



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 24, 2018 – 10:46 AM EST

PDB ID : 6C24
EMDB ID: : EMD-7335
Title : Cryo-EM structure of PRC2 bound to cofactors AEBP2 and JARID2 in the
Extended Active State
Authors : Kasinath, V.; Faini, M.; Poepsel, S.; Reif, D.; Feng, A.; Stjepanovic, G.;
Aebersold, R.; Nogales, E.
Deposited on : 2018-01-06
Resolution : 3.50 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

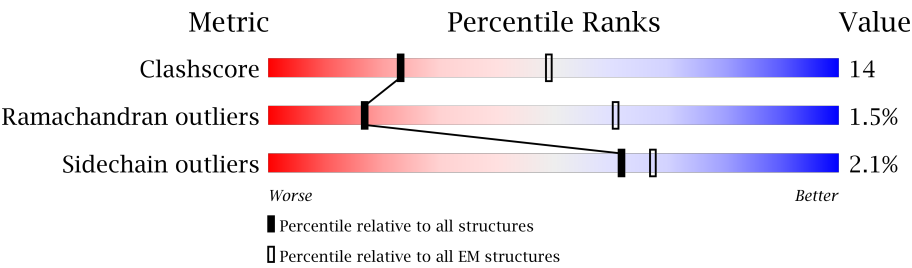
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

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 3.50 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	739	13% .. 83%
1	M	739	13% . 83%
1	Q	739	7% . 91%
2	B	345	. 98%
3	E	345	5% .. 92%
4	C	746	17% . 80%
4	K	746	35% 9% 56%
5	L	441	54% 27% . 18%
6	N	425	65% 24% . 9%

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Mol	Chain	Length	Quality of chain
7	O	7	<div><div></div><div>86%</div><div>14%</div></div>
8	P	295	<div><div></div><div>19%</div><div>..</div><div>78%</div></div>
9	Z	135	<div><div></div><div>80%</div><div>20%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13346 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 Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	123	Total	C	N	O	S	0	0
			867	555	157	149	6		
1	M	122	Total	C	N	O	S	0	0
			962	609	169	175	9		
1	Q	66	Total	C	N	O	S	0	0
			496	315	94	85	2		

- Molecule 2 is a protein called Protein Jumonji.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	7	Total	C	N	O	0	0
			52	35	9	8		

- Molecule 3 is a protein called Protein Jumonji.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	27	Total	C	N	O	S	0	0
			184	112	32	39	1		

- Molecule 4 is a protein called Histone-lysine N-methyltransferase EZH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	325	Total	C	N	O	S	0	0
			2406	1514	426	436	30		
4	C	148	Total	C	N	O	S	0	0
			1227	779	218	223	7		

- Molecule 5 is a protein called Polycomb protein EED.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	362	Total	C	N	O	S	0	0
			2881	1829	506	526	20		

- Molecule 6 is a protein called Histone-binding protein RBBP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	386	Total	C	N	O	S	0	0
			3062	1933	524	595	10		

- Molecule 7 is a protein called JARID2-substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	7	Total	C	N	O	0	0
			51	33	11	7		

- Molecule 8 is a protein called Zinc finger protein AEBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	64	Total	C	N	O	S	0	0
			484	304	91	87	2		

