

# wwPDB EM Validation Summary Report (i)

#### Apr 4, 2024 – 05:29 pm BST

PDB ID : 8RBZ EMDB ID : EMD-19040 Title Structure of Integrator-PP2A-SOSS-CTD post-termination complex : Authors : Fianu, I.; Ochmann, M.; Walshe, J.L.; Cramer, P. Deposited on 2023-12-05 : 3.70 Å(reported) Resolution : Based on initial model ? :

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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1. dev 92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{MapQ}$	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive	EM structures
	$(\# { m Entries})$	$(\# { m Entries})$
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  $\geq=3, 2, 1$  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	Quality of chain						
1	1	9	100%							
2	В	213	<b>48%</b> • 50%							
3	С	106	37% 63%							
4	Y	13	100%							
5	a	2192	49% 51%							
6	b	1204	87%	• 13%						
7	С	1042	44% 56%							
8	d	963	85%	15%						

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Mol	Chain	Length	Quality of chain	
9	е	1021	83%	16%
10	f	889	61% 39%	)
11	g	964	91%	• 8%
12	h	995	88%	• 11%
13	i	658	95%	• 5%
14	j	710	94%	6%
15	k	602	90%	• 8%
16	n	518	24% 39% 61%	
17	О	451	81%	19%
18	р	591	97%	••
19	q	311	93%	• 7%
20	r	27	100%	
21	m	706	5% 95%	

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# 2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 74102 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 UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	9	Total 45	С 27	N 9	0 9	0	0

• Molecule 2 is a protein called SOSS complex subunit B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	В	107	Total 806	C 516	N 135	0 151	${f S}$ $4$	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	-1	SER	-	expression tag	UNP Q9BQ15
В	0	ASN	-	expression tag	UNP Q9BQ15

• Molecule 3 is a protein called SOSS complex subunit C.

Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
3	С	39	Total 296	C 190	N 56	O 50	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	-1	SER	-	expression tag	UNP Q9NRY2
С	0	ASN	-	expression tag	UNP Q9NRY2

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

Mol	Chain	Residues	L	Ator	$\mathbf{ns}$	AltConf	Trace	
4	Y	13	Total 95	C 60	N 13	O 22	0	0



• Molecule 5 is a protein called Integrator complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	1085	Total 8525	C 5425	N 1502	0 1547	S 51	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-1	SER	-	expression tag	UNP Q8N201
a	0	ASN	-	expression tag	UNP Q8N201

• Molecule 6 is a protein called Integrator complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	1051	Total 7988	C 5120	N 1352	0 1454	S 62	0	0

• Molecule 7 is a protein called Integrator complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	с	463	Total 3717	C 2380	N 646	O 662	S 29	0	0

• Molecule 8 is a protein called Integrator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	818	Total 6395	C 4081	N 1091	0 1189	S 34	0	0

• Molecule 9 is a protein called Integrator complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	е	855	Total 6253	C 3974	N 1139	0 1114	S 26	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
е	-1	SER	-	expression tag	UNP Q6P9B9
e	0	ASN	-	expression tag	UNP Q6P9B9

• Molecule 10 is a protein called Integrator complex subunit 6.



Mol	Chain	Residues		Atoms					Trace
10	f	544	Total 4137	C 2653	N 701	O 758	S 25	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	-1	SER	-	expression tag	UNP Q9UL03
f	0	ASN	-	expression tag	UNP Q9UL03

• Molecule 11 is a protein called Integrator complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	g	886	Total 6725	C 4261	N 1169	O 1255	S 40	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Residue Modelled Actual Comment		Comment	Reference
g	-1	SER	-	expression tag	UNP Q9NVH2
g	0	ASN	-	expression tag	UNP Q9NVH2

• Molecule 12 is a protein called Integrator complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	h	887	Total 6748	C 4333	N 1156	0 1221	S 38	0	0

• Molecule 13 is a protein called Integrator complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	i	626	Total 4867	C 3134	N 792	O 908	S 33	0	0

• Molecule 14 is a protein called Integrator complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	j	668	Total 3313	C 1976	N 668	O 669	0	0

• Molecule 15 is a protein called Integrator complex subunit 11.



Mol	Chain	Residues		At	AltConf	Trace			
15	k	551	Total 4079	C 2613	N 706	О 734	S 26	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	-1	SER	-	expression tag	UNP Q5TA45
k	0	ASN	-	expression tag	UNP Q5TA45
k	203	GLN	GLU	engineered mutation	UNP Q5TA45
k	487	GLU	ASP	conflict	UNP Q5TA45

• Molecule 16 is a protein called Integrator complex subunit 14.

Mol	Chain	Residues		Ato	ms		AltConf	Trace
16	n	204	Total 1007	C 599	N 204	O 204	0	0

• Molecule 17 is a protein called Integrator complex subunit 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	О	367	Total 1824	C 1090	N 367	O 367	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	-1	SER	-	expression tag	UNP Q96N11
0	0	ASN	-	expression tag	UNP Q96N11

• Molecule 18 is a protein called Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	р	580	Total 4432	C 2822	N 753	0 831	S 26	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
р	-1	SER	-	expression tag	UNP P30153
р	0	ASN	-	expression tag	UNP P30153



• Molecule 19 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	q	290	Total 2322	C 1467	N 403	0 437	S 15	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	-1	SER	-	expression tag	UNP P67775
q	0	ASN	-	expression tag	UNP P67775
q	88	ASN	ASP	engineered mutation	UNP P67775

• Molecule 20 is a protein called DSS1.

Mol	Chain	Residues	Atoms				AltConf	Trace	
20	r	27	Total 237	C 146	N 37	O 53	S 1	0	0

• Molecule 21 is a protein called Integrator complex subunit 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	m	35	Total 287	C 175	N 61	O 51	0	0

• Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
22	k	2	Total Zn 2 2	0

• Molecule 23 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	AltConf
23	q	2	Total Mn 2 2	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-

Chain 1: 100%	
There are no outlier residues recorded for this chain.	
• Molecule 2: SOSS complex subunit B1	
Chain B: 48% • 50%	
SER MET THR THR THR THR THR THR THR THR THR TH	ASN GLN ASN GLY ASN
CLV SLEU SLEU SLEU CLV CLV CLV CLV CLV CLV CLV CLV CLV CLV	SER LYS ARG
• Molecule 3: SOSS complex subunit C	
Chain C: 37% 63%	
SER MET AIIA ASIN MET ASIN ASIN ASIN ASIN CLI CLI CLI ASIN ASIN ASIN ASIN ASIN ASIN ASIN ASI	ASP PHE ARG ASP HIS
• Molecule 4: DNA-directed RNA polymerase subunit	
Chain Y: 100%	I
There are no outlier residues recorded for this chain.	
• Molecule 5: Integrator complex subunit 1	
Chain a: 49% 51%	
SER MET MET MET MET MET AIN AIN AIN AIN AIN AIN AIN AIN AIN AIN	PRO SER GLU ARG LYS







# 

• Molecule 6: Integrator complex subunit 2



• Molecule 8: Integrator complex subunit 4





• Molecule 11: Integrator complex subunit 7



Chain k:

• 8%

# 



• Molecule 16: Integrator complex subunit 14





 $\bullet$  Molecule 18: Serine/threenine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform

Chain p:

97%



#### SER MET MET MET MET MET ASP ASP BS ME ME ME ME SS SS SS ME SS SS ME ALA

• Molecule 19: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain q:	93% • 7%	-
SER ASIN MET MET ASIN ASIP ALU VAL 1/YS 1/49 1/49 1/49 1/49 1/49 1/49 1/49 1/49	ALY CLU VAL HIS ARG ARG ARG PRD PRD LEU LEU	
• Molecule 20: DS	S1	
Chain r:	100%	I
There are no outlie	er residues recorded for this chain.	
• Molecule 21: Int	egrator complex subunit 13	
Chain m: 5%	95%	-
MET LYS LYS LIE PHE SER GLU SER HIS LYS THR VAL VAL	ARE ARE TYR. TYR. TYR. TYR. ALA ALA ALA ARE ALA ARE ARE ARE ARE ARE ARE ARE ARE ARE AR	VAL GLU SER SER MET
GLU TYR CYS ARG ARG TYR TYR TYR TYR TLE PHE PHE LYS TYS	LEU VAL VAL VAL VAL VAL SER SER SER SER ASP CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	ASP PRO GLU CYS CYS
SER ILE LEU LEU HIS GLY VAL ALA ALA ALA ALA CLU CLU	CINC LIVE TYR TYR GLU GLU GLU GLU HRR GLU AALA AALA AALA AALA AALA AALA AALA	GLU ASP CYS VAL GLN
GLU THR ILE HIS HIS GLU GLU LYS LYS LEU ALA ALA SSR	AAS HAS HAS HAS HAS HAS HAS CYS CYS CYS CYS CYS CYS CYS CYS CYS CY	SER VAL ARG ALA GLY
ARG HIS LEU LEU LEU LYS LYS LYS LEU ASN ILE LEU VAL LEU CLN GLN GLN	ALA ASP ASP ASP ASP ASP THR THR THR THR ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	SER GLY ASP SER HIS
LEU GLY GLY GLY GLY SER ARC GLU GLU CLU CLU CLU CLU CLU CLU	THER LEEU CYS CYS CYS THR ASN ASN ASN ASN ASN CYS THR ALU CYS CYS ALU CYS CYS ALU CYS CYS ALU CYS CYS CYS CYS CYS CYS CYS CYS CYS CYS	ASN GLY ARG SER VAL
LEU LEU GLU GLU GLU GLN PRO RLY SER SER SER SER SER SER SER SER SER SER	HIRE HIRE SER SER SER SER SER SER SER CLU VAL LEU VAL LEU VAL LEU VAL LEU VAL CLU SER SER SER SER SER SER SER SER SER SER	THR ASP PHE GLY GLU
PHE MET ARG GLU GLU ASN ARG LEU PHR PHR PHR ASP PRC	TANA TYN TYN TILE ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	PRO LEU ALA SER VAL
ILE VAL LYS CLU SER CLU SER LEU CLU ASN CYS	CIUS CIN CIN TYR TYR TYR TYR ASN ASN ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	LEU GLU LEU LEU VAL
ARG ALA HIS HIE HIE ASN ASN ASN GLU LYS HIS GLN VAL	CLU CVS CVS CVS CVS CVS ALA ALA CVS CVS ALA PRO CVS PRO GLU GLU CVS GLU CVS ARG GLU CVS ARG GLU CVS ARG GLU CVS CVS FRO GLU CVS CVS ALA CVS CVS ALA C C C C C C C C C C C C C C C C C C	SER TRP GLN ASP SER
GLU ARG LEU LYS CLY CLY GLU GLU GLU GLU FII	ALA ALA ALA ALA ALA ALA ALA ALA ALA ALA	L489 GLU GLU GLU
ASN GLY GLV GLU THR GLU ASN ASS ALA SER ARG CIN		



# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	236382	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 $(e^-/\text{\AA}^2)$	39.93	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.195	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.00308	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor



# 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, 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		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
2	В	0.29	0/820	0.61	0/1109	
3	С	0.26	0/304	0.49	0/413	
4	Y	0.27	0/100	0.46	0/139	
5	a	0.28	0/8682	0.58	2/11763~(0.0%)	
6	b	0.31	0/8128	0.59	1/11072~(0.0%)	
7	с	0.28	0/3791	0.57	0/5134	
8	d	0.29	0/6519	0.57	2/8853~(0.0%)	
9	е	0.29	0/6390	0.54	0/8706	
10	f	0.28	0/4240	0.58	0/5784	
11	g	0.29	0/6835	0.55	1/9271~(0.0%)	
12	h	0.28	0/6867	0.52	0/9330	
13	i	0.29	0/4986	0.60	1/6798~(0.0%)	
14	j	0.24	0/3309	0.36	0/4608	
15	k	0.28	0/4168	0.57	0/5665	
16	n	0.24	0/1006	0.41	0/1399	
17	0	0.24	0/1821	0.36	0/2538	
18	р	0.31	0/4506	0.61	1/6130~(0.0%)	
19	q	0.28	0/2378	0.59	0/3228	
20	r	0.27	0/241	0.48	0/327	
21	m	0.25	0/292	0.62	0/393	
All	All	0.29	0/75383	0.56	8/102660~(0.0%)	

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
18	р	421	LEU	CA-CB-CG	5.94	128.95	115.30
6	b	54	LEU	CA-CB-CG	5.84	128.73	115.30
5	a	1835	LEU	CA-CB-CG	5.49	127.94	115.30
11	g	235	LEU	CA-CB-CG	5.34	127.59	115.30

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Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
13	i	309	LEU	CA-CB-CG	5.29	127.46	115.30

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	1	45	0	12	0	0
2	В	806	0	806	3	0
3	С	296	0	286	0	0
4	Y	95	0	82	0	0
5	a	8525	0	8673	0	0
6	b	7988	0	8032	0	0
7	с	3717	0	3806	0	0
8	d	6395	0	6420	0	0
9	е	6253	0	6063	0	0
10	f	4137	0	3989	0	0
11	g	6725	0	6694	0	0
12	h	6748	0	6613	0	0
13	i	4867	0	4840	0	0
14	j	3313	0	1464	0	0
15	k	4079	0	3873	0	0
16	n	1007	0	439	0	0
17	0	1824	0	802	0	0
18	р	4432	0	4487	0	0
19	q	2322	0	2215	0	0
20	r	237	0	201	0	0
21	m	287	0	275	0	0
22	k	2	0	0	0	0
23	q	2	0	0	0	0
All	All	74102	0	70072	3	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 2.

All (3) close contacts within the same asymmetric unit are listed below, sorted by their clash



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:ASP:N	2:B:91:ASP:OD1	2.49	0.46
2:B:67:ILE:HG22	2:B:95:ILE:HD13	1.99	0.44
2:B:97:GLU:OE1	2:B:98:PHE:N	2.52	0.42

magnitude.

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	ntiles
2	В	105/213~(49%)	100~(95%)	5 (5%)	0	100	100
3	С	37/106~(35%)	37~(100%)	0	0	100	100
4	Y	11/13~(85%)	11 (100%)	0	0	100	100
5	a	1061/2192~(48%)	1031 (97%)	29 (3%)	1 (0%)	51	83
6	b	1033/1204~(86%)	981~(95%)	52~(5%)	0	100	100
7	с	461/1042~(44%)	447 (97%)	14 (3%)	0	100	100
8	d	806/963~(84%)	787~(98%)	19 (2%)	0	100	100
9	e	833/1021~(82%)	800 (96%)	33~(4%)	0	100	100
10	f	530/889~(60%)	512 (97%)	18 (3%)	0	100	100
11	g	876/964~(91%)	848 (97%)	27 (3%)	1 (0%)	51	83
12	h	865/995~(87%)	837 (97%)	28 (3%)	0	100	100
13	i	618/658~(94%)	595 (96%)	23 (4%)	0	100	100
14	j	660/710~(93%)	643 (97%)	17 (3%)	0	100	100
15	k	539/602~(90%)	513 (95%)	25~(5%)	1 (0%)	47	78
16	n	202/518~(39%)	197 (98%)	5 (2%)	0	100	100
17	0	$36\overline{1/451}$ (80%)	$3\overline{43}\ (95\%)$	17 (5%)	1 (0%)	41	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
18	р	578/591~(98%)	561~(97%)	17 (3%)	0	100	100
19	q	288/311~(93%)	275~(96%)	13~(4%)	0	100	100
20	r	25/27~(93%)	24 (96%)	1 (4%)	0	100	100
21	m	33/706~(5%)	30~(91%)	3~(9%)	0	100	100
All	All	9922/14176~(70%)	9572 (96%)	346 (4%)	4 (0%)	100	100

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All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	a	1630	VAL
11	g	885	ASN
15	k	305	ILE
17	0	318	LEU

#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
2	В	87/181~(48%)	86~(99%)	1 (1%)	73	85
3	С	28/87~(32%)	28 (100%)	0	100	100
4	Y	13/13~(100%)	13 (100%)	0	100	100
5	a	946/1909~(50%)	940 (99%)	6 (1%)	86	93
6	b	869/1072~(81%)	861~(99%)	8 (1%)	78	88
7	с	414/927~(45%)	409 (99%)	5 (1%)	71	84
8	d	702/845~(83%)	700~(100%)	2~(0%)	92	96
9	е	616/814~(76%)	612~(99%)	4 (1%)	86	93
10	f	438/798~(55%)	436 (100%)	2~(0%)	88	94
11	g	723/842~(86%)	720 (100%)	3~(0%)	91	95
12	h	700/896~(78%)	693~(99%)	7(1%)	76	86
13	i	554/600~(92%)	551 (100%)	3 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
15	k	403/522~(77%)	397~(98%)	6~(2%)	65	81
18	р	485/514~(94%)	479~(99%)	6 (1%)	71	84
19	q	251/276~(91%)	249~(99%)	2(1%)	81	89
20	r	27/27~(100%)	27~(100%)	0	100	100
21	m	30/639~(5%)	30 (100%)	0	100	100
All	All	7286/10962~(66%)	7231 (99%)	55 (1%)	82	89

Continued from previous page...

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	g	672	LYS
12	h	430	LYS
19	q	86	TYR
18	р	245	MET
11	g	808	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
9	е	690	GLN
11	g	145	GLN
12	h	988	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis. 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-19040. 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: 240



Y Index: 240



Z Index: 240

#### 6.2.2 Raw map



X Index: 240

Y Index: 240

Z Index: 240  $\,$ 

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: 230



Y Index: 280



Z Index: 282

#### 6.3.2 Raw map



X Index: 230

Y Index: 240



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 0.00308. 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 2799  $\text{nm}^3$ ; this corresponds to an approximate mass of 2528 kDa.

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



#### 7.3 Rotationally averaged power spectrum (i)



\*Reported resolution corresponds to spatial frequency of 0.270  ${\rm \AA^{-1}}$ 



## 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 0.270  ${\rm \AA^{-1}}$ 



#### 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	3.70	-	-
Author-provided FSC curve	3.80	5.48	3.86
Unmasked-calculated*	4.37	7.53	4.50

\*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 4.37 differs from the reported value 3.7 by more than 10 %



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-19040 and PDB model 8RBZ. 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 0.00308 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 (0.00308).



#### 9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

### 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.00308) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9770	0.2930
1	1.0000	0.3650
В	1.0000	0.0960
С	0.9630	0.0550
Y	0.9890	0.5060
a	0.9830	0.2600
b	0.9930	0.3820
С	0.9850	0.1360
d	0.9970	0.3340
е	0.9940	0.3530
f	0.9950	0.3430
g	0.9930	0.4080
h	0.9950	0.3840
i	0.9960	0.2720
j	0.8400	0.0330
k	0.9950	0.1930
m	0.9890	0.0910
n	0.3880	0.0150
0	0.9750	0.0730
р	0.9980	0.2470
q	0.9940	0.4750
r	0.9910	0.3220

