



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 12:30 PM UTC

PDB ID : 7VDV / pdb_00007vdv
EMDB ID : EMD-31926
Title : The overall structure of human chromatin remodeling PBAF-nucleosome complex
Authors : Chen, Z.C.; Chen, K.J.; Yuan, J.J.
Deposited on : 2021-09-07
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

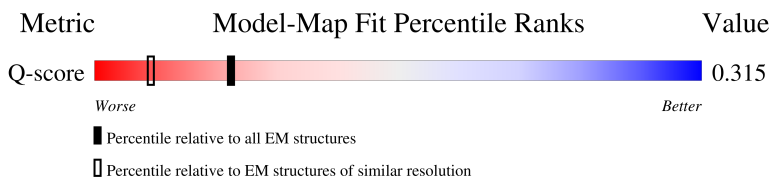
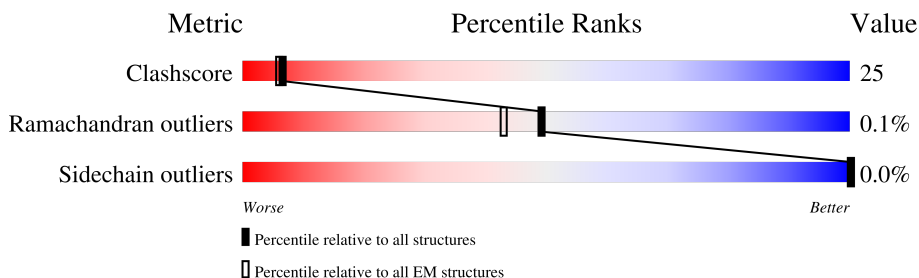
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	103	
1	F	103	
2	C	130	
2	G	130	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	126	
3	H	126	
4	E	136	
4	K	136	
5	I	207	
6	J	207	
7	A	1485	
8	N	429	
9	P	375	
10	Q	870	
11	R	514	
12	T	652	
13	U	7	
14	V	385	
15	W	1214	
15	X	1214	
16	Y	529	
17	Z	411	
18	a	1020	
19	M	16	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	BEF	A	1701	-	-	X	-
22	ADP	A	1703	-	-	X	-

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 40028 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 Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
1	F	86	Total	C	N	O	S	0	0
			672	424	130	117	1		

- Molecule 2 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	107	Total	C	N	O	0	0
			811	510	158	143		
2	G	108	Total	C	N	O	0	0
			828	522	162	144		

- Molecule 3 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	93	Total	C	N	O	S	0	0
			717	450	128	137	2		
3	H	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

- Molecule 4 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	95	Total	C	N	O	S	0	0
			779	492	148	136	3		
4	K	98	Total	C	N	O	S	0	0
			801	506	153	139	3		

- Molecule 5 is a DNA chain called DNA (207-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	135	Total	C	N	O	P	0	0
			2752	1307	499	811	135		

- Molecule 6 is a DNA chain called DNA (207-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	137	Total	C	N	O	P	0	0
			2827	1337	532	821	137		

- Molecule 7 is a protein called Isoform 2 of Transcription activator BRG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	809	Total	C	N	O	S	0	0
			6652	4216	1208	1196	32		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	MET	-	initiating methionine	UNP P51532
A	1615	ALA	-	expression tag	UNP P51532
A	1616	SER	-	expression tag	UNP P51532
A	1617	GLY	-	expression tag	UNP P51532
A	1618	GLY	-	expression tag	UNP P51532
A	1619	SER	-	expression tag	UNP P51532
A	1620	TRP	-	expression tag	UNP P51532
A	1621	SER	-	expression tag	UNP P51532
A	1622	HIS	-	expression tag	UNP P51532
A	1623	PRO	-	expression tag	UNP P51532
A	1624	GLN	-	expression tag	UNP P51532
A	1625	PHE	-	expression tag	UNP P51532
A	1626	GLU	-	expression tag	UNP P51532
A	1627	LYS	-	expression tag	UNP P51532
A	1628	TRP	-	expression tag	UNP P51532
A	1629	SER	-	expression tag	UNP P51532
A	1630	HIS	-	expression tag	UNP P51532
A	1631	PRO	-	expression tag	UNP P51532
A	1632	GLN	-	expression tag	UNP P51532
A	1633	PHE	-	expression tag	UNP P51532
A	1634	GLU	-	expression tag	UNP P51532
A	1635	LYS	-	expression tag	UNP P51532
A	1636	TRP	-	expression tag	UNP P51532
A	1637	SER	-	expression tag	UNP P51532
A	1638	HIS	-	expression tag	UNP P51532

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1639	PRO	-	expression tag	UNP P51532
A	1640	GLN	-	expression tag	UNP P51532
A	1641	PHE	-	expression tag	UNP P51532
A	1642	GLU	-	expression tag	UNP P51532
A	1643	LYS	-	expression tag	UNP P51532

- Molecule 8 is a protein called Actin-like protein 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	334	Total	C	N	O	S	0	0
			2612	1656	441	495	20		

- Molecule 9 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	317	Total	C	N	O	S	0	0
			2482	1575	409	480	18		

- Molecule 10 is a protein called AT-rich interactive domain-containing protein 2,AT-rich interactive domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	500	Total	C	N	O	S	0	0
			3981	2540	670	748	23		

- Molecule 11 is a protein called PHD finger protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	92	Total	C	N	O	S	0	0
			771	498	132	140	1		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-15	MET	-	expression tag	UNP Q8WUB8
R	-14	HIS	-	expression tag	UNP Q8WUB8
R	-13	HIS	-	expression tag	UNP Q8WUB8
R	-12	HIS	-	expression tag	UNP Q8WUB8
R	-11	HIS	-	expression tag	UNP Q8WUB8
R	-10	HIS	-	expression tag	UNP Q8WUB8
R	-9	HIS	-	expression tag	UNP Q8WUB8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	-8	HIS	-	expression tag	UNP Q8WUB8
R	-7	HIS	-	expression tag	UNP Q8WUB8
R	-6	HIS	-	expression tag	UNP Q8WUB8
R	-5	HIS	-	expression tag	UNP Q8WUB8
R	-4	HIS	-	expression tag	UNP Q8WUB8
R	-3	HIS	-	expression tag	UNP Q8WUB8
R	-2	GLY	-	expression tag	UNP Q8WUB8
R	-1	GLU	-	expression tag	UNP Q8WUB8
R	0	PHE	-	expression tag	UNP Q8WUB8

- Molecule 12 is a protein called Isoform 2 of Bromodomain-containing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	267	Total	C	N	O	S	3	0
			2166	1368	367	416	15		

- Molecule 13 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	U	7	Total	C	N	O	0	0
			35	21	7	7		

- Molecule 14 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily B member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	238	Total	C	N	O	S	0	0
			1910	1191	336	370	13		

- Molecule 15 is a protein called SWI/SNF complex subunit SMARCC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	248	Total	C	N	O	S	0	0
			2056	1305	362	379	10		
15	X	252	Total	C	N	O	S	0	0
			2072	1320	363	378	11		

- Molecule 16 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily D member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	245	Total	C	N	O	S	0	0
			2057	1308	368	370	11		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	516	ALA	-	expression tag	UNP Q96GM5
Y	517	SER	-	expression tag	UNP Q96GM5
Y	518	HIS	-	expression tag	UNP Q96GM5
Y	519	HIS	-	expression tag	UNP Q96GM5
Y	520	HIS	-	expression tag	UNP Q96GM5
Y	521	HIS	-	expression tag	UNP Q96GM5
Y	522	HIS	-	expression tag	UNP Q96GM5
Y	523	HIS	-	expression tag	UNP Q96GM5
Y	524	HIS	-	expression tag	UNP Q96GM5
Y	525	HIS	-	expression tag	UNP Q96GM5
Y	526	HIS	-	expression tag	UNP Q96GM5
Y	527	HIS	-	expression tag	UNP Q96GM5
Y	528	HIS	-	expression tag	UNP Q96GM5
Y	529	HIS	-	expression tag	UNP Q96GM5

- Molecule 17 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	92	Total	C	N	O	S	0	0
			757	469	147	137	4		

- Molecule 18 is a protein called Protein polybromo-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	a	92	Total	C	N	O	S	0	0
			750	471	141	135	3		

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	670	MET	-	initiating methionine	UNP Q86U86
a	?	-	ALA	deletion	UNP Q86U86
a	?	-	ALA	deletion	UNP Q86U86
a	?	-	GLN	deletion	UNP Q86U86
a	?	-	GLN	deletion	UNP Q86U86
a	?	-	GLN	deletion	UNP Q86U86

Continued on next page...

