



## Full wwPDB EM Validation Report ⓘ

Dec 7, 2022 – 11:22 AM JST

PDB ID : 6JYL  
EMDB ID : EMD-9718  
Title : The crosslinked complex of ISWI-nucleosome in the ADP.BeF-bound state  
Authors : Yan, L.J.; Wu, H.; Li, X.M.; Gao, N.; Chen, Z.C.  
Deposited on : 2019-04-26  
Resolution : 3.37 Å(reported)  
Based on initial model : 5X0Y

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

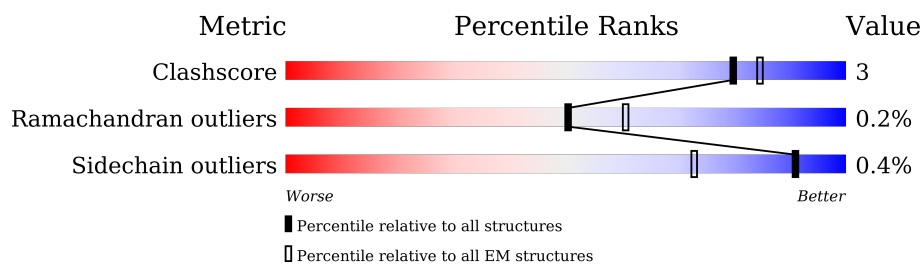
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.37 Å.

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





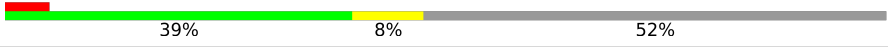
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	135	
1	E	135	
2	B	102	
2	F	102	
3	C	129	
3	G	129	
4	D	122	
4	H	122	

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Mol	Chain	Length	Quality of chain
5	I	167	
6	J	167	
7	K	1061	

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 16136 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 H3.

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

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	88	Total	C	N	O	S	0	0
			707	445	143	118	1		
2	F	80	Total	C	N	O	S	0	0
			632	398	122	111	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	107	Total	C	N	O	0	0
			811	510	158	143		
3	G	107	Total	C	N	O	0	0
			815	513	159	143		

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	93	Total	C	N	O	S	0	0
			718	451	128	137	2		
4	H	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	conflict	UNP P02281

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Chain	Residue	Modelled	Actual	Comment	Reference
H	29	THR	SER	conflict	UNP P02281

- Molecule 5 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		

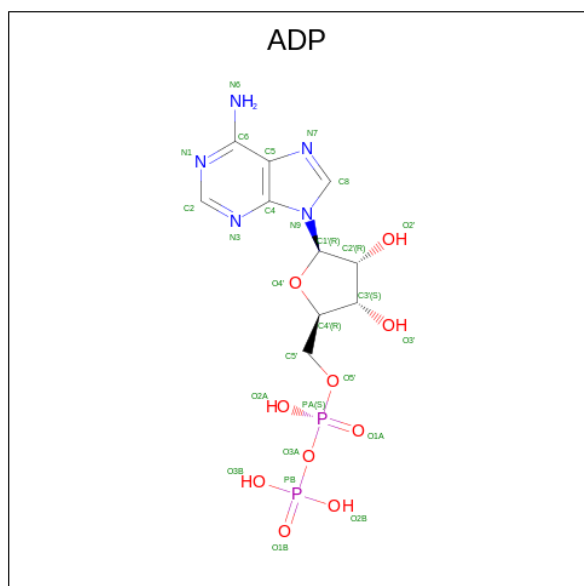
- Molecule 6 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		

- Molecule 7 is a protein called ISWI chromatin-remodeling complex ATPase ISW1.

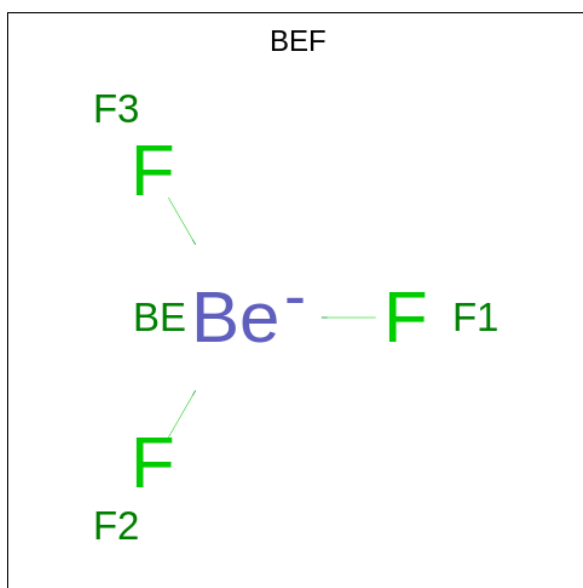
Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	504	Total	C	N	O	S	0	0
			4129	2639	709	768	13		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

- Molecule 9 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula:  $\text{BeF}_3$ ).



Mol	Chain	Residues	Atoms			AltConf
9	K	1	Total	Be	F	0
			4	1	3	

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula:  $\text{Mg}$ ).

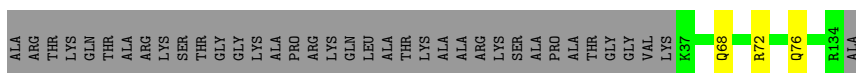
Mol	Chain	Residues	Atoms		AltConf
10	K	1	Total	Mg	0
			1	1	

### 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.

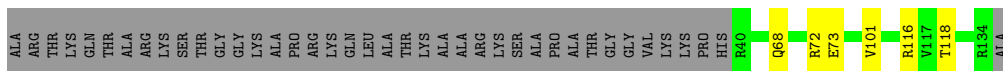
- Molecule 1: Histone H3

Chain A:  70% 27%




- Molecule 1: Histone H3

Chain E:  66% 30%



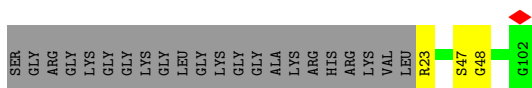
- Molecule 2: Histone H4

Chain B:  82% 14%




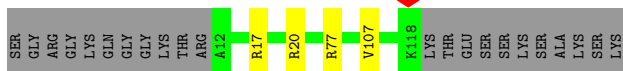
- Molecule 2: Histone H4

Chain F:  75% 22%



- Molecule 3: Histone H2A

Chain C:  80% 17%



- Molecule 3: Histone H2A

SER	GLY	ARG	GLY	LYS	GLN	GLY	GLY	LYS	THR	ARG	A12	R77	K118	LYS	THR	GLU	SER	SER	SER	LYS	SER	ALA	LYS	SER	LYS
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- Chain D:  76% 24%