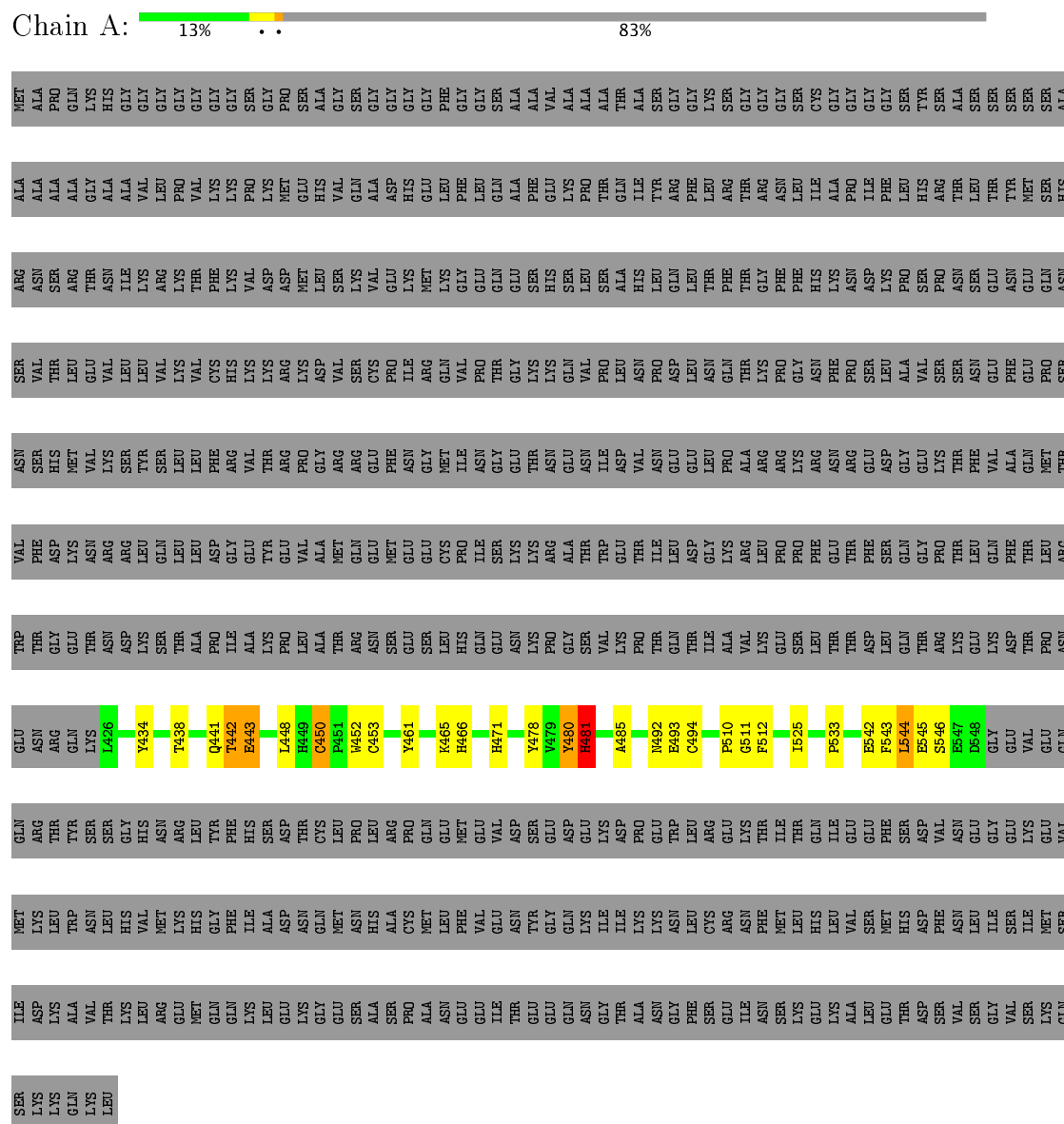
- Molecule 9 is a protein called SUZ12.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	Z	135	Total	C	N	O	0	0
			674	404	135	135		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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: Polycomb protein SUZ12