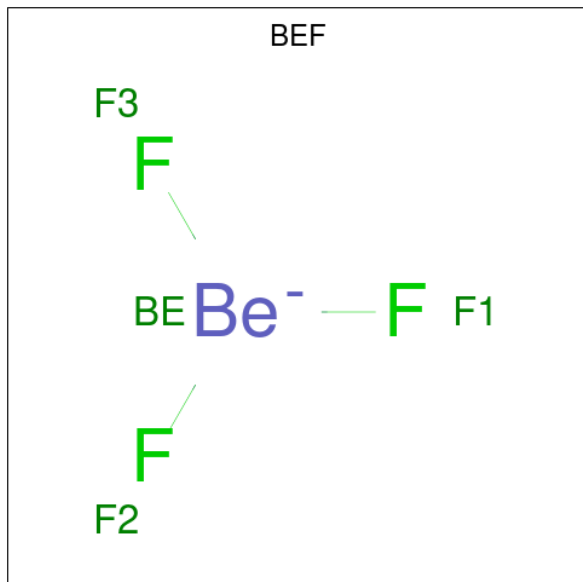
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
a	?	-	GLN	deletion	UNP Q86U86
a	?	-	PRO	deletion	UNP Q86U86
a	?	-	SER	deletion	UNP Q86U86
a	?	-	ALA	deletion	UNP Q86U86
a	?	-	SER	deletion	UNP Q86U86
a	?	-	PRO	deletion	UNP Q86U86
a	?	-	ARG	deletion	UNP Q86U86
a	?	-	ALA	deletion	UNP Q86U86
a	?	-	GLY	deletion	UNP Q86U86
a	?	-	THR	deletion	UNP Q86U86
a	?	-	PRO	deletion	UNP Q86U86
a	?	-	VAL	deletion	UNP Q86U86
a	?	-	GLY	deletion	UNP Q86U86
a	?	-	ALA	deletion	UNP Q86U86
a	?	-	LEU	deletion	UNP Q86U86
a	?	-	MET	deletion	UNP Q86U86
a	?	-	GLY	deletion	UNP Q86U86
a	?	-	VAL	deletion	UNP Q86U86
a	?	-	VAL	deletion	UNP Q86U86
a	?	-	PRO	deletion	UNP Q86U86
a	?	-	PRO	deletion	UNP Q86U86
a	?	-	PRO	deletion	UNP Q86U86
a	?	-	THR	deletion	UNP Q86U86
a	?	-	PRO	deletion	UNP Q86U86
a	?	-	MET	deletion	UNP Q86U86
a	?	-	GLY	deletion	UNP Q86U86
a	?	-	MET	deletion	UNP Q86U86
a	?	-	LEU	deletion	UNP Q86U86
a	?	-	ASN	deletion	UNP Q86U86
a	?	-	GLN	deletion	UNP Q86U86
a	?	-	GLN	deletion	UNP Q86U86
a	?	-	LEU	deletion	UNP Q86U86
a	?	-	THR	deletion	UNP Q86U86
a	?	-	PRO	deletion	UNP Q86U86
a	?	-	VAL	deletion	UNP Q86U86

- Molecule 19 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	M	16	Total	C	N	O	0	0
			80	48	16	16		

- Molecule 20 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).