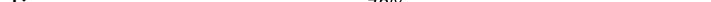
ALA	LYS	SER	ALA	PRO	PRO	LYS	LYS	GLY	SER	LYS	LYS	ALA	VAL	THR	LYS	THR	GLN	LYS	LYS	ASP	GLY	LYS	LYS	ARG	ARG	LYS	T29	A121	LYS
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- Chain H:  72% 0 24%

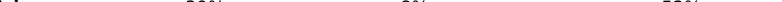
ALA
LYS
SER
ALA
PRO
ALA
PRO
LYS
GLY
SER
LYS
LYS
ALA
VAL
THR
LYS
THR
GLN
LYS
LYS
ASP
GLY
LYS
LYS
ARG
ARG
LYS
T29
E68
E73
R76
L99
P100
A121
LYS

- Chain I:  83% 13%

Category	Number of Genes
DC	10
T2	10
C47	10
T48	10
A97	10
A98	10
C123	10
A124	10
G132	10
T147	10
DA	10
DG	10
DC	10
DG	10
DT	10
DT	10
DT	10
DT	10
DT	10
DT	10
DC	10
DC	10
DA	10
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DA	10
DA	10
DA	10
DA	10
DT	10
DT	10
DC	10
DC	10
DT	10
DA	10
DA	10
DG	10

- Chain J:  78% 9% 13%

DC	DT	DA	DG	DT	DT	DA	DC	DC	DC	DC	DC	DC	DC	DC	DC	DC	DC	DT	A1	C20	A21	T50	T51	T57	T58	G65	G66	G95	T96	C123	G124	C132	A133	C134	C135	A146	DC
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- Chain K:  5% 39% 8% 52%

GLU	ASN	LEU	LYS	PRO	PHE	GLN	VAL	GLY	LEU	PRO	PRO	HIS	ASP	PRO	GLU	SER	ASN	LYS	LYS	ARG	TYR	LEU	LEU	LYS	ASP	ALA	ASN	GLY	LYS	PHE	D101	D102	E103	G104	K107	R108	F109	E110	L113	S114	G117	H121	E124	S125	K126	A127	ALA	LYS	D130	P131	K132	F133	S134	K135	S136	K137	S138	K139	S140	K141	S142	K143	S144	K145	S146	K147	S148	K149	S150	K151	S152	K153	S154	K155	S156	K157	S158	K159	S160	K161	S162	K163	S164	K165	S166	K167	S168	K169	S170	K171	S172	K173	S174	K175	S176	K177	S178	K179	S180	K181	S182	K183	S184	K185	S186	K187	S188	K189	S190	K191	S192	K193	S194	K195	S196	K197	S198	K199	S200	K201	S202	K203	S204	K205	S206	K207	S208	K209	S210	K211	S212	K213	S214	K215	S216	K217	S218	K219	S220	K221	S222	K223	S224	K225	S226	K227	S228	K229	S230	K231	S232	K233	S234	K235	S236	K237	S238	K239	S240	K241	S242	K243	S244	K245	S246	K247	S248	K249	S250	K251	S252	K253	S254	K255	S256	K257	S258	K259	S260	K261	S262	K263	S264	K265	S266	K267	S268	K269	S270	K271	S272	K273	S274	K275	S276	K277	S278	K279	S280	K281	S282	K283	S284	K285	S286	K287	S288	K289	S290	K291	S292	K293	S294	K295	S296	K297	S298	K299	S300	K301	S302	K303	S304	K305	S306	K307	S308	K309	S310	K311	S312	K313	S314	K315	S316	K317	S318	K319	S320	K321	S322	K323	S324	K325	S326	K327	S328	K329	S330	K331	S332	K333	S334	K335	S336	K337	S338	K339	S340	K341	S342	K343	S344	K345	S346	K347	S348	K349	S350	K351	S352	K353	S354	K355	S356	K357	S358	K359	S360	K361	S362	K363	S364	K365	S366	K367	S368	K369	S370	K371	S372	K373	S374	K375	S376	K377	S378	K379	S380	K381	S382	K383	S384	K385	S386	K387	S388	K389	S390	K391	S392	K393	S394	K395	S396	K397	S398	K399	S400	K401	S402	K403	S404	K405	S406	K407	S408	K409	S410	K411	S412	K413	S414	K415	S416	K417	S418	K419	S420	K421	S422	K423	S424	K425	S426	K427	S428	K429	S430	K431	S432	K433	S434	K435	S436	K437	S438	K439	S440	K441	S442	K443	S444	K445	S446	K447	S448	K449	S450	K451	S452	K453	S454	K455	S456	K457	S458	K459	S460	K461	S462	K463	S464	K465	S466	K467	S468	K469	S470	K471	S472	K473	S474	K475	S476	K477	S478	K479	S480	K481	S482	K483	S484	K485	S486	K487	S488	K489	S490	K491	S492	K493	S494	K495	S496	K497	S498	K499	S500	K501	S502	K503	S504	K505	S506	K507	S508	K509	S510	K511	S512	K513	S514	K515	S516	K517	S518	K519	S520	K521	S522	K523	S524	K525	S526	K527	S528	K529	S530	K531	S532	K533	S534	K535	S536	K537	S538	K539	S540	K541	S542	K543	S544	K545	S546	K547	S548	K549	S550	K551	S552	K553	S554	K555	S556	K557	S558	K559	S560	K561	S562	K563	S564	K565	S566	K567	S568	K569	S570	K571	S572	K573	S574	K575	S576	K577	S578	K579	S580	K581	S582	K583	S584	K585	S586	K587	S588	K589	S590	K591	S592	K593	S594	K595	S596	K597
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Q135	V136	L137	D138	V139	L140	E141	E142	N143	LYS	ALA	ASN	GLY	LYS	GLY	GLY	LYS	GLY	GLY	HIS	HIS	GLN	ASP	ASP	VAL	ARG	ARG	ARG	ARG	LYS	THR	GLU	GLU	GLU	HIS	GLY	GLU	ASP	ALA	ALA	GLU	LEU	LEU	LEU	LYS	LYS	GLU	GLU	ASP	ASP	ASP	SER	SER	ASP	ASP	ASP	GLU	SER	SER	ILE	GLU	PHE	Q154	S158	L156	Q200	N205	V206
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T215	Q230	L238	T244	V250	L257	L261	R262	N272	T275	L276	Q277	G278	R283	T287	L291	D295	S302	R308	L322	A326	H327	K330	R341	S345	R348	T352	G353	T354	P355	L356	Q357	L363	W364	L367
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	316230	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.5	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.120	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0216	Depositor
Map size (Å)	256.80002, 256.80002, 256.80002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.42	0/813	0.52	0/1093
1	E	0.42	0/789	0.51	0/1059
2	B	0.45	0/715	0.58	0/955
2	F	0.48	0/639	0.57	0/855
3	C	0.41	0/821	0.52	0/1112
3	G	0.42	0/825	0.51	0/1116
4	D	0.42	0/729	0.50	0/985
4	H	0.44	0/737	0.52	0/993
5	I	0.89	0/3333	0.99	0/5137
6	J	0.88	0/3381	0.97	0/5221
7	K	0.30	0/4207	0.51	0/5678
All	All	0.63	0/16989	0.75	0/24204

