

# wwPDB EM Validation Summary Report (i)

#### May 6, 2023 – 01:39 PM EDT

PDB ID : 8EBW EMDB ID : EMD-28000 Title : Initial DNA-lesion (AP) binding by XPC and TFIIH complex2 Authors : Kim, J.; Yang, W. Deposited on : 2022-08-31 Resolution : 5.60 Å(reported) Based on initial model : 6NMI

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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

EMDB validation analysis	:	0.0.1. dev 50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
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)	:	2.32.2

# 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 5.60 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)	${ m EM~structures} \ (\#{ m Entries})$
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 >=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 c	chain
1	А	782	53%	<b>24% 21%</b>
2	В	768	46% 71%	27% ••
3	С	548	20% 41% 14% •	44%
4	D	462	<b>67</b> %	28% • •
5	Е	417	13%	25% · 15%
6	F	308	57%	27% • 15%
7	G	71	<u>8%</u> 59%	30% 6% 6%
8	Н	950	30% 40% 16%	44%

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Contre	naca fron	i previous	puye		
Mol	Chain	Length		Quality of chain	
9	Ι	417	11%	85%	
10	J	172	46%	66%	20% 13%
11	L	53	32%	64%	36%
19	м	52	34%	<b>0</b> //	
14	111	- 55	5	8%	42%

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# 2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 30759 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 TFIIH basal transcription factor complex helicase XPB subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	А	614	Total 4955	C 3163	N 857	O 905	S 30	0	0

• Molecule 2 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	В	760	Total 6120	C 3907	N 1067	0 1117	S 29	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	761	ASP	-	expression tag	UNP P18074
В	762	TYR	-	expression tag	UNP P18074
В	763	LYS	-	expression tag	UNP P18074
В	764	ASP	-	expression tag	UNP P18074
В	765	ASP	-	expression tag	UNP P18074
В	766	ASP	-	expression tag	UNP P18074
В	767	ASP	-	expression tag	UNP P18074
В	768	LYS	-	expression tag	UNP P18074

• Molecule 3 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	С	309	Total 2511	C 1596	N 441	0 461	S 13	0	0

• Molecule 4 is a protein called General transcription factor IIH subunit 4, p52.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	446	$\begin{array}{c} \text{Total} \\ 3557 \end{array}$	C 2289	N 620	O 635	S 13	0	0



• Molecule 5 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Е	355	Total 2792	C 1760	N 483	O 522	S 27	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Е	-21	MET	-	initiating methionine	UNP Q13888
Е	-20	GLY	-	expression tag	UNP Q13888
Е	-19	SER	-	expression tag	UNP Q13888
Е	-18	SER	-	expression tag	UNP Q13888
E	-17	HIS	-	expression tag	UNP Q13888
Е	-16	HIS	-	expression tag	UNP Q13888
Е	-15	HIS	-	expression tag	UNP Q13888
Е	-14	HIS	-	expression tag	UNP Q13888
Е	-13	HIS	-	expression tag	UNP Q13888
Е	-12	HIS	-	expression tag	UNP Q13888
Е	-11	SER	-	expression tag	UNP Q13888
E	-10	SER	-	expression tag	UNP Q13888
Е	-9	GLY	-	expression tag	UNP Q13888
Е	-8	LEU	-	expression tag	UNP Q13888
E	-7	GLU	-	expression tag	UNP Q13888
E	-6	VAL	-	expression tag	UNP Q13888
E	-5	LEU	-	expression tag	UNP Q13888
Ε	-4	PHE	-	expression tag	UNP Q13888
Е	-3	GLN	-	expression tag	UNP Q13888
E	-2	GLY	-	expression tag	UNP Q13888
E	-1	PRO	-	expression tag	UNP Q13888
E	0	HIS	-	expression tag	UNP Q13888

• Molecule 6 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	261	Total 2057	C 1316	N 341	0 381	S 19	0	0

• Molecule 7 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	67	Total 530	C 342	N 84	0 101	${ m S} { m 3}$	0	0



• Molecule 8 is a protein called Xeroderma pigmentosum, complementation group C, isoform CRA\_a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Н	532	Total 4364	C 2790	N 772	0 782	S 20	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Н	-9	MET	-	initiating methionine	UNP A0A024R2M8
Н	-8	ASP	-	expression tag	UNP A0A024R2M8
Н	-7	TYR	-	expression tag	UNP A0A024R2M8
Н	-6	LYS	-	expression tag	UNP A0A024R2M8
Н	-5	ASP	-	expression tag	UNP A0A024R2M8
Н	-4	ASP	-	expression tag	UNP A0A024R2M8
Н	-3	ASP	-	expression tag	UNP A0A024R2M8
Н	-2	ASP	-	expression tag	UNP A0A024R2M8
Н	-1	LYS	-	expression tag	UNP A0A024R2M8
Н	0	HIS	-	expression tag	UNP A0A024R2M8
Н	499	VAL	ALA	conflict	UNP A0A024R2M8