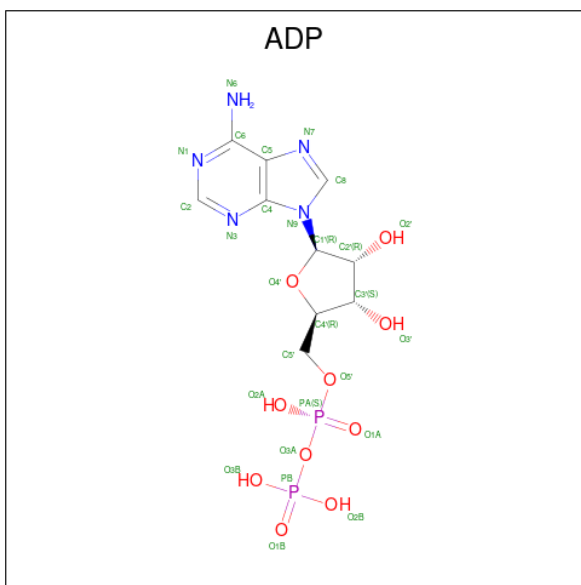


Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	Be	F	0
			4	1	3	

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	Mg	0
			1	1	

- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

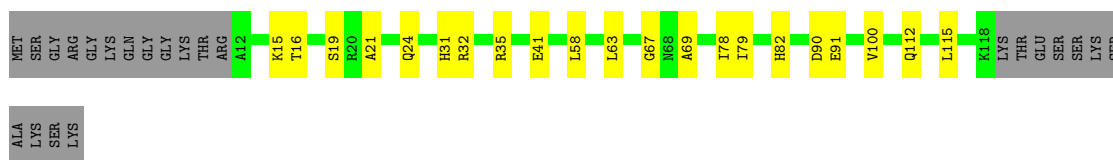
- Molecule 1: Histone H4



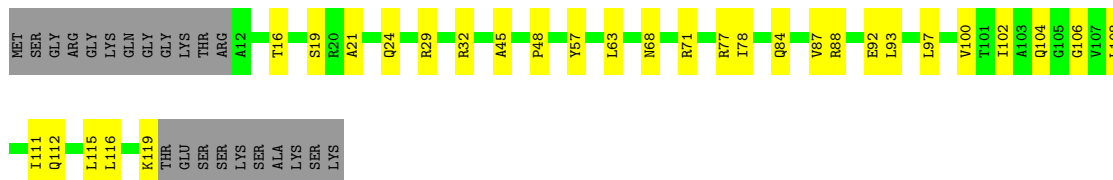
- Molecule 1: Histone H4



- Molecule 2: Histone H2A

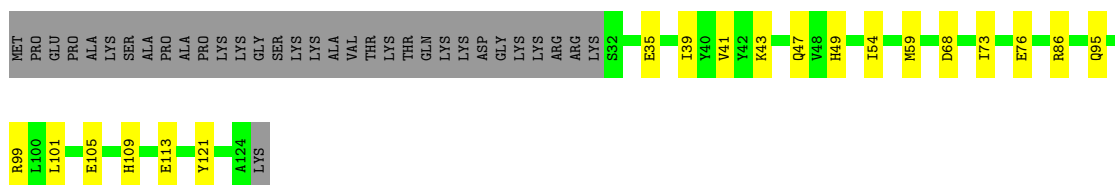


- Molecule 2: Histone H2A



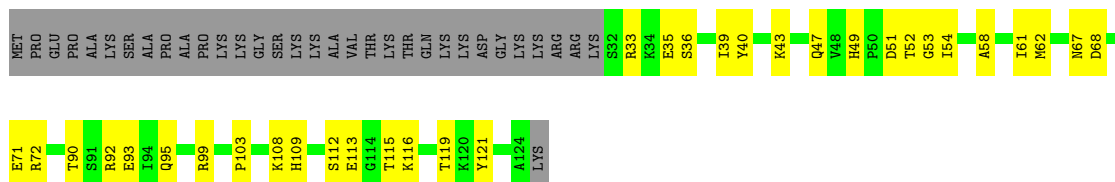
- Molecule 3: Histone H2B 1.1





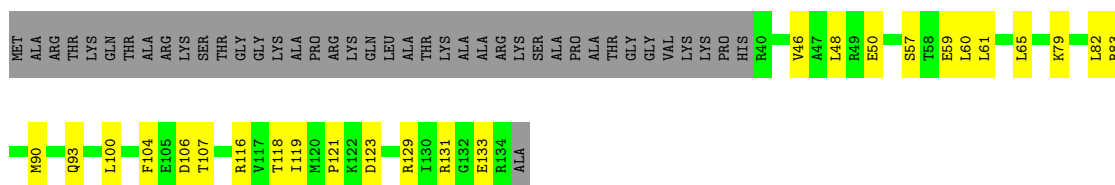
• Molecule 3: Histone H2B 1.1

Chain H: 48% 26% 26%



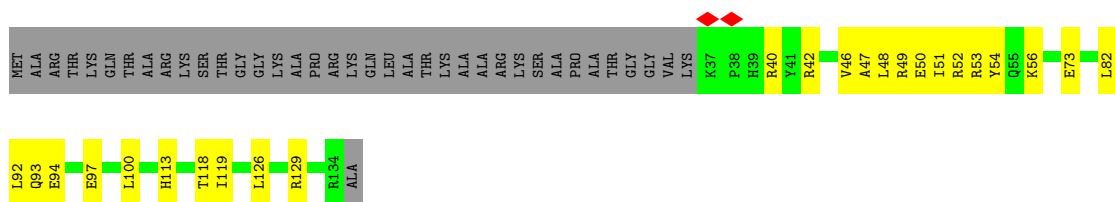
• Molecule 4: Histone H3

Chain E: 51% 18% 30%



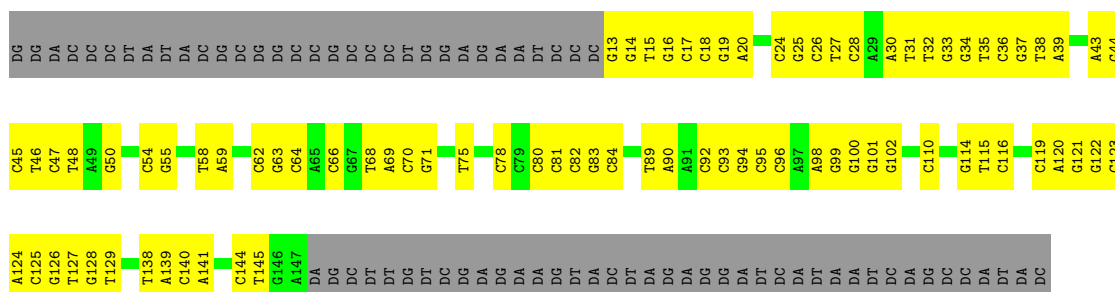
• Molecule 4: Histone H3

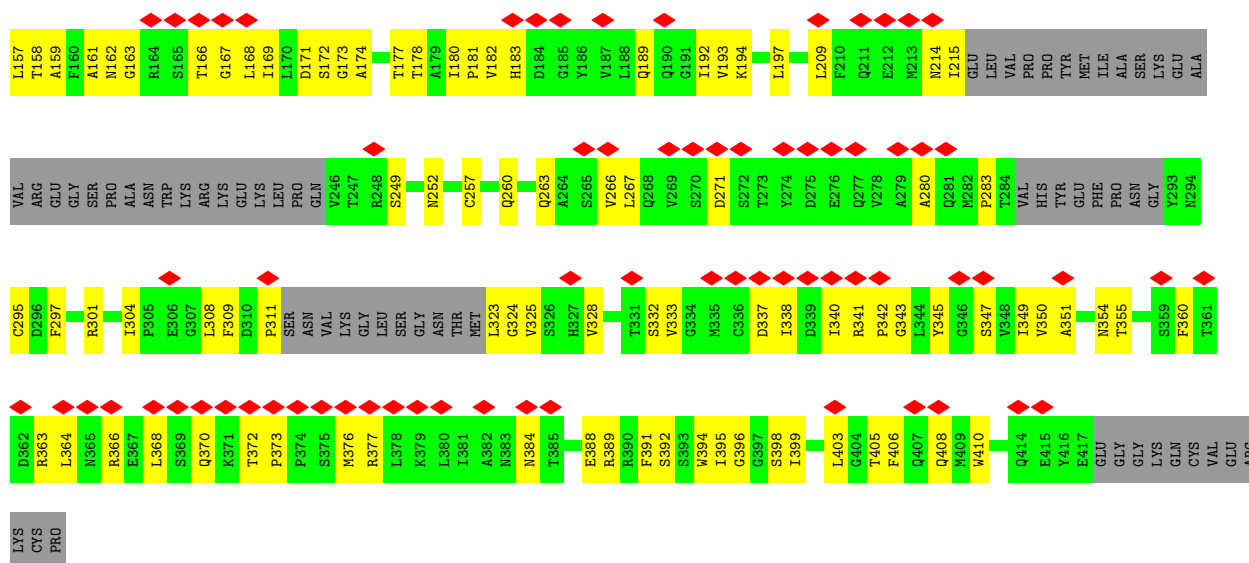
Chain K: 54% 18% 28%



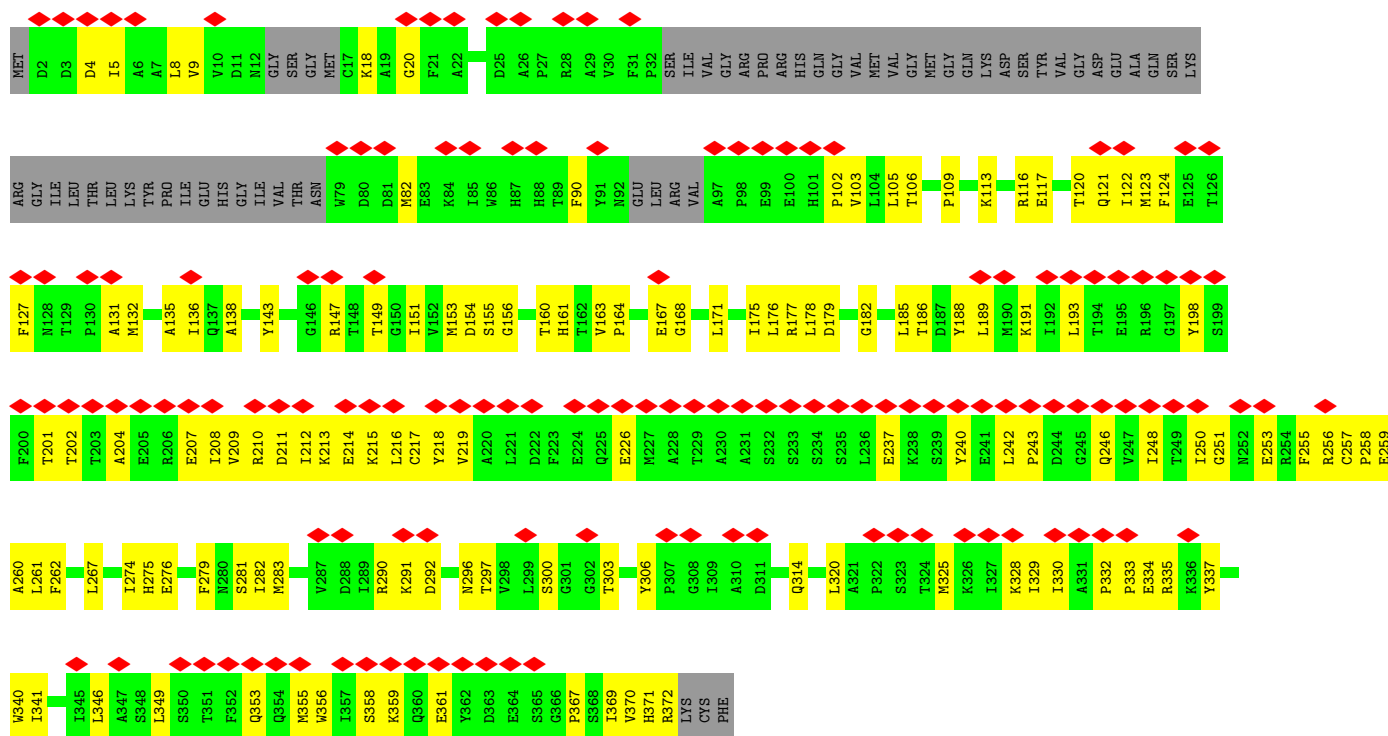
• Molecule 5: DNA (207-MER)

Chain I: 26% 40% 35%

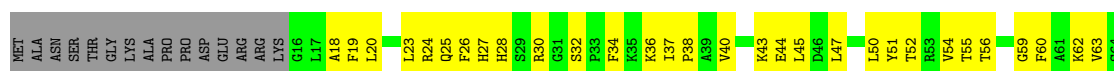
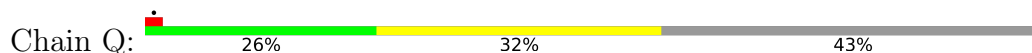




• Molecule 9: Actin, cytoplasmic 1

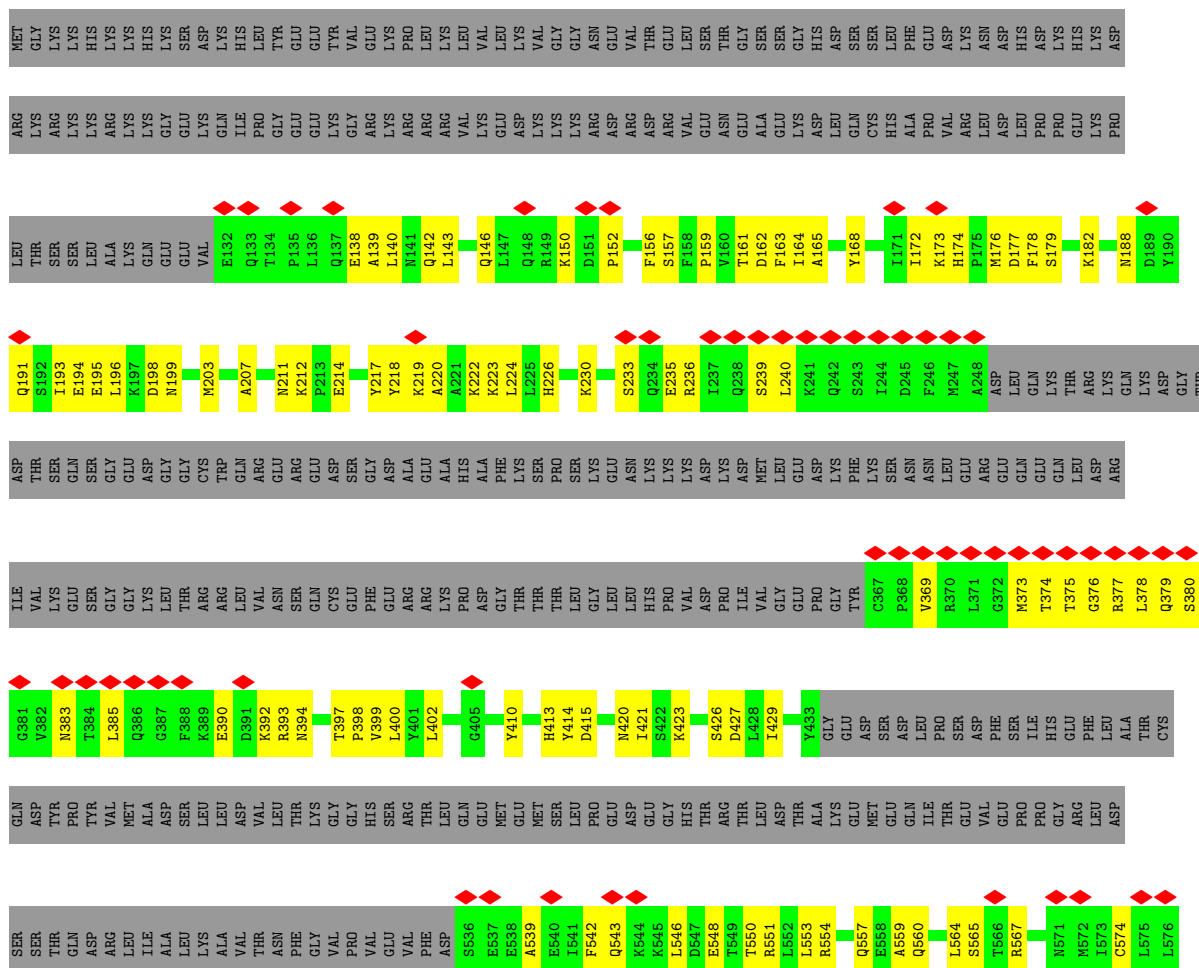


• Molecule 10: AT-rich interactive domain-containing protein 2, AT-rich interactive domain-containing protein 2





- Molecule 12: Isoform 2 of Bromodomain-containing protein 7







[illegible]

- Molecule 16: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily D member 1

[illegible]