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	A	801	0	831	2	0
1	E	779	0	815	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	707	0	760	4	0
2	F	632	0	665	2	0
3	C	811	0	849	3	0
3	G	815	0	860	1	0
4	D	718	0	725	0	0
4	H	726	0	747	3	0
5	I	2975	0	1639	5	0
6	J	3011	0	1639	9	0
7	K	4129	0	4168	58	0
8	K	27	0	12	2	0
9	K	4	0	0	0	0
10	K	1	0	0	0	0
All	All	16136	0	13710	79	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (79) 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)
7:K:611:ARG:HH21	7:K:611:ARG:HA	1.13	1.07
7:K:611:ARG:HA	7:K:611:ARG:NH2	1.76	0.99
2:B:18:HIS:CE1	7:K:491:TYR:CD1	2.73	0.77
3:C:77:ARG:HH21	5:I:132:DG:H5'	1.64	0.63
7:K:594:VAL:HG12	7:K:624:PHE:HB2	1.83	0.60
7:K:431:VAL:HG11	7:K:506:VAL:HG21	1.87	0.57
7:K:614:ARG:NH1	8:K:1201:ADP:O1B	2.39	0.56
7:K:356:LEU:HB3	7:K:363:LEU:HB2	1.88	0.56
7:K:262:ARG:NH2	7:K:562:ASP:OD2	2.37	0.56
7:K:498:VAL:HG12	7:K:504:LEU:HB3	1.89	0.55
4:H:73:GLU:OE2	4:H:76:ARG:NH2	2.40	0.55
7:K:326:ALA:HB3	7:K:352:THR:HB	1.90	0.53
7:K:272:ASN:ND2	7:K:295:ASP:O	2.42	0.53
7:K:250:VAL:HG12	7:K:322:ILE:HB	1.90	0.53
7:K:345:SER:OG	7:K:348:ARG:NH1	2.40	0.53
7:K:443:LYS:HD3	7:K:460:GLU:HG3	1.90	0.53
7:K:480:TYR:OH	7:K:500:ASN:ND2	2.42	0.52
5:I:97:DA:OP1	7:K:601:ASN:ND2	2.38	0.52
7:K:261:LEU:HD13	7:K:275:ILE:HG13	1.92	0.52
7:K:586:ASN:ND2	8:K:1201:ADP:O3'	2.42	0.51
7:K:364:TRP:O	7:K:368:ASN:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:200:GLN:HG2	7:K:230:GLN:HE21	1.75	0.51
7:K:590:ALA:O	7:K:617:GLN:NE2	2.44	0.51
7:K:566:ALA:HB3	7:K:569:SER:HB2	1.92	0.50
1:A:68:GLN:HE21	1:A:72:ARG:HH21	1.60	0.50
1:E:68:GLN:HE21	1:E:72:ARG:HH21	1.60	0.49
7:K:524:PHE:HE1	7:K:576:LEU:HD12	1.78	0.48
7:K:603:GLN:NE2	7:K:647:ASP:OD2	2.46	0.48
7:K:104:GLY:HA2	7:K:107:LYS:HB2	1.96	0.48
1:E:73:GLU:OE2	2:F:23:ARG:N	2.46	0.48
7:K:508:ASP:OD2	7:K:541:ARG:NH2	2.43	0.48
7:K:602:PRO:HG3	7:K:640:ALA:HB1	1.95	0.48
7:K:188:SER:HA	7:K:196:LEU:HD12	1.95	0.47
7:K:521:VAL:HG23	7:K:592:VAL:HG23	1.96	0.47
7:K:364:TRP:HA	7:K:367:LEU:HB3	1.95	0.47
2:B:18:HIS:ND1	7:K:491:TYR:CD1	2.82	0.47
6:J:58:DT:OP1	7:K:283:ARG:NH2	2.41	0.47
7:K:238:LEU:O	7:K:244:ILE:N	2.41	0.46
5:I:97:DA:H2'	5:I:98:DA:C8	2.50	0.46
1:A:76:GLN:HE21	7:K:464:ARG:HG3	1.80	0.46
7:K:108:ARG:HG2	7:K:215:ILE:HG22	1.97	0.46
6:J:57:DT:O3'	7:K:308:ARG:NH2	2.49	0.46
6:J:134:DC:H2''	6:J:135:DC:H5'	1.98	0.46
7:K:611:ARG:HH21	7:K:611:ARG:CA	2.05	0.45
7:K:108:ARG:HD2	7:K:374:ILE:HD11	1.98	0.45
6:J:123:DC:H2''	6:J:124:DG:C8	2.52	0.45
7:K:275:ILE:HG22	7:K:277:GLN:HG2	1.99	0.45
2:F:47:SER:OG	2:F:48:GLY:N	2.50	0.45
3:G:77:ARG:HH21	6:J:132:DC:H5'	1.82	0.44
2:B:91:LYS:NZ	4:H:68:GLU:OE1	2.50	0.44
7:K:548:ILE:HD11	7:K:560:ALA:HB3	1.99	0.44
7:K:611:ARG:O	7:K:614:ARG:HD2	2.17	0.44
7:K:524:PHE:HB2	7:K:595:LEU:HD23	1.99	0.44
7:K:531:LEU:HD23	7:K:534:LEU:HD12	2.00	0.44
3:C:17:ARG:HA	3:C:20:ARG:HG2	1.99	0.43
1:E:116:ARG:NH1	1:E:118:THR:O	2.51	0.43
6:J:20:DC:H2''	6:J:21:DA:C8	2.54	0.43
6:J:50:DT:H2'	6:J:51:DT:H71	1.99	0.43
7:K:104:GLY:O	7:K:108:ARG:N	2.46	0.43
7:K:205:ASN:HA	7:K:208:VAL:HG22	2.01	0.42
6:J:65:DC:H2''	6:J:66:DG:C8	2.54	0.42
7:K:278:GLY:O	7:K:283:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:330:LYS:NZ	7:K:357:GLN:OE1	2.47	0.42
7:K:287:ILE:HA	7:K:291:LEU:HB3	2.01	0.41
2:B:15:ALA:N	7:K:536:ASP:OD1	2.53	0.41
3:C:107:VAL:HG21	1:E:101:VAL:HG11	2.02	0.41
5:I:123:DC:H2''	5:I:124:DA:C8	2.55	0.41
7:K:327:HIS:HE2	7:K:354:THR:HG1	1.62	0.41
7:K:478:HIS:HA	7:K:479:PRO:HD3	1.93	0.41
7:K:503:LYS:HB3	7:K:626:LEU:HD13	2.02	0.41
7:K:544:GLU:HB3	7:K:571:LYS:HG2	2.02	0.41
6:J:95:DG:H2'	6:J:96:DT:H71	2.02	0.41
4:H:99:LEU:HA	4:H:100:PRO:HD3	1.88	0.40
7:K:257:LEU:HD11	7:K:302:SER:HB3	2.03	0.40
7:K:434:SER:H	7:K:437:GLN:HE21	1.68	0.40
5:I:47:DC:H2''	5:I:48:DT:H71	2.04	0.40
7:K:429:LEU:HB2	7:K:626:LEU:HD23	2.03	0.40
7:K:547:ARG:HE	7:K:549:ASP:HB2	1.86	0.40
7:K:549:ASP:OD1	7:K:550:GLY:N	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	A	96/135 (71%)	96 (100%)	0	0	100	100
1	E	93/135 (69%)	93 (100%)	0	0	100	100
2	B	86/102 (84%)	81 (94%)	5 (6%)	0	100	100
2	F	78/102 (76%)	76 (97%)	2 (3%)	0	100	100
3	C	105/129 (81%)	104 (99%)	1 (1%)	0	100	100
3	G	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
4	D	91/122 (75%)	89 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	91/122 (75%)	88 (97%)	3 (3%)	0	100	100
7	K	496/1061 (47%)	450 (91%)	44 (9%)	2 (0%)	34	68
All	All	1241/2037 (61%)	1179 (95%)	60 (5%)	2 (0%)	50	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	K	493	THR
7	K	355	PRO

