6-N1	5.66	125.53	122.70
20	a	1095	C	N3-C2-O2	-5.66	117.94	121.90
23	v	167	PHE	CB-CG-CD2	-5.66	116.83	120.80
26	8	330	LYS	N-CA-CB	5.66	120.79	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	a	410	U	N3-C2-O2	-5.63	118.26	122.20
20	a	1453	G	C5-C6-O6	-5.63	125.22	128.60
20	a	410	U	N1-C2-O2	5.63	126.74	122.80
20	a	1459	C	C6-N1-C2	-5.63	118.05	120.30
20	a	299	C	N1-C2-O2	5.62	122.27	118.90
20	a	765	C	N1-C2-O2	5.61	122.27	118.90
20	a	559	C	N1-C2-O2	5.61	122.27	118.90
20	a	19	C	C6-N1-C2	-5.59	118.06	120.30
20	a	1446	G	C4-N9-C1'	5.59	133.76	126.50
26	8	280	ILE	CB-CA-C	5.58	122.77	111.60
20	a	976	C	C5-C6-N1	5.58	123.79	121.00
26	8	300	ILE	N-CA-C	-5.58	95.94	111.00
20	a	371	C	N3-C4-N4	5.57	121.90	118.00
20	a	808	U	N1-C2-O2	5.57	126.70	122.80
20	a	1172	G	N1-C6-O6	-5.56	116.56	119.90
20	a	1374	C	N3-C2-O2	-5.56	118.01	121.90
26	8	73	GLU	CA-CB-CG	5.56	125.63	113.40
20	a	131	G	N1-C6-O6	-5.54	116.57	119.90
20	a	1081	C	N3-C4-N4	5.54	121.88	118.00
20	a	1438	G	C8-N9-C4	-5.54	104.18	106.40
20	a	637	C	N1-C2-O2	5.54	122.22	118.90
20	a	1087	G	C2-N3-C4	-5.54	109.13	111.90
8	j	135	LEU	CA-CB-CG	5.53	128.02	115.30
20	a	909	U	C2-N1-C1'	5.53	124.33	117.70
20	a	1358	C	N1-C2-O2	5.52	122.21	118.90
20	a	462	U	C5-C6-N1	5.52	125.46	122.70
20	a	1058	C	C6-N1-C2	-5.51	118.09	120.30
20	a	1238	C	C2-N3-C4	-5.50	117.15	119.90
20	a	7	G	N9-C4-C5	5.50	107.60	105.40
20	a	1005	U	C2-N3-C4	5.49	130.30	127.00
20	a	1330	U	N1-C2-O2	5.49	126.64	122.80
20	a	900	G	N3-C2-N2	5.48	123.74	119.90
20	a	1106	C	N1-C2-O2	5.48	122.19	118.90
20	a	484	C	C2-N1-C1'	5.47	124.82	118.80
20	a	1296	U	N1-C2-O2	5.47	126.63	122.80
20	a	285	C	N3-C4-N4	5.47	121.83	118.00
20	a	912	G	C5-C6-O6	5.47	131.88	128.60
20	a	1442	A	N7-C8-N9	5.46	116.53	113.80
20	a	83	C	C5-C6-N1	5.45	123.73	121.00
20	a	910	U	C2-N3-C4	-5.45	123.73	127.00
20	a	152	G	C4-C5-N7	5.44	112.98	110.80
20	a	779	C	C6-N1-C2	-5.44	118.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	a	962	G	N1-C6-O6	-5.44	116.63	119.90
20	a	1290	C	N3-C4-C5	-5.44	119.72	121.90
20	a	454	G	C6-C5-N7	-5.44	127.14	130.40
20	a	121	C	C2-N1-C1'	5.43	124.77	118.80
21	w	164	THR	CA-CB-CG2	-5.43	104.80	112.40
20	a	932	A	C8-N9-C1'	-5.43	117.93	127.70
20	a	986	C	C6-N1-C2	-5.42	118.13	120.30
20	a	1486	U	C6-N1-C2	-5.42	117.75	121.00
20	a	1352	C	C6-N1-C2	-5.42	118.13	120.30
20	a	147	C	C5-C4-N4	-5.42	116.41	120.20
20	a	342	G	N3-C2-N2	-5.42	116.11	119.90
20	a	1256	U	N3-C4-C5	-5.41	111.36	114.60
20	a	1331	C	N1-C2-O2	5.41	122.14	118.90
3	e	303	MET	CB-CG-SD	5.40	128.59	112.40
23	v	129	LEU	CA-CB-CG	5.40	127.71	115.30
20	a	209	G	N1-C6-O6	-5.39	116.66	119.90
20	a	493	C	N3-C4-C5	5.39	124.06	121.90
20	a	1226	U	N1-C2-O2	5.39	126.58	122.80
20	a	1439	U	C5-C4-O4	-5.39	122.67	125.90
20	a	566	C	N1-C2-O2	5.38	122.13	118.90
20	a	1087	G	C5-C6-N1	-5.38	108.81	111.50
20	a	784	U	C6-N1-C2	-5.37	117.78	121.00
20	a	850	A	N1-C6-N6	5.37	121.82	118.60
20	a	134	C	C6-N1-C2	-5.37	118.15	120.30
20	a	670	A	N3-C4-N9	5.37	131.69	127.40
20	a	1353	C	C6-N1-C2	-5.36	118.16	120.30
20	a	472	G	N3-C2-N2	5.34	123.64	119.90
20	a	1106	C	N3-C2-O2	-5.33	118.17	121.90
20	a	295	G	N7-C8-N9	5.33	115.77	113.10
20	a	139	G	C5-C6-N1	5.33	114.16	111.50
20	a	784	U	C5-C6-N1	5.33	125.36	122.70
20	a	1029	A	C5-N7-C8	-5.32	101.24	103.90
20	a	1150	U	C2-N1-C1'	5.32	124.09	117.70
20	a	1238	C	C2-N1-C1'	5.32	124.65	118.80
20	a	1353	C	N3-C2-O2	-5.32	118.18	121.90
20	a	255	C	C5-C4-N4	-5.32	116.48	120.20
20	a	301	C	C6-N1-C2	-5.31	118.17	120.30
20	a	1195	G	N3-C4-N9	5.31	129.19	126.00
20	a	246	G	C4-N9-C1'	5.31	133.40	126.50
20	a	881	C	C5-C4-N4	-5.31	116.48	120.20
20	a	1106	C	C6-N1-C1'	-5.31	114.43	120.80
20	a	1035	U	N1-C2-O2	5.30	126.51	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	a	987	G	C5-C6-O6	5.30	131.78	128.60
21	w	159	LEU	CB-CG-CD1	-5.30	102.00	111.00
20	a	1211	C	N1-C2-O2	5.28	122.07	118.90
21	w	136	ASP	CB-CG-OD2	-5.27	113.56	118.30
20	a	938	G	C5-C6-O6	-5.26	125.44	128.60
26	8	303	VAL	N-CA-C	5.26	125.21	111.00
20	a	229	A	N1-C2-N3	-5.26	126.67	129.30
20	a	90	C	C2-N1-C1'	5.26	124.59	118.80
20	a	800	C	C2-N1-C1'	5.25	124.58	118.80
20	a	139	G	N1-C2-N2	5.25	120.92	116.20
20	a	1295	G	C2-N3-C4	-5.25	109.28	111.90
20	a	239	U	N3-C2-O2	-5.24	118.53	122.20
20	a	566	C	C6-N1-C2	-5.24	118.20	120.30
20	a	1256	U	N1-C2-N3	-5.24	111.76	114.90
20	a	727	C	N1-C2-O2	5.24	122.04	118.90
20	a	1057	G	C8-N9-C1'	-5.24	120.19	127.00
20	a	204	C	C6-N1-C2	-5.24	118.21	120.30
20	a	336	U	C2-N1-C1'	5.24	123.98	117.70
20	a	912	G	N9-C4-C5	5.24	107.49	105.40
20	a	444	A	O4'-C1'-N9	5.23	112.38	108.20
20	a	987	G	N1-C2-N2	5.23	120.91	116.20
20	a	523	G	N3-C4-C5	5.22	131.21	128.60
20	a	361	C	N3-C4-N4	5.22	121.66	118.00
20	a	1290	C	N3-C4-N4	5.22	121.66	118.00
20	a	1446	G	N3-C4-N9	5.22	129.13	126.00
20	a	1099	G	O4'-C1'-N9	5.22	112.38	108.20
20	a	299	C	N3-C2-O2	-5.22	118.25	121.90
20	a	786	C	C5-C4-N4	-5.22	116.55	120.20
20	a	493	C	C2-N3-C4	-5.22	117.29	119.90
20	a	88	G	C8-N9-C1'	-5.21	120.22	127.00
20	a	1446	G	C8-N9-C1'	-5.21	120.22	127.00
20	a	909	U	N1-C2-O2	5.21	126.45	122.80
20	a	1334	G	C5-C6-N1	5.21	114.11	111.50
20	a	560	C	N3-C2-O2	-5.20	118.26	121.90
20	a	1348	C	C2-N3-C4	-5.20	117.30	119.90
20	a	523	G	N1-C6-O6	5.20	123.02	119.90
20	a	572	C	N3-C4-N4	5.19	121.63	118.00
20	a	933	C	C6-N1-C2	-5.19	118.22	120.30
18	u	103	PHE	CB-CG-CD2	-5.19	117.17	120.80
20	a	372	C	C6-N1-C2	-5.19	118.23	120.30
20	a	1234	A	C2-N3-C4	5.18	113.19	110.60
20	a	806	U	N3-C2-O2	-5.18	118.58	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	a	131	G	C5-C6-N1	5.17	114.09	111.50
20	a	470	C	N1-C2-O2	5.17	122.00	118.90
20	a	568	C	N3-C2-O2	-5.17	118.28	121.90
20	a	702	C	N1-C2-O2	5.17	122.00	118.90
20	a	1453	G	N3-C2-N2	5.16	123.52	119.90
20	a	1017	G	C4-N9-C1'	5.16	133.21	126.50
20	a	1458	C	C6-N1-C2	-5.16	118.24	120.30
20	a	1459	C	N3-C4-N4	5.15	121.61	118.00
25	x	85	PRO	C-N-CD	5.15	139.22	128.40
20	a	287	C	N3-C2-O2	-5.15	118.30	121.90
20	a	83	C	N3-C4-C5	-5.14	119.84	121.90
23	v	25	TYR	CB-CG-CD1	5.14	124.09	121.00
20	a	190	C	N3-C2-O2	-5.13	118.31	121.90
20	a	1095	C	C2-N1-C1'	5.13	124.44	118.80
20	a	1272	C	N3-C2-O2	-5.13	118.31	121.90
11	m	127	LEU	CA-CB-CG	-5.13	103.50	115.30
20	a	255	C	C6-N1-C2	-5.13	118.25	120.30
20	a	406	U	C5-C6-N1	5.12	125.26	122.70
20	a	1353	C	C5-C6-N1	5.12	123.56	121.00
20	a	453	G	C4-N9-C1'	5.12	133.16	126.50
20	a	496	G	C4-C5-N7	5.12	112.85	110.80
20	a	800	C	C6-N1-C2	-5.11	118.25	120.30
20	a	797	G	C5-C6-O6	5.11	131.67	128.60
20	a	1244	C	C6-N1-C2	-5.11	118.25	120.30
20	a	83	C	N3-C4-N4	5.11	121.58	118.00
26	8	346	PHE	CB-CG-CD1	-5.11	117.22	120.80
20	a	1163	G	C5-C6-O6	-5.11	125.54	128.60
20	a	295	G	O5'-P-OP2	-5.09	101.12	105.70
20	a	1185	C	C6-N1-C2	-5.09	118.26	120.30
20	a	529	G	C4-C5-N7	5.08	112.83	110.80
20	a	911	C	C6-N1-C2	-5.08	118.27	120.30
20	a	293	C	C5-C6-N1	5.08	123.54	121.00
20	a	1486	U	C4-C5-C6	-5.08	116.65	119.70
20	a	1332	C	C6-N1-C2	-5.07	118.27	120.30
20	a	35	C	C5-C6-N1	5.07	123.54	121.00
20	a	88	G	N1-C6-O6	5.07	122.94	119.90
20	a	293	C	N3-C2-O2	-5.07	118.35	121.90
20	a	1081	C	N1-C2-N3	5.07	122.75	119.20
20	a	1438	G	N1-C6-O6	-5.06	116.86	119.90
20	a	271	A	N7-C8-N9	5.06	116.33	113.80
20	a	493	C	N3-C4-N4	-5.06	114.46	118.00
20	a	88	G	C6-C5-N7	-5.06	127.36	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	a	394	G	N3-C4-N9	5.06	129.03	126.00
20	a	90	C	C5-C6-N1	5.05	123.53	121.00
20	a	1106	C	C6-N1-C2	-5.05	118.28	120.30
10	l	5	LYS	CD-CE-NZ	-5.05	100.09	111.70
21	w	136	ASP	N-CA-CB	-5.04	101.52	110.60
20	a	1318	C	C6-N1-C2	-5.04	118.29	120.30
20	a	983	G	C5-C6-N1	5.03	114.02	111.50
20	a	806	U	N1-C2-O2	5.03	126.32	122.80
20	a	1092	G	N3-C2-N2	-5.03	116.38	119.90
21	w	149	PRO	N-CA-C	5.03	125.17	112.10
20	a	150	C	C5-C6-N1	5.02	123.51	121.00
20	a	1304	G	N3-C4-N9	5.02	129.01	126.00
20	a	881	C	C5-C6-N1	5.02	123.51	121.00
23	v	99	GLU	CA-CB-CG	-5.02	102.36	113.40
20	a	999	G	N1-C6-O6	5.02	122.91	119.90
23	v	37	GLU	CG-CD-OE1	5.02	128.33	118.30
11	m	118	ARG	NE-CZ-NH1	5.01	122.81	120.30
20	a	423	A	C2-N3-C4	5.01	113.11	110.60
20	a	1189	G	N1-C6-O6	-5.01	116.89	119.90
20	a	1029	A	C5-C6-N6	-5.00	119.70	123.70

There are no chirality outliers.

All (58) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	8	273	PRO	Peptide
26	8	277	PHE	Peptide
26	8	298	SER	Peptide
26	8	299	ASP	Peptide
26	8	302	THR	Peptide
26	8	303	VAL	Peptide
26	8	304	LEU	Peptide
26	8	315	LEU	Peptide
26	8	329	LYS	Peptide
26	8	346	PHE	Sidechain
26	8	359	ARG	Peptide
26	8	366	MET	Mainchain
26	8	369	ALA	Peptide
26	8	370	ASP	Peptide
26	8	69	ASN	Peptide
26	8	71	PRO	Peptide
26	8	72	MET	Peptide

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Mol	Chain	Res	Type	Group
1	b	168	VAL	Peptide
1	b	201	ASP	Sidechain
2	c	168	ILE	Peptide
2	c	86	GLU	Peptide
2	c	88	ARG	Peptide
22	d	155	SER	Peptide
22	d	23	ASN	Peptide
3	e	147	LYS	Peptide
4	f	102	PRO	Peptide
5	g	8	GLU	Peptide
7	i	78	ARG	Peptide
7	i	96	ILE	Peptide
8	j	135	LEU	Peptide
10	l	24	LEU	Peptide
10	l	27	CYS	Peptide
10	l	8	ILE	Peptide
11	m	137	LYS	Peptide
11	m	34	LYS	Peptide
18	u	103	PHE	Sidechain
23	v	100	LYS	Peptide
23	v	101	PRO	Peptide
23	v	104	GLY	Peptide
23	v	120	SER	Mainchain
23	v	147	LYS	Peptide
23	v	158	GLY	Peptide
23	v	159	THR	Peptide
23	v	165	PHE	Sidechain
23	v	168	VAL	Peptide
23	v	184	ASN	Peptide
23	v	185	ASN	Peptide
23	v	187	VAL	Peptide
23	v	188	LEU	Peptide
23	v	194	ARG	Sidechain
23	v	33	LEU	Peptide
21	w	108	LYS	Peptide
21	w	110	ILE	Peptide
21	w	126	LEU	Peptide
21	w	130	TYR	Peptide
21	w	148	LYS	Peptide
21	w	176	ASN	Peptide
21	w	98	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	b	1787	0	1828	0	0
2	c	1719	0	1807	0	0
3	e	1292	0	1355	0	0
4	f	886	0	888	0	0
5	g	1161	0	1237	0	0
6	h	1088	0	1149	0	0
7	i	1020	0	1072	0	0
8	j	796	0	841	0	0
9	k	887	0	933	0	0
10	l	967	0	1046	0	0
11	m	898	0	950	0	0
12	o	525	0	572	0	0
13	p	664	0	703	0	0
14	q	635	0	667	0	0
15	r	518	0	544	0	0
16	s	627	0	653	0	0
17	t	832	0	883	0	0
18	u	393	0	406	0	0
19	y	845	0	892	0	0
20	a	31777	0	16007	0	0
21	w	689	0	706	0	0
22	d	1633	0	1727	0	0
23	v	1464	0	1456	0	0
24	n	819	0	858	0	0
25	x	289	0	301	0	0
26	8	1201	0	1220	46	0
All	All	55412	0	40701	46	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 12.

All (46) 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)
26:8:317:HIS:HA	26:8:324:VAL:HA	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:8:291:GLN:HB3	26:8:327:SER:HA	1.60	0.83
26:8:342:PRO:HA	26:8:345:VAL:HB	1.61	0.83
26:8:63:ALA:O	26:8:66:ARG:C	2.22	0.78
26:8:365:ALA:O	26:8:366:MET:O	2.03	0.74
26:8:354:GLN:OE1	26:8:357:ARG:NH1	2.18	0.73
26:8:64:TYR:HA	26:8:67:CYS:HB2	1.72	0.72
26:8:318:ASP:HB3	26:8:323:ARG:HB2	1.74	0.68
26:8:359:ARG:HG3	26:8:360:ILE:HG13	1.75	0.68
26:8:257:GLN:HE22	26:8:283:ILE:HA	1.60	0.67
26:8:304:LEU:HD13	26:8:306:PRO:HD3	1.82	0.60
26:8:268:VAL:HG21	26:8:305:GLN:HB3	1.84	0.59
26:8:316:SER:HB3	26:8:325:SER:HB2	1.86	0.57
26:8:262:SER:OG	26:8:281:GLY:O	2.22	0.56
26:8:366:MET:SD	26:8:366:MET:N	2.78	0.56
26:8:320:GLU:OE1	26:8:323:ARG:NH2	2.35	0.56
26:8:280:ILE:HG23	26:8:283:ILE:HG12	1.90	0.54
26:8:363:ALA:O	26:8:364:GLU:HB3	2.09	0.52
26:8:285:GLY:HA2	26:8:324:VAL:O	2.09	0.52
26:8:342:PRO:O	26:8:346:PHE:N	2.40	0.51
26:8:257:GLN:NE2	26:8:283:ILE:HA	2.25	0.51
26:8:317:HIS:HB3	26:8:324:VAL:HG12	1.93	0.51
26:8:291:GLN:CD	26:8:327:SER:HB2	2.31	0.50
26:8:365:ALA:C	26:8:366:MET:O	2.50	0.50
26:8:63:ALA:HA	26:8:66:ARG:HB2	1.94	0.49
26:8:315:LEU:O	26:8:317:HIS:N	2.45	0.49
26:8:288:HIS:O	26:8:292:ILE:HG13	2.12	0.48
26:8:63:ALA:O	26:8:66:ARG:O	2.33	0.47
26:8:61:GLU:O	26:8:65:GLU:HG3	2.15	0.47
26:8:257:GLN:NE2	26:8:282:GLY:O	2.48	0.47
26:8:343:LYS:HA	26:8:346:PHE:CE2	2.50	0.46
26:8:318:ASP:OD2	26:8:323:ARG:NH2	2.45	0.45
26:8:356:PHE:O	26:8:359:ARG:HG2	2.16	0.45
26:8:264:VAL:HG22	26:8:281:GLY:H	1.81	0.45
26:8:329:LYS:HE2	26:8:332:GLU:OE2	2.16	0.45
26:8:317:HIS:CA	26:8:324:VAL:HA	2.33	0.44
26:8:329:LYS:HB3	26:8:332:GLU:OE2	2.17	0.44
26:8:69:ASN:HB3	26:8:73:GLU:HG2	1.99	0.44
26:8:354:GLN:HA	26:8:357:ARG:NH1	2.33	0.44
26:8:364:GLU:HA	26:8:364:GLU:OE1	2.18	0.44
26:8:367:ALA:HB3	26:8:368:ARG:HG2	2.00	0.43
26:8:369:ALA:O	26:8:371:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:8:271:LEU:CD1	26:8:304:LEU:HA	2.50	0.41
26:8:280:ILE:HD13	26:8:280:ILE:HG21	1.69	0.41
26:8:268:VAL:HG11	26:8:305:GLN:HB3	2.03	0.41
26:8:315:LEU:HD23	26:8:327:SER:H	1.85	0.41

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	
1	b	225/236 (95%)	195 (87%)	29 (13%)	1 (0%)	34	69
2	c	211/218 (97%)	181 (86%)	28 (13%)	2 (1%)	17	54
3	e	169/253 (67%)	150 (89%)	17 (10%)	2 (1%)	13	48
4	f	109/146 (75%)	85 (78%)	24 (22%)	0	100	100
5	g	147/155 (95%)	130 (88%)	16 (11%)	1 (1%)	22	59
6	h	132/134 (98%)	116 (88%)	16 (12%)	0	100	100
7	i	131/157 (83%)	107 (82%)	23 (18%)	1 (1%)	19	56
8	j	96/122 (79%)	83 (86%)	13 (14%)	0	100	100
9	k	116/138 (84%)	104 (90%)	12 (10%)	0	100	100
10	l	121/123 (98%)	100 (83%)	21 (17%)	0	100	100
11	m	108/126 (86%)	90 (83%)	18 (17%)	0	100	100
12	o	60/90 (67%)	59 (98%)	1 (2%)	0	100	100
13	p	78/88 (89%)	61 (78%)	17 (22%)	0	100	100
14	q	76/108 (70%)	64 (84%)	12 (16%)	0	100	100
15	r	62/101 (61%)	58 (94%)	4 (6%)	0	100	100
16	s	76/92 (83%)	61 (80%)	15 (20%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	t	103/108 (95%)	93 (90%)	10 (10%)	0	100	100
18	u	42/137 (31%)	39 (93%)	3 (7%)	0	100	100
19	y	106/236 (45%)	96 (91%)	10 (9%)	0	100	100
21	w	82/121 (68%)	79 (96%)	0	3 (4%)	3	28
22	d	197/201 (98%)	173 (88%)	22 (11%)	2 (1%)	15	51
23	v	188/198 (95%)	171 (91%)	14 (7%)	3 (2%)	9	43
24	n	97/100 (97%)	90 (93%)	7 (7%)	0	100	100
25	x	35/47 (74%)	30 (86%)	4 (11%)	1 (3%)	4	32
26	8	150/370 (40%)	116 (77%)	18 (12%)	16 (11%)	0	6
All	All	2917/3805 (77%)	2531 (87%)	354 (12%)	32 (1%)	18	50

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	e	148	ILE
21	w	149	PRO
23	v	105	MET
26	8	72	MET
26	8	73	GLU
26	8	299	ASP
26	8	300	ILE
26	8	303	VAL
26	8	316	SER
26	8	330	LYS
26	8	366	MET
26	8	367	ALA
26	8	370	ASP
26	8	371	MET
2	c	89	PRO
22	d	5	ARG
23	v	121	PRO
26	8	360	ILE
26	8	368	ARG
1	b	169	ASP
7	i	159	ALA
21	w	150	TRP
2	c	88	ARG
3	e	302	PRO
25	x	90	ILE

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Mol	Chain	Res	Type
26	8	306	PRO
26	8	364	GLU
5	g	9	GLU
22	d	168	PRO
23	v	120	SER
21	w	119	PRO
26	8	307	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	192/201 (96%)	188 (98%)	4 (2%)	53	74
2	c	185/188 (98%)	185 (100%)	0	100	100
3	e	132/203 (65%)	128 (97%)	4 (3%)	41	66
4	f	98/125 (78%)	98 (100%)	0	100	100
5	g	120/126 (95%)	120 (100%)	0	100	100
6	h	117/117 (100%)	115 (98%)	2 (2%)	60	79
7	i	103/123 (84%)	102 (99%)	1 (1%)	76	86
8	j	90/110 (82%)	90 (100%)	0	100	100
9	k	92/109 (84%)	92 (100%)	0	100	100
10	l	106/106 (100%)	106 (100%)	0	100	100
11	m	97/109 (89%)	97 (100%)	0	100	100
12	o	58/85 (68%)	58 (100%)	0	100	100
13	p	71/79 (90%)	70 (99%)	1 (1%)	67	82
14	q	70/95 (74%)	70 (100%)	0	100	100
15	r	56/96 (58%)	56 (100%)	0	100	100
16	s	67/81 (83%)	67 (100%)	0	100	100
17	t	86/89 (97%)	84 (98%)	2 (2%)	50	71
18	u	40/118 (34%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	y	97/213 (46%)	94 (97%)	3 (3%)	40	65
21	w	75/109 (69%)	74 (99%)	1 (1%)	69	83
22	d	178/180 (99%)	175 (98%)	3 (2%)	60	79
23	v	160/168 (95%)	158 (99%)	2 (1%)	69	83
24	n	89/90 (99%)	89 (100%)	0	100	100
25	x	28/37 (76%)	28 (100%)	0	100	100
26	8	129/310 (42%)	125 (97%)	4 (3%)	40	65
All	All	2536/3267 (78%)	2509 (99%)	27 (1%)	74	85

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	30	ARG
1	b	40	LYS
1	b	94	HIS
1	b	201	ASP
3	e	144	LYS
3	e	266	LEU
3	e	303	MET
3	e	305	GLU
6	h	67	ARG
6	h	79	LEU
7	i	176	ARG
13	p	46	THR
17	t	103	ARG
17	t	162	ARG
19	y	91	ARG
19	y	119	ARG
19	y	159	LEU
21	w	103	PHE
22	d	27	ARG
22	d	40	LYS
22	d	160	LEU
23	v	24	LEU
23	v	37	GLU
26	8	283	ILE
26	8	304	LEU
26	8	314	ILE
26	8	368	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
2	c	18	HIS
2	c	34	GLN
2	c	187	GLN
3	e	225	HIS
3	e	264	ASN
6	h	19	ASN
6	h	51	HIS
6	h	68	ASN
7	i	127	ASN
7	i	161	HIS
8	j	126	ASN
8	j	149	HIS
8	j	151	HIS
9	k	127	HIS
9	k	128	ASN
10	l	77	HIS
11	m	56	ASN
11	m	65	GLN
11	m	83	ASN
11	m	125	HIS
15	r	59	GLN
15	r	83	GLN
16	s	23	ASN
18	u	124	ASN
19	y	165	GLN
21	w	155	GLN
21	w	162	GLN
21	w	172	GLN
22	d	57	HIS
22	d	112	ASN
22	d	115	HIS
22	d	142	GLN
23	v	45	HIS
23	v	96	ASN
23	v	163	ASN
23	v	196	ASN
26	8	58	GLN
26	8	269	GLN
26	8	294	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	a	1477/1491 (99%)	310 (20%)	0

All (310) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	a	5	A
20	a	6	U
20	a	7	G
20	a	10	G
20	a	31	U
20	a	32	G
20	a	33	A
20	a	40	G
20	a	45	A
20	a	48	C
20	a	49	U
20	a	50	U
20	a	52	A
20	a	55	C
20	a	62	G
20	a	72	A
20	a	75	U
20	a	82	U
20	a	83	C
20	a	85	A
20	a	90	C
20	a	92	G
20	a	100	A
20	a	104	A
20	a	105	C
20	a	106	G
20	a	114	A
20	a	115	C
20	a	121	C
20	a	127	A
20	a	130	G
20	a	143	G
20	a	147	C
20	a	148	G
20	a	150	C
20	a	152	G

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Mol	Chain	Res	Type
20	a	166	G
20	a	167	G
20	a	174	A
20	a	180	A
20	a	191	G
20	a	202	G
20	a	216	U
20	a	218	G
20	a	221	A
20	a	222	G
20	a	230	G
20	a	237	G
20	a	238	C
20	a	252	G
20	a	260	G
20	a	269	A
20	a	277	A
20	a	287	C
20	a	296	A
20	a	299	C
20	a	300	A
20	a	303	G
20	a	315	A
20	a	317	G
20	a	322	G
20	a	323	C
20	a	324	A
20	a	325	G
20	a	338	U
20	a	343	C
20	a	344	A
20	a	349	G
20	a	353	A
20	a	355	G
20	a	358	U
20	a	360	A
20	a	369	U
20	a	377	G
20	a	382	C
20	a	383	A
20	a	384	G
20	a	392	A

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Mol	Chain	Res	Type
20	a	393	C
20	a	395	G
20	a	399	G
20	a	400	U
20	a	410	U
20	a	411	U
20	a	416	G
20	a	423	A
20	a	424	G
20	a	426	A
20	a	429	G
20	a	432	G
20	a	433	G
20	a	434	U
20	a	443	A
20	a	444	A
20	a	447	A
20	a	453	G
20	a	456	U
20	a	459	C
20	a	466	C
20	a	469	G
20	a	472	G
20	a	475	G
20	a	478	G
20	a	479	U
20	a	481	A
20	a	495	A
20	a	507	A
20	a	510	G
20	a	511	A
20	a	512	U
20	a	514	G
20	a	520	A
20	a	521	A
20	a	524	C
20	a	525	G
20	a	536	G
20	a	543	A
20	a	544	A
20	a	566	C
20	a	577	A

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Mol	Chain	Res	Type
20	a	578	C
20	a	579	A
20	a	580	G
20	a	600	U
20	a	601	G
20	a	602	G
20	a	613	G
20	a	630	G
20	a	650	A
20	a	651	G
20	a	659	A
20	a	660	A
20	a	669	A
20	a	670	A
20	a	671	C
20	a	672	G
20	a	695	A
20	a	696	C
20	a	697	A
20	a	703	A
20	a	725	A
20	a	741	U
20	a	742	A
20	a	757	G
20	a	762	A
20	a	763	A
20	a	765	C
20	a	766	G
20	a	768	U
20	a	769	G
20	a	775	U
20	a	776	A
20	a	780	G
20	a	784	U
20	a	790	U
20	a	791	C
20	a	794	C
20	a	795	C
20	a	796	C
20	a	797	G
20	a	798	U
20	a	799	G

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Mol	Chain	Res	Type
20	a	821	A
20	a	822	A
20	a	825	A
20	a	834	G
20	a	838	A
20	a	849	A
20	a	851	G
20	a	863	A
20	a	875	G
20	a	876	G
20	a	883	C
20	a	884	A
20	a	909	U
20	a	915	G
20	a	918	A
20	a	920	G
20	a	924	A
20	a	925	G
20	a	926	A
20	a	938	G
20	a	941	U
20	a	942	G
20	a	945	A
20	a	946	U
20	a	948	C
20	a	953	A
20	a	954	A
20	a	958	U
20	a	961	U
20	a	963	A
20	a	964	A
20	a	969	A
20	a	973	G
20	a	974	U
20	a	975	G
20	a	978	U
20	a	980	C
20	a	981	G
20	a	982	G
20	a	985	A
20	a	986	C
20	a	992	C

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Mol	Chain	Res	Type
20	a	994	C
20	a	995	A
20	a	1003	C
20	a	1005	U
20	a	1014	U
20	a	1027	U
20	a	1034	U
20	a	1038	G
20	a	1041	A
20	a	1043	G
20	a	1044	U
20	a	1047	C
20	a	1050	A
20	a	1057	G
20	a	1066	G
20	a	1073	G
20	a	1074	U
20	a	1075	U
20	a	1079	A
20	a	1080	A
20	a	1082	G
20	a	1088	U
20	a	1089	U
20	a	1091	G
20	a	1095	C
20	a	1099	G
20	a	1100	A
20	a	1105	A
20	a	1107	U
20	a	1114	G
20	a	1115	A
20	a	1116	U
20	a	1119	G
20	a	1130	G
20	a	1131	U
20	a	1132	G
20	a	1144	A
20	a	1149	A
20	a	1150	U
20	a	1160	U
20	a	1161	A
20	a	1162	U

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Mol	Chain	Res	Type
20	a	1163	G
20	a	1174	C
20	a	1175	A
20	a	1184	A
20	a	1186	A
20	a	1187	A
20	a	1188	U
20	a	1189	G
20	a	1195	G
20	a	1198	A
20	a	1204	U
20	a	1205	C
20	a	1206	G
20	a	1208	G
20	a	1222	G
20	a	1223	A
20	a	1227	A
20	a	1229	C
20	a	1233	A
20	a	1234	A
20	a	1235	A
20	a	1243	C
20	a	1246	C
20	a	1247	A
20	a	1248	G
20	a	1250	U
20	a	1253	G
20	a	1265	C
20	a	1266	A
20	a	1267	A
20	a	1271	G
20	a	1280	A
20	a	1288	A
20	a	1294	A
20	a	1295	G
20	a	1311	C
20	a	1312	A
20	a	1317	G
20	a	1319	G
20	a	1327	C
20	a	1328	G
20	a	1346	C

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Mol	Chain	Res	Type
20	a	1347	A
20	a	1351	C
20	a	1368	G
20	a	1371	G
20	a	1390	A
20	a	1395	A
20	a	1397	C
20	a	1400	C
20	a	1401	A
20	a	1402	A
20	a	1403	G
20	a	1405	A
20	a	1418	A
20	a	1441	A
20	a	1443	G
20	a	1452	A
20	a	1454	G
20	a	1455	U
20	a	1466	G
20	a	1478	G
20	a	1479	G
20	a	1480	A

There are no RNA pucker outliers to report.

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 monosaccharides 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.

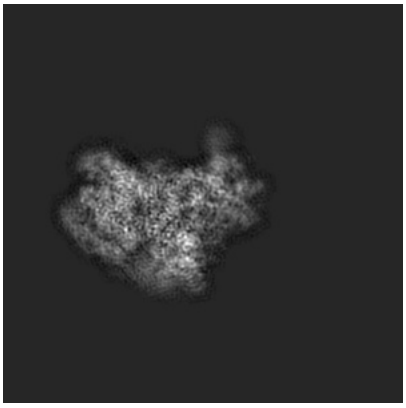
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6710. These allow visual inspection of the internal detail of the map and identification of artifacts.

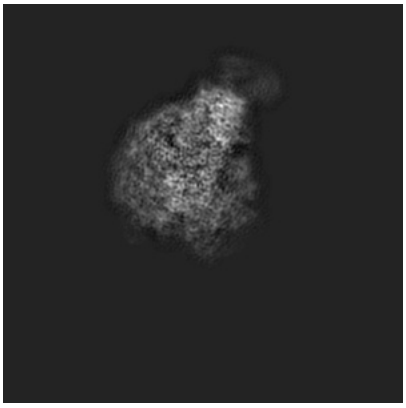
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

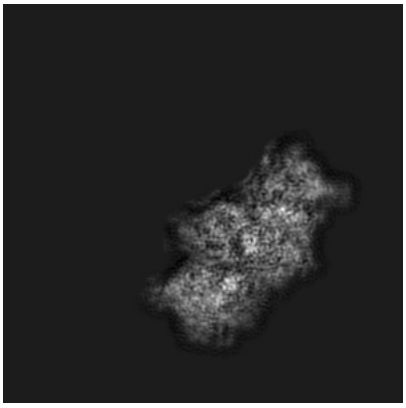
6.1.1 Primary map



X



Y

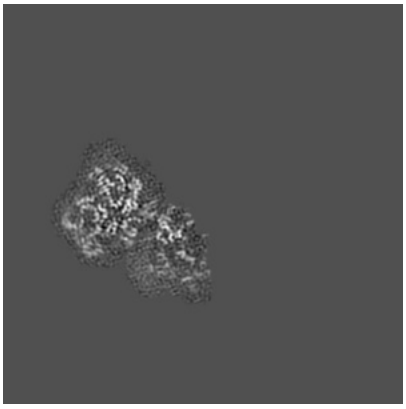


Z

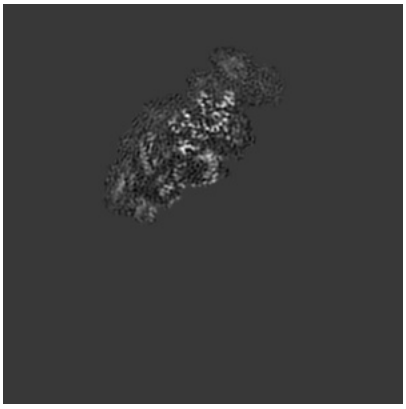
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

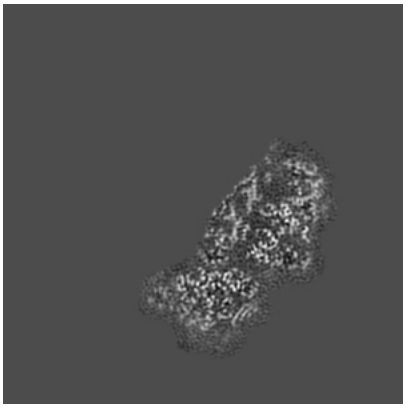
6.2.1 Primary map



X Index: 192



Y Index: 192

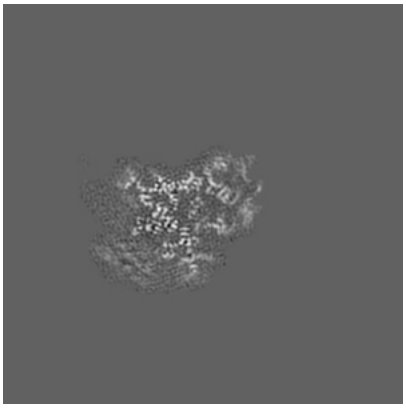


Z Index: 192

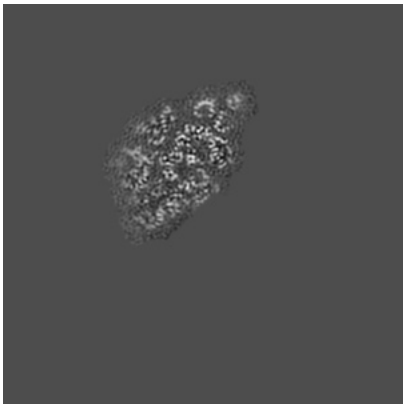
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

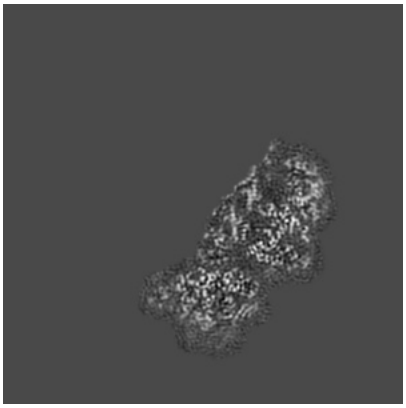
6.3.1 Primary map



X Index: 253



Y Index: 160

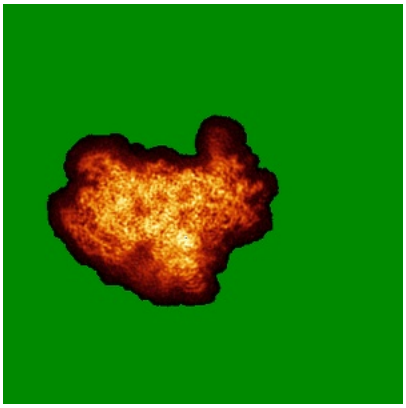


Z Index: 191

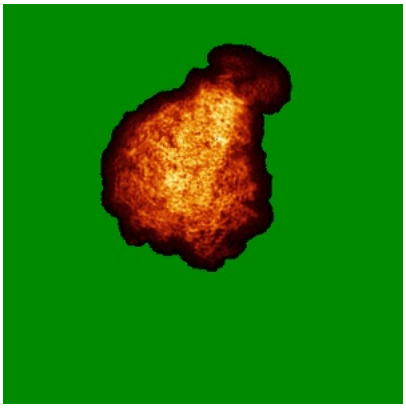
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

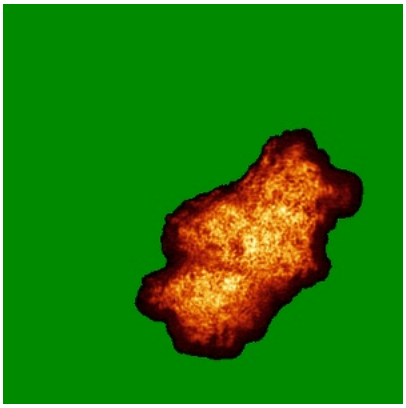
6.4.1 Primary map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

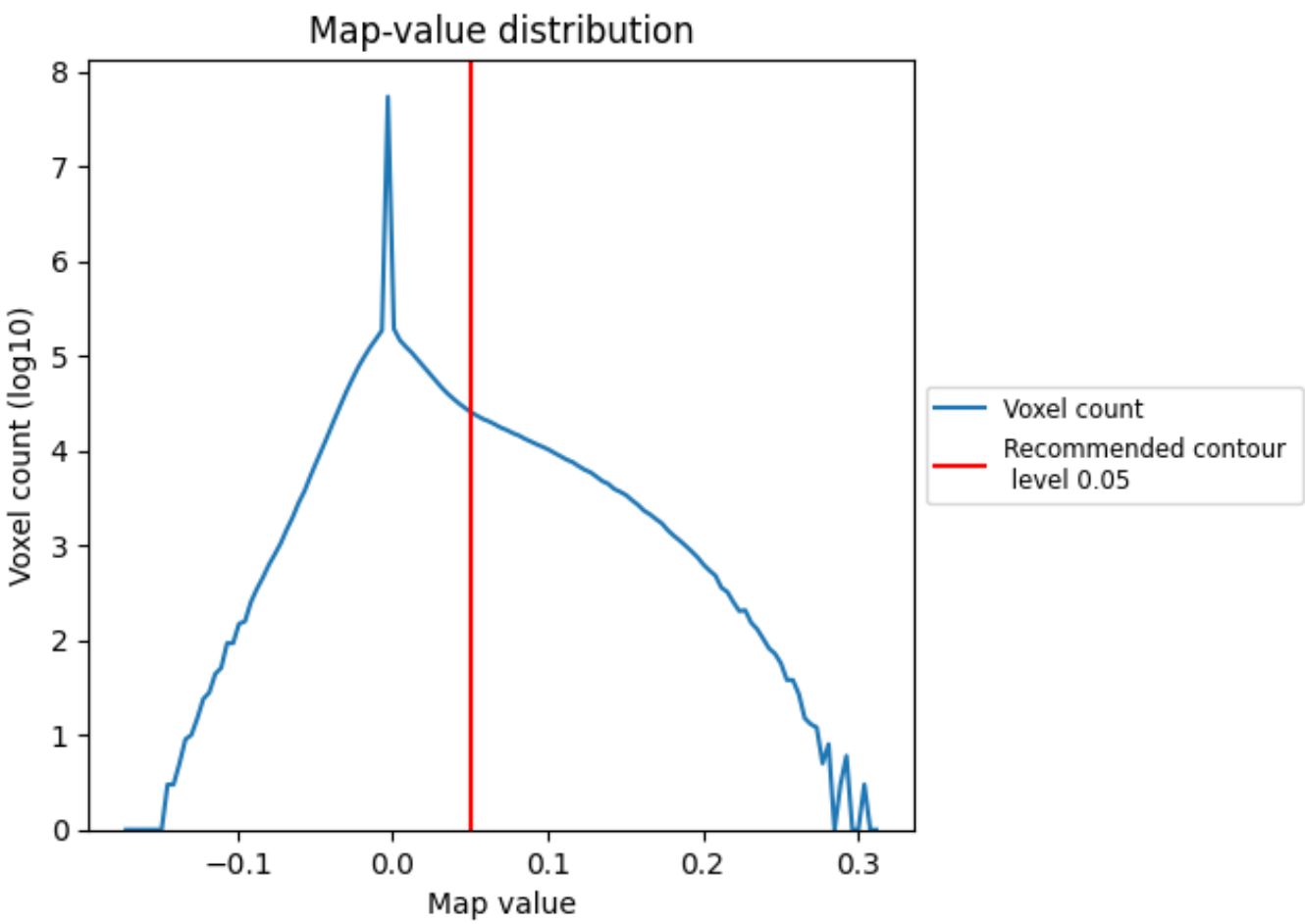
6.6 Mask visualisation (i)

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

7 Map analysis (i)

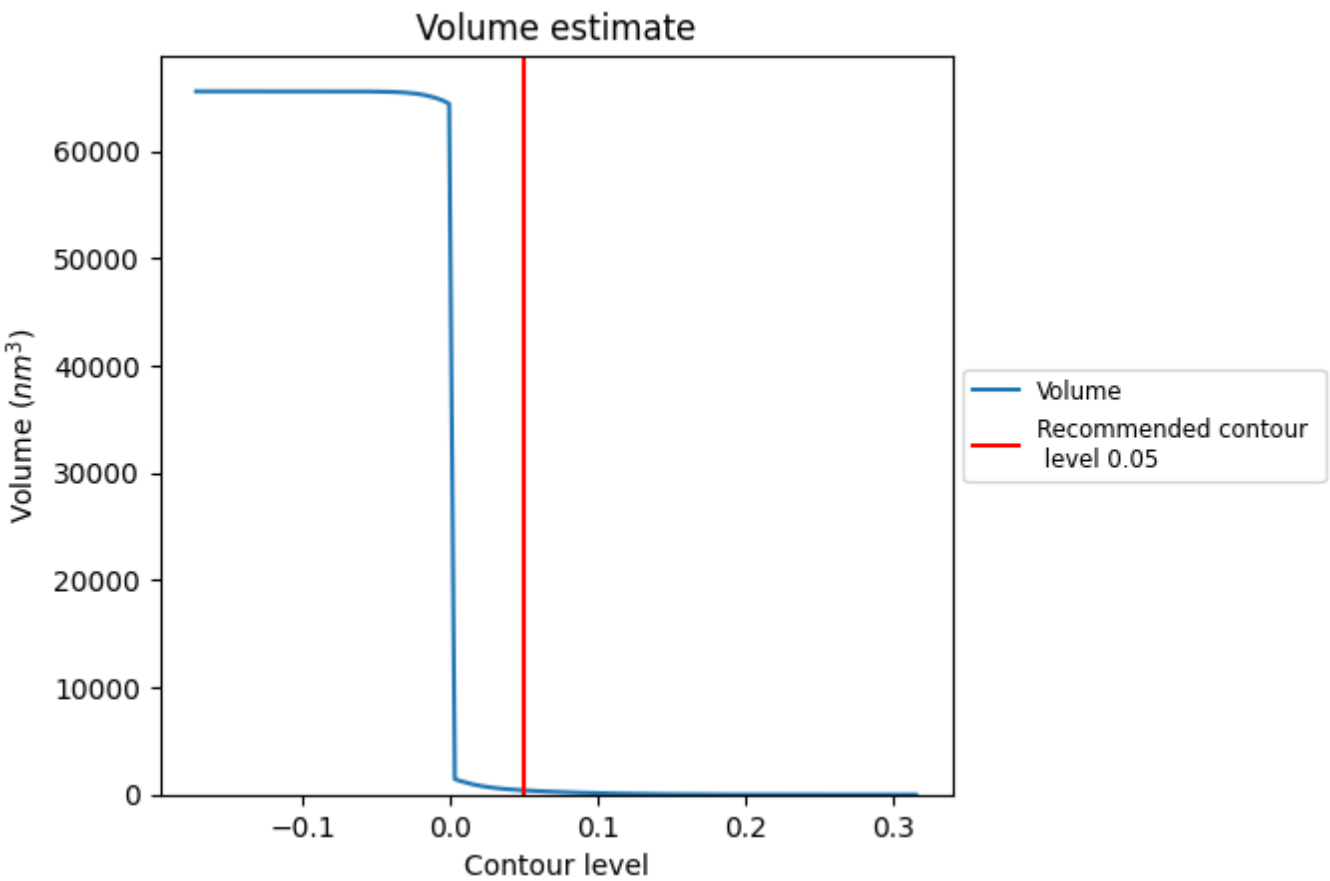
This section contains the results of statistical analysis of the map.

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.

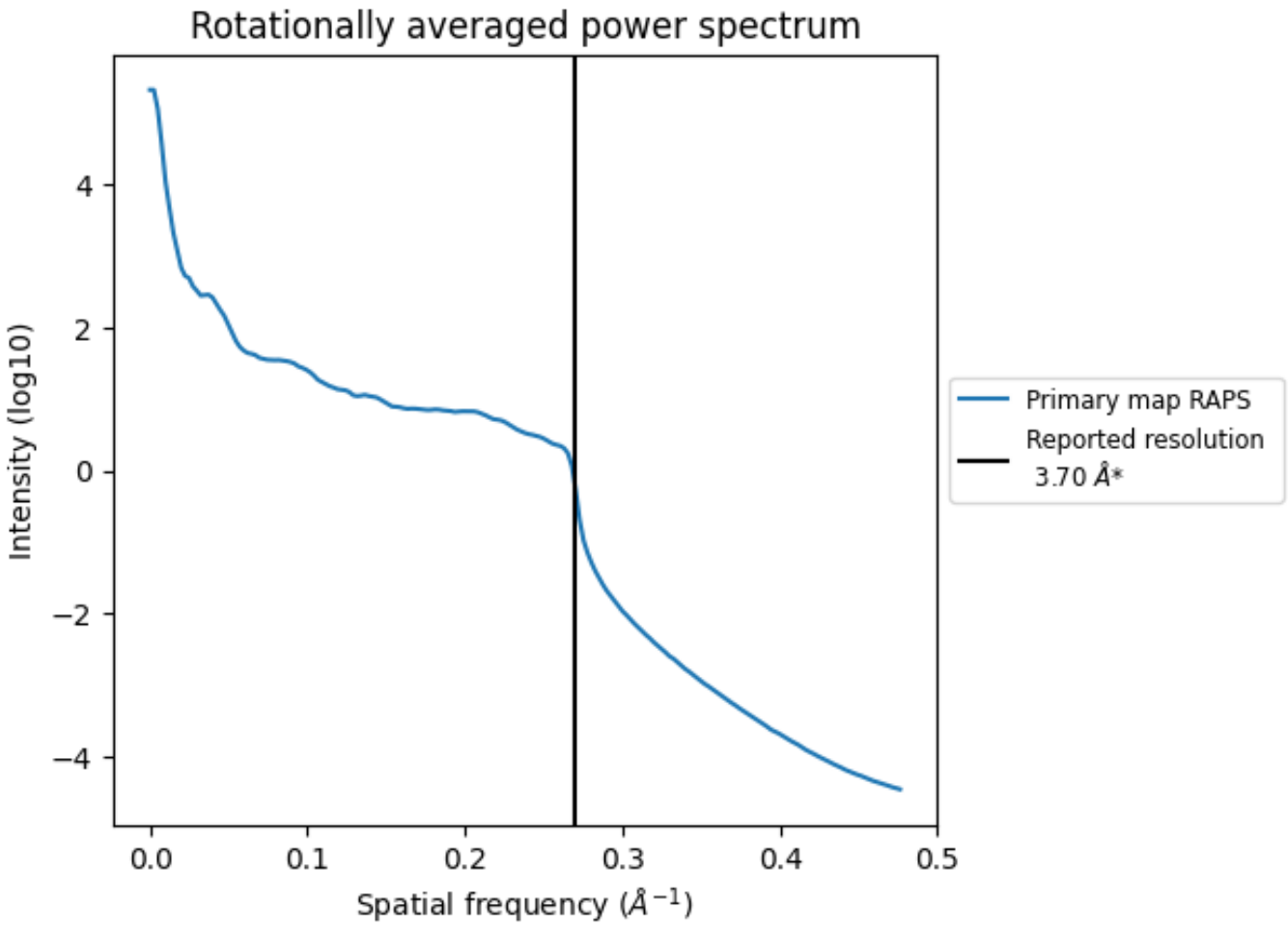
7.2 Volume estimate (i)



The volume at the recommended contour level is 393 nm^3; this corresponds to an approximate mass of 355 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 (i)



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

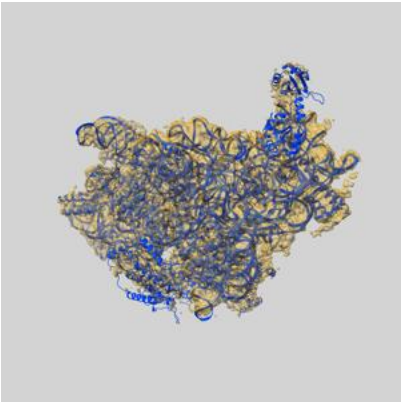
8 Fourier-Shell correlation (i)

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

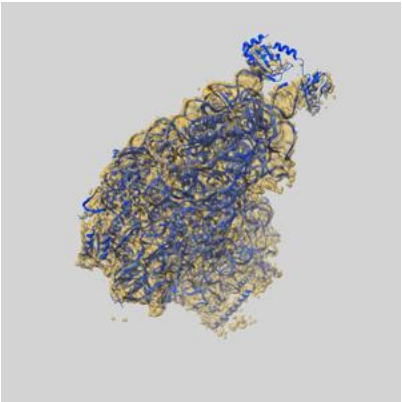
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6710 and PDB model 5X8R. Per-residue inclusion information can be found in section 3 on page 8.

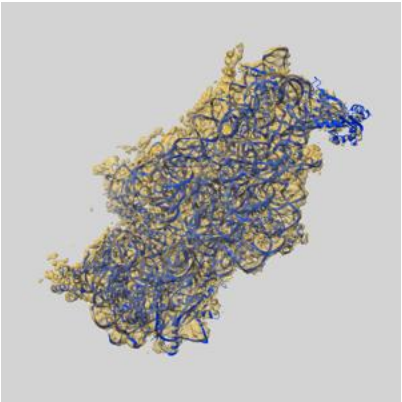
9.1 Map-model overlay (i)



X



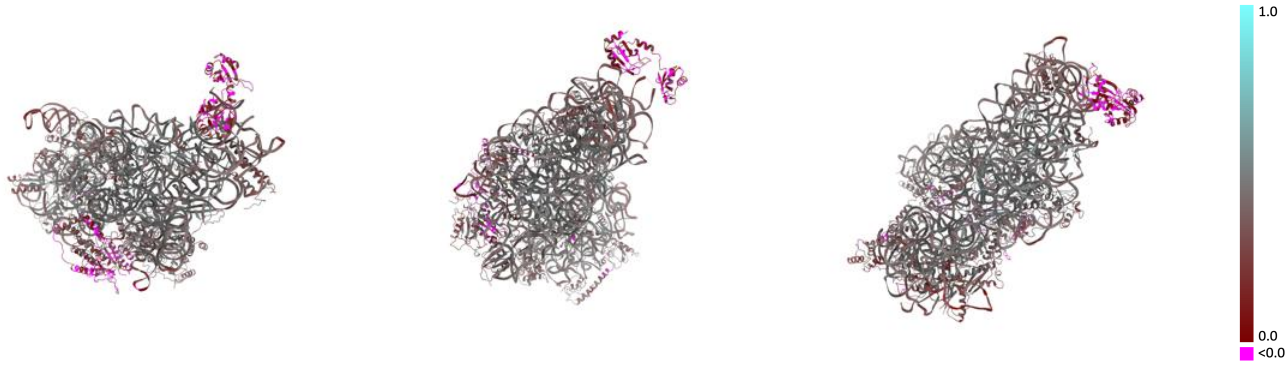
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

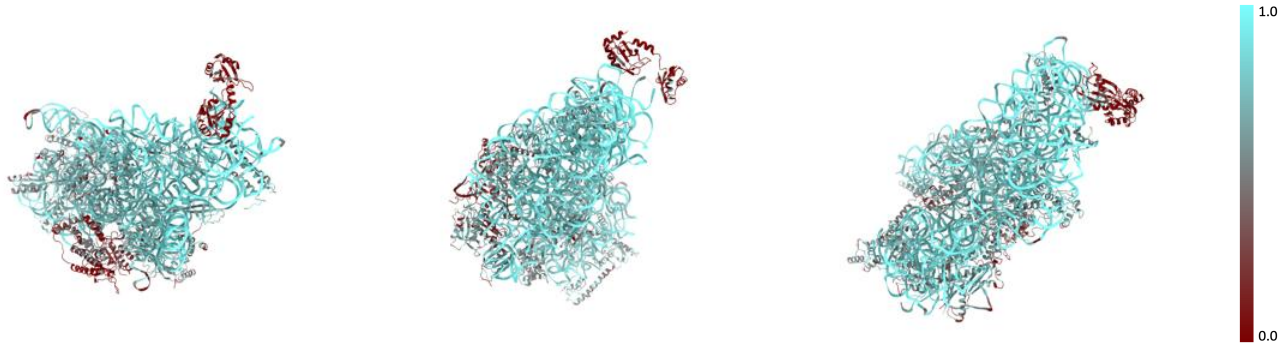
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

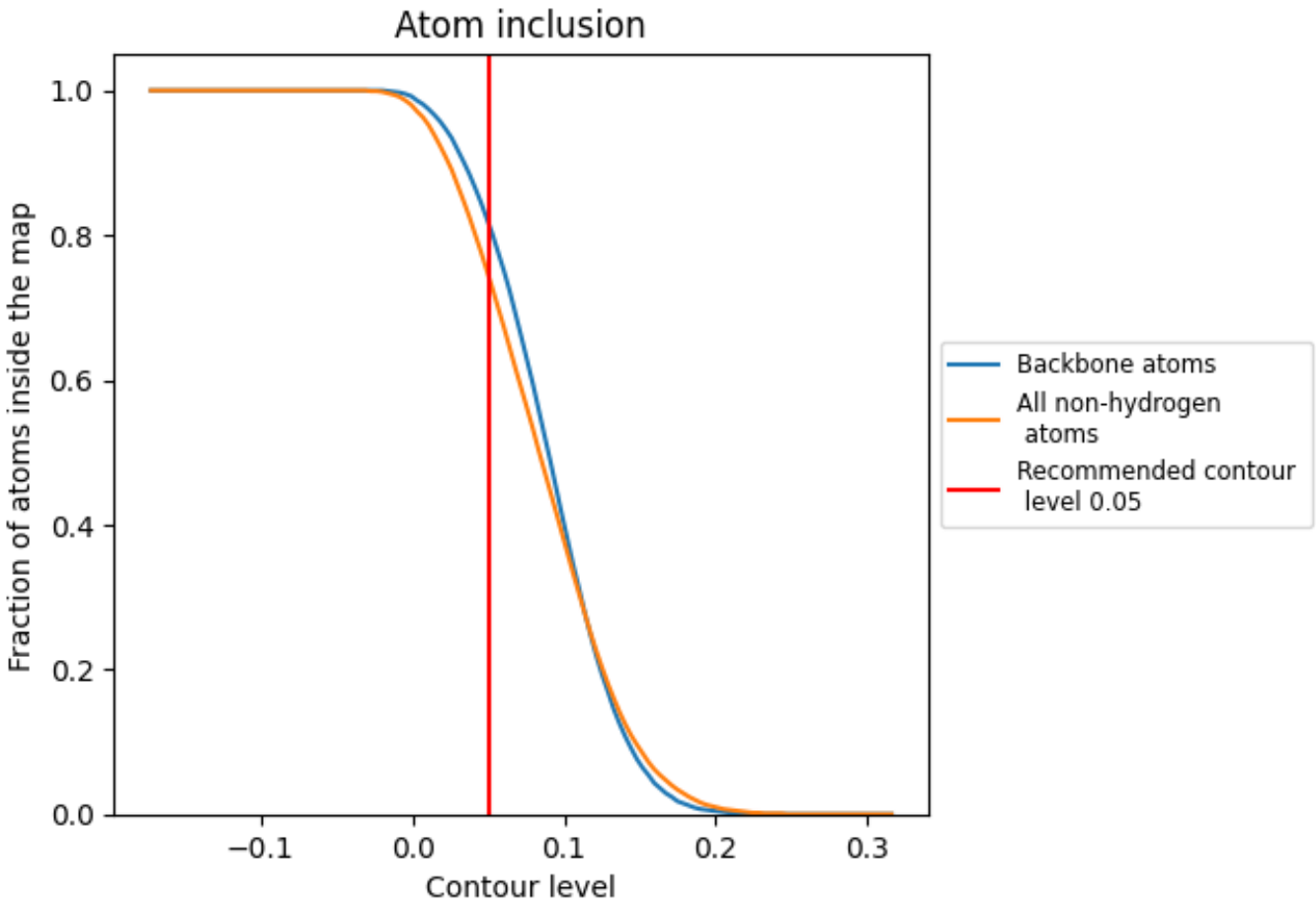
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7460	0.3930
8	0.0280	0.0120
a	0.9010	0.4330
b	0.3430	0.3270
c	0.6460	0.4160
d	0.6610	0.4040
e	0.6890	0.4310
f	0.5410	0.3560
g	0.5160	0.3730
h	0.6780	0.4220
i	0.6850	0.4000
j	0.6210	0.4020
k	0.6330	0.3940
l	0.7070	0.4640
m	0.6100	0.3210
n	0.6470	0.3870
o	0.5350	0.3860
p	0.7280	0.4350
q	0.6890	0.4520
r	0.6290	0.3840
s	0.6500	0.3850
t	0.6510	0.3400
u	0.4920	0.3180
v	0.0850	0.0540
w	0.0620	-0.0250
x	0.6880	0.4150
y	0.5960	0.4000