H7S	ASN	ALA	LVS	LVS	K126	L133	P134	Q135	R136	I137	R138	E139	L140	V141	P142	E143	S144	Q145	A146	I147	M148	D149	L150	L151	A152	F153	E154	R155	K156	L157	D158	I161	M162	R163	K164	R165	L166	D167	I168	Q169	E170	A171	L172	K173	R174	P175	I176	K177	GLN	LVS	ARG	LVS	LEU	ARG	ILE	PRO	ILE
-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	ASN	THR	THR	PHE	ASN	PRO	ALA	LYS	SER	ASP	GLU	GLY	GLY	THR	VAL	ALA	SER	TRP	GLU	LEU	ARG	VAL	GLU	GLY	ARG	LEU	LEU	GLU	ASP	LYS	TYR	ASP	THR	THR	LYS	GLN	LYS	ARG	LYS	PHE	SER	SER	PHE	PHE	LYS	LYS	LEU	VAL	ILE	GLU	LEU	GLY	ASP	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASP	LEU	TYR	GLY	PRO	ASP	ASN	HIS	LEU	VAL	GLU	TRP	HTS	ARG	THR	ALA	THR	THR	GLN	GLU	THR	ASP	GLY	PHE	GLN	VAL	LYS	ARG	PRO	GLY	ASP	VAL	ASN	VAL	ARG	CYS	THR	VAL	LEU	LEU	MET	LEU	ASP	ASP	TYR	Q291	P292	P293	Q294	P295	K296	P299	R300	L301	A302	R303	L304	L305	G306	I307
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

H308	H309	Q310	Q310	Q311	R312	P313	V314	I315	I316	Q317	A318	L319	W320	Q321	Q322	I323	K324	T325	H326	K327	L328	Q329	D330	P331	H332	E333	R334	E335	F336	V337	I338	C339	D340	K341	Y342	L343	Q344	Q345	I346	F347	E348	S349	Q350	R351	M352	K353	F354	S355	E356	I357	P358	Q359	R360	L361	H362	A363	L364	L365	M366	Q367
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

P368	E369	PRO	ILE	ILE	ILE	ASN	HIS	VAL	ILE	SER	VAL	ASP	PRO	ASN	ASP	GLN	LYS	THR	CYS	TYR	ASP	ILE	ASP	VAL	GLU	VAL	ASP	T399	L400	K401	T402	Q403	M404	N405	L408	L409	A412	A413	E416	I417	A418	T419	N422	E426	T427	E428	I429	T430	I431	N432	Q433
------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

L434	K435	T436	Q437	R438	E439	F440	M441	L442	S443	F444	A445	R446	D447	W455	L456	Q459	L463	K464	T465	M466	V469	V470	G471	N472	E476	A479	E480	F481	Y482	F483	E489	A490	V491	C492	C493	Y494	F495	Y496	S497	K498	V499	Q500	Q501	R502	S503	Q504	E505	L506	E507	Q508
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

[illegible]

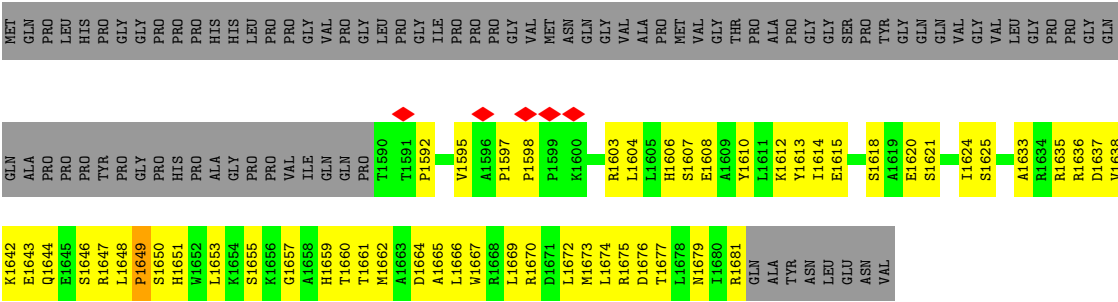
- Molecule 17: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1



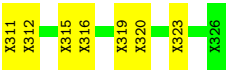
MET	LYS	ARG	PRO	SER	TYR	ALA	PRO	PRO	PRO	THR	PRO	ALA	ALA	ALA	GLN	MET	PRO	SER	THR	PRO	GLY	PHE	VAL	GLY	TYR	ASN	PRO	TYR	SER	HIS	LEU	ALA	ALA	ASN	ASN	TYR	ARG	LEU	GLY	GLY	ASN	PRO	GLY	THR	ASN	SER	ARG	VAL	THR	ALA	SER	SER	GLY	ILE	THR	ILE	PRO
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

[illegible]

ALA	GLU	LYS	ILE	GLU	TYR	ASN	SER	MET	LYS	ALA	ALA	TYR	HIS	ASN	SER	PRO	PRO	ALA	TYR	LEU	LEU	ALA	ALA	GLU	GLU	GLU	SER	ARG	GLN	ARG	GLN	SER	ARG	MET	GLU	LYS	GLY	GLU	GLU	PRO	PRO	TYR	MET	SER	ILE	GLN	PRO	ALA	ALA	GLU	ASP	PRO	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



● Molecule 19: unknown



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137659	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0062	Depositor
Map size ($\text{\AA}$)	389.69998, 389.69998, 389.69998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BEF, ADP

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	0.81	0/711	0.71	0/950
1	F	0.77	0/680	0.79	2/912 (0.2%)
2	C	0.66	0/821	0.56	0/1112
2	G	0.65	0/838	0.59	0/1131
3	D	0.73	0/728	0.63	0/983
3	H	0.73	0/736	0.68	0/991
4	E	0.72	0/789	0.67	0/1059
4	K	0.75	0/813	0.60	0/1093
5	I	0.59	0/3083	0.47	0/4752
6	J	0.59	0/3175	0.46	0/4903
7	A	0.30	0/6771	0.54	0/9102
8	N	0.19	0/2667	0.43	0/3615
9	P	0.16	0/2535	0.42	0/3436
10	Q	0.33	0/4051	0.53	0/5466
11	R	0.36	0/792	0.56	0/1072
12	T	0.20	0/2210	0.48	0/2977
14	V	0.43	0/1947	0.54	0/2638
15	W	0.38	0/2097	0.50	0/2831
15	X	0.26	0/2120	0.50	0/2869
16	Y	0.22	0/2097	0.44	0/2822
17	Z	0.24	0/765	0.50	0/1021
18	a	0.29	0/767	0.65	0/1037
All	All	0.44	0/41193	0.52	2/56772 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	63	GLU	N-CA-CB	6.07	119.04	110.12
1	F	63	GLU	CB-CA-C	-5.43	101.78	110.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	703	0	757	22	0
1	F	672	0	698	21	0
2	C	811	0	849	19	0
2	G	828	0	884	30	0
3	D	717	0	723	20	0
3	H	725	0	745	30	0
4	E	779	0	815	22	0
4	K	801	0	831	28	0
5	I	2752	0	1516	116	0
6	J	2827	0	1537	123	0
7	A	6652	0	6786	390	0
8	N	2612	0	2557	111	0
9	P	2482	0	2432	101	0
10	Q	3981	0	4002	259	0
11	R	771	0	774	77	0
12	T	2166	0	2163	99	0
13	U	35	0	10	2	0
14	V	1910	0	1860	129	0
15	W	2056	0	2028	119	0
15	X	2072	0	2052	160	0
16	Y	2057	0	2088	109	0
17	Z	757	0	786	50	0
18	a	750	0	761	57	0
19	M	80	0	18	4	0
20	A	4	0	0	3	0
21	A	1	0	0	0	0
22	A	27	0	12	11	0
All	All	40028	0	37684	1807	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 25.

The worst 5 of 1807 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)
12:T:377:ARG:C	12:T:378:LEU:HD23	1.31	1.49
12:T:377:ARG:O	12:T:378:LEU:HD23	1.10	1.25
12:T:377:ARG:O	12:T:378:LEU:CD2	1.96	1.13
12:T:377:ARG:C	12:T:378:LEU:CD2	2.23	1.11
7:A:426:ARG:HA	11:R:262:PHE:HE1	1.27	0.98

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	85/103 (82%)	78 (92%)	7 (8%)	0	100	100
1	F	84/103 (82%)	81 (96%)	3 (4%)	0	100	100
2	C	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
2	G	106/130 (82%)	103 (97%)	3 (3%)	0	100	100
3	D	91/126 (72%)	89 (98%)	2 (2%)	0	100	100
3	H	91/126 (72%)	89 (98%)	2 (2%)	0	100	100
4	E	93/136 (68%)	90 (97%)	3 (3%)	0	100	100
4	K	96/136 (71%)	91 (95%)	5 (5%)	0	100	100
7	A	797/1485 (54%)	714 (90%)	82 (10%)	1 (0%)	48	78
8	N	324/429 (76%)	300 (93%)	24 (7%)	0	100	100
9	P	309/375 (82%)	295 (96%)	14 (4%)	0	100	100
10	Q	490/870 (56%)	432 (88%)	56 (11%)	2 (0%)	30	59
11	R	90/514 (18%)	83 (92%)	7 (8%)	0	100	100
12	T	264/652 (40%)	236 (89%)	28 (11%)	0	100	100
14	V	234/385 (61%)	215 (92%)	19 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	W	242/1214 (20%)	230 (95%)	12 (5%)	0	100	100
15	X	246/1214 (20%)	231 (94%)	15 (6%)	0	100	100
16	Y	239/529 (45%)	229 (96%)	10 (4%)	0	100	100
17	Z	90/411 (22%)	88 (98%)	2 (2%)	0	100	100
18	a	90/1020 (9%)	75 (83%)	14 (16%)	1 (1%)	11	38
All	All	4166/10088 (41%)	3851 (92%)	311 (8%)	4 (0%)	49	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	Q	455	GLN
10	Q	451	SER
18	a	1649	PRO
7	A	169	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	72/79 (91%)	72 (100%)	0	100	100
1	F	67/79 (85%)	67 (100%)	0	100	100
2	C	81/102 (79%)	81 (100%)	0	100	100
2	G	84/102 (82%)	84 (100%)	0	100	100
3	D	77/106 (73%)	77 (100%)	0	100	100
3	H	79/106 (74%)	79 (100%)	0	100	100
4	E	82/111 (74%)	82 (100%)	0	100	100
4	K	84/111 (76%)	84 (100%)	0	100	100
7	A	720/1303 (55%)	720 (100%)	0	100	100
8	N	287/364 (79%)	287 (100%)	0	100	100
9	P	270/318 (85%)	270 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	Q	446/765 (58%)	446 (100%)	0	100	100
11	R	83/452 (18%)	83 (100%)	0	100	100
12	T	245/587 (42%)	245 (100%)	0	100	100
14	V	214/346 (62%)	214 (100%)	0	100	100
15	W	216/1030 (21%)	216 (100%)	0	100	100
15	X	222/1030 (22%)	222 (100%)	0	100	100
16	Y	227/455 (50%)	227 (100%)	0	100	100
17	Z	86/361 (24%)	85 (99%)	1 (1%)	63	72
18	a	82/912 (9%)	82 (100%)	0	100	100
All	All	3724/8719 (43%)	3723 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Z	232	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
8	N	370	GLN
18	a	1602	GLN
12	T	148	GLN
17	Z	268	ASN
16	Y	432	ASN

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

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	BEF	A	1701	-	0,3,3	-	-	-		
22	ADP	A	1703	21	28,29,29	1.37	5 (17%)	43,45,45	1.90	10 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	ADP	A	1703	21	-	7/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1703	ADP	C5-C4	4.57	1.47	1.39
22	A	1703	ADP	C5-C6	2.47	1.47	1.41
22	A	1703	ADP	C5-N7	-2.42	1.34	1.39
22	A	1703	ADP	C8-N7	2.19	1.35	1.31
22	A	1703	ADP	C4-N9	-2.01	1.33	1.37

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1703	ADP	C5-C4-N3	-5.69	118.88	126.72
22	A	1703	ADP	N3-C4-N9	4.64	135.07	127.17
22	A	1703	ADP	C2-N3-C4	3.54	120.48	111.83
22	A	1703	ADP	C4-C5-N7	-3.28	106.83	110.58
22	A	1703	ADP	N3-C2-N1	-3.07	123.94	128.58

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

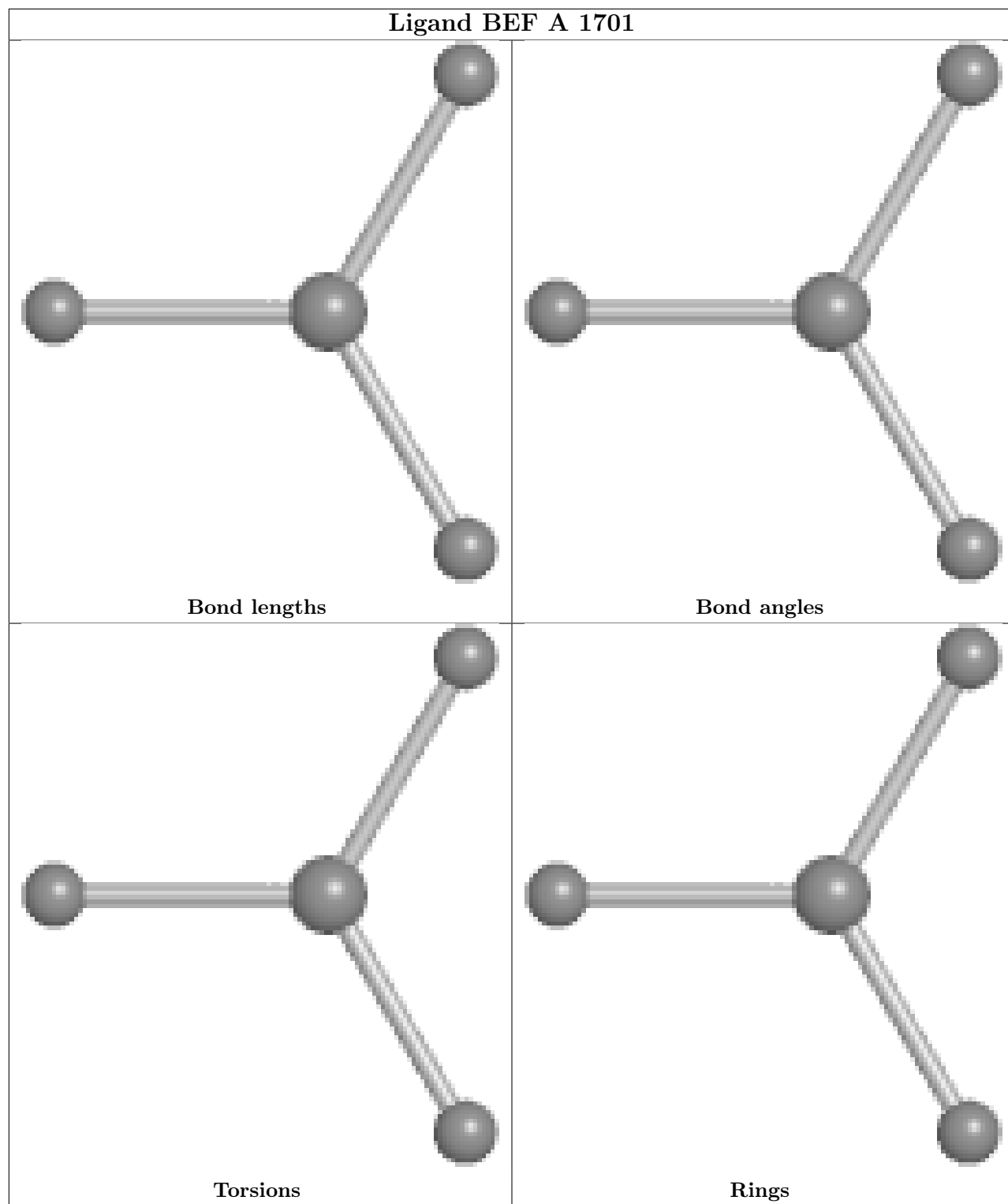
Mol	Chain	Res	Type	Atoms
22	A	1703	ADP	C5'-O5'-PA-O2A
22	A	1703	ADP	O4'-C4'-C5'-O5'
22	A	1703	ADP	C3'-C4'-C5'-O5'
22	A	1703	ADP	PB-O3A-PA-O1A
22	A	1703	ADP	C5'-O5'-PA-O1A

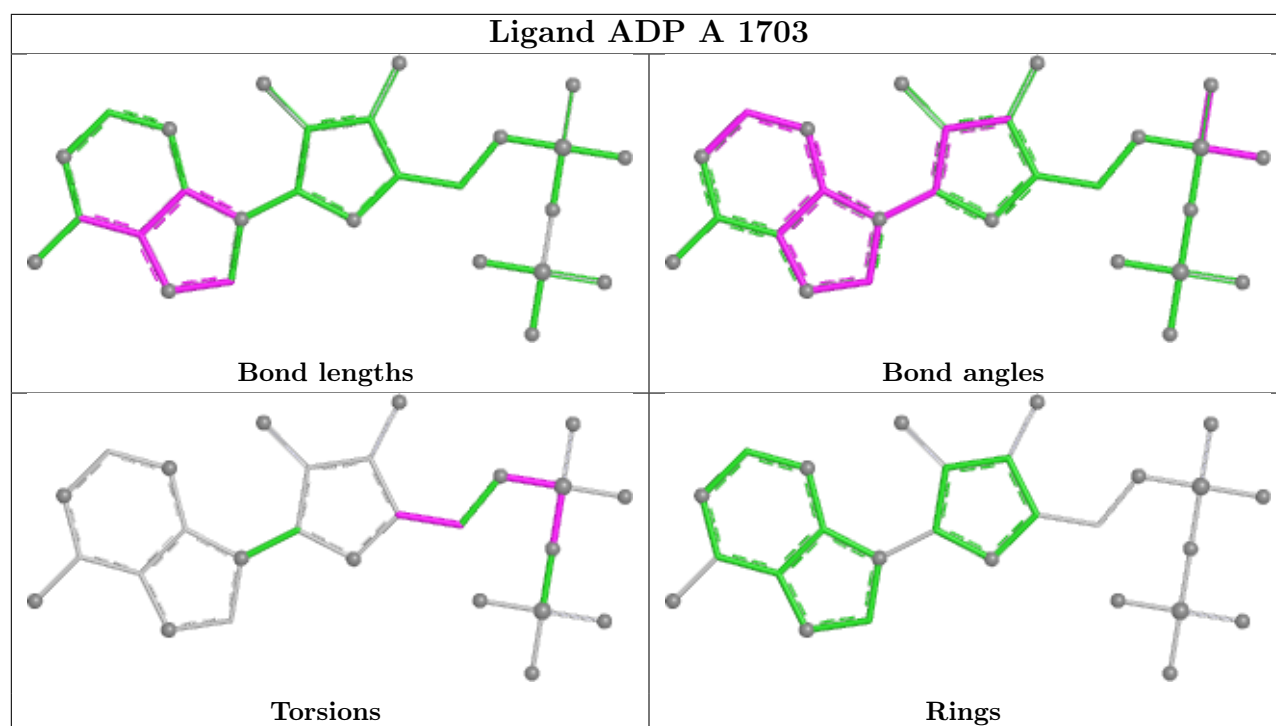
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	1701	BEF	3	0
22	A	1703	ADP	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

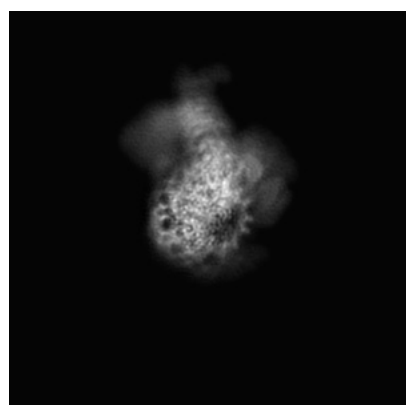
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31926. These allow visual inspection of the internal detail of the map and identification of artifacts.