### 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	A	84/110 (76%)	84 (100%)	0	100	100
1	E	82/110 (74%)	82 (100%)	0	100	100
2	B	72/78 (92%)	71 (99%)	1 (1%)	67	83
2	F	64/78 (82%)	64 (100%)	0	100	100
3	C	81/101 (80%)	81 (100%)	0	100	100
3	G	82/101 (81%)	82 (100%)	0	100	100
4	D	77/102 (76%)	77 (100%)	0	100	100
4	H	79/102 (78%)	79 (100%)	0	100	100
7	K	459/958 (48%)	456 (99%)	3 (1%)	84	92
All	All	1080/1740 (62%)	1076 (100%)	4 (0%)	91	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	45	ARG
7	K	547	ARG
7	K	611	ARG
7	K	614	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	76	GLN
4	D	81	ASN
1	E	68	GLN
4	H	81	ASN
7	K	272	ASN
7	K	437	GLN
7	K	500	ASN
7	K	526	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
8	ADP	K	1201	10	24,29,29	0.95	1 (4%)	29,45,45	1.58	4 (13%)
9	BEF	K	1202	-	0,3,3	-	-	-		



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
8	ADP	K	1201	10	-	4/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	1201	ADP	C5-C4	2.36	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	1201	ADP	PA-O3A-PB	-4.48	117.45	132.83
8	K	1201	ADP	N3-C2-N1	-3.29	123.53	128.68
8	K	1201	ADP	C3'-C2'-C1'	3.01	105.51	100.98
8	K	1201	ADP	C4-C5-N7	-2.72	106.56	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	K	1201	ADP	C3'-C4'-C5'-O5'
8	K	1201	ADP	O4'-C4'-C5'-O5'
8	K	1201	ADP	C5'-O5'-PA-O3A
8	K	1201	ADP	C5'-O5'-PA-O2A

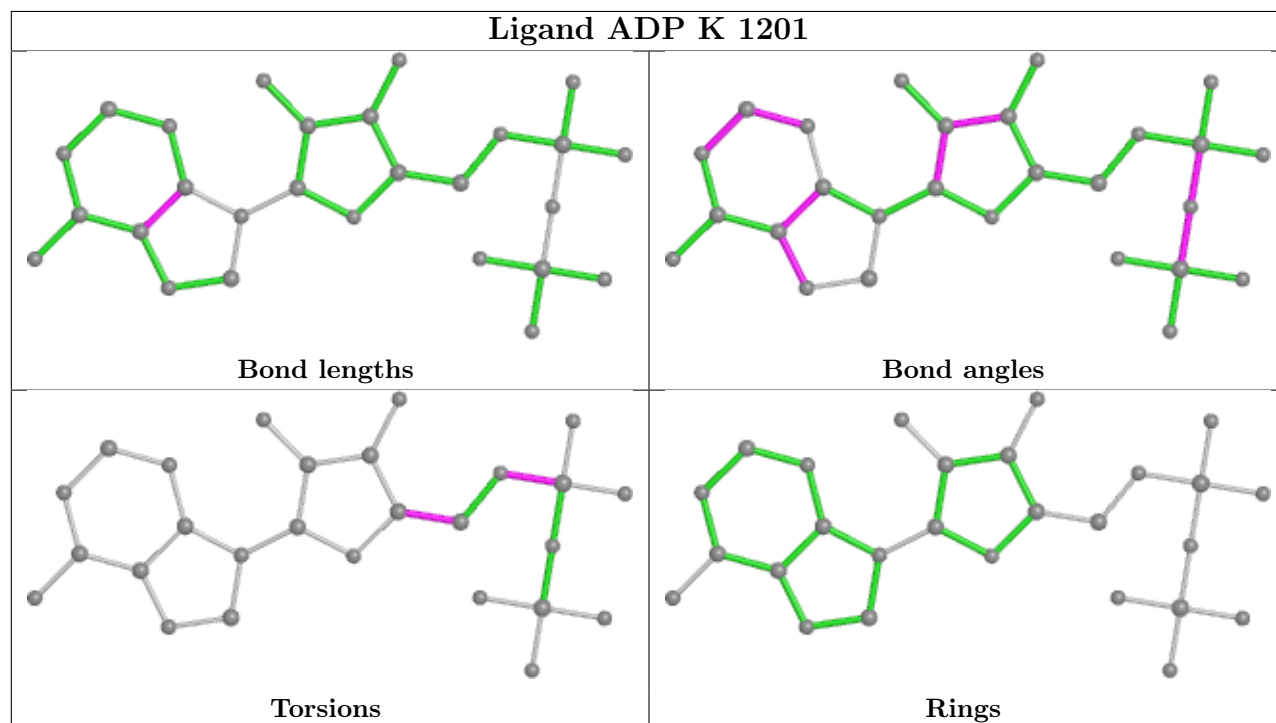
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	K	1201	ADP	2	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.

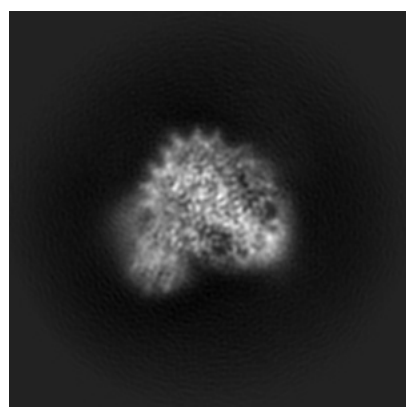
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9718. These allow visual inspection of the internal detail of the map and identification of artifacts.