- Molecule 1: Polycomb protein SUZ12



Met	Ser	His	Glu	Thr	Val	Asn	Ser	Ser	Val	Ala	Met
Pro	Glu	Pro	Asn	Thr	Phe	Ser	His	Ser	Val	Ala	Pro
Gln	Phe	Lys	Arg	Gly	Asp	His	His	Thr	Thr	Ala	Gln
Lys	Leu	Gly	Gln	Glu	Lys	Met	Val	Leu	Arg	Ala	Lys
Leu	Leu	Ala	Lys	Thr	Asn	Val	Lys	Glu	Asn	Ala	His
Glu	Ser	Arg	Leu	Asn	Arg	Lys	Val	Val	Asn	Ala	Lys
Lys	Glu	Ile	Lys	Asp	Arg	Ser	Leu	Leu	Ile	Ala	Gly
Glu	Asp	Ile	Ile	Lys	Leu	Thr	Thr	Val	Lys	Val	Gly
Glu	Gly	Val	Phe	Ser	Gln	Ser	Leu	Val	Arg	Leu	Gly
Ser	Gly	Ile	Thr	Thr	Leu	Leu	Leu	Lys	Lys	Pro	Gly
Val	Val	Ile	Gln	Ala	Leu	Leu	Leu	Val	Thr	Val	Gly
Ala	Glu	Asn	Phe	Pro	Asp	Phe	Arg	Cys	Phe	Lys	Gly
Ser	Gln	Asn	Glu	Ile	Gly	Arg	Arg	His	Lys	Lys	Gly
Pro	Gln	Cys	Leu	Ala	Glu	Val	Val	His	Val	Lys	Gly
Ala	Gln	Cys	Thr	Ala	Thr	Arg	Arg	Lys	Val	Pro	Gly
Asn	Arg	Thr	Asn	Lys	Tyr	Arg	Thr	Arg	Lys	Asp	Gly
Glu	Thr	Gly	Asn	Lys	Glu	Pro	Asn	Arg	Val	Met	Ser
Glu	Tyr	Asp	Asn	Leu	Val	Pro	Lys	Lys	Asp	Glu	Ser
Ile	Ser	Ser	Thr	Ala	Ala	Gly	Asp	Asp	Leu	His	Ala
Thr	Ser	Thr	Arg	Thr	Met	Arg	Arg	Val	Val	Val	Gly
Glu	Gly	Ala	Gln	Arg	Gln	Glu	Glu	Ser	Ser	Gln	Gly
Glu	Gly	Gly	Gln	Thr	Asn	Arg	Arg	Thr	Val	Val	Gly
Gln	Hs61	Asn	Thr	Ser	Met	Phe	Phe	Pro	Pro	His	Gly
Asn	Hs62	Asn	Glu	Glu	Glu	Asn	Asn	Ile	Arg	Gly	Gly
Gly	Hs63	Pro	Ala	Ser	Glu	Gly	Gly	Arg	Met	His	Gly
Thr	Hs64	Gln	Ala	Ser	Glu	Gly	Gly	Met	Arg	Glu	Gly
Thr	Hs65	Asp	Arg	Leu	Cys	Met	Met	Gln	Lys	Phe	Gly
Ala	Ls74	Ile	Asp	His	Ile	Ile	Asn	Pro	Val	Phe	Gly
Gly	Hs75	Arg	Leu	Glu	Lys	Ser	Gly	Thr	Gln	Gln	Gly
Phe	Hs76	Gln	His	Asn	Lys	Thr	Glu	Gly	Glu	Ala	Ala
Ser	Hs79	Pro	Cys	Lys	Lys	Thr	Thr	Lys	Ser	Phe	Ala
Glu	Hs80	Thr	Pro	Pro	Arg	Asn	Asn	Lys	His	Glu	Val
Ile	Hs81	Phe	Thr	Gly	Ala	Glu	Glu	Gln	Ser	Lys	Val
Asn	Hs82	Ala	Cys	Ser	Thr	Asn	Asn	Pro	Leu	Pro	Ala
Ser	Hs83	Phe	Thr	Val	Thr	Ile	Ile	Pro	Ser	Thr	Ala
Lys	Hs85	Ser	Leu	Lys	Lys	Asp	Asp	Leu	Ala	Gln	Thr
Glu	Hs86	Arg	Asn	Pro	Thr	Val	Val	Asn	His	Ile	Ala
Lys	Hs87	Asn	Cys	Thr	Ile	Asn	Asn	Pro	Tyr	Thr	Ser
Ala	Hs88	Gly	Arg	Gln	Leu	Glu	Glu	Arg	Arg	Arg	Gly
Ala	Hs89	Thr	Leu	Thr	Asp	Leu	Leu	Leu	Thr	Thr	Ser
Leu	Hs90	Pro	Lys	Thr	Asp	Glu	Glu	Asp	Thr	Thr	Gly
Glu	Hs91	Val	Val	Ile	Gly	Gly	Glu	Leu	Leu	Leu	Gly
Thr	Hs92	Lys	Leu	Thr	Asp	Leu	Leu	Asn	Phe	Leu	Gly
Thr	Hs93	Thr	His	Leu	Phe	Arg	Arg	Asn	Lys	Ala	Gly
Val	Hs94	His	Leu	Thr	Glu	Asn	Asn	Phe	Pro	Pro	Gly
Ser	Hs95	Ile	Lys	Thr	Thr	Arg	Arg	Pro	Asn	Asn	Gly
Lys	Hs96	Leu	Leu	Asp	Phe	Glu	Glu	Ser	Asp	Ile	Gly
Gln	Hs97	Val	Cys	Leu	Ser	Leu	Leu	Pro	Phe	Phe	Gly
Ser	Hs98	Cys	His	Gln	Ser	Asp	Asp	Lys	Lys	Lys	Gly
Lys	Hs99	Val	Arg	Thr	Gly	Lys	Arg	Pro	Val	His	Ser
Lys	Hs100	Pro	Ser	Arg	Thr	Thr	Lys	Thr	Pro	Arg	Ser
Gln	Hs101	Lys	Phe	Lys	Thr	Thr	Glu	Val	Ser	Thr	Ala
Lys	Hs102	Arg	Ile	Lys	Glu	Phe	Val	Asn	Ser	Leu	Ser
Leu	Hs103	Thr	Phe	Lys	Gln	Thr	Gly	Glu	Thr	Thr	Ser
Leu	Hs104	Lys	Asn	Asp	Phe	Ala	Asn	Phe	Asn	Tyr	Ser
Leu	Hs105	Ala	Thr	Thr	Thr	Gln	Glu	Glu	Met	Ser	Ser
Leu	Hs106	Ala	Tyr	Pro	Arg	Met	Thr	Pro	Gln	His	Ala
Leu	Hs107	Met	Val	Asn	Leu	Thr	Thr	Thr	Asn	Ser	Ala