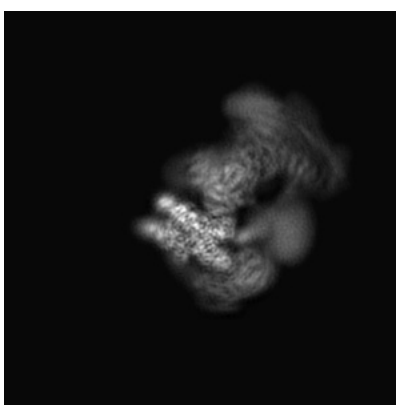
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

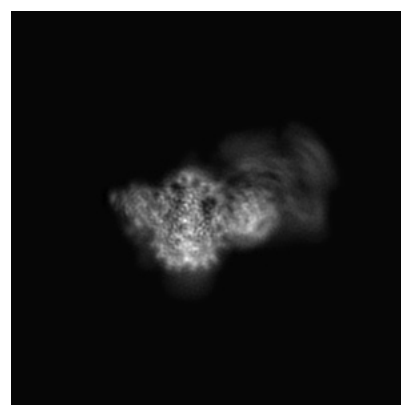
6.1.1 Primary map



X



Y

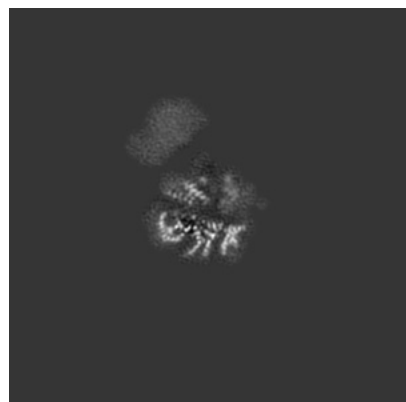


Z

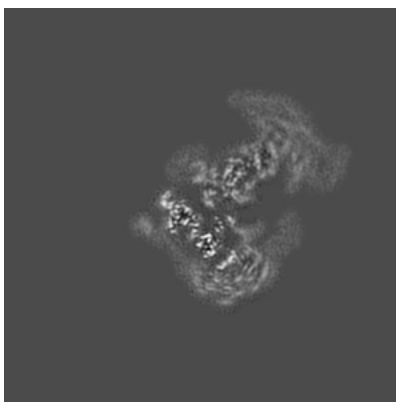
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 180



Y Index: 180

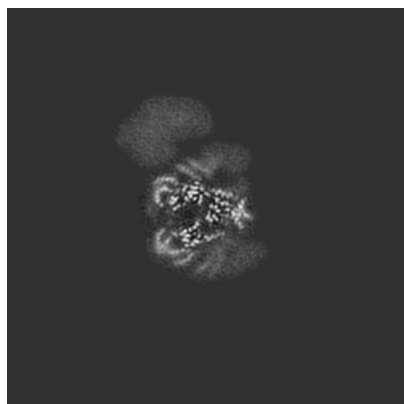


Z Index: 180

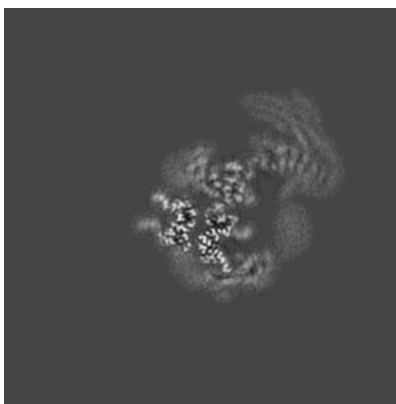
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

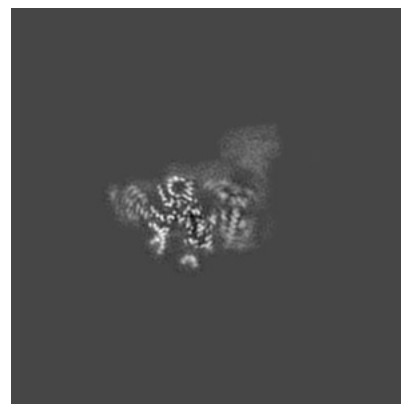
6.3.1 Primary map



X Index: 159



Y Index: 169

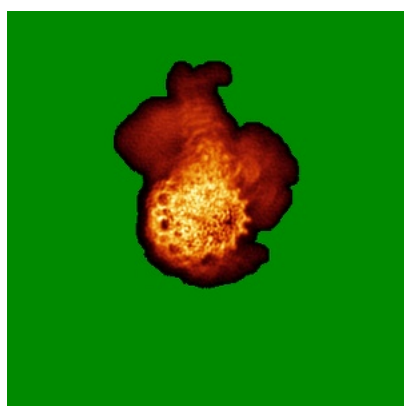


Z Index: 192

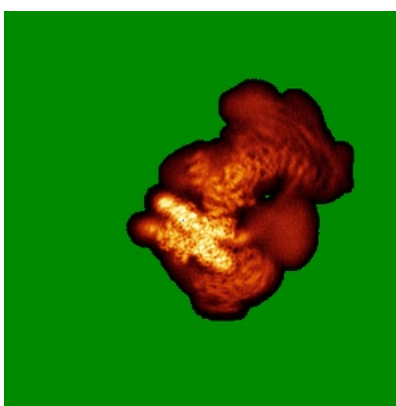
The images above show the largest variance slices of the map in three orthogonal directions.

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

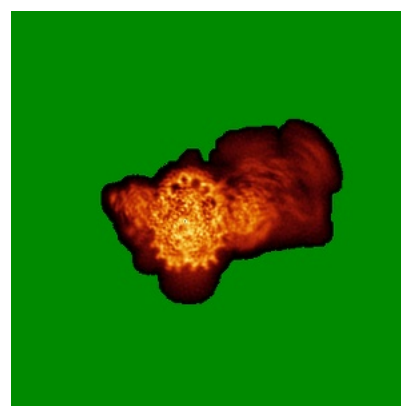
6.4.1 Primary map



X



Y

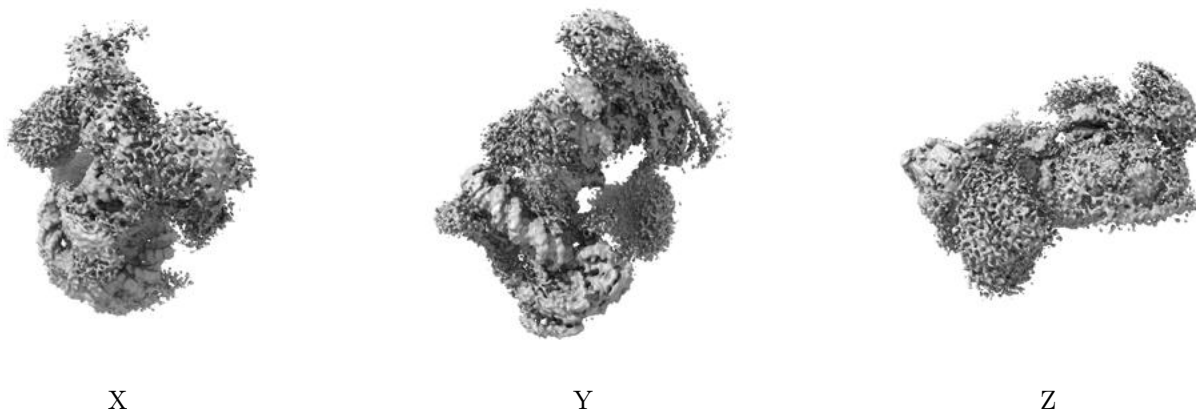


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0062. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

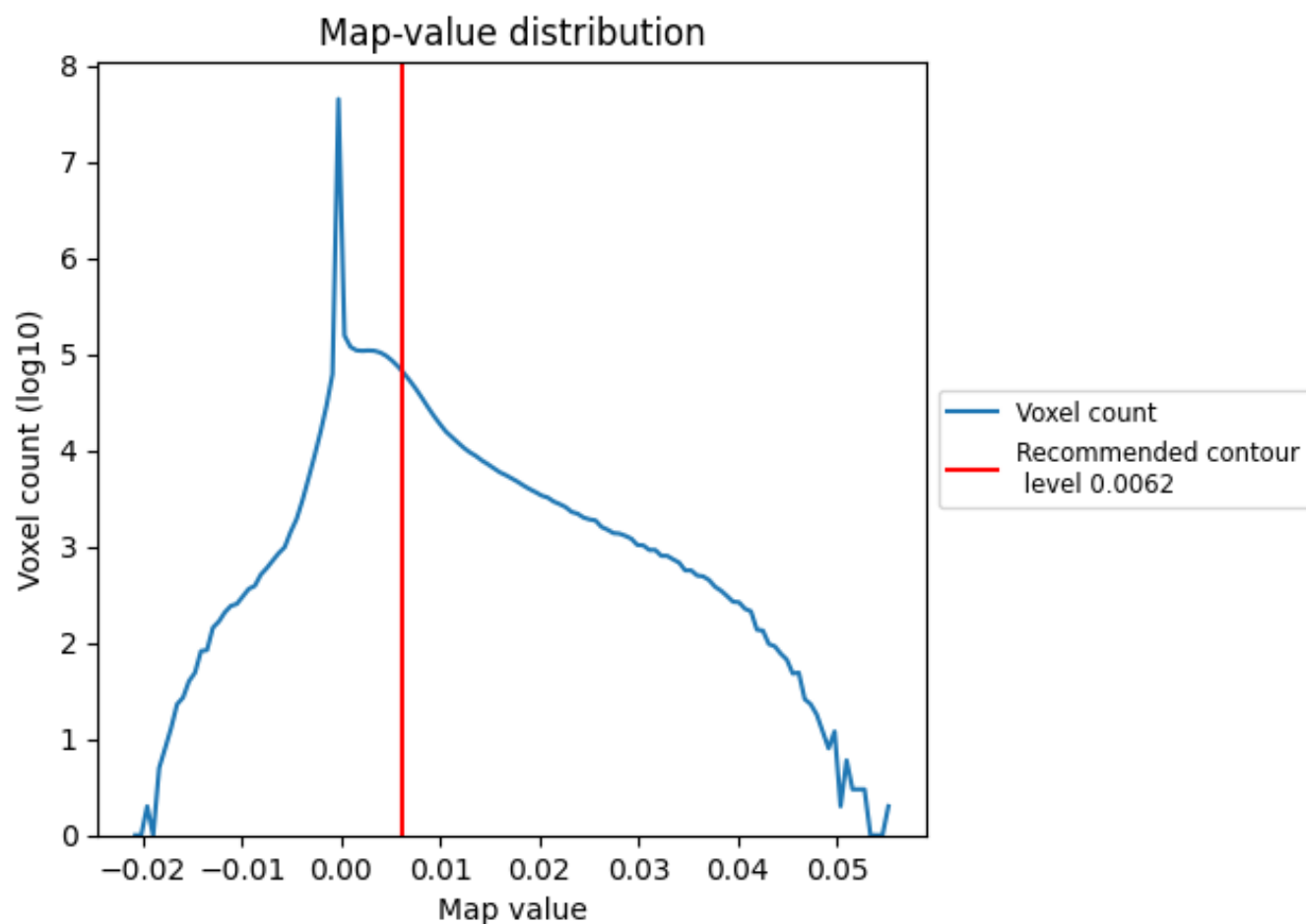
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