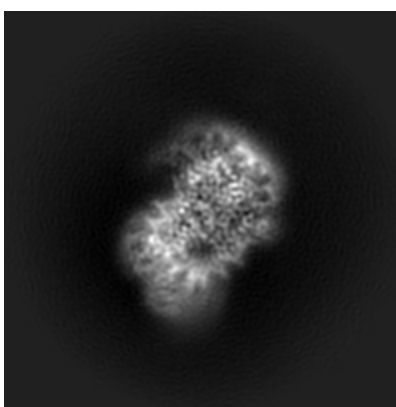
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

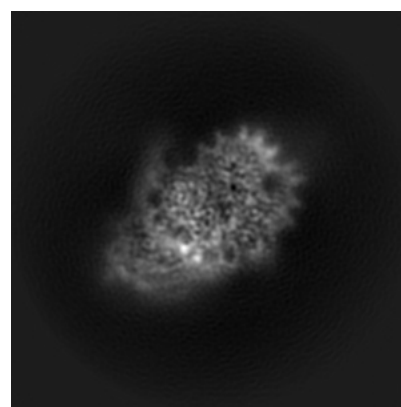
#### 6.1.1 Primary map



X



Y

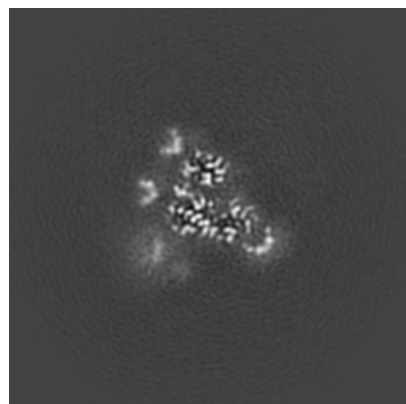


Z

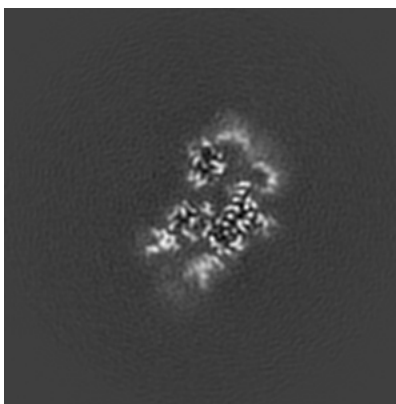
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

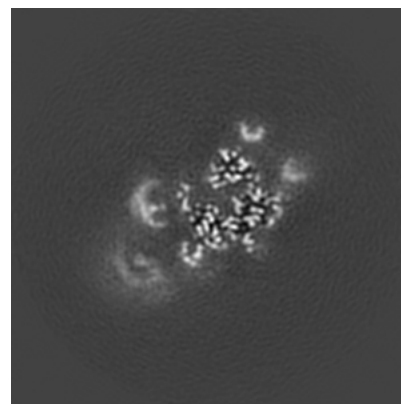
#### 6.2.1 Primary map



X Index: 120



Y Index: 120

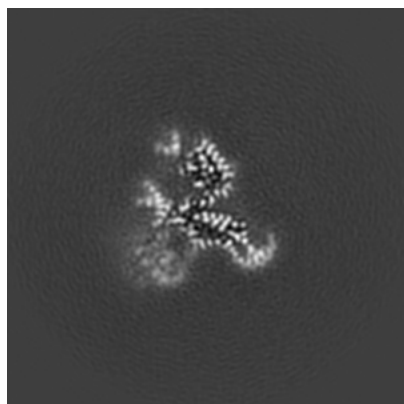


Z Index: 120

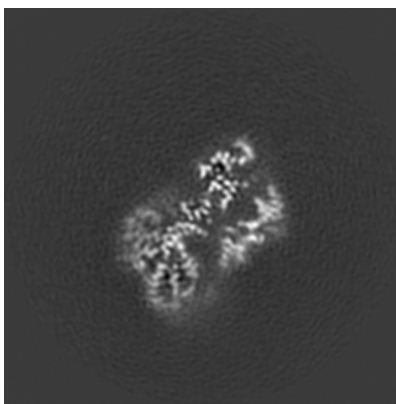
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

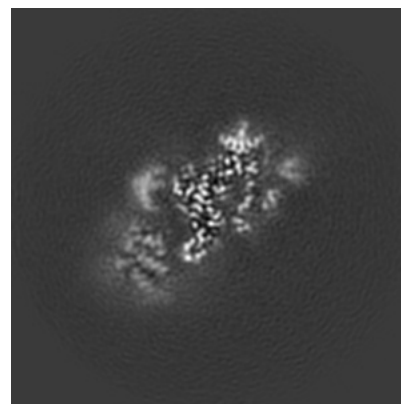
### 6.3.1 Primary map



X Index: 113



Y Index: 99



Z Index: 112

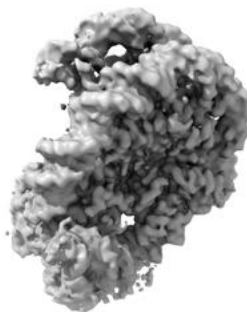
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0216. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