- Molecule 1: Polycomb protein SUZ12

Chain Q: 7% . 91%

[illegible]

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

- Molecule 2: Protein Jumonji

Chain B:  98%

[illegible]

- Molecule 3: Protein Jumonji

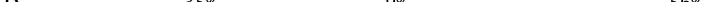
Chain E: 5% .. 92%

[illegible]

LYS ARG GLU LEU VAL LYS ASP THR PRO LYS ASN HIS LYS PRO SER SER ALA VAL ASN HIS THR ILE SER GLY LYS THR GLU SER SER ASN ALA LYS THR ARG LYS GLN VAL LEU SER LEU GLY GLY ALA GLY SER SER LYS SER THR GLY PRO VAL VAL ASN GLY LYS VAL SER GLY

LEU ASN PRO LYS SER CYS THR LYS GLU VAL GLY ARG GLN LEU ARG GLU GLY LEU GLN LEU ARG GLU GLY LEU ASN SER LYS ARG ARG LEU GLU GLU ALA HIS GLN ALA

- Molecule 4: Histone-lysine N-methyltransferase EZH2

Chain K:  35% 9% 56%

NET	GLY	GLN	THR	GLY	LYS	LYS	SER	GLY	LYS	GLY	PRO	VAL	CYS	TRP	ARG	LYS	ARG	ARG	VAL	LYS	SER	GLU	GLU	TYR	MET	ARG	ARG	LEU	LEU	GLN	GLN	LYS	LYS	LYS	ARG	ARG	PHE	ASP	ALA	ASP	GLU	GLU	VAL	LYS	LYS	SER	SER	SER	ASN	ARG	ARG	GLN	LYS	LYS	ILE	LEU	LEU	GLU	GLU	ARG	THR	GLU	GLU	ILE	LEU	LEU	ASN	ASN	GLN	GLU	TYR
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LYS GLN ARG ARG ARG ILE GLN PRO VAL HIS HIS ILE LEU LEU THR SER VAL VAL SER SER SER LEU LEU ARG GLY THR THR ARG GLU GLU CYS SER VAL VAL THR SER ASP ASP ASP PHE PRO PRO THR THR GLN GLN VAL ILE ILE PRO PRO LEU LEU LYS LYS THR THR LEU LEU ASN ALA VAL VAL ALA ALA SER SER VAL VAL PRO PRO ILE ILE MET MET TYR TYR SER SER TRP TRP SER PRO PRO LEU LEU GLN GLN GLN ASN

NET	VAL	GLU	GLU	ASP	GLU	THR	VAL	VAL	HIS	ASN	ILE	PRO	TYR	MET	GLY	ASP	GLU	VAL	LEU	ASP	GLN	GLY	THR	PHE	ILE	GLU	GLU	ILE	LYS	ASN	TYR	ASP	GLY	LYS	VAL	VAL	HIS	GLY	ASP	ARG	GLU	CYS	GLY	PHE	ILE	ILE	ASN	ASP	GLU	GLU	ASN	ALA	LEU	GLY
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Tyr	Asn	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	PRO	GLU	GLU	ARG	ARG	LEU	GLU	GLY	GLN	Lys	ASP	HIS	Arg	SER	ARG	PRO	PRO	ARG	LYS	PHE	PRO	ILE	LYS	PHE	GLU	ALA	ILE	SER	SER	NET	PHE	PRO	ASP	Lys	GLY	THR	ALA	GLU	GLU	V
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[illegible][illegible]