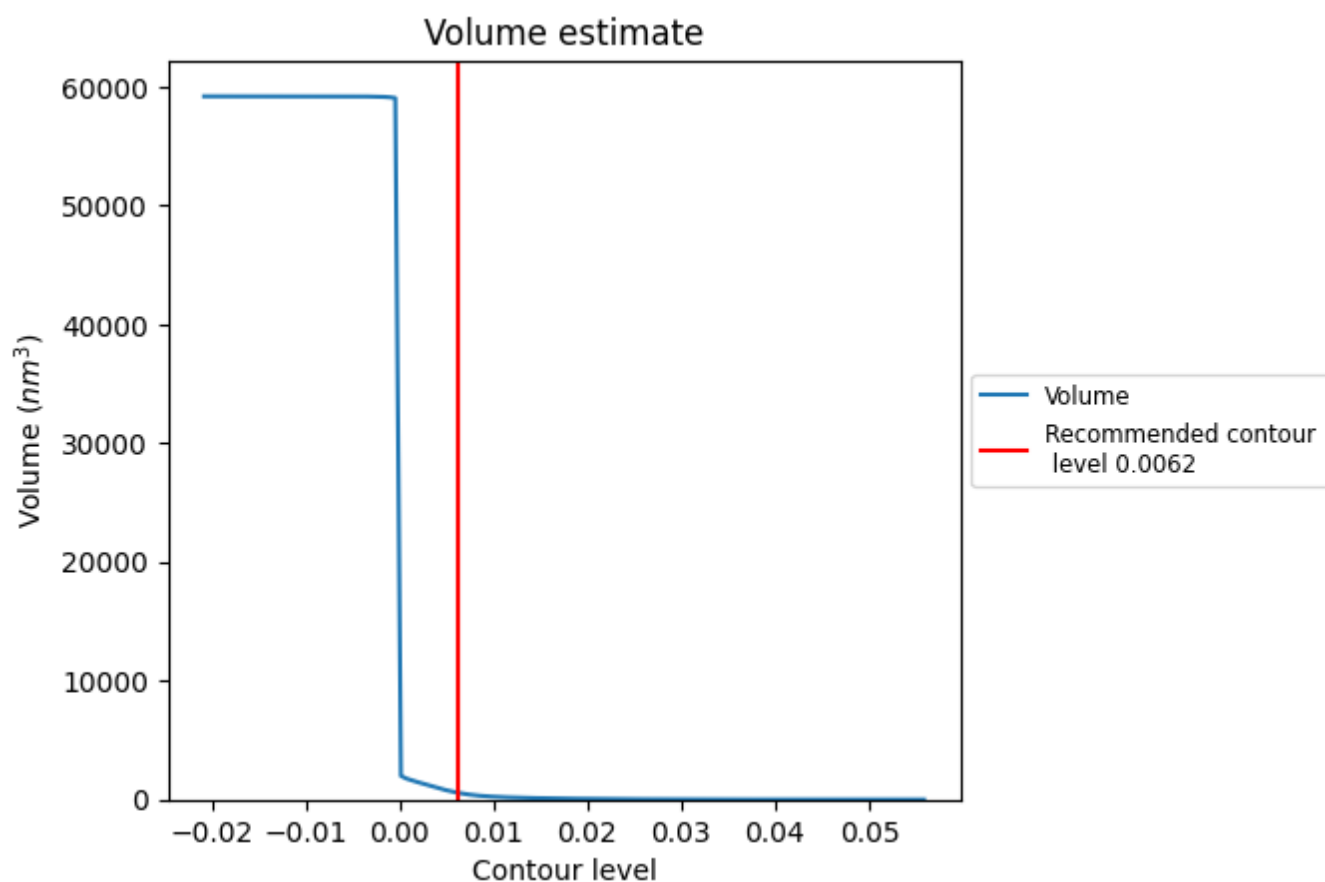
This section contains the results of statistical analysis of the map.

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.

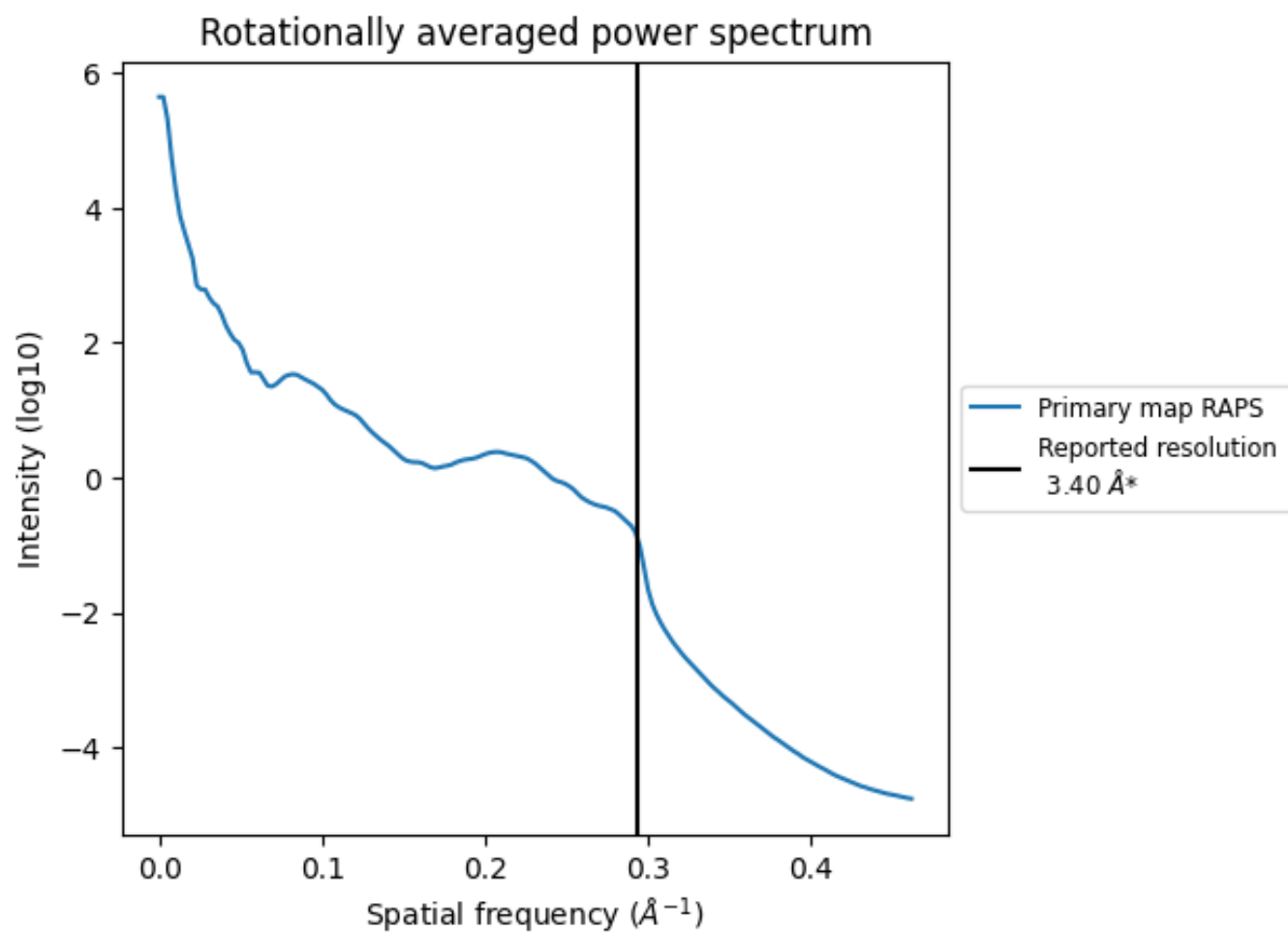
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 575 nm³; this corresponds to an approximate mass of 519 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

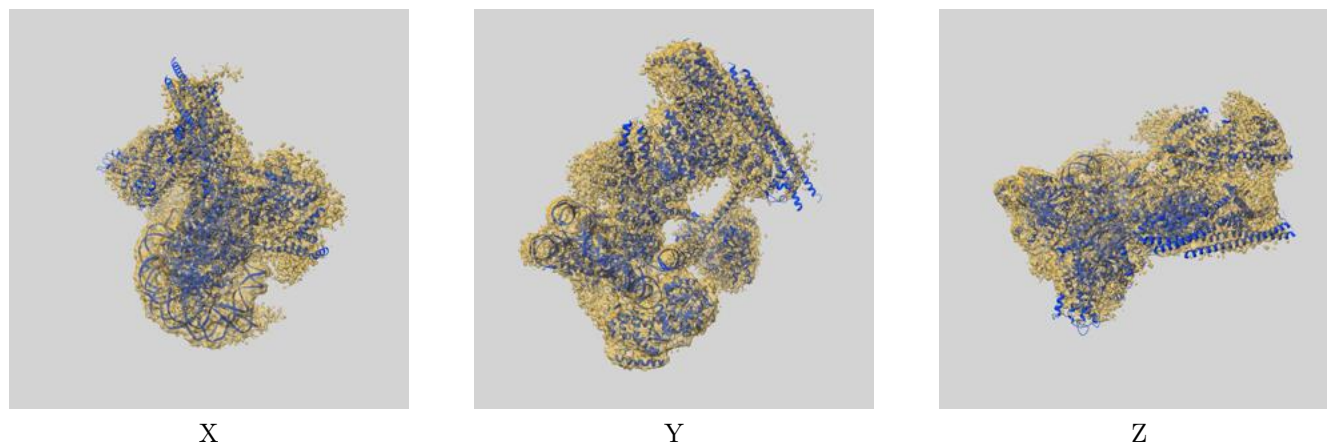
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

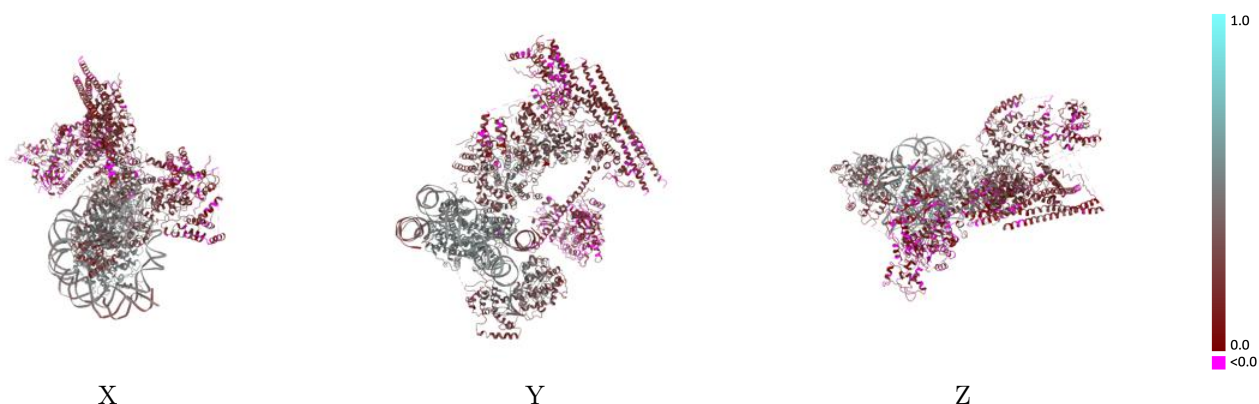
This section contains information regarding the fit between EMDB map EMD-31926 and PDB model 7VDV. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



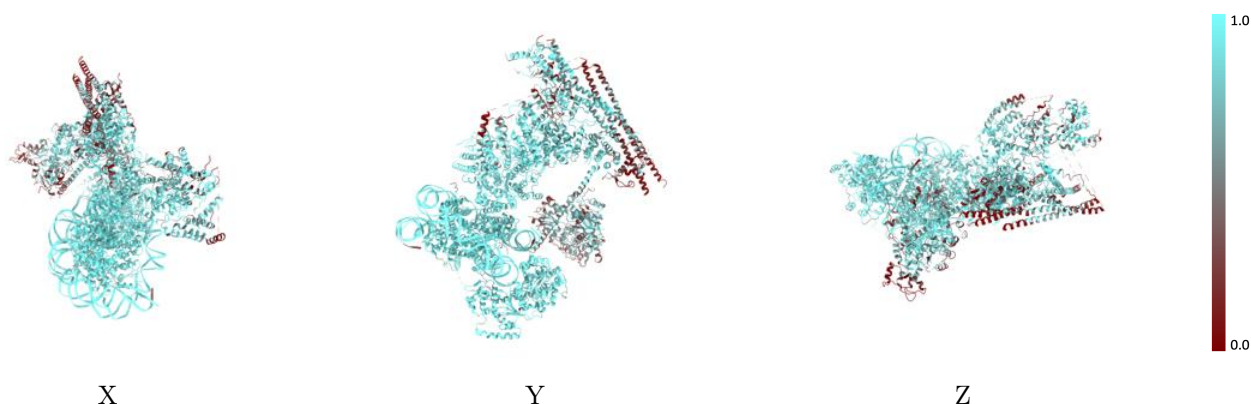
The images above show the 3D surface view of the map at the recommended contour level 0.0062 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



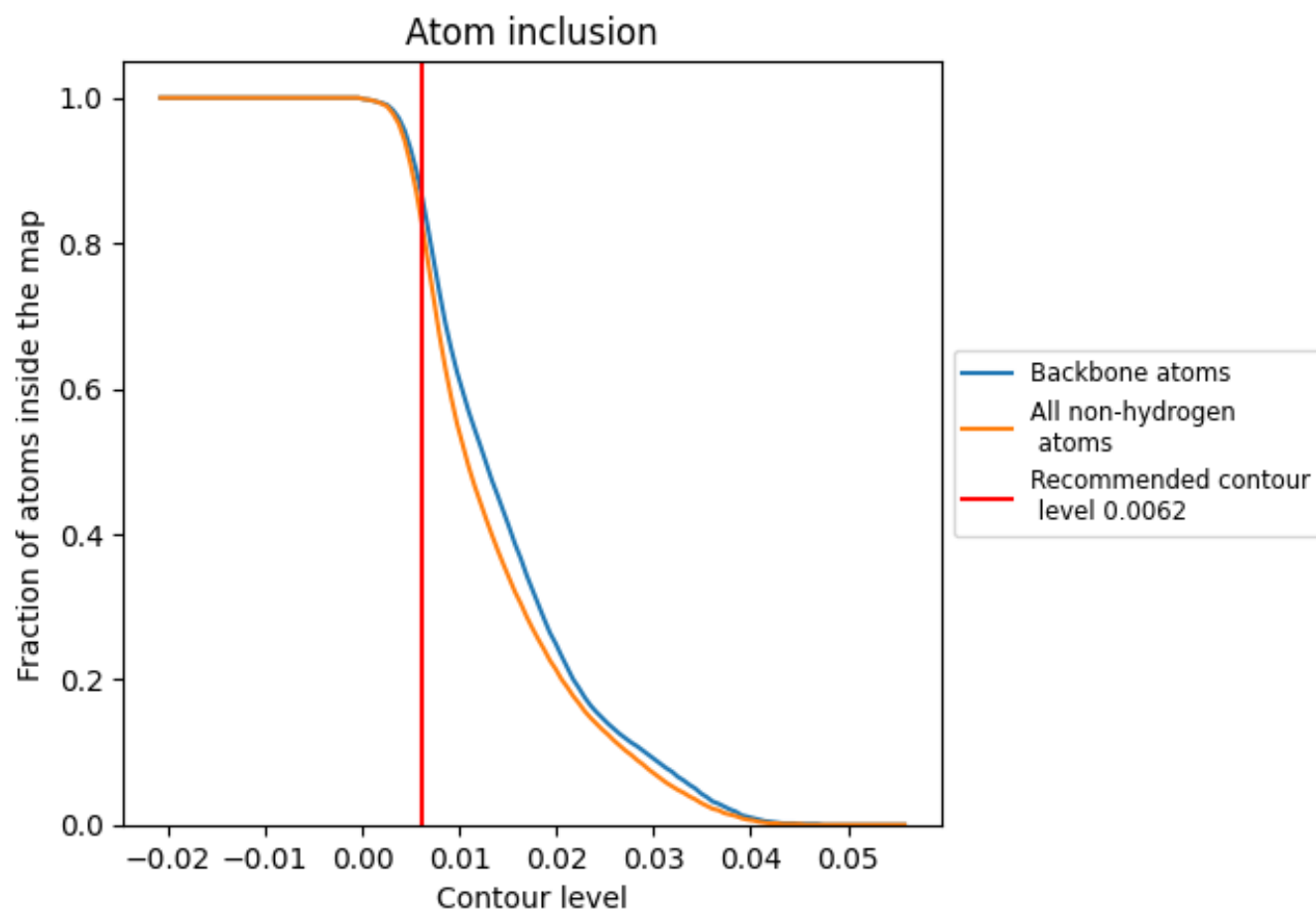
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0062).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 82% 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 (0.0062) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8210	 0.3150
A	 0.8640	 0.3170
B	 0.9570	 0.5090
C	 0.9940	 0.5150
D	 0.9940	 0.5110
E	 0.9920	 0.5150
F	 0.9520	 0.5190
G	 0.9780	 0.5090
H	 0.9850	 0.5050
I	 0.9980	 0.4350
J	 0.9680	 0.4190
K	 0.9550	 0.4920
M	 0.7750	 0.1560
N	 0.6510	 0.1120
P	 0.4900	 0.1020
Q	 0.8730	 0.3070
R	 0.9730	 0.3480
T	 0.6500	 0.1690
U	 0.7710	 0.2360
V	 0.9660	 0.3910
W	 0.7650	 0.3070
X	 0.7280	 0.2340
Y	 0.5600	 0.1990
Z	 0.4600	 0.1730
a	 0.8380	 0.3010