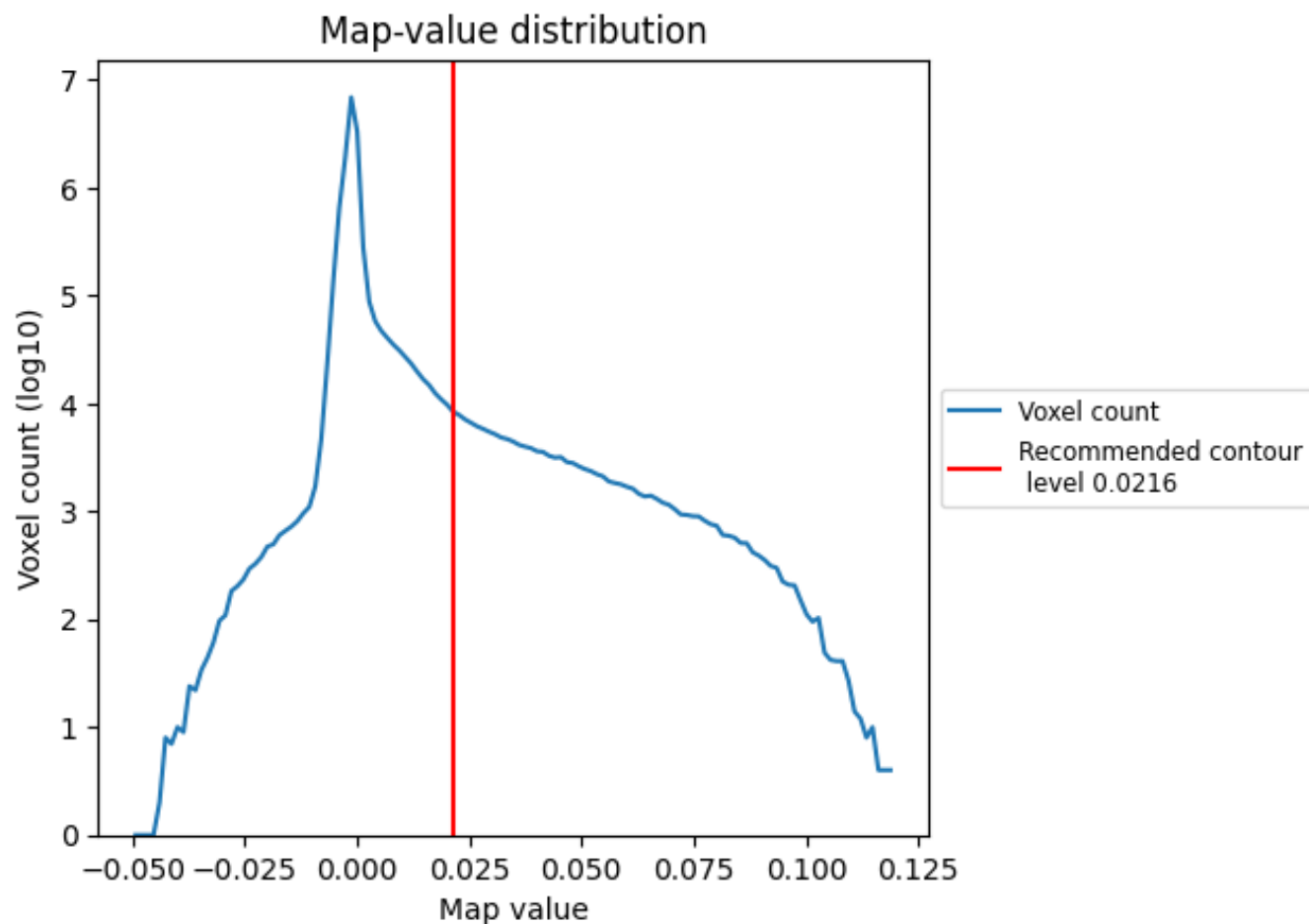
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

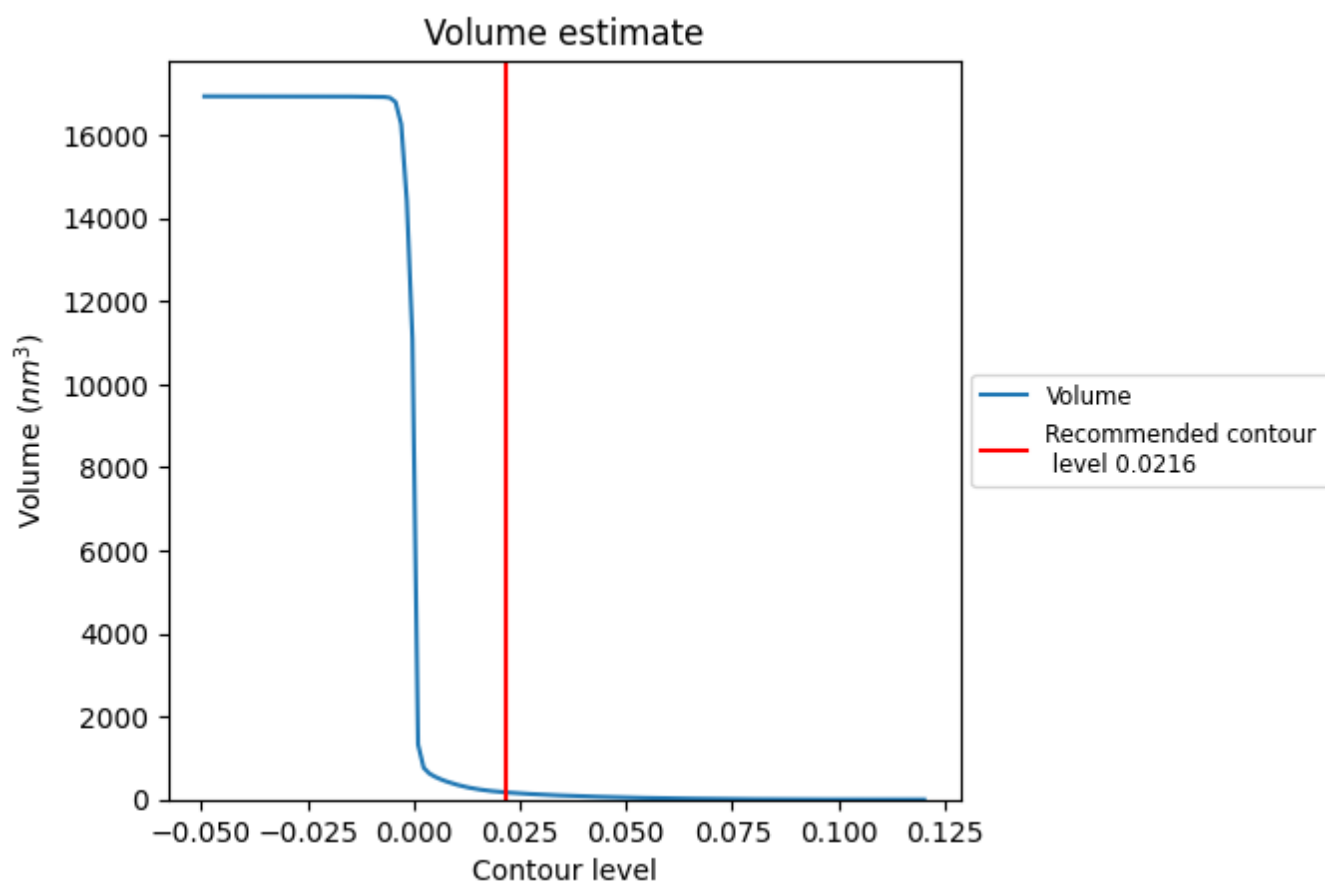
This section contains the results of statistical analysis of the map.

### 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.

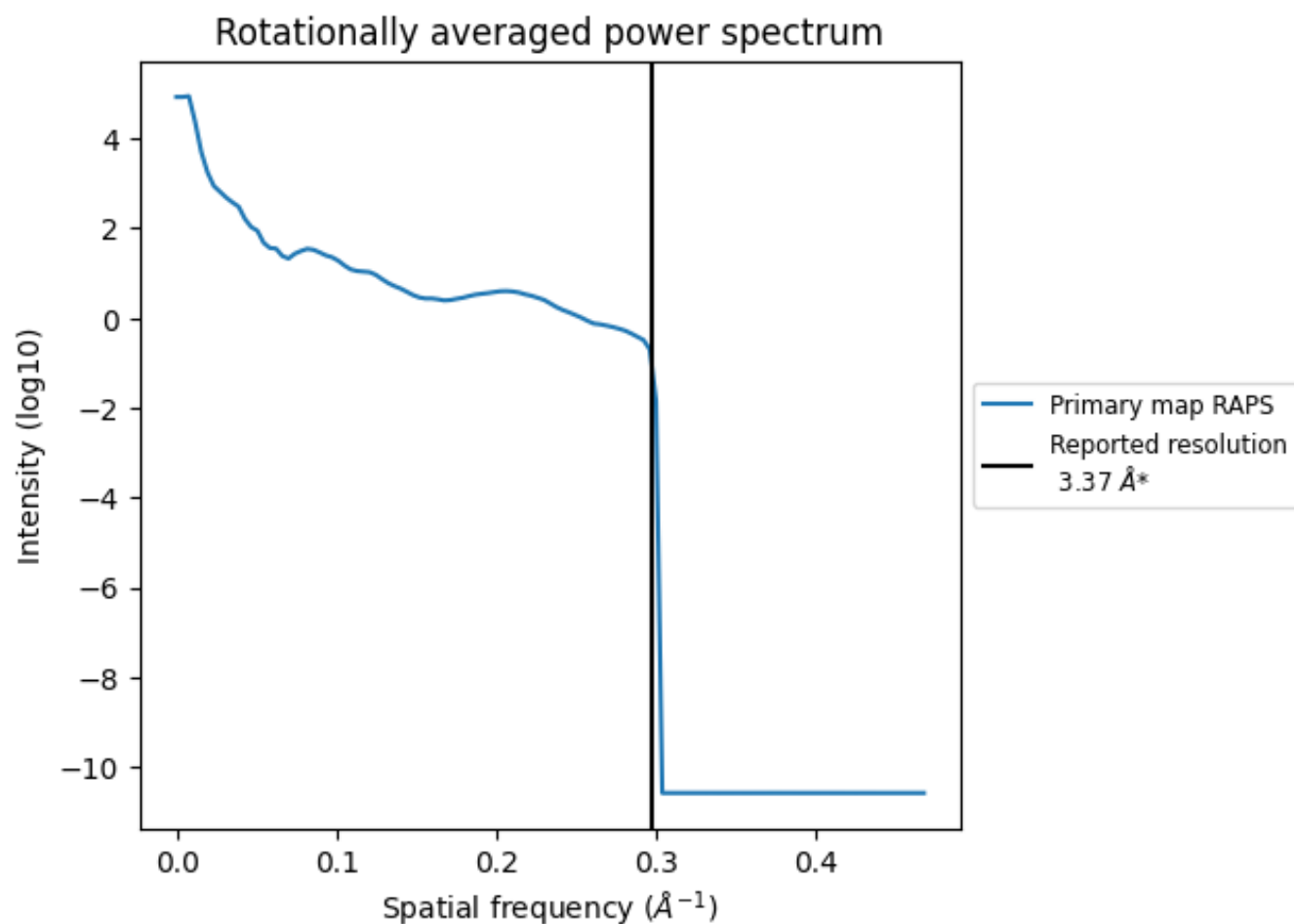
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 174 nm<sup>3</sup>; this corresponds to an approximate mass of 157 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 0.297  $\text{\AA}^{-1}$



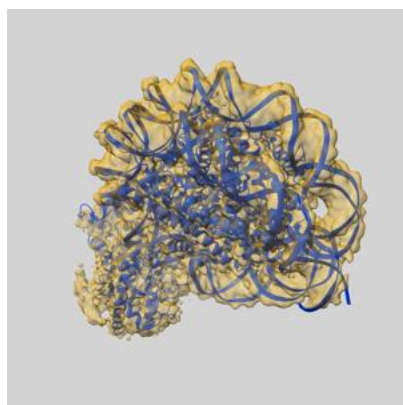
## 8 Fourier-Shell correlation ⓘ

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

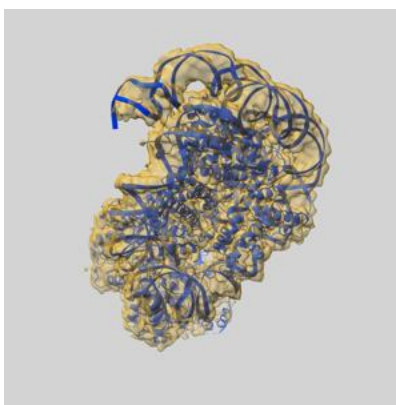
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9718 and PDB model 6JYL. Per-residue inclusion information can be found in section [3](#) on page [7](#).

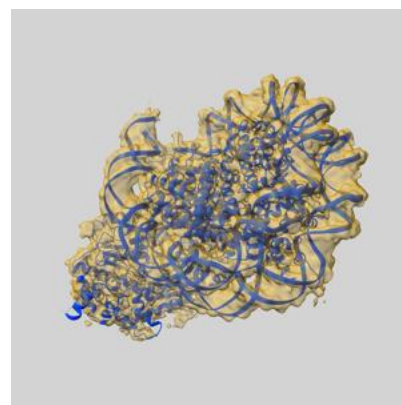
### 9.1 Map-model overlay [i](#)



X



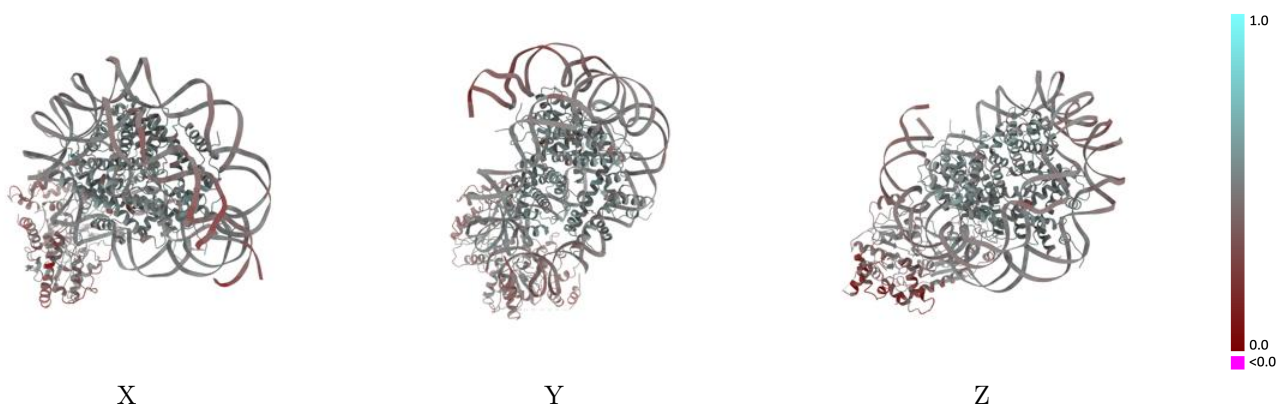
Y



Z

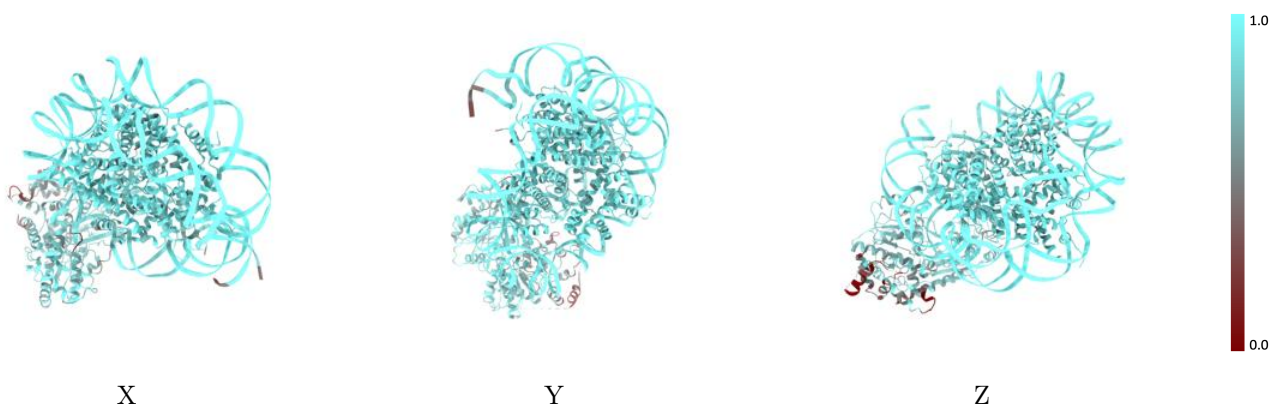
The images above show the 3D surface view of the map at the recommended contour level 0.0216 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



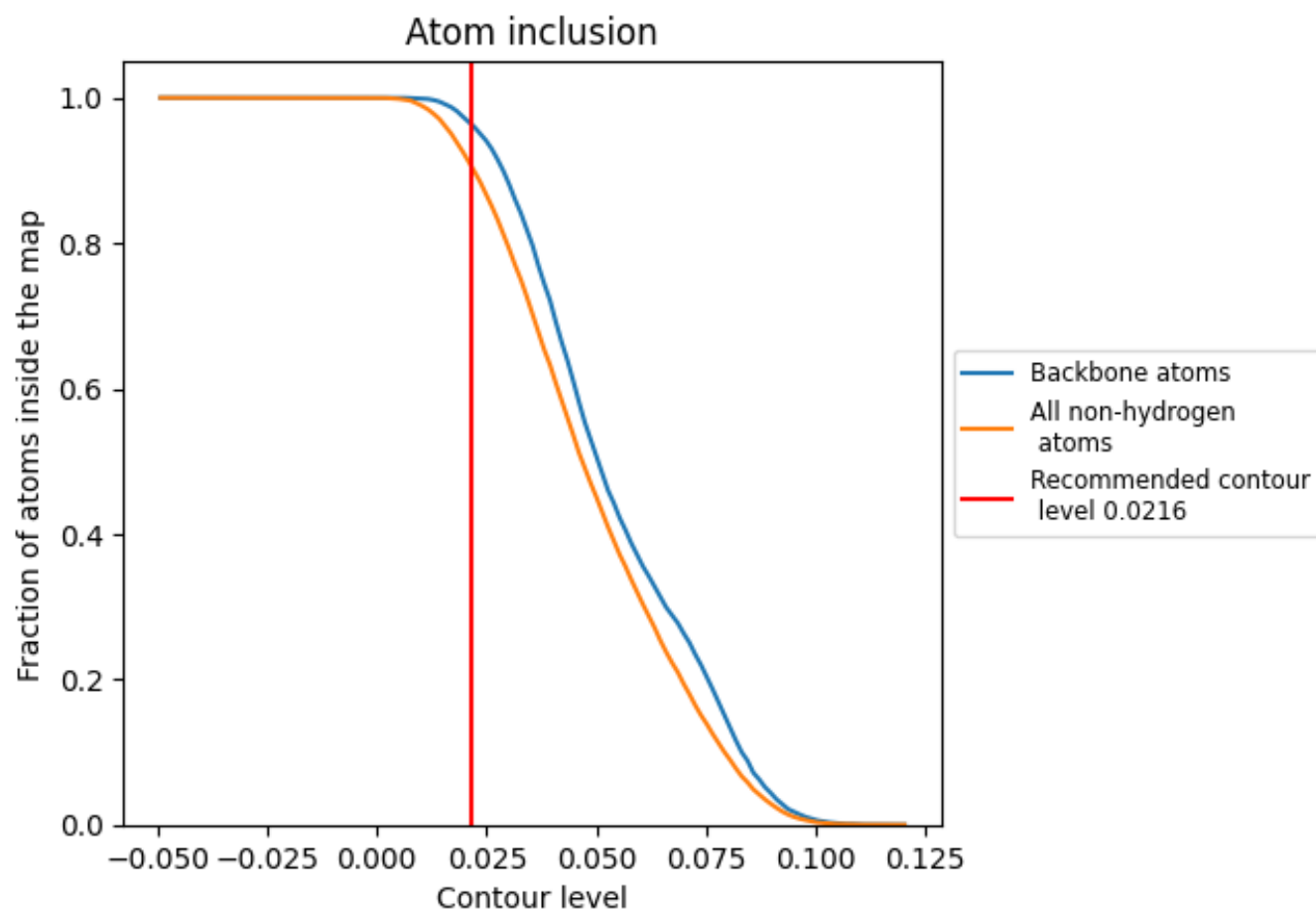
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0216).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 91% 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 (0.0216) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9052	<div><div></div></div> 0.4520
A	<div><div></div></div> 0.9288	<div><div></div></div> 0.5230
B	<div><div></div></div> 0.9247	<div><div></div></div> 0.5040
C	<div><div></div></div> 0.9198	<div><div></div></div> 0.5110
D	<div><div></div></div> 0.9444	<div><div></div></div> 0.5110
E	<div><div></div></div> 0.9227	<div><div></div></div> 0.5170
F	<div><div></div></div> 0.9457	<div><div></div></div> 0.5220
G	<div><div></div></div> 0.9392	<div><div></div></div> 0.5210
H	<div><div></div></div> 0.9436	<div><div></div></div> 0.5040
I	<div><div></div></div> 0.9866	<div><div></div></div> 0.4470
J	<div><div></div></div> 0.9817	<div><div></div></div> 0.4450
K	<div><div></div></div> 0.7496	<div><div></div></div> 0.3730

1.0

0.0

<0.0