GLU	GLU	GLU	LVS	ASP	GLU	THR	SER	SER	SER	GLU	ALA	ASN	SER	ARG	CYS	GLN	THR	PRO	ILE	LVS	MET	PRO	G423	F440	R441	V442	L443	I444	G445	T446	Y447	F451	G452	G459	L477	PRO	ALA	PRO	PRO	GLU	GLU	ASP	VAL	ASP	THR	PRO	ARG	ARG	LVS	LVS
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LVS	HIS	ARG	TRP	ALA	ALA	HIS	CYS	ARG	LVS	GLN	LVS	LVS	ASP	GLY	SER	SS14	G523	G547	Q548	P558	Q665	G580	G588	G589	AS90	AS91	D592	H593	W594	D595	SS96	K597	H598	W599	SE00	R608	K611	L614	A617	P618	SE19	D620	W621	A622	W623
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F627		S639	E640	S647	Q648	D649	E650	A651	D652	R653	Y658	M662	N670	F673	R679	R685	F686	A687	N688	H689	S690	V691	C695	Q717	L722	F723	Y726	R727	F728	S729	Q730	A731	D732	K735	Tra	Val	Gly	ILE	ILE	GLU	ARG	GLU	Met	GLU	Met	ILE	Pro
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- Molecule 4: Histone-lysine N-methyltransferase EZH2

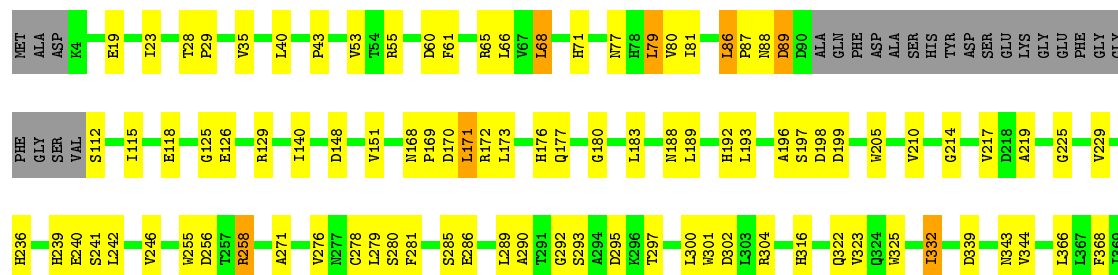
Chain C: 17% 3% 80%

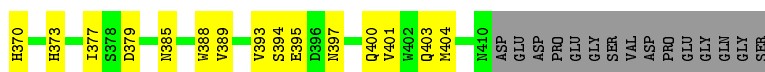
NET	GLY	GLN	GLY	GLY	LYS	LYS	SER	GLU	LYS	GLY	PRO	VAL	G14	W15	V19	I49	R52	T53	K61	R64	L71	T72	S73	V74	S75	S76	L77	C83	S84	VAL	THR	SER	ASP	LEU	ASP	PHE	PRO	THR	GLN	G95	I96	L101	V104	D124	GLU	THR	VAL	LEU
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ASN	ILE	PRO	TYR	MET	GLY	ASP	GLU	VAL	LEU	ASN	GLN	ASP	GLY	THR	PHE	LYS	LYS	ASN	TYR	TRP	GLY	ASP	ARG	ARG	GLU	CYS	G164	H76	Q180	Y181	ASN	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLY	GLY	ARG	GLU	GLU	LVS	GLN
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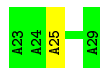
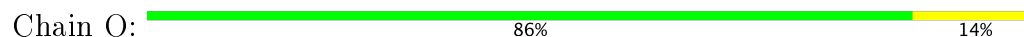
[illegible]

CYS ARG ARG ARG CYS PHE LYS TYR ASP CYS PHE CYS HIS HIS HIS HIS THR ALA THR PRO ASN THR TYR LYS ARG ARG LYS ASN ASN THR GLU THR ALA THR LEU ASP ASN ASN LYS TYR CYS CYS GLY PRO PRO GLN CYS TYR TYR GLN HIS LEU LEU GLU GLY GