Full wwPDB EM Validation Report ⓘ

Oct 26, 2024 – 03:21 PM EDT

PDB ID	:	6N4C
EMDB ID	:	EMD-0340
Title	:	EM structure of the DNA wrapping in bacterial open transcription initiation complex
Authors	:	Florez-Ariza, A.; Cassago, A.; de Oliveira, P.S.L.; Guerra, D.G.; Portugal, R.V.
Deposited on	:	2018-11-19
Resolution	:	17.00 Å(reported)
Based on initial model	:	4YLN

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:

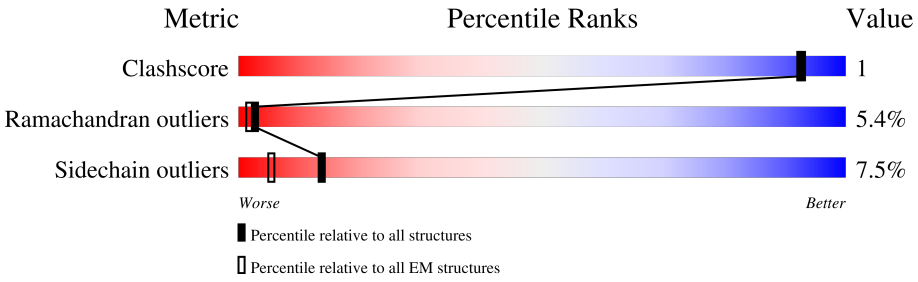
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 17.00 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	F	558	19% 80% 15%
2	C	1341	14% 84% 14%
3	D	1358	6% 85% 12%
4	A	316	11% 78% 19%
5	B	310	13% 76% 19%
6	E	90	34% 70% 26%
7	a	94	12% 57% 31%
8	b	94	15% 51% 34%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 68774 atoms, of which 33722 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 RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	F	558	9018	2799	4523	794	875	27	0	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLU	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	LEU	deletion	UNP P00579
F	?	-	ALA	deletion	UNP P00579
F	?	-	PRO	deletion	UNP P00579
F	?	-	THR	deletion	UNP P00579
F	?	-	ALA	deletion	UNP P00579
F	?	-	THR	deletion	UNP P00579
F	?	-	HIS	deletion	UNP P00579
F	?	-	VAL	deletion	UNP P00579
F	?	-	GLY	deletion	UNP P00579
F	?	-	SER	deletion	UNP P00579
F	?	-	GLU	deletion	UNP P00579
F	?	-	LEU	deletion	UNP P00579
F	?	-	SER	deletion	UNP P00579
F	?	-	GLN	deletion	UNP P00579
F	?	-	GLU	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	LEU	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	GLU	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	GLU	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	GLU	deletion	UNP P00579
F	?	-	GLU	deletion	UNP P00579

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ASP	deletion	UNP P00579
F	?	-	GLY	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	SER	deletion	UNP P00579
F	?	-	ALA	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	ILE	deletion	UNP P00579
F	?	-	ALA	deletion	UNP P00579
F	?	-	LYS	deletion	UNP P00579
F	?	-	GLU	deletion	UNP P00579
F	?	-	PRO	deletion	UNP P00579
F	521	ILE	-	insertion	UNP P00579
F	?	-	LEU	deletion	UNP P00579
F	?	-	GLU	deletion	UNP P00579
F	?	-	LEU	deletion	UNP P00579
F	?	-	PRO	deletion	UNP P00579
F	?	-	LEU	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	1341	Total	C	H	N	O	S	0	0
			21172	6636	10595	1842	2056	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	1358	Total	C	H	N	O	S	0	0
			21296	6615	10758	1882	1991	50		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLU	deletion	UNP A0A369F490
D	?	-	GLY	deletion	UNP A0A369F490
D	?	-	LYS	deletion	UNP A0A369F490
D	?	-	GLU	deletion	UNP A0A369F490

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	A	316	Total	C	H	N	O	S	0	0
			5001	1545	2528	436	484	8		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	B	310	Total	C	H	N	O	S	0	0
			4883	1508	2471	422	475	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	255	LEU	ARG	conflict	UNP P0A7Z4

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	E	90	Total	C	H	N	O	S	0	0
			1431	430	722	136	142	1		

- Molecule 7 is a DNA chain called DNA (94-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	a	94	Total	C	H	N	O	P	0	0
			2995	923	1064	349	566	93		

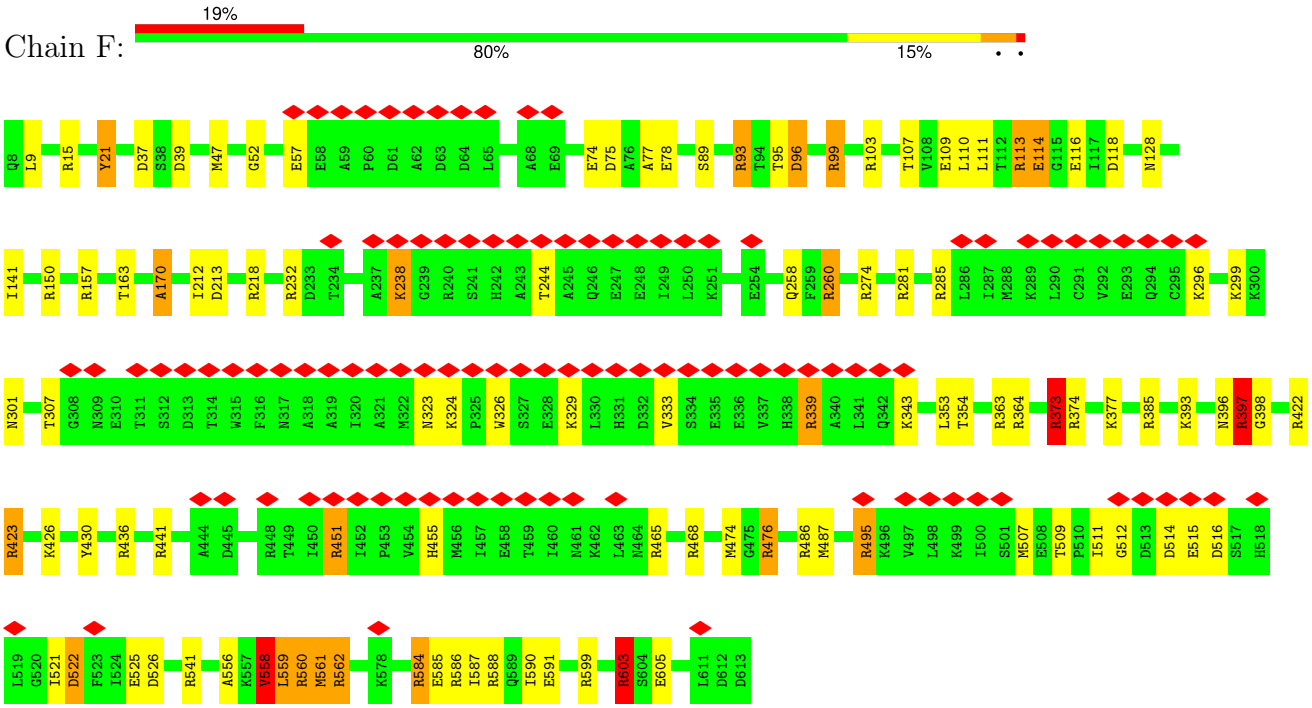
- Molecule 8 is a DNA chain called DNA (94-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
8	b	94	Total	C	H	N	O	P	0	0
			2978	917	1061	349	558	93		

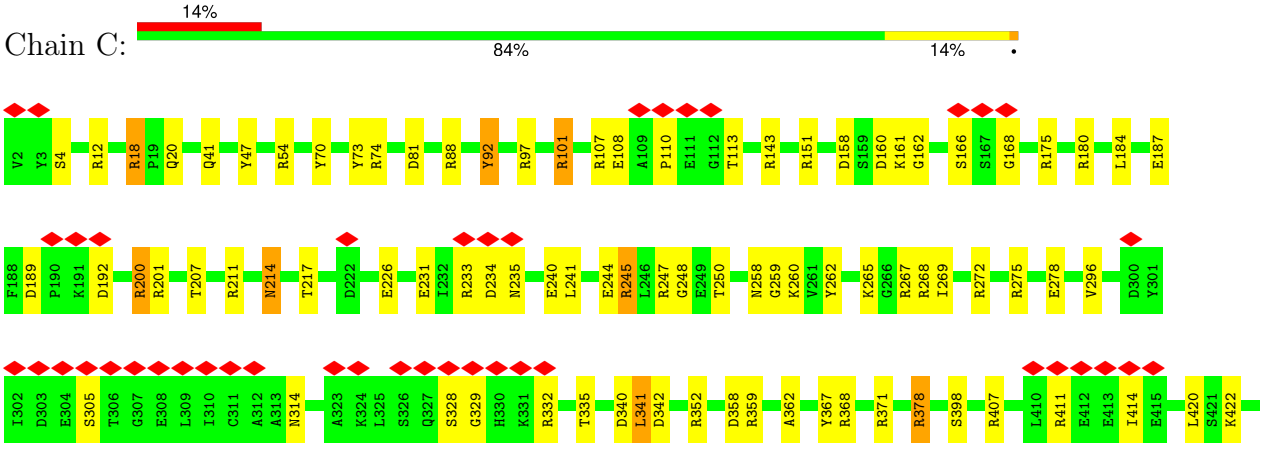
3 Residue-property plots (i)

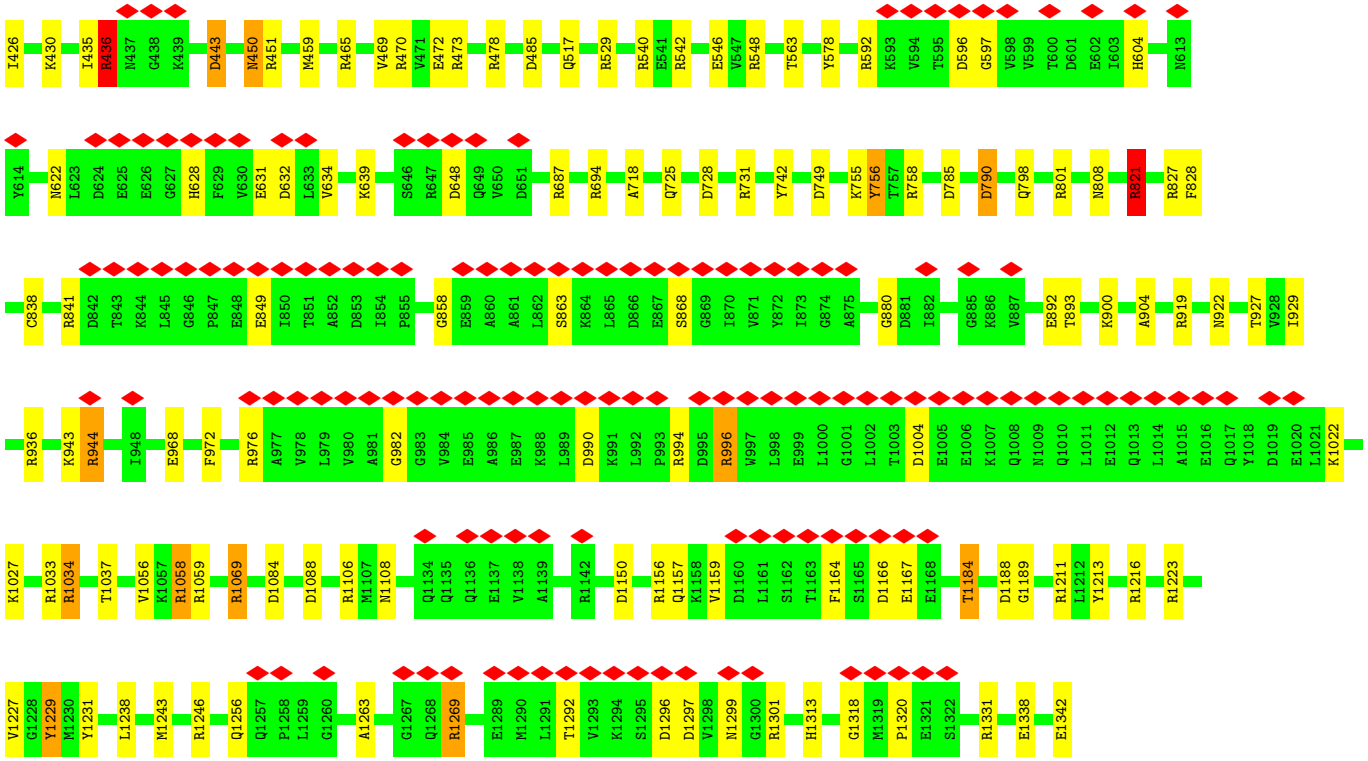
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



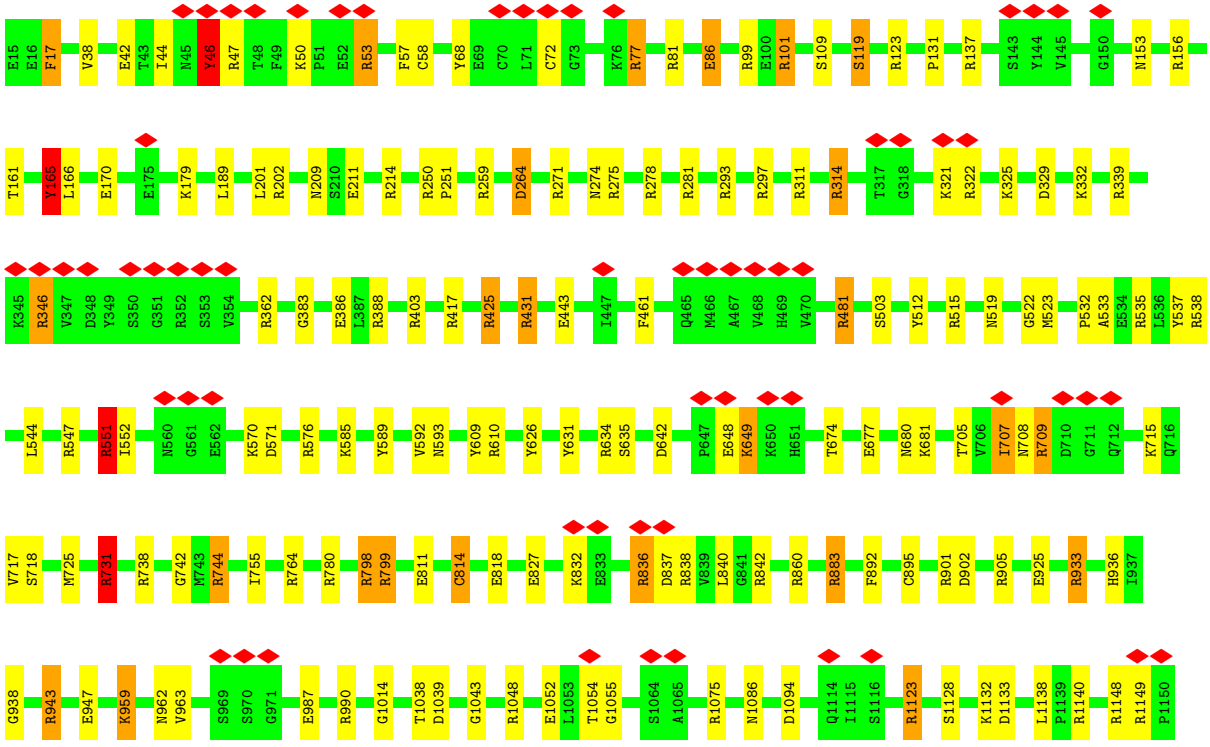
• Molecule 2: DNA-directed RNA polymerase subunit beta

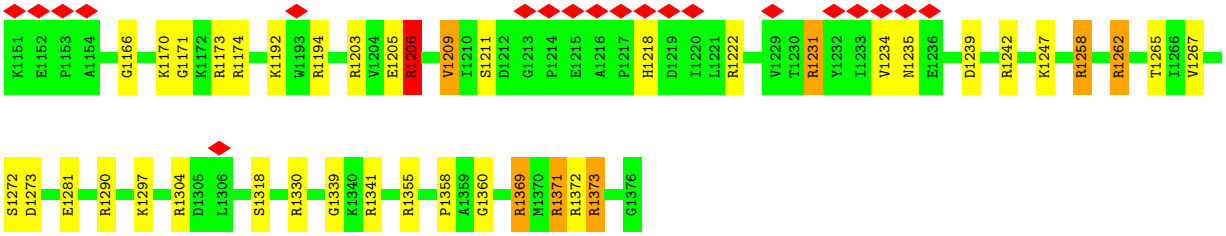




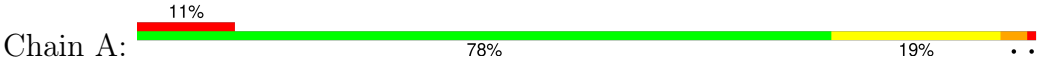
• Molecule 3: DNA-directed RNA polymerase subunit beta'

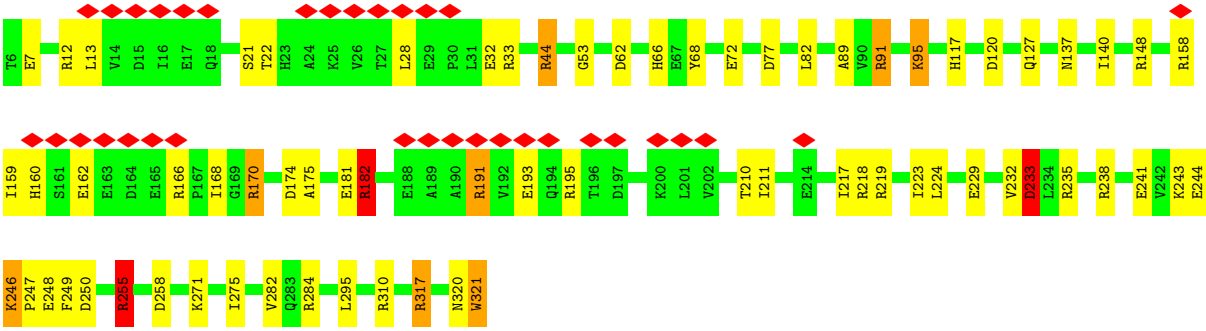
Chain D:



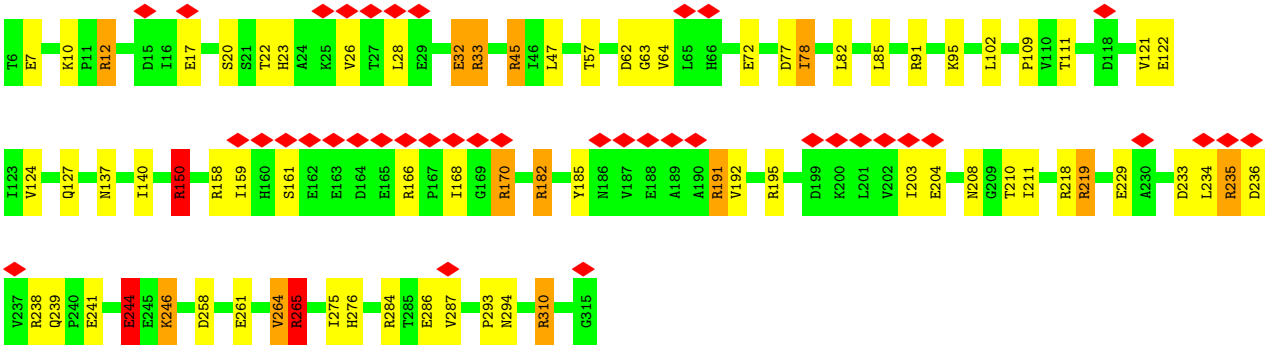


• Molecule 4: DNA-directed RNA polymerase subunit alpha

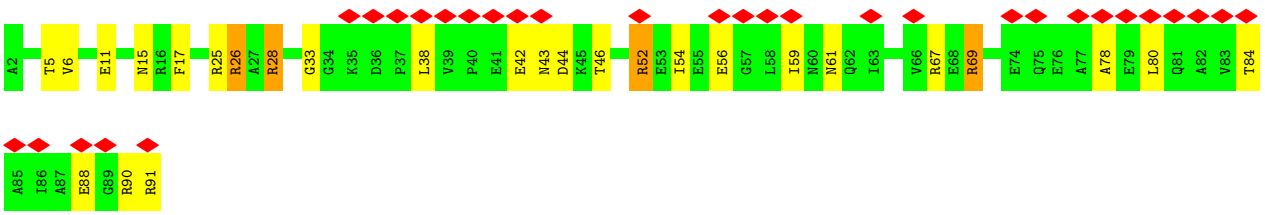




• Molecule 5: DNA-directed RNA polymerase subunit alpha

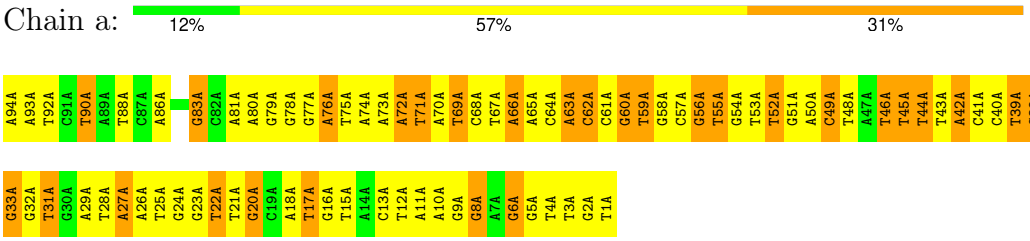


• Molecule 6: DNA-directed RNA polymerase subunit omega



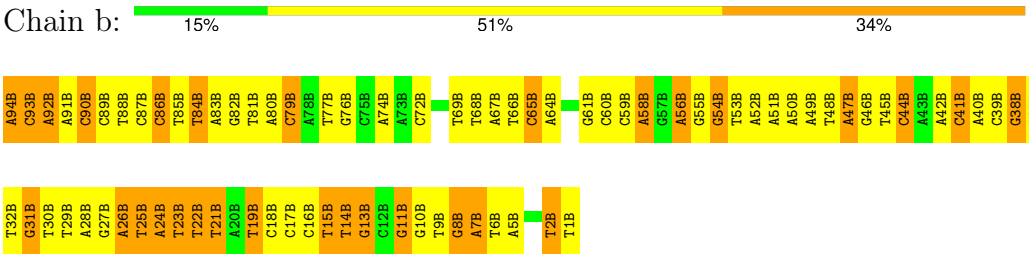
• Molecule 7: DNA (94-MER)

Chain a:



• Molecule 8: DNA (94-MER)

Chain b:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	16015	Depositor
Resolution determination method	FSC 1/2 BIT CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL 2100	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	14.200	Depositor
Minimum map value	-6.374	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	0.42	Depositor
Map size (Å)	320.4, 320.4, 320.4	wwPDB
Map dimensions	90, 90, 90	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.56, 3.56, 3.56	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	F	0.80	4/4553 (0.1%)	1.26	41/6127 (0.7%)
2	C	0.73	0/10746	1.18	76/14499 (0.5%)
3	D	0.72	0/10699	1.20	91/14447 (0.6%)
4	A	0.74	0/2505	1.26	20/3392 (0.6%)
5	B	0.74	0/2442	1.30	18/3308 (0.5%)
6	E	0.73	0/711	1.76	10/956 (1.0%)
7	a	1.26	0/2166	1.97	118/3344 (3.5%)
8	b	1.78	16/2150 (0.7%)	2.41	148/3314 (4.5%)
All	All	0.88	20/35972 (0.1%)	1.40	522/49387 (1.1%)

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	F	0	19
2	C	0	25
3	D	0	29
4	A	0	10
5	B	0	10
6	E	0	4
7	a	0	45
8	b	0	44
All	All	0	186

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	b	5(B)	DA	N7-C5	42.03	1.64	1.39
8	b	49(B)	DA	C2-N3	-23.01	1.12	1.33
8	b	50(B)	DA	P-O5'	14.36	1.74	1.59
8	b	92(B)	DA	O3'-P	10.89	1.74	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	b	51(B)	DA	O3'-P	10.04	1.73	1.61
8	b	48(B)	DT	O3'-P	9.04	1.72	1.61
8	b	90(B)	DC	P-O5'	8.88	1.68	1.59
1	F	560	ARG	C-N	8.29	1.53	1.34
8	b	47(B)	DA	C5'-C4'	8.13	1.60	1.51
8	b	49(B)	DA	P-O5'	8.04	1.67	1.59
8	b	47(B)	DA	P-O5'	7.84	1.67	1.59
1	F	562	ARG	C-N	7.16	1.50	1.34
8	b	47(B)	DA	O3'-P	-6.90	1.52	1.61
8	b	49(B)	DA	C5'-C4'	6.23	1.58	1.51
1	F	559	LEU	C-N	6.20	1.48	1.34
8	b	47(B)	DA	N7-C5	6.00	1.42	1.39
8	b	51(B)	DA	C3'-O3'	5.77	1.51	1.44
1	F	561	MET	N-CA	5.56	1.57	1.46
8	b	49(B)	DA	O3'-P	5.45	1.67	1.61
8	b	47(B)	DA	C3'-O3'	-5.10	1.37	1.44

All (522) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	78	ALA	O-C-N	30.92	172.18	122.70
8	b	47(B)	DA	O4'-C1'-N9	30.91	129.63	108.00
8	b	91(B)	DA	O5'-P-OP2	-30.64	73.94	110.70
8	b	47(B)	DA	N1-C6-N6	-18.52	107.49	118.60
8	b	50(B)	DA	P-O3'-C3'	17.60	140.82	119.70
8	b	92(B)	DA	OP2-P-O3'	17.38	143.44	105.20
8	b	92(B)	DA	P-O3'-C3'	-16.77	99.57	119.70
8	b	49(B)	DA	N1-C6-N6	-16.40	108.76	118.60
6	E	78	ALA	CA-C-O	-16.04	86.41	120.10
8	b	91(B)	DA	OP1-P-OP2	-15.21	96.78	119.60
8	b	49(B)	DA	C4-C5-C6	-15.04	109.48	117.00
6	E	78	ALA	CA-C-N	-14.29	85.77	117.20
8	b	91(B)	DA	P-O5'-C5'	-14.08	98.37	120.90
8	b	91(B)	DA	P-O3'-C3'	13.87	136.35	119.70
8	b	47(B)	DA	O5'-C5'-C4'	13.49	144.72	111.00
8	b	92(B)	DA	O3'-P-O5'	-11.73	81.72	104.00
2	C	473	ARG	NE-CZ-NH1	11.55	126.08	120.30
3	D	943	ARG	NE-CZ-NH1	11.46	126.03	120.30
8	b	51(B)	DA	P-O3'-C3'	11.30	133.26	119.70
8	b	51(B)	DA	O3'-P-O5'	11.10	125.09	104.00
8	b	91(B)	DA	O5'-C5'-C4'	11.09	138.72	111.00
5	B	91	ARG	NE-CZ-NH2	-11.03	114.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	91	ARG	NE-CZ-NH1	10.80	125.70	120.30
5	B	150	ARG	NE-CZ-NH1	10.78	125.69	120.30
8	b	47(B)	DA	C4-C5-C6	-10.56	111.72	117.00
2	C	411	ARG	NE-CZ-NH1	10.54	125.57	120.30
8	b	48(B)	DT	P-O3'-C3'	10.46	132.26	119.70
8	b	49(B)	DA	O4'-C1'-N9	10.38	115.26	108.00
4	A	219	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	F	599	ARG	NE-CZ-NH1	10.36	125.48	120.30
5	B	33	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	F	486	ARG	NE-CZ-NH1	10.26	125.43	120.30
8	b	7(B)	DA	O4'-C1'-N9	10.11	115.08	108.00
8	b	47(B)	DA	C1'-O4'-C4'	-10.10	100.00	110.10
8	b	49(B)	DA	C6-C5-N7	10.06	139.34	132.30
3	D	547	ARG	NE-CZ-NH1	10.04	125.32	120.30
5	B	310	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	F	285	ARG	NE-CZ-NH1	9.98	125.29	120.30
3	D	481	ARG	NE-CZ-NH1	9.97	125.29	120.30
1	F	397	ARG	NE-CZ-NH1	9.85	125.22	120.30
2	C	12	ARG	NE-CZ-NH1	9.85	125.22	120.30
8	b	47(B)	DA	C5-C6-N1	9.85	122.62	117.70
8	b	5(B)	DA	C8-N9-C4	9.78	109.71	105.80
1	F	423	ARG	NE-CZ-NH1	9.75	125.17	120.30
3	D	798	ARG	NE-CZ-NH1	9.71	125.15	120.30
2	C	268	ARG	NE-CZ-NH2	9.70	125.15	120.30
3	D	293	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	F	274	ARG	NE-CZ-NH1	9.64	125.12	120.30
2	C	470	ARG	NE-CZ-NH1	9.55	125.07	120.30
2	C	801	ARG	NE-CZ-NH1	9.48	125.04	120.30
3	D	535	ARG	NE-CZ-NH2	9.46	125.03	120.30
1	F	339	ARG	NE-CZ-NH1	9.43	125.01	120.30
3	D	576	ARG	NE-CZ-NH1	9.29	124.95	120.30
3	D	271	ARG	NE-CZ-NH1	9.27	124.94	120.30
3	D	1371	ARG	NE-CZ-NH1	9.24	124.92	120.30
8	b	46(B)	DG	O4'-C1'-N9	9.14	114.40	108.00
2	C	1106	ARG	NE-CZ-NH1	9.13	124.86	120.30
3	D	297	ARG	NE-CZ-NH1	9.13	124.86	120.30
3	D	551	ARG	NE-CZ-NH2	9.12	124.86	120.30
1	F	260	ARG	NE-CZ-NH1	8.99	124.80	120.30
2	C	175	ARG	NE-CZ-NH1	8.97	124.79	120.30
8	b	35(B)	DC	O4'-C1'-N1	8.94	114.26	108.00
8	b	56(B)	DA	O4'-C1'-N9	8.93	114.25	108.00
3	D	339	ARG	NE-CZ-NH1	8.92	124.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	b	47(B)	DA	C5'-C4'-O4'	8.88	126.17	109.30
3	D	1372	ARG	NE-CZ-NH1	8.85	124.72	120.30
2	C	200	ARG	NE-CZ-NH1	8.84	124.72	120.30
2	C	371	ARG	NE-CZ-NH1	8.83	124.72	120.30
2	C	332	ARG	NE-CZ-NH2	8.83	124.71	120.30
3	D	860	ARG	NE-CZ-NH1	8.81	124.71	120.30
1	F	93	ARG	NE-CZ-NH1	8.77	124.69	120.30
3	D	99	ARG	NE-CZ-NH1	8.76	124.68	120.30
3	D	610	ARG	NE-CZ-NH1	8.76	124.68	120.30
8	b	38(B)	DG	O4'-C1'-N9	8.75	114.12	108.00
3	D	780	ARG	NE-CZ-NH1	8.74	124.67	120.30
3	D	905	ARG	NE-CZ-NH1	8.70	124.65	120.30
7	a	74(A)	DA	O4'-C1'-N9	8.68	114.08	108.00
3	D	53	ARG	NE-CZ-NH1	8.65	124.63	120.30
8	b	5(B)	DA	C5-N7-C8	-8.57	99.61	103.90
4	A	235	ARG	NE-CZ-NH1	8.54	124.57	120.30
2	C	1211	ARG	NE-CZ-NH1	8.43	124.51	120.30
3	D	836	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	F	436	ARG	NE-CZ-NH1	8.30	124.45	120.30
3	D	311	ARG	NE-CZ-NH1	8.29	124.45	120.30
8	b	47(B)	DA	C6-C5-N7	8.26	138.08	132.30
7	a	83(A)	DG	O4'-C1'-N9	8.25	113.77	108.00
8	b	37(B)	DC	O4'-C1'-N1	8.24	113.77	108.00
8	b	66(B)	DT	O4'-C1'-N1	8.22	113.75	108.00
1	F	15	ARG	NE-CZ-NH1	8.20	124.40	120.30
3	D	744	ARG	NE-CZ-NH1	8.18	124.39	120.30
4	A	148	ARG	NE-CZ-NH1	8.16	124.38	120.30
8	b	32(B)	DT	O4'-C1'-N1	8.12	113.68	108.00
3	D	1330	ARG	NE-CZ-NH1	8.10	124.35	120.30
2	C	540	ARG	NE-CZ-NH1	8.08	124.34	120.30
7	a	24(A)	DG	O4'-C1'-N9	8.07	113.65	108.00
3	D	933	ARG	NE-CZ-NH1	7.95	124.27	120.30
5	B	191	ARG	NE-CZ-NH1	7.94	124.27	120.30
2	C	478	ARG	NE-CZ-NH1	7.93	124.26	120.30
8	b	34(B)	DG	O4'-C1'-N9	7.90	113.53	108.00
3	D	77	ARG	NE-CZ-NH1	7.89	124.25	120.30
3	D	1206	ARG	NE-CZ-NH1	7.85	124.22	120.30
2	C	368	ARG	NE-CZ-NH1	7.84	124.22	120.30
7	a	56(A)	DG	O4'-C1'-N9	7.82	113.47	108.00
5	B	45	ARG	NE-CZ-NH1	7.81	124.20	120.30
7	a	22(A)	DT	O4'-C1'-N1	7.80	113.46	108.00
1	F	603	ARG	NE-CZ-NH1	7.79	124.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	107	ARG	NE-CZ-NH1	7.74	124.17	120.30
4	A	182	ARG	NE-CZ-NH1	7.72	124.16	120.30
8	b	49(B)	DA	C5-C6-N6	7.68	129.84	123.70
4	A	91	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	F	364	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	F	451	ARG	NE-CZ-NH1	7.63	124.12	120.30
2	C	1246	ARG	NE-CZ-NH1	7.61	124.11	120.30
7	a	64(A)	DC	O4'-C1'-N1	7.59	113.31	108.00
3	D	799	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	F	99	ARG	NE-CZ-NH2	-7.52	116.54	120.30
2	C	548	ARG	NE-CZ-NH1	7.50	124.05	120.30
8	b	64(B)	DA	O4'-C1'-N9	7.49	113.24	108.00
2	C	758	ARG	NE-CZ-NH2	7.47	124.03	120.30
8	b	93(B)	DC	O4'-C1'-N1	7.45	113.22	108.00
8	b	2(B)	DT	O4'-C1'-N1	7.43	113.20	108.00
8	b	5(B)	DA	O4'-C1'-N9	7.42	113.20	108.00
8	b	90(B)	DC	O4'-C1'-N1	7.42	113.19	108.00
8	b	26(B)	DA	O4'-C1'-N9	7.41	113.19	108.00
2	C	245	ARG	NE-CZ-NH1	7.41	124.00	120.30
2	C	473	ARG	NE-CZ-NH2	-7.40	116.60	120.30
8	b	5(B)	DA	C4-C5-N7	-7.40	107.00	110.70
3	D	281	ARG	NE-CZ-NH1	7.40	124.00	120.30
2	C	272	ARG	NE-CZ-NH1	7.39	123.99	120.30
5	B	12	ARG	NE-CZ-NH1	7.39	123.99	120.30
3	D	1355	ARG	NE-CZ-NH2	7.37	123.99	120.30
2	C	529	ARG	NE-CZ-NH1	7.36	123.98	120.30
3	D	738	ARG	NE-CZ-NH1	7.35	123.97	120.30
7	a	57(A)	DC	O4'-C1'-N1	7.35	113.14	108.00
2	C	451	ARG	NE-CZ-NH1	7.32	123.96	120.30
2	C	996	ARG	NE-CZ-NH1	7.18	123.89	120.30
5	B	195	ARG	NE-CZ-NH1	7.17	123.88	120.30
3	D	764	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	F	363	ARG	NE-CZ-NH1	7.14	123.87	120.30
8	b	90(B)	DC	P-O5'-C5'	7.14	132.32	120.90
1	F	588	ARG	NE-CZ-NH1	7.12	123.86	120.30
3	D	431	ARG	NE-CZ-NH1	7.10	123.85	120.30
7	a	6(A)	DG	O4'-C1'-N9	7.09	112.96	108.00
2	C	1216	ARG	NE-CZ-NH1	7.08	123.84	120.30
2	C	1033	ARG	NE-CZ-NH1	7.08	123.84	120.30
6	E	52	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	F	113	ARG	NE-CZ-NH1	7.07	123.83	120.30
7	a	69(A)	DT	O4'-C1'-N1	7.06	112.94	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	156	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	F	422	ARG	NE-CZ-NH1	7.05	123.82	120.30
8	b	84(B)	DT	O4'-C1'-N1	7.04	112.93	108.00
2	C	976	ARG	NE-CZ-NH1	7.03	123.81	120.30
3	D	842	ARG	NE-CZ-NH1	7.02	123.81	120.30
7	a	13(A)	DC	O4'-C1'-N1	7.00	112.90	108.00
8	b	47(B)	DA	C5-C6-N6	6.99	129.29	123.70
6	E	26	ARG	NE-CZ-NH2	6.99	123.80	120.30
7	a	76(A)	DA	O4'-C1'-N9	6.97	112.88	108.00
2	C	542	ARG	NE-CZ-NH1	6.95	123.78	120.30
2	C	97	ARG	NE-CZ-NH1	6.95	123.78	120.30
4	A	158	ARG	NE-CZ-NH1	6.94	123.77	120.30
7	a	20(A)	DG	O4'-C1'-N9	6.94	112.86	108.00
7	a	71(A)	DT	O4'-C1'-N1	6.93	112.85	108.00
2	C	407	ARG	NE-CZ-NH1	6.92	123.76	120.30
2	C	694	ARG	NE-CZ-NH1	6.89	123.75	120.30
5	B	170	ARG	NE-CZ-NH1	6.88	123.74	120.30
8	b	49(B)	DA	C4'-C3'-C2'	-6.88	96.91	103.10
8	b	21(B)	DT	O4'-C1'-N1	6.88	112.81	108.00
1	F	591	GLU	OE1-CD-OE2	-6.87	115.05	123.30
2	C	994	ARG	NE-CZ-NH1	6.85	123.73	120.30
7	a	66(A)	DA	O4'-C1'-N9	6.83	112.78	108.00
3	D	214	ARG	NE-CZ-NH1	6.82	123.71	120.30
2	C	88	ARG	NE-CZ-NH1	6.82	123.71	120.30
5	B	284	ARG	NE-CZ-NH1	6.82	123.71	120.30
2	C	731	ARG	NE-CZ-NH1	6.81	123.71	120.30
8	b	22(B)	DT	O4'-C1'-N1	6.80	112.76	108.00
1	F	476	ARG	NE-CZ-NH1	6.80	123.70	120.30
2	C	151	ARG	NE-CZ-NH1	6.78	123.69	120.30
8	b	49(B)	DA	C5-C6-N1	6.77	121.08	117.70
8	b	19(B)	DT	O4'-C1'-N1	6.75	112.73	108.00
8	b	15(B)	DT	O4'-C1'-N1	6.74	112.72	108.00
3	D	81	ARG	NE-CZ-NH1	6.73	123.66	120.30
2	C	944	ARG	NE-CZ-NH1	6.72	123.66	120.30
8	b	5(B)	DA	C6-C5-N7	6.71	136.99	132.30
8	b	66(B)	DT	C6-C5-C7	-6.69	118.88	122.90
3	D	1290	ARG	NE-CZ-NH1	6.67	123.64	120.30
7	a	53(A)	DT	C6-C5-C7	-6.67	118.90	122.90
3	D	278	ARG	NE-CZ-NH2	-6.66	116.97	120.30
3	D	538	ARG	NE-CZ-NH1	6.65	123.62	120.30
3	D	990	ARG	NE-CZ-NH1	6.63	123.62	120.30
8	b	27(B)	DG	O4'-C1'-N9	6.63	112.64	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	310	ARG	NE-CZ-NH1	6.61	123.61	120.30
7	a	41(A)	DC	O4'-C1'-N1	6.61	112.63	108.00
3	D	1373	ARG	NE-CZ-NH1	6.61	123.60	120.30
3	D	403	ARG	NE-CZ-NH1	6.57	123.59	120.30
3	D	314	ARG	NE-CZ-NH1	6.56	123.58	120.30
8	b	49(B)	DA	C2-N3-C4	6.55	113.88	110.60
5	B	158	ARG	NE-CZ-NH1	6.54	123.57	120.30
3	D	1242	ARG	NE-CZ-NH1	6.54	123.57	120.30
7	a	15(A)	DT	O4'-C1'-N1	6.53	112.57	108.00
3	D	1174	ARG	NE-CZ-NH1	6.52	123.56	120.30
3	D	1262	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	C	18	ARG	NE-CZ-NH1	6.51	123.56	120.30
8	b	53(B)	DT	O4'-C1'-N1	6.51	112.56	108.00
4	A	166	ARG	NE-CZ-NH1	6.50	123.55	120.30
2	C	1034	ARG	NE-CZ-NH1	6.49	123.54	120.30
2	C	211	ARG	NE-CZ-NH1	6.48	123.54	120.30
2	C	592	ARG	NE-CZ-NH1	6.47	123.53	120.30
3	D	901	ARG	NE-CZ-NH1	6.46	123.53	120.30
3	D	1123	ARG	NE-CZ-NH1	6.45	123.52	120.30
8	b	25(B)	DT	C6-C5-C7	-6.44	119.04	122.90
1	F	468	ARG	NE-CZ-NH2	-6.42	117.09	120.30
3	D	1148	ARG	NE-CZ-NH1	6.41	123.50	120.30
2	C	180	ARG	NE-CZ-NH1	6.40	123.50	120.30
7	a	48(A)	DT	C6-C5-C7	-6.40	119.06	122.90
7	a	23(A)	DG	O4'-C1'-N9	6.40	112.48	108.00
8	b	56(B)	DA	O4'-C1'-C2'	-6.40	100.78	105.90
7	a	43(A)	DT	C6-C5-C7	-6.38	119.07	122.90
2	C	1069	ARG	NE-CZ-NH2	-6.38	117.11	120.30
2	C	201	ARG	NE-CZ-NH1	6.37	123.49	120.30
8	b	14(B)	DT	C6-C5-C7	-6.37	119.08	122.90
2	C	101	ARG	NE-CZ-NH1	6.36	123.48	120.30
5	B	166	ARG	NE-CZ-NH1	6.36	123.48	120.30
3	D	425	ARG	NE-CZ-NH1	6.35	123.47	120.30
7	a	92(A)	DT	C6-C5-C7	-6.35	119.09	122.90
4	A	44	ARG	NE-CZ-NH1	6.34	123.47	120.30
6	E	67	ARG	NE-CZ-NH1	6.33	123.47	120.30
7	a	39(A)	DT	C6-C5-C7	-6.32	119.11	122.90
7	a	37(A)	DT	C6-C5-C7	-6.32	119.11	122.90
4	A	12	ARG	NE-CZ-NH1	6.31	123.45	120.30
8	b	49(B)	DA	C4'-C3'-O3'	6.30	125.46	109.70
8	b	30(B)	DT	C6-C5-C7	-6.30	119.12	122.90
8	b	35(B)	DC	O4'-C1'-C2'	-6.29	100.86	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	a	45(A)	DT	O4'-C1'-N1	6.29	112.41	108.00
7	a	46(A)	DT	O4'-C1'-N1	6.29	112.40	108.00
4	A	284	ARG	NE-CZ-NH1	6.29	123.44	120.30
8	b	25(B)	DT	O4'-C1'-N1	6.27	112.39	108.00
2	C	1269	ARG	NE-CZ-NH1	6.27	123.44	120.30
7	a	17(A)	DT	C6-C5-C7	-6.27	119.14	122.90
7	a	75(A)	DT	C6-C5-C7	-6.26	119.14	122.90
1	F	541	ARG	NE-CZ-NH1	6.26	123.43	120.30
7	a	77(A)	DG	P-O3'-C3'	6.24	127.19	119.70
8	b	53(B)	DT	C6-C5-C7	-6.24	119.16	122.90
2	C	267	ARG	NE-CZ-NH1	6.22	123.41	120.30
4	A	33	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	F	103	ARG	NE-CZ-NH1	6.22	123.41	120.30
7	a	88(A)	DT	C6-C5-C7	-6.21	119.17	122.90
7	a	67(A)	DT	C6-C5-C7	-6.21	119.18	122.90
6	E	69	ARG	NE-CZ-NH1	6.20	123.40	120.30
8	b	47(B)	DA	O3'-P-O5'	-6.20	92.22	104.00
7	a	12(A)	DT	C6-C5-C7	-6.20	119.18	122.90
3	D	101	ARG	NE-CZ-NH1	6.19	123.39	120.30
4	A	317	ARG	NE-CZ-NH1	6.18	123.39	120.30
7	a	48(A)	DT	O4'-C1'-N1	6.18	112.33	108.00
8	b	88(B)	DT	O4'-C1'-N1	6.18	112.33	108.00
7	a	62(A)	DC	O4'-C1'-N1	6.18	112.33	108.00
2	C	919	ARG	NE-CZ-NH1	6.17	123.39	120.30
7	a	54(A)	DG	O4'-C1'-N9	6.16	112.31	108.00
8	b	1(B)	DT	C6-C5-C7	-6.15	119.21	122.90
7	a	44(A)	DT	C6-C5-C7	-6.15	119.21	122.90
7	a	22(A)	DT	C6-C5-C7	-6.15	119.21	122.90
8	b	77(B)	DT	C6-C5-C7	-6.14	119.21	122.90
7	a	3(A)	DT	C6-C5-C7	-6.14	119.22	122.90
8	b	68(B)	DT	C6-C5-C7	-6.14	119.22	122.90
5	B	182	ARG	NE-CZ-NH1	6.13	123.37	120.30
8	b	2(B)	DT	C6-C5-C7	-6.13	119.22	122.90
8	b	33(B)	DG	O4'-C1'-N9	6.12	112.29	108.00
7	a	36(A)	DG	O4'-C1'-N9	6.12	112.28	108.00
3	D	137	ARG	NE-CZ-NH1	6.12	123.36	120.30
7	a	4(A)	DT	C6-C5-C7	-6.12	119.23	122.90
2	C	687	ARG	NE-CZ-NH1	6.11	123.36	120.30
3	D	278	ARG	NE-CZ-NH1	6.11	123.35	120.30
8	b	88(B)	DT	C6-C5-C7	-6.11	119.24	122.90
2	C	275	ARG	NE-CZ-NH1	6.10	123.35	120.30
7	a	45(A)	DT	C6-C5-C7	-6.10	119.24	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	b	29(B)	DT	C6-C5-C7	-6.10	119.24	122.90
8	b	9(B)	DT	C6-C5-C7	-6.10	119.24	122.90
2	C	758	ARG	NH1-CZ-NH2	-6.09	112.70	119.40
3	D	1075	ARG	NE-CZ-NH1	6.08	123.34	120.30
3	D	1341	ARG	NE-CZ-NH1	6.08	123.34	120.30
8	b	60(B)	DC	O4'-C1'-N1	6.08	112.26	108.00
1	F	150	ARG	NE-CZ-NH1	6.07	123.33	120.30
6	E	91	ARG	NE-CZ-NH1	6.07	123.33	120.30
7	a	21(A)	DT	C6-C5-C7	-6.06	119.26	122.90
7	a	15(A)	DT	C6-C5-C7	-6.06	119.26	122.90
8	b	81(B)	DT	C6-C5-C7	-6.06	119.26	122.90
7	a	25(A)	DT	C6-C5-C7	-6.05	119.27	122.90
8	b	45(B)	DT	C6-C5-C7	-6.05	119.27	122.90
8	b	45(B)	DT	O4'-C1'-N1	6.05	112.24	108.00
7	a	59(A)	DT	C6-C5-C7	-6.05	119.27	122.90
7	a	94(A)	DA	O4'-C1'-N9	6.05	112.23	108.00
2	C	74	ARG	NE-CZ-NH1	6.04	123.32	120.30
7	a	68(A)	DC	O4'-C1'-N1	6.04	112.23	108.00
3	D	1222	ARG	NE-CZ-NH1	6.04	123.32	120.30
7	a	69(A)	DT	C6-C5-C7	-6.04	119.28	122.90
7	a	52(A)	DT	C6-C5-C7	-6.04	119.28	122.90
8	b	23(B)	DT	O4'-C1'-N1	6.04	112.22	108.00
7	a	34(A)	DC	O4'-C1'-N1	6.03	112.22	108.00
8	b	15(B)	DT	C6-C5-C7	-6.03	119.28	122.90
7	a	31(A)	DT	C6-C5-C7	-6.03	119.28	122.90
1	F	339	ARG	CD-NE-CZ	6.03	132.04	123.60
8	b	59(B)	DC	O4'-C1'-N1	6.02	112.22	108.00
5	B	219	ARG	NE-CZ-NH1	6.02	123.31	120.30
7	a	3(A)	DT	O4'-C1'-N1	6.02	112.21	108.00
8	b	23(B)	DT	C6-C5-C7	-6.02	119.29	122.90
8	b	22(B)	DT	C6-C5-C7	-6.02	119.29	122.90
7	a	28(A)	DT	C6-C5-C7	-6.01	119.30	122.90
7	a	52(A)	DT	O4'-C1'-N1	6.00	112.20	108.00
1	F	441	ARG	NE-CZ-NH1	6.00	123.30	120.30
8	b	84(B)	DT	C6-C5-C7	-6.00	119.30	122.90
7	a	4(A)	DT	O4'-C1'-N1	6.00	112.20	108.00
7	a	1(A)	DT	C6-C5-C7	-5.99	119.31	122.90
2	C	352	ARG	NE-CZ-NH1	5.98	123.29	120.30
8	b	86(B)	DC	O4'-C1'-N1	5.97	112.18	108.00
7	a	71(A)	DT	C6-C5-C7	-5.95	119.33	122.90
7	a	58(A)	DG	O4'-C1'-N9	5.95	112.16	108.00
8	b	21(B)	DT	C6-C5-C7	-5.94	119.34	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	b	58(B)	DA	O4'-C1'-N9	5.93	112.15	108.00
2	C	758	ARG	NE-CZ-NH1	5.93	123.26	120.30
3	D	1149	ARG	NE-CZ-NH1	5.93	123.26	120.30
3	D	538	ARG	NE-CZ-NH2	5.92	123.26	120.30
8	b	54(B)	DG	O4'-C1'-N9	5.91	112.14	108.00
7	a	90(A)	DT	C6-C5-C7	-5.90	119.36	122.90
4	A	195	ARG	NE-CZ-NH1	5.89	123.25	120.30
8	b	85(B)	DT	C6-C5-C7	-5.89	119.36	122.90
2	C	233	ARG	NE-CZ-NH1	5.89	123.25	120.30
3	D	275	ARG	NE-CZ-NH1	5.89	123.25	120.30
2	C	1331	ARG	NE-CZ-NH1	5.87	123.24	120.30
8	b	11(B)	DG	O4'-C4'-C3'	5.87	109.52	106.00
2	C	54	ARG	NE-CZ-NH1	5.87	123.23	120.30
8	b	19(B)	DT	C6-C5-C7	-5.84	119.39	122.90
2	C	378	ARG	NE-CZ-NH1	5.84	123.22	120.30
3	D	883	ARG	NE-CZ-NH1	5.81	123.21	120.30
8	b	41(B)	DC	O4'-C1'-N1	5.81	112.07	108.00
7	a	43(A)	DT	O4'-C4'-C3'	5.79	109.47	106.00
7	a	50(A)	DA	O4'-C4'-C3'	5.78	109.47	106.00
3	D	634	ARG	NE-CZ-NH1	5.78	123.19	120.30
8	b	83(B)	DA	O4'-C1'-N9	5.77	112.04	108.00
8	b	49(B)	DA	C5-N7-C8	-5.77	101.02	103.90
8	b	18(B)	DC	O4'-C1'-N1	5.76	112.03	108.00
2	C	1059	ARG	NE-CZ-NH1	5.76	123.18	120.30
3	D	47	ARG	NE-CZ-NH2	5.75	123.18	120.30
4	A	238	ARG	NE-CZ-NH1	5.75	123.18	120.30
2	C	540	ARG	NE-CZ-NH2	-5.75	117.42	120.30
3	D	731	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	F	218	ARG	NE-CZ-NH1	5.73	123.16	120.30
8	b	92(B)	DA	OP1-P-O3'	5.73	117.80	105.20
3	D	538	ARG	NH1-CZ-NH2	-5.72	113.10	119.40
7	a	42(A)	DA	O4'-C1'-N9	5.72	112.00	108.00
2	C	841	ARG	NE-CZ-NH1	5.71	123.16	120.30
8	b	69(B)	DT	C6-C5-C7	-5.71	119.47	122.90
3	D	738	ARG	NE-CZ-NH2	-5.70	117.45	120.30
8	b	6(B)	DT	C6-C5-C7	-5.70	119.48	122.90
8	b	87(B)	DC	O4'-C1'-N1	5.69	111.98	108.00
3	D	123	ARG	NE-CZ-NH1	5.68	123.14	120.30
7	a	43(A)	DT	O4'-C1'-N1	5.68	111.98	108.00
5	B	150	ARG	NE-CZ-NH2	-5.68	117.46	120.30
2	C	1223	ARG	NE-CZ-NH1	5.67	123.14	120.30
8	b	94(B)	DA	O4'-C1'-N9	5.67	111.97	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	a	79(A)	DG	O4'-C1'-N9	5.67	111.97	108.00
3	D	322	ARG	NE-CZ-NH1	5.66	123.13	120.30
3	D	1355	ARG	NE-CZ-NH1	-5.66	117.47	120.30
7	a	38(A)	DC	O4'-C1'-N1	5.64	111.95	108.00
1	F	558	VAL	CA-CB-CG2	-5.64	102.44	110.90
3	D	1203	ARG	NE-CZ-NH1	5.63	123.12	120.30
3	D	838	ARG	NE-CZ-NH1	5.63	123.12	120.30
8	b	32(B)	DT	C6-C5-C7	-5.63	119.52	122.90
2	C	436	ARG	NE-CZ-NH1	5.62	123.11	120.30
8	b	24(B)	DA	O4'-C1'-N9	5.62	111.93	108.00
1	F	374	ARG	NE-CZ-NH1	5.61	123.11	120.30
7	a	28(A)	DT	O4'-C4'-C3'	5.61	109.37	106.00
7	a	46(A)	DT	O4'-C4'-C3'	5.61	109.37	106.00
2	C	1231	TYR	CB-CG-CD1	-5.61	117.63	121.00
8	b	29(B)	DT	O4'-C1'-N1	5.61	111.92	108.00
3	D	814	CYS	CA-CB-SG	5.61	124.09	114.00
3	D	1304	ARG	NE-CZ-NH1	5.61	123.10	120.30
8	b	16(B)	DC	O4'-C1'-N1	5.60	111.92	108.00
7	a	46(A)	DT	C6-C5-C7	-5.59	119.54	122.90
7	a	9(A)	DG	O4'-C1'-N9	5.59	111.91	108.00
3	D	259	ARG	NE-CZ-NH1	5.58	123.09	120.30
8	b	47(B)	DA	P-O5'-C5'	5.57	129.82	120.90
3	D	362	ARG	NE-CZ-NH1	5.57	123.08	120.30
2	C	200	ARG	NE-CZ-NH2	-5.55	117.52	120.30
3	D	1140	ARG	NE-CZ-NH1	5.55	123.07	120.30
7	a	55(A)	DT	C4-C5-C6	5.55	121.33	118.00
3	D	709	ARG	NE-CZ-NH1	5.55	123.07	120.30
2	C	821	ARG	NE-CZ-NH1	5.54	123.07	120.30
4	A	235	ARG	NH1-CZ-NH2	-5.54	113.31	119.40
8	b	66(B)	DT	C4-C5-C6	5.53	121.32	118.00
7	a	53(A)	DT	O4'-C4'-C3'	5.53	109.32	106.00
7	a	55(A)	DT	C6-C5-C7	-5.52	119.59	122.90
7	a	32(A)	DG	O4'-C1'-N9	5.51	111.86	108.00
7	a	27(A)	DA	O4'-C4'-C3'	5.51	109.31	106.00
4	A	255	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	F	15	ARG	NH1-CZ-NH2	-5.50	113.35	119.40
6	E	28	ARG	NE-CZ-NH1	5.49	123.04	120.30
8	b	30(B)	DT	O4'-C1'-N1	5.47	111.83	108.00
1	F	21	TYR	CB-CG-CD2	-5.47	117.72	121.00
2	C	936	ARG	NE-CZ-NH1	5.47	123.03	120.30
8	b	1(B)	DT	C4-C5-C6	5.46	121.28	118.00
8	b	79(B)	DC	O4'-C1'-N1	5.46	111.82	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	a	52(A)	DT	C4-C5-C6	5.46	121.27	118.00
2	C	1106	ARG	CD-NE-CZ	5.45	131.24	123.60
8	b	31(B)	DG	O4'-C1'-N9	5.45	111.82	108.00
8	b	8(B)	DG	O4'-C1'-N9	5.45	111.82	108.00
7	a	25(A)	DT	C4-C5-C6	5.44	121.27	118.00
2	C	1301	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	F	385	ARG	NE-CZ-NH1	5.43	123.01	120.30
2	C	268	ARG	CD-NE-CZ	5.42	131.19	123.60
7	a	59(A)	DT	O4'-C1'-N1	5.41	111.78	108.00
1	F	468	ARG	NE-CZ-NH1	5.40	123.00	120.30
8	b	14(B)	DT	C4-C5-C6	5.40	121.24	118.00
7	a	45(A)	DT	C4-C5-C6	5.39	121.24	118.00
7	a	15(A)	DT	C4-C5-C6	5.39	121.23	118.00
8	b	44(B)	DC	O4'-C1'-N1	5.39	111.77	108.00
7	a	44(A)	DT	C4-C5-C6	5.38	121.23	118.00
8	b	21(B)	DT	C4-C5-C6	5.38	121.23	118.00
7	a	40(A)	DC	O4'-C1'-N1	5.37	111.76	108.00
2	C	465	ARG	NE-CZ-NH1	5.37	122.98	120.30
8	b	13(B)	DG	O4'-C1'-N9	5.36	111.75	108.00
3	D	1371	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	F	558	VAL	CB-CA-C	-5.36	101.22	111.40
7	a	60(A)	DG	O4'-C4'-C3'	5.35	109.21	106.00
4	A	218	ARG	NE-CZ-NH1	5.35	122.97	120.30
7	a	53(A)	DT	C4-C5-C6	5.34	121.21	118.00
7	a	37(A)	DT	C4-C5-C6	5.34	121.20	118.00
7	a	3(A)	DT	C4-C5-C6	5.34	121.20	118.00
2	C	158	ASP	CB-CG-OD1	5.33	123.10	118.30
8	b	85(B)	DT	O4'-C4'-C3'	5.33	109.20	106.00
8	b	23(B)	DT	C5-C6-N1	-5.32	120.51	123.70
3	D	1330	ARG	NE-CZ-NH2	-5.32	117.64	120.30
7	a	81(A)	DA	O4'-C4'-C3'	5.32	109.19	106.00
7	a	46(A)	DT	C5-C6-N1	-5.31	120.52	123.70
7	a	48(A)	DT	C4-C5-C6	5.30	121.18	118.00
8	b	50(B)	DA	O5'-C5'-C4'	5.29	124.23	111.00
3	D	943	ARG	NE-CZ-NH2	-5.29	117.66	120.30
8	b	68(B)	DT	C4-C5-C6	5.29	121.17	118.00
8	b	25(B)	DT	C4-C5-C6	5.29	121.17	118.00
8	b	85(B)	DT	C4-C5-C6	5.28	121.17	118.00
1	F	373	ARG	NE-CZ-NH1	5.27	122.94	120.30
7	a	17(A)	DT	C4-C5-C6	5.27	121.16	118.00
7	a	61(A)	DC	O4'-C4'-C3'	5.27	109.16	106.00
3	D	1149	ARG	NE-CZ-NH2	-5.27	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	a	74(A)	DA	O4'-C1'-C2'	-5.26	101.69	105.90
6	E	90	ARG	NE-CZ-NH1	5.26	122.93	120.30
8	b	46(B)	DG	O5'-P-OP2	5.25	117.01	110.70
2	C	143	ARG	NE-CZ-NH1	5.25	122.92	120.30
7	a	29(A)	DA	O4'-C4'-C3'	5.25	109.15	106.00
8	b	53(B)	DT	C4-C5-C6	5.24	121.14	118.00
7	a	4(A)	DT	C4-C5-C6	5.24	121.14	118.00
8	b	69(B)	DT	C4-C5-C6	5.23	121.14	118.00
8	b	22(B)	DT	C4-C5-C6	5.23	121.14	118.00
8	b	88(B)	DT	C4-C5-C6	5.23	121.14	118.00
8	b	77(B)	DT	C4-C5-C6	5.22	121.13	118.00
7	a	67(A)	DT	C4-C5-C6	5.21	121.13	118.00
1	F	281	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	F	423	ARG	NE-CZ-NH2	-5.21	117.70	120.30
3	D	1231	ARG	NE-CZ-NH1	5.21	122.90	120.30
8	b	29(B)	DT	C4-C5-C6	5.21	121.12	118.00
7	a	59(A)	DT	C4-C5-C6	5.20	121.12	118.00
3	D	1258	ARG	NE-CZ-NH1	5.19	122.90	120.30
7	a	1(A)	DT	C4-C5-C6	5.19	121.12	118.00
3	D	346	ARG	NE-CZ-NH1	5.19	122.89	120.30
3	D	1133	ASP	C-N-CA	5.19	134.67	121.70
7	a	61(A)	DC	O4'-C1'-N1	5.19	111.63	108.00
3	D	1194	ARG	NE-CZ-NH1	5.19	122.89	120.30
3	D	1369	ARG	NE-CZ-NH1	5.18	122.89	120.30
8	b	45(B)	DT	C4-C5-C6	5.18	121.11	118.00
8	b	17(B)	DC	O4'-C1'-N1	5.18	111.62	108.00
8	b	80(B)	DA	O4'-C4'-C3'	5.17	109.10	106.00
8	b	9(B)	DT	C4-C5-C6	5.17	121.10	118.00
8	b	65(B)	DC	O4'-C4'-C3'	5.16	109.10	106.00
5	B	218	ARG	NE-CZ-NH1	5.16	122.88	120.30
8	b	74(B)	DA	P-O3'-C3'	5.16	125.89	119.70
8	b	30(B)	DT	C4-C5-C6	5.15	121.09	118.00
7	a	69(A)	DT	C4-C5-C6	5.15	121.09	118.00
3	D	314	ARG	NE-CZ-NH2	-5.15	117.73	120.30
7	a	75(A)	DT	C4-C5-C6	5.15	121.09	118.00
7	a	55(A)	DT	O4'-C1'-N1	5.15	111.60	108.00
8	b	66(B)	DT	P-O3'-C3'	5.15	125.88	119.70
7	a	43(A)	DT	C4-C5-C6	5.14	121.09	118.00
7	a	22(A)	DT	C4-C5-C6	5.14	121.09	118.00
3	D	515	ARG	NE-CZ-NH1	5.14	122.87	120.30
8	b	2(B)	DT	C4-C5-C6	5.14	121.08	118.00
7	a	8(A)	DG	O4'-C4'-C3'	5.14	109.08	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	a	67(A)	DT	O4'-C1'-N1	5.13	111.59	108.00
1	F	584	ARG	NE-CZ-NH1	5.13	122.87	120.30
3	D	202	ARG	NE-CZ-NH1	5.13	122.87	120.30
8	b	84(B)	DT	C4-C5-C6	5.13	121.08	118.00
7	a	31(A)	DT	C4-C5-C6	5.12	121.07	118.00
8	b	14(B)	DT	O4'-C4'-C3'	5.12	109.07	106.00
7	a	28(A)	DT	C4-C5-C6	5.12	121.07	118.00
8	b	48(B)	DT	O3'-P-O5'	5.11	113.71	104.00
8	b	49(B)	DA	O4'-C4'-C3'	5.11	109.07	106.00
7	a	88(A)	DT	C4-C5-C6	5.10	121.06	118.00
8	b	76(B)	DG	O4'-C1'-N9	5.10	111.57	108.00
2	C	359	ARG	NE-CZ-NH2	5.10	122.85	120.30
7	a	92(A)	DT	C4-C5-C6	5.09	121.06	118.00
7	a	49(A)	DC	O4'-C1'-N1	5.09	111.56	108.00
8	b	32(B)	DT	C4-C5-C6	5.09	121.05	118.00
8	b	92(B)	DA	O4'-C1'-N9	5.08	111.56	108.00
7	a	27(A)	DA	N1-C6-N6	-5.08	115.55	118.60
3	D	610	ARG	NE-CZ-NH2	-5.07	117.76	120.30
4	A	170	ARG	NE-CZ-NH1	5.07	122.83	120.30
8	b	15(B)	DT	C4-C5-C6	5.07	121.04	118.00
3	D	417	ARG	NE-CZ-NH1	5.06	122.83	120.30
7	a	39(A)	DT	C4-C5-C6	5.06	121.04	118.00
8	b	21(B)	DT	C5-C6-N1	-5.06	120.66	123.70
7	a	12(A)	DT	C4-C5-C6	5.06	121.03	118.00
8	b	19(B)	DT	C4-C5-C6	5.05	121.03	118.00
7	a	71(A)	DT	C4-C5-C6	5.05	121.03	118.00
2	C	1269	ARG	CD-NE-CZ	5.04	130.66	123.60
1	F	95	THR	C-N-CA	5.04	134.30	121.70
7	a	63(A)	DA	O4'-C1'-N9	5.04	111.53	108.00
2	C	790	ASP	CB-CG-OD1	5.03	122.83	118.30
7	a	46(A)	DT	C4-C5-C6	5.03	121.02	118.00
1	F	495	ARG	NE-CZ-NH1	5.03	122.81	120.30
7	a	33(A)	DG	O4'-C1'-N9	5.03	111.52	108.00
7	a	17(A)	DT	O4'-C1'-N1	5.02	111.51	108.00
7	a	44(A)	DT	O4'-C1'-N1	5.01	111.51	108.00
7	a	72(A)	DA	O4'-C4'-C3'	5.01	109.00	106.00
4	A	321	TRP	CB-CG-CD2	5.01	133.11	126.60
5	B	238	ARG	NE-CZ-NH2	5.00	122.80	120.30

There are no chirality outliers.

All (186) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	13	LEU	Peptide
4	A	160	HIS	Peptide
4	A	162	GLU	Peptide
4	A	170	ARG	Sidechain
4	A	182	ARG	Sidechain
4	A	191	ARG	Sidechain
4	A	233	ASP	Peptide
4	A	246	LYS	Peptide
4	A	255	ARG	Sidechain
4	A	77	ASP	Peptide
5	B	102	LEU	Peptide
5	B	12	ARG	Sidechain
5	B	150	ARG	Sidechain
5	B	170	ARG	Sidechain
5	B	208	ASN	Peptide
5	B	235	ARG	Sidechain
5	B	244	GLU	Peptide
5	B	310	ARG	Sidechain
5	B	7	GLU	Peptide
5	B	85	LEU	Peptide
2	C	1027	LYS	Peptide
2	C	1034	ARG	Peptide
2	C	1058	ARG	Sidechain
2	C	1069	ARG	Sidechain
2	C	1156	ARG	Sidechain
2	C	1188	ASP	Peptide
2	C	1213	TYR	Sidechain
2	C	1229	TYR	Sidechain
2	C	168	GLY	Peptide
2	C	18	ARG	Sidechain
2	C	200	ARG	Sidechain
2	C	240	GLU	Peptide
2	C	245	ARG	Sidechain
2	C	247	ARG	Sidechain
2	C	342	ASP	Peptide
2	C	367	TYR	Sidechain
2	C	435	ILE	Peptide
2	C	450	ASN	Peptide
2	C	578	TYR	Sidechain
2	C	742	TYR	Sidechain
2	C	756	TYR	Sidechain
2	C	821	ARG	Sidechain
2	C	892	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	C	92	TYR	Sidechain
2	C	944	ARG	Sidechain
3	D	101	ARG	Sidechain
3	D	1014	GLY	Peptide
3	D	1048	ARG	Sidechain
3	D	1054	THR	Peptide
3	D	109	SER	Peptide
3	D	1173	ARG	Sidechain
3	D	1206	ARG	Sidechain
3	D	1258	ARG	Sidechain
3	D	1262	ARG	Sidechain
3	D	1339	GLY	Peptide
3	D	1369	ARG	Sidechain
3	D	153	ASN	Peptide
3	D	165	TYR	Peptide
3	D	250	ARG	Peptide
3	D	346	ARG	Sidechain
3	D	38	VAL	Peptide
3	D	388	ARG	Sidechain
3	D	46	TYR	Sidechain
3	D	481	ARG	Sidechain
3	D	503	SER	Peptide
3	D	523	MET	Peptide
3	D	571	ASP	Peptide
3	D	642	ASP	Peptide
3	D	744	ARG	Sidechain
3	D	799	ARG	Sidechain
3	D	933	ARG	Sidechain
3	D	943	ARG	Sidechain
3	D	962	ASN	Peptide
3	D	963	VAL	Peptide
6	E	15	ASN	Peptide
6	E	17	PHE	Peptide
6	E	28	ARG	Sidechain
6	E	52	ARG	Sidechain
1	F	157	ARG	Sidechain
1	F	170	ALA	Peptide
1	F	232	ARG	Sidechain
1	F	260	ARG	Peptide
1	F	343	LYS	Peptide
1	F	353	LEU	Peptide
1	F	373	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	F	430	TYR	Sidechain
1	F	465	ARG	Sidechain
1	F	474	MET	Peptide
1	F	476	ARG	Sidechain
1	F	495	ARG	Sidechain
1	F	514	ASP	Peptide
1	F	584	ARG	Sidechain
1	F	585	GLU	Peptide
1	F	586	ARG	Sidechain
1	F	603	ARG	Sidechain
1	F	93	ARG	Sidechain
1	F	99	ARG	Sidechain
7	a	10(A)	DA	Sidechain
7	a	11(A)	DA	Sidechain
7	a	16(A)	DG	Sidechain
7	a	17(A)	DT	Sidechain
7	a	18(A)	DA	Sidechain
7	a	2(A)	DG	Sidechain
7	a	20(A)	DG	Sidechain
7	a	22(A)	DT	Sidechain
7	a	26(A)	DA	Sidechain
7	a	27(A)	DA	Sidechain
7	a	31(A)	DT	Sidechain
7	a	33(A)	DG	Sidechain
7	a	35(A)	DG	Sidechain
7	a	38(A)	DC	Sidechain
7	a	39(A)	DT	Sidechain
7	a	42(A)	DA	Sidechain
7	a	44(A)	DT	Sidechain
7	a	45(A)	DT	Sidechain
7	a	46(A)	DT	Sidechain
7	a	49(A)	DC	Sidechain
7	a	5(A)	DG	Sidechain
7	a	51(A)	DG	Sidechain
7	a	52(A)	DT	Sidechain
7	a	55(A)	DT	Sidechain
7	a	56(A)	DG	Sidechain
7	a	59(A)	DT	Sidechain
7	a	6(A)	DG	Sidechain
7	a	60(A)	DG	Sidechain
7	a	62(A)	DC	Sidechain
7	a	63(A)	DA	Sidechain