• Molecule 9 is a protein called UV excision repair protein RAD23 homolog B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Ι	61	Total 504	C 316	N 95	0 91	${S \over 2}$	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ι	410	LEU	-	expression tag	UNP P54727
Ι	411	GLU	-	expression tag	UNP P54727
Ι	412	HIS	-	expression tag	UNP P54727
Ι	413	HIS	-	expression tag	UNP P54727
Ι	414	HIS	-	expression tag	UNP P54727
Ι	415	HIS	-	expression tag	UNP P54727
Ι	416	HIS	-	expression tag	UNP P54727
Ι	417	HIS	-	expression tag	UNP P54727

• Molecule 10 is a protein called Centrin-2.



Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	149	Total 1201	C 749	N 194	0 251	${ m S} 7$	1	0

• Molecule 11 is a DNA chain called DNA (Ap).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	53	Total 1075	C 510	N 196	0 316	Р 53	0	0

• Molecule 12 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	М	53	Total 1078	C 515	N 190	O 320	Р 53	0	0

• Molecule 13 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $Fe_4S_4$ ).



Mol	Chain	Residues	Atoms	AltConf
13	В	1	TotalFeS844	0

• Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
14	Ε	3	Total 3	Zn 3	0

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Mol	Chain	Residues	Atoms	AltConf
14	F	2	Total Zn 2 2	0

• Molecule 15 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
15	J	2	Total Ca 2 2	0



Chain B:

# 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: TFIIH basal transcription factor complex helicase XPB subunit



<sup>•</sup> Molecule 2: General transcription and DNA repair factor IIH helicase subunit XPD

46% 71% 27%

























# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66841	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	54.1	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	103000	Depositor
Image detector	GATAN K3 $(6k \ge 4k)$	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	373.5, 373.5, 373.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.245, 1.245, 1.245	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: 3DR, SF4, CA, ZN

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).

Mal	Chain	Bond	lengths	Bond	angles
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.26	0/5059	0.39	0/6833
2	В	0.24	0/6247	0.38	0/8457
3	С	0.24	0/2564	0.37	0/3460
4	D	0.25	0/3641	0.38	0/4934
5	Ε	0.24	0/2857	0.39	0/3870
6	F	0.25	0/2093	0.38	0/2833
7	G	0.25	0/536	0.40	0/724
8	Н	0.24	0/4467	0.37	0/6041
9	Ι	0.25	0/515	0.37	0/696
10	J	0.24	0/1211	0.38	0/1605
11	L	0.48	0/1181	0.87	0/1820
12	М	0.48	0/1206	0.89	0/1857
All	All	0.27	0/31577	0.45	0/43130

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	А	4955	0	4997	141	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	6120	0	6164	134	0
3	С	2511	0	2502	57	0
4	D	3557	0	3596	91	0
5	Е	2792	0	2735	75	0
6	F	2057	0	2079	67	0
7	G	530	0	539	23	0
8	Н	4364	0	4363	117	0
9	Ι	504	0	497	10	0
10	J	1201	0	1185	19	0
11	L	1075	0	591	13	0
12	М	1078	0	599	19	0
13	В	8	0	0	0	0
14	Е	3	0	0	0	0
14	F	2	0	0	0	0
15	J	2	0	0	0	0
All	All	30759	0	29847	693	0

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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 11.

The worst 5 of 693 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:E:382:CYS:HB3	5:E:385:CYS:SG	2.15	0.86
2:B:349:VAL:HA	2:B:418:ILE:O	1.76	0.84
8:H:711:SER:H	8:H:715:ARG:HE	1.30	0.80
7:G:14:PRO:O	7:G:18:GLN:NE2	2.17	0.76
2:B:622:GLY:HA2	2:B:681:ASP:HB2	1.69	0.75

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	Perce	entiles
1	А	610/782~(78%)	$591 \ (97\%)$	19 (3%)	0	100	100
2	В	758/768~(99%)	748 (99%)	10 (1%)	0	100	100
3	С	301/548~(55%)	295~(98%)	6 (2%)	0	100	100
4	D	444/462~(96%)	439 (99%)	5 (1%)	0	100	100
5	Е	351/417~(84%)	342~(97%)	9~(3%)	0	100	100
6	F	257/308~(83%)	249~(97%)	8 (3%)	0	100	100
7	G	65/71~(92%)	64 (98%)	1 (2%)	0	100	100
8	Н	524/950~(55%)	505~(96%)	19 (4%)	0	100	100
9	Ι	59/417~(14%)	56~(95%)	3~(5%)	0	100	100
10	J	148/172~(86%)	146 (99%)	2 (1%)	0	100	100
All	All	3517/4895~(72%)	3435 (98%)	82 (2%)	0	100	100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	543/688~(79%)	528~(97%)	15 (3%)	43 65
2	В	664/672~(99%)	645~(97%)	19 (3%)	42 64
3	С	277/484~(57%)	267~(96%)	10 (4%)	35 59
4	D	384/399~(96%)	370~(96%)	14 (4%)	35 59
5	Ε	317/371~(85%)	307~(97%)	10 (3%)	39 61
6	F	233/272~(86%)	230~(99%)	3~(1%)	69 82
7	G	60/64~(94%)	55~(92%)	5 (8%)	11 36
8	Н	467/815~(57%)	461 (99%)	6 (1%)	69 82
9	Ι	57/336~(17%)	56~(98%)	1 (2%)	59 77
10	J	130/152~(86%)	125 (96%)	5(4%)	33 57
All	All	3132/4253~(74%)	3044 (97%)	88 (3%)	46 65



5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
4	D	434	GLU
7	G	6	LYS
5	Е	21	ILE
5	Ε	304	GLU
7	G	59	GLU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such side chains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
6	F	258	HIS
7	G	18	GLN
9	Ι	293	GLN
5	Е	365	ASN
6	F	25	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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).

Mal	Mal Trung Chain Dag I		Type Chain Bes Link		B	ond leng	$\operatorname{gths}$	Bond angles		
IVIOI	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
11	3DR	L	31	11	8,11,12	6.27	4 (50%)	9,14,17	1.53	2 (22%)
11	3DR	L	30	11	8,11,12	6.25	4 (50%)	9,14,17	1.68	3 (33%)

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
11	3DR	L	31	11	-	2/3/15/16	0/1/1/1
11	3DR	L	30	11	-	0/3/15/16	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
11	L	31	3DR	C2'-C3'	-13.26	1.29	1.52
11	L	30	3DR	C2'-C3'	-12.93	1.30	1.52
11	L	30	3DR	O4'-C4'	-9.93	1.28	1.44
11	L	31	3DR	O4'-C4'	-9.58	1.28	1.44
11	L	31	3DR	C3'-C4'	4.52	1.65	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
11	L	31	3DR	O4'-C4'-C3'	3.16	108.38	103.73
11	L	30	3DR	C1'-C2'-C3'	2.73	106.28	103.20
11	L	30	3DR	C2'-C3'-C4'	2.61	108.15	102.75
11	L	30	3DR	C1'-O4'-C4'	-2.56	104.35	108.48
11	L	31	3DR	C2'-C3'-C4'	2.12	107.15	102.75

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	L	31	3DR	O4'-C4'-C5'-O5'
11	L	31	3DR	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 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).

Mal	Tuno	Chain	Dog	Link	Bond lengths			Bond angles		
WIOI	Type	e Chain Res Link			Counts	RMSZ	# Z >2	Counts	RMSZ   #  Z  > 2	
13	SF4	В	1000	2	0,12,12	-	-	-		

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
13	SF4	В	1000	2	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 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-28000. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections (i)

#### 6.1.1 Primary map



6.1.2 Raw map



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



### 6.2 Central slices (i)

### 6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

#### 6.2.2 Raw map



X Index: 150

Y Index: 150

Z Index: 150

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: 141



Y Index: 183



Z Index: 152

#### 6.3.2 Raw map



X Index: 141

Y Index: 170



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



#### 6.4.2 Raw map



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

#### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

#### 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 236  $\rm nm^3;$  this corresponds to an approximate mass of 213 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 0.179  ${\rm \AA^{-1}}$ 



# 8 Fourier-Shell correlation (i)

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 (i)



\*Reported resolution corresponds to spatial frequency of 0.179  $\mathrm{\AA^{-1}}$ 



## 8.2 Resolution estimates (i)

$\mathbf{Bosolution} \text{ ostimato } (\mathbf{\hat{\lambda}})$	Estimation criterion (FSC cut-off)				
Resolution estimate (A)	0.143	0.5	Half-bit		
Reported by author	5.60	-	-		
Author-provided FSC curve	5.52	7.86	6.00		
Unmasked-calculated*	7.49	8.76	7.74		

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.49 differs from the reported value 5.6 by more than 10 %



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-28000 and PDB model 8EBW. Per-residue inclusion information can be found in section 3 on page 9.

## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



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



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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).



### 9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

	Q-score	Atom inclusion	Chain
	0.2080	0.5520	All
1.0	0.2640	0.6910	А
	0.1970	0.4320	В
	0.1880	0.5160	С
	0.2490	0.7260	D
	0.2490	0.6210	Е
	0.2530	0.6390	F
	0.2460	0.6740	G
	0.1330	0.3890	Н
0.0	0.1080	0.2470	I
<0.0	0.1330	0.4080	J
	0.1750	0.5800	L
	0.1830	0.6260	М