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Mol	Chain	Res	Type	Group
7	a	65(A)	DA	Sidechain
7	a	66(A)	DA	Sidechain
7	a	69(A)	DT	Sidechain
7	a	70(A)	DA	Sidechain
7	a	71(A)	DT	Sidechain
7	a	72(A)	DA	Sidechain
7	a	73(A)	DA	Sidechain
7	a	76(A)	DA	Sidechain
7	a	78(A)	DG	Sidechain
7	a	8(A)	DG	Sidechain
7	a	80(A)	DA	Sidechain
7	a	83(A)	DG	Sidechain
7	a	86(A)	DA	Sidechain
7	a	90(A)	DT	Sidechain
7	a	93(A)	DA	Sidechain
8	b	10(B)	DG	Sidechain
8	b	11(B)	DG	Sidechain
8	b	13(B)	DG	Sidechain
8	b	14(B)	DT	Sidechain
8	b	15(B)	DT	Sidechain
8	b	19(B)	DT	Sidechain
8	b	2(B)	DT	Sidechain
8	b	21(B)	DT	Sidechain
8	b	22(B)	DT	Sidechain
8	b	23(B)	DT	Sidechain
8	b	24(B)	DA	Sidechain
8	b	25(B)	DT	Sidechain
8	b	26(B)	DA	Sidechain
8	b	28(B)	DA	Sidechain
8	b	31(B)	DG	Sidechain
8	b	33(B)	DG	Sidechain
8	b	34(B)	DG	Sidechain
8	b	38(B)	DG	Sidechain
8	b	39(B)	DC	Sidechain
8	b	40(B)	DA	Sidechain
8	b	41(B)	DC	Sidechain
8	b	42(B)	DA	Sidechain
8	b	44(B)	DC	Sidechain
8	b	47(B)	DA	Sidechain
8	b	52(B)	DA	Sidechain
8	b	54(B)	DG	Sidechain
8	b	55(B)	DG	Sidechain

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Mol	Chain	Res	Type	Group
8	b	56(B)	DA	Sidechain
8	b	58(B)	DA	Sidechain
8	b	61(B)	DG	Sidechain
8	b	65(B)	DC	Sidechain
8	b	67(B)	DA	Sidechain
8	b	7(B)	DA	Sidechain
8	b	72(B)	DC	Sidechain
8	b	79(B)	DC	Sidechain
8	b	8(B)	DG	Sidechain
8	b	82(B)	DG	Sidechain
8	b	84(B)	DT	Sidechain
8	b	86(B)	DC	Sidechain
8	b	89(B)	DC	Sidechain
8	b	90(B)	DC	Sidechain
8	b	92(B)	DA	Sidechain
8	b	93(B)	DC	Sidechain
8	b	94(B)	DA	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4495	4523	4521	2	0
2	C	10577	10595	10591	6	0
3	D	10538	10758	10755	6	0
4	A	2473	2528	2525	1	0
5	B	2412	2471	2468	2	0
6	E	709	722	719	5	0
7	a	1931	1064	1065	0	0
8	b	1917	1061	1061	0	0
All	All	35052	33722	33705	22	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 1.

All (22) 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)
5:B:264:VAL:HG12	5:B:265:ARG:H	1.56	0.71
2:C:546:GLU:H	2:C:546:GLU:CD	2.11	0.53
2:C:1184:THR:HG23	2:C:1189:GLY:HA2	1.91	0.53
6:E:38:LEU:H	6:E:59:ILE:HD13	1.76	0.51
4:A:232:VAL:HG22	4:A:233:ASP:H	1.78	0.49
2:C:426:ILE:HG22	2:C:430:LYS:HE3	1.96	0.48
6:E:25:ARG:HH11	6:E:61:ASN:ND2	2.12	0.47
6:E:59:ILE:HG22	6:E:59:ILE:O	2.16	0.45
3:D:86:GLU:CD	3:D:86:GLU:H	2.20	0.45
1:F:558:VAL:C	1:F:560:ARG:H	2.18	0.44
6:E:38:LEU:HB2	6:E:59:ILE:HG12	1.99	0.44
3:D:325:LYS:HE3	3:D:329:ASP:CB	2.47	0.44
1:F:558:VAL:HG21	1:F:590:ILE:HG22	2.00	0.44
5:B:234:LEU:HD12	5:B:234:LEU:H	1.83	0.43
3:D:959:LYS:HE2	3:D:959:LYS:HA	2.01	0.43
3:D:570:LYS:HE2	3:D:589:TYR:CD2	2.54	0.42
2:C:81:ASP:HA	2:C:92:TYR:CE1	2.54	0.41
2:C:798:GLN:HE22	2:C:827:ARG:HG2	1.85	0.41
2:C:1184:THR:HG23	2:C:1189:GLY:CA	2.51	0.40
6:E:26:ARG:NH2	6:E:59:ILE:HG22	2.37	0.40
3:D:544:LEU:HD11	3:D:631:TYR:CD1	2.57	0.40
3:D:512:TYR:CE2	3:D:635:SER:HA	2.57	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
1	F	556/558 (100%)	421 (76%)	103 (18%)	32 (6%)	1 14
2	C	1339/1341 (100%)	1085 (81%)	193 (14%)	61 (5%)	2 17
3	D	1356/1358 (100%)	1089 (80%)	203 (15%)	64 (5%)	2 16
4	A	314/316 (99%)	223 (71%)	71 (23%)	20 (6%)	1 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	B	308/310 (99%)	202 (66%)	73 (24%)	33 (11%)	0 6
6	E	88/90 (98%)	71 (81%)	12 (14%)	5 (6%)	1 14
All	All	3961/3973 (100%)	3091 (78%)	655 (16%)	215 (5%)	3 15

All (215) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	9	LEU
1	F	37	ASP
1	F	89	SER
1	F	96	ASP
1	F	110	LEU
1	F	111	LEU
1	F	299	LYS
1	F	515	GLU
1	F	522	ASP
1	F	558	VAL
1	F	559	LEU
2	C	110	PRO
2	C	113	THR
2	C	192	ASP
2	C	234	ASP
2	C	296	VAL
2	C	328	SER
2	C	341	LEU
2	C	596	ASP
2	C	1056	VAL
2	C	1238	LEU
2	C	1313	HIS
3	D	264	ASP
3	D	321	LYS
3	D	551	ARG
3	D	585	LYS
3	D	832	LYS
3	D	947	GLU
3	D	1094	ASP
3	D	1206	ARG
3	D	1273	ASP
4	A	22	THR
4	A	159	ILE
4	A	168	ILE

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Mol	Chain	Res	Type
4	A	247	PRO
5	B	20	SER
5	B	77	ASP
5	B	150	ARG
5	B	161	SER
5	B	185	TYR
5	B	192	VAL
5	B	236	ASP
5	B	244	GLU
5	B	264	VAL
5	B	286	GLU
5	B	294	ASN
1	F	107	THR
1	F	238	LYS
1	F	333	VAL
1	F	396	ASN
1	F	398	GLY
1	F	562	ARG
2	C	214	ASN
2	C	265	LYS
2	C	340	ASP
2	C	443	ASP
2	C	472	GLU
2	C	634	VAL
2	C	828	PHE
2	C	904	ALA
2	C	922	ASN
2	C	1004	ASP
2	C	1243	MET
2	C	1297	ASP
3	D	17	PHE
3	D	58	CYS
3	D	72	CYS
3	D	552	ILE
3	D	649	LYS
3	D	708	ASN
3	D	840	LEU
3	D	1055	GLY
3	D	1138	LEU
3	D	1209	VAL
4	A	21	SER
4	A	174	ASP

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Mol	Chain	Res	Type
4	A	175	ALA
5	B	22	THR
5	B	72	GLU
5	B	124	VAL
5	B	159	ILE
5	B	210	THR
1	F	114	GLU
1	F	324	LYS
2	C	41	GLN
2	C	161	LYS
2	C	162	GLY
2	C	166	SER
2	C	269	ILE
2	C	362	ALA
2	C	398	SER
2	C	420	LEU
2	C	648	ASP
2	C	718	ALA
2	C	756	TYR
2	C	858	GLY
2	C	900	LYS
2	C	982	GLY
2	C	990	ASP
2	C	1058	ARG
2	C	1256	GLN
3	D	46	TYR
3	D	165	TYR
3	D	166	LEU
3	D	189	LEU
3	D	201	LEU
3	D	431	ARG
3	D	519	ASN
3	D	522	GLY
3	D	533	ALA
3	D	681	LYS
3	D	707	ILE
3	D	717	VAL
3	D	742	GLY
3	D	814	CYS
3	D	1128	SER
3	D	1170	LYS
3	D	1192	LYS

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Mol	Chain	Res	Type
3	D	1360	GLY
4	A	62	ASP
4	A	193	GLU
4	A	223	ILE
5	B	17	GLU
5	B	26	VAL
5	B	78	ILE
5	B	246	LYS
5	B	261	GLU
5	B	265	ARG
6	E	33	GLY
6	E	46	THR
1	F	78	GLU
1	F	323	ASN
1	F	339	ARG
1	F	397	ARG
2	C	259	GLY
2	C	414	ILE
2	C	436	ARG
2	C	517	GLN
2	C	639	LYS
2	C	808	ASN
2	C	880	GLY
2	C	1166	ASP
2	C	1263	ALA
3	D	53	ARG
3	D	68	TYR
3	D	77	ARG
3	D	119	SER
3	D	251	PRO
3	D	715	LYS
3	D	718	SER
3	D	731	ARG
3	D	892	PHE
3	D	936	HIS
3	D	1166	GLY
3	D	1297	LYS
3	D	1318	SER
3	D	1358	PRO
3	D	1373	ARG
4	A	68	TYR
4	A	95	LYS

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Mol	Chain	Res	Type
4	A	224	LEU
4	A	275	ILE
5	B	62	ASP
5	B	233	ASP
1	F	77	ALA
1	F	377	LYS
1	F	509	THR
1	F	556	ALA
2	C	248	GLY
2	C	250	THR
2	C	329	GLY
2	C	450	ASN
2	C	631	GLU
2	C	1084	ASP
3	D	50	LYS
3	D	131	PRO
3	D	161	THR
3	D	827	GLU
3	D	1234	VAL
3	D	1247	LYS
4	A	72	GLU
4	A	120	ASP
4	A	217	ILE
5	B	32	GLU
6	E	42	GLU
6	E	44	ASP
1	F	170	ALA
2	C	4	SER
2	C	1184	THR
3	D	383	GLY
3	D	461	PHE
3	D	1171	GLY
4	A	89	ALA
5	B	47	LEU
5	B	109	PRO
6	E	5	THR
1	F	52	GLY
1	F	512	GLY
2	C	1159	VAL
2	C	1318	GLY
2	C	1320	PRO
3	D	938	GLY

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Mol	Chain	Res	Type
3	D	1043	GLY
4	A	246	LYS
5	B	63	GLY
5	B	275	ILE
3	D	532	PRO
5	B	168	ILE
1	F	511	ILE
4	A	53	GLY
5	B	64	VAL
5	B	287	VAL
2	C	597	GLY
5	B	293	PRO
1	F	521	ILE

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	F	491/491 (100%)	448 (91%)	43 (9%)	8 25
2	C	1156/1156 (100%)	1083 (94%)	73 (6%)	15 36
3	D	1132/1132 (100%)	1067 (94%)	65 (6%)	17 38
4	A	276/276 (100%)	243 (88%)	33 (12%)	4 16
5	B	270/270 (100%)	239 (88%)	31 (12%)	4 16
6	E	74/74 (100%)	65 (88%)	9 (12%)	4 15
All	All	3399/3399 (100%)	3145 (92%)	254 (8%)	14 31

All (254) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	21	TYR
1	F	39	ASP
1	F	47	MET
1	F	57	GLU
1	F	74	GLU

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Mol	Chain	Res	Type
1	F	75	ASP
1	F	96	ASP
1	F	109	GLU
1	F	113	ARG
1	F	114	GLU
1	F	116	GLU
1	F	118	ASP
1	F	128	ASN
1	F	141	ILE
1	F	163	THR
1	F	212	ILE
1	F	213	ASP
1	F	238	LYS
1	F	244	THR
1	F	258	GLN
1	F	296	LYS
1	F	301	ASN
1	F	307	THR
1	F	326	TRP
1	F	329	LYS
1	F	354	THR
1	F	373	ARG
1	F	393	LYS
1	F	397	ARG
1	F	423	ARG
1	F	426	LYS
1	F	451	ARG
1	F	455	HIS
1	F	487	MET
1	F	507	MET
1	F	516	ASP
1	F	522	ASP
1	F	525	GLU
1	F	526	ASP
1	F	561	MET
1	F	587	ILE
1	F	603	ARG
1	F	605	GLU
2	C	20	GLN
2	C	47	TYR
2	C	70	TYR
2	C	73	TYR

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Mol	Chain	Res	Type
2	C	101	ARG
2	C	108	GLU
2	C	160	ASP
2	C	184	LEU
2	C	187	GLU
2	C	189	ASP
2	C	207	THR
2	C	214	ASN
2	C	217	THR
2	C	226	GLU
2	C	231	GLU
2	C	235	ASN
2	C	241	LEU
2	C	244	GLU
2	C	258	ASN
2	C	260	LYS
2	C	262	TYR
2	C	278	GLU
2	C	305	SER
2	C	314	ASN
2	C	335	THR
2	C	341	LEU
2	C	358	ASP
2	C	378	ARG
2	C	422	LYS
2	C	436	ARG
2	C	443	ASP
2	C	459	MET
2	C	469	VAL
2	C	485	ASP
2	C	563	THR
2	C	604	HIS
2	C	622	ASN
2	C	628	HIS
2	C	632	ASP
2	C	725	GLN
2	C	728	ASP
2	C	749	ASP
2	C	755	LYS
2	C	785	ASP
2	C	790	ASP
2	C	821	ARG

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Mol	Chain	Res	Type
2	C	838	CYS
2	C	849	GLU
2	C	863	SER
2	C	868	SER
2	C	893	THR
2	C	927	THR
2	C	929	ILE
2	C	943	LYS
2	C	968	GLU
2	C	972	PHE
2	C	996	ARG
2	C	1022	LYS
2	C	1037	THR
2	C	1088	ASP
2	C	1108	ASN
2	C	1150	ASP
2	C	1157	GLN
2	C	1164	PHE
2	C	1167	GLU
2	C	1227	VAL
2	C	1229	TYR
2	C	1269	ARG
2	C	1292	THR
2	C	1296	ASP
2	C	1299	ASN
2	C	1338	GLU
2	C	1342	GLU
3	D	17	PHE
3	D	42	GLU
3	D	44	ILE
3	D	46	TYR
3	D	57	PHE
3	D	86	GLU
3	D	119	SER
3	D	165	TYR
3	D	170	GLU
3	D	179	LYS
3	D	209	ASN
3	D	211	GLU
3	D	264	ASP
3	D	274	ASN
3	D	314	ARG

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Mol	Chain	Res	Type
3	D	332	LYS
3	D	386	GLU
3	D	425	ARG
3	D	443	GLU
3	D	537	TYR
3	D	551	ARG
3	D	592	VAL
3	D	593	ASN
3	D	609	TYR
3	D	626	TYR
3	D	648	GLU
3	D	649	LYS
3	D	674	THR
3	D	677	GLU
3	D	680	ASN
3	D	705	THR
3	D	707	ILE
3	D	709	ARG
3	D	725	MET
3	D	731	ARG
3	D	755	ILE
3	D	798	ARG
3	D	811	GLU
3	D	818	GLU
3	D	836	ARG
3	D	837	ASP
3	D	883	ARG
3	D	895	CYS
3	D	902	ASP
3	D	925	GLU
3	D	959	LYS
3	D	987	GLU
3	D	1038	THR
3	D	1039	ASP
3	D	1052	GLU
3	D	1086	ASN
3	D	1123	ARG
3	D	1132	LYS
3	D	1205	GLU
3	D	1209	VAL
3	D	1211	SER
3	D	1218	HIS

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Mol	Chain	Res	Type
3	D	1231	ARG
3	D	1235	ASN
3	D	1239	ASP
3	D	1265	THR
3	D	1267	VAL
3	D	1272	SER
3	D	1281	GLU
3	D	1371	ARG
4	A	7	GLU
4	A	28	LEU
4	A	32	GLU
4	A	44	ARG
4	A	66	HIS
4	A	82	LEU
4	A	91	ARG
4	A	95	LYS
4	A	117	HIS
4	A	127	GLN
4	A	137	ASN
4	A	140	ILE
4	A	181	GLU
4	A	182	ARG
4	A	191	ARG
4	A	210	THR
4	A	211	ILE
4	A	229	GLU
4	A	233	ASP
4	A	241	GLU
4	A	243	LYS
4	A	244	GLU
4	A	248	GLU
4	A	249	PHE
4	A	250	ASP
4	A	255	ARG
4	A	258	ASP
4	A	271	LYS
4	A	282	VAL
4	A	295	LEU
4	A	317	ARG
4	A	320	ASN
4	A	321	TRP
5	B	10	LYS

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Mol	Chain	Res	Type
5	B	23	HIS
5	B	28	LEU
5	B	32	GLU
5	B	33	ARG
5	B	45	ARG
5	B	57	THR
5	B	78	ILE
5	B	82	LEU
5	B	95	LYS
5	B	111	THR
5	B	121	VAL
5	B	122	GLU
5	B	127	GLN
5	B	137	ASN
5	B	140	ILE
5	B	182	ARG
5	B	191	ARG
5	B	203	ILE
5	B	204	GLU
5	B	211	ILE
5	B	219	ARG
5	B	229	GLU
5	B	235	ARG
5	B	239	GLN
5	B	241	GLU
5	B	244	GLU
5	B	246	LYS
5	B	258	ASP
5	B	265	ARG
5	B	276	HIS
6	E	6	VAL
6	E	11	GLU
6	E	43	ASN
6	E	54	ILE
6	E	56	GLU
6	E	69	ARG
6	E	80	LEU
6	E	84	THR
6	E	88	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	446	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0340. 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

6.1.1 Primary map

X

Y

Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 45

Y Index: 45

Z Index: 45

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: 47

Y Index: 40

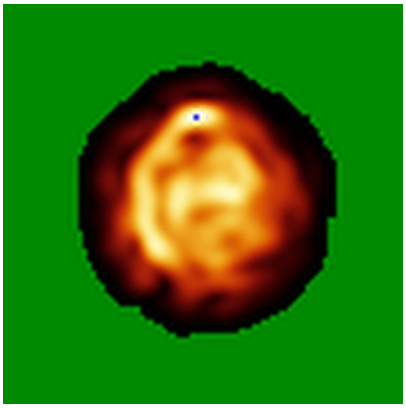
Z Index: 48

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

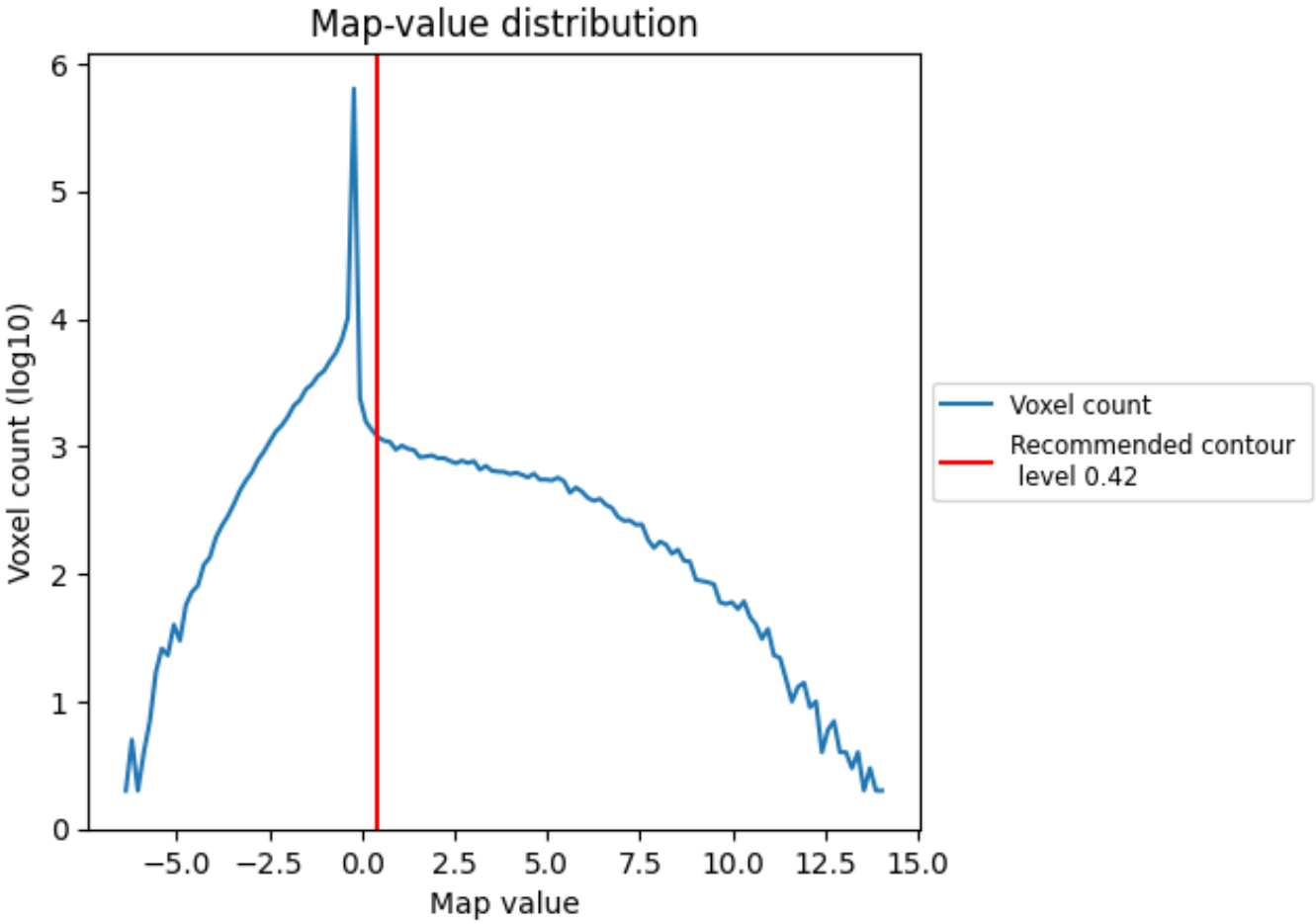
6.6 Mask visualisation (i)

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

7 Map analysis

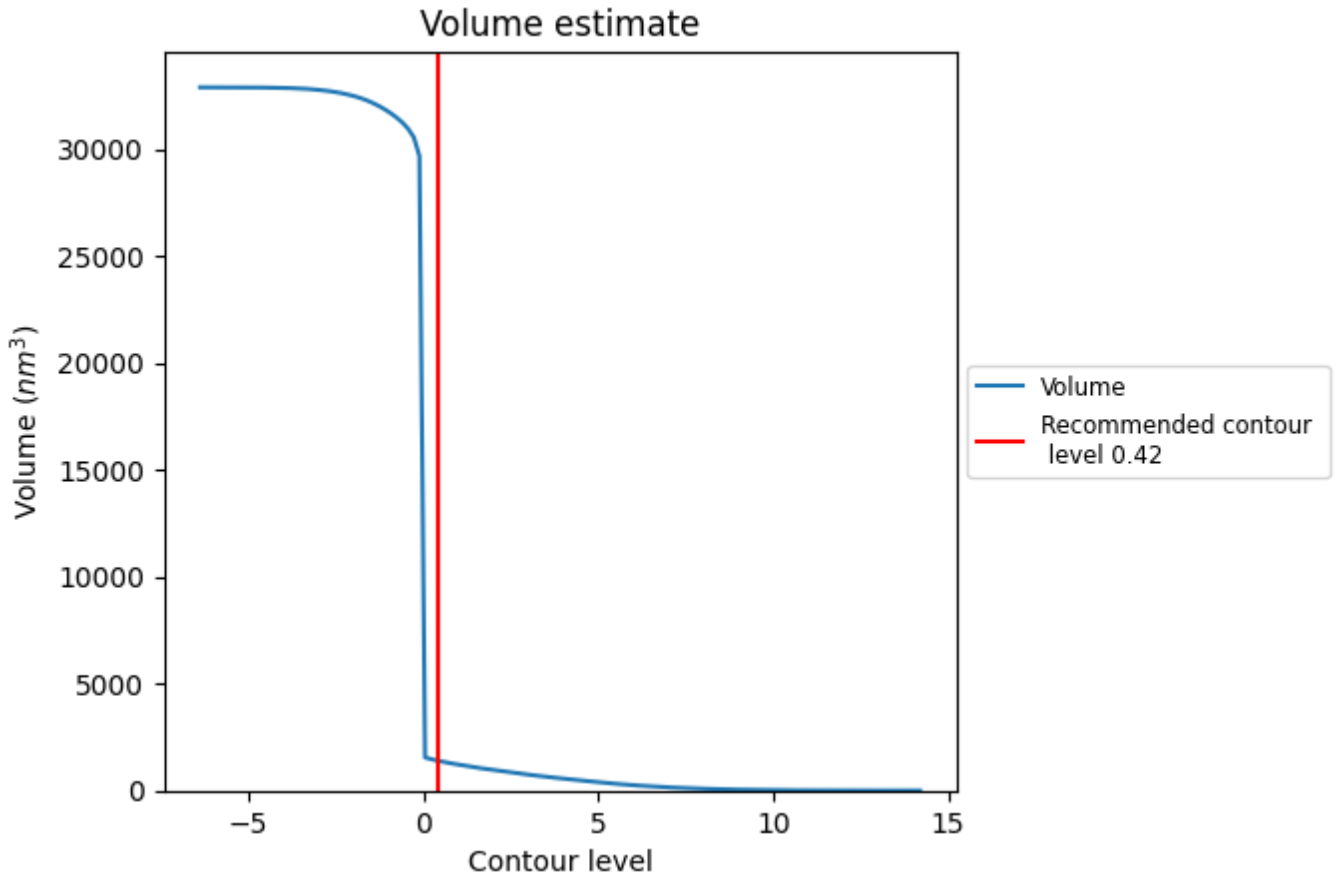
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

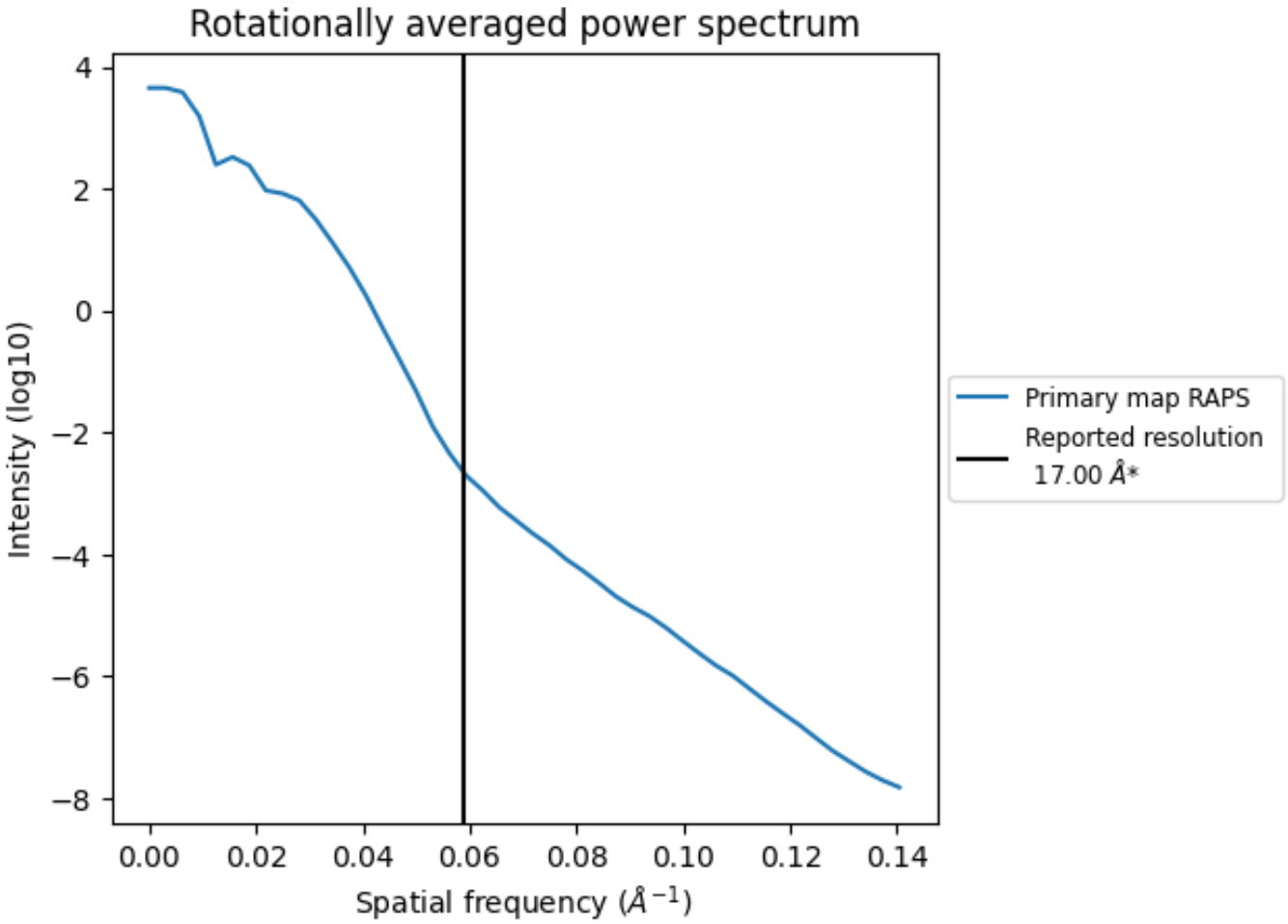
7.2 Volume estimate



The volume at the recommended contour level is 1394 nm^3; this corresponds to an approximate mass of 1259 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)

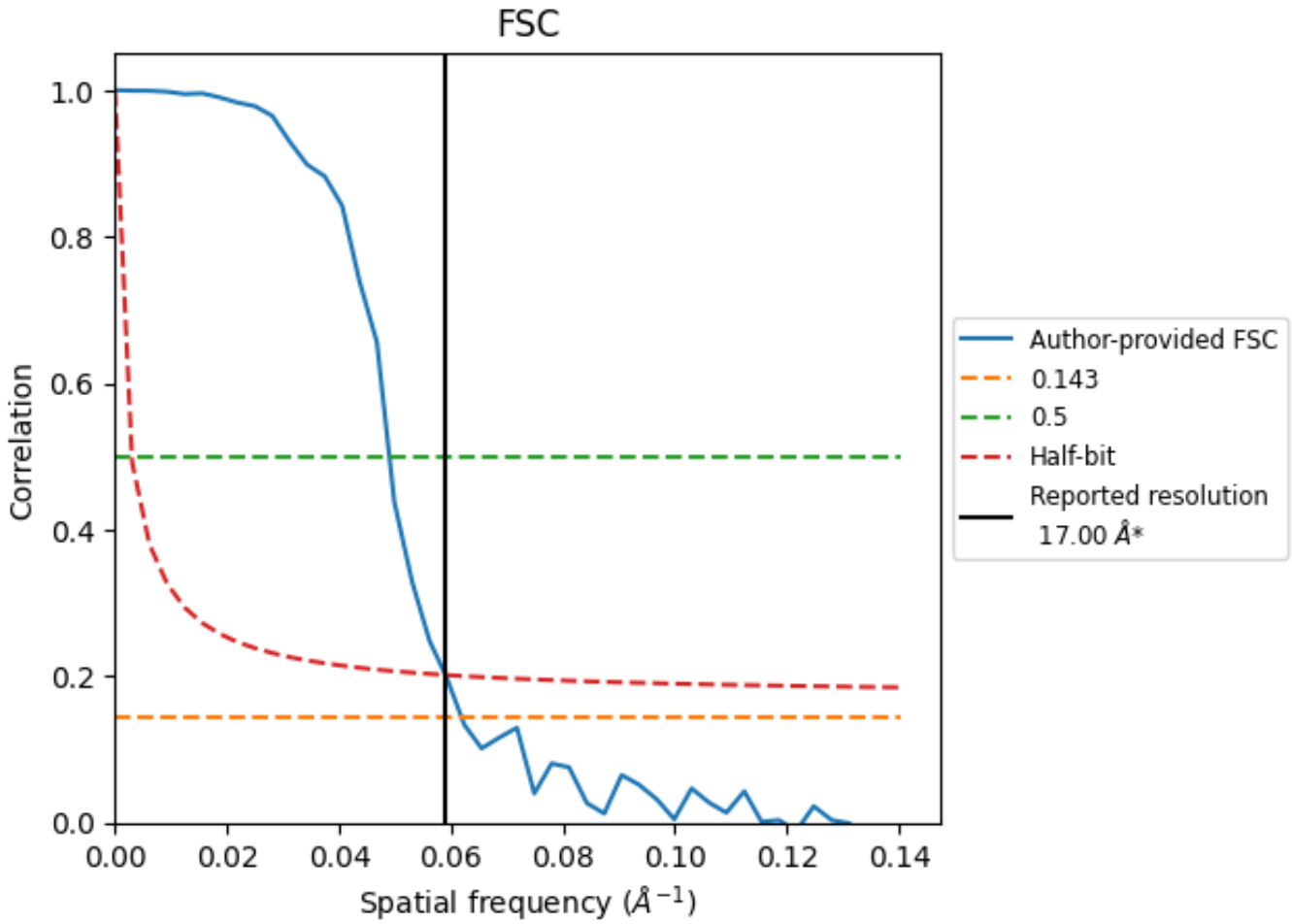


*Reported resolution corresponds to spatial frequency of 0.059 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.059 Å^{-1}

8.2 Resolution estimates (i)

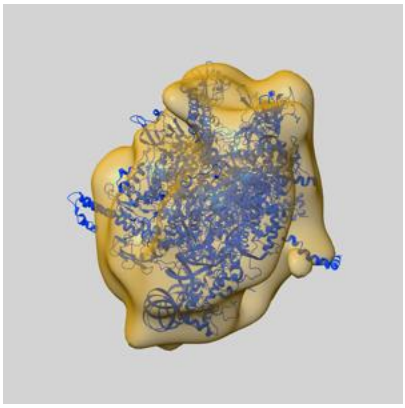
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	17.00
Author-provided FSC curve	16.16	20.41	16.95
Unmasked-calculated*	-	-	-

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

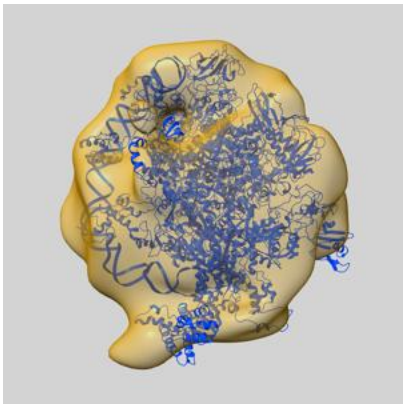
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0340 and PDB model 6N4C. Per-residue inclusion information can be found in section 3 on page 6.

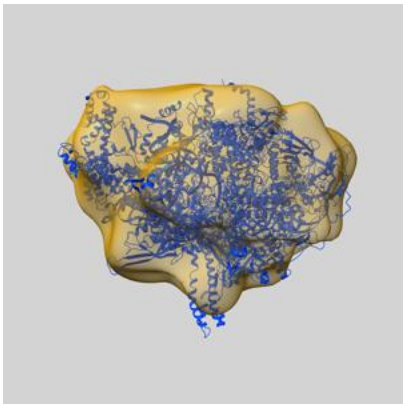
9.1 Map-model overlay



X



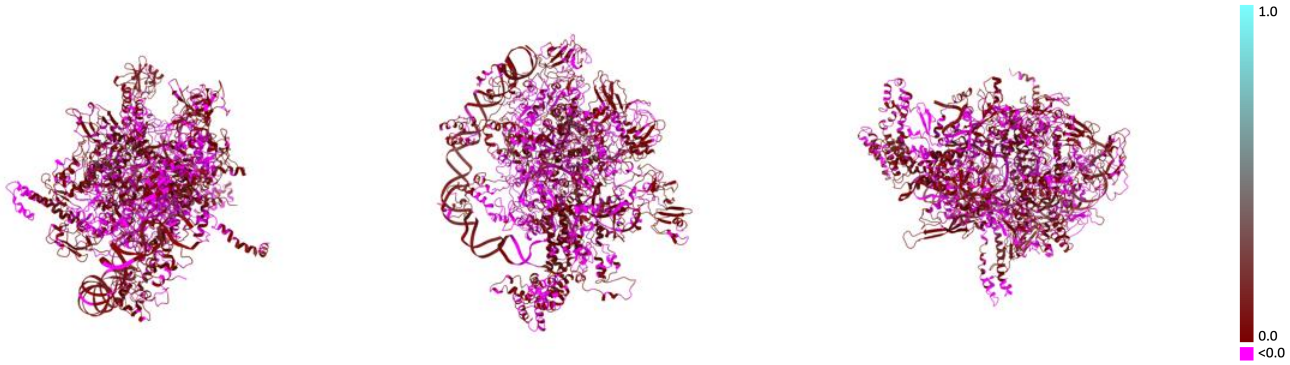
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.42 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.

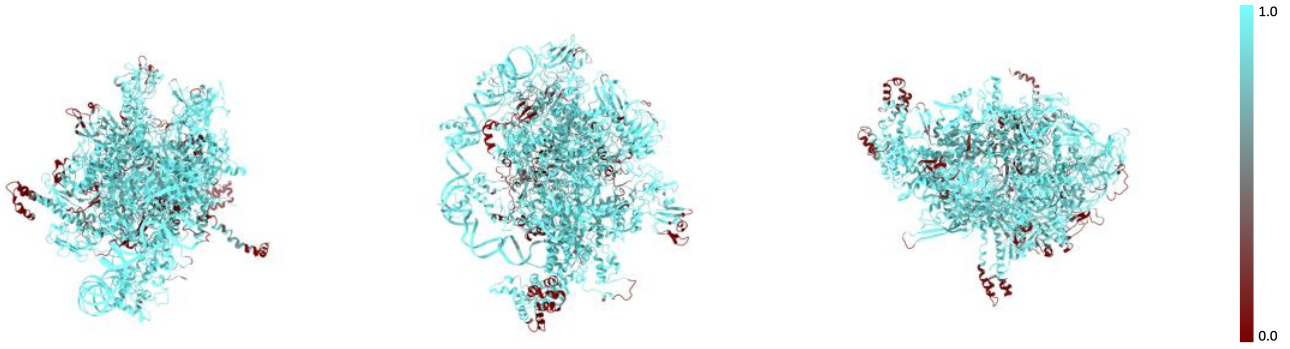
9.2 Q-score mapped to coordinate model



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.

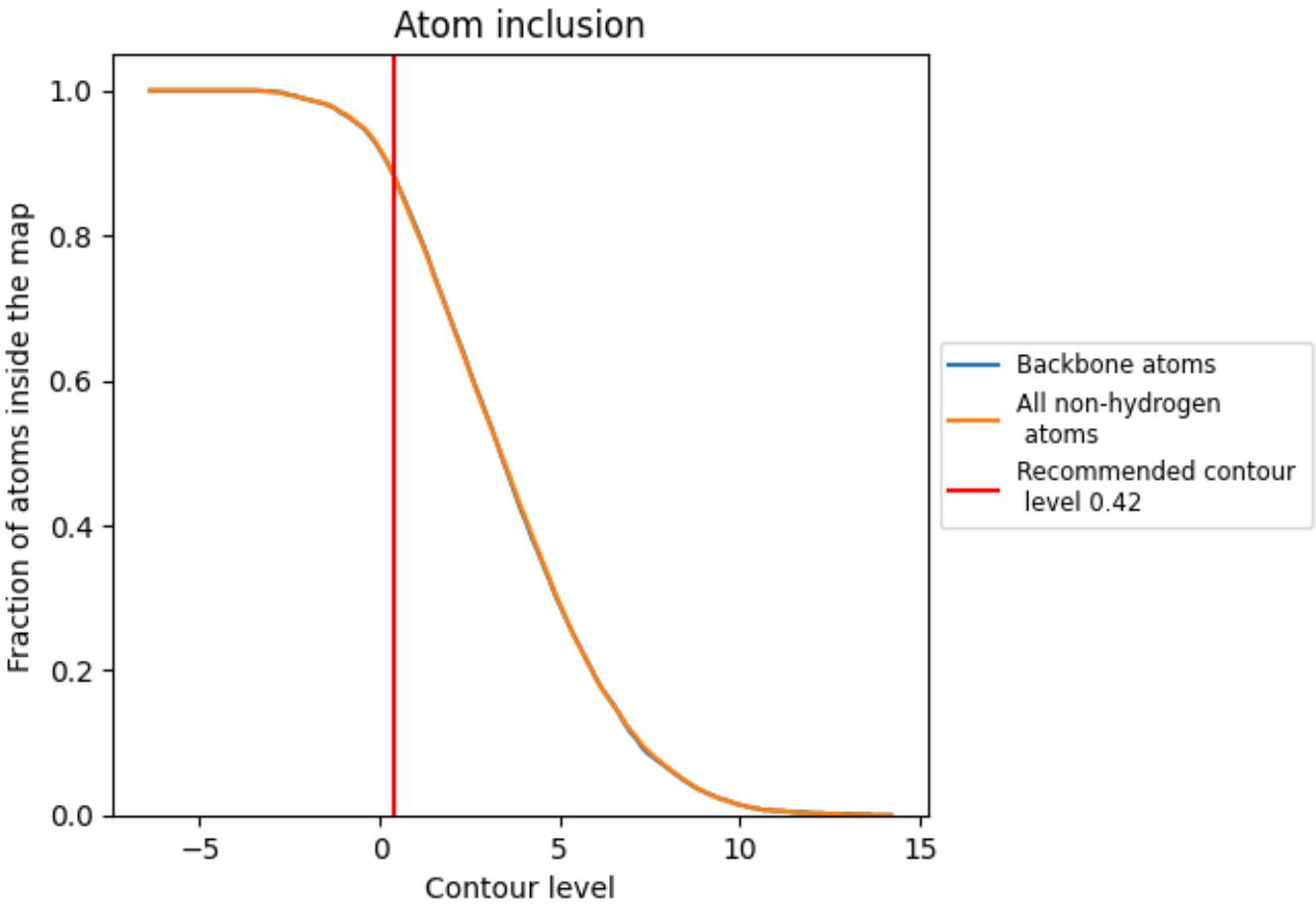
9.3 Atom inclusion mapped to coordinate model



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 (0.42).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.42) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8790	0.0190
A	0.8800	0.0210
B	0.8460	0.0110
C	0.8480	0.0190
D	0.9260	0.0140
E	0.6310	0.0120
F	0.8030	0.0170
a	0.9870	0.0410
b	0.9530	0.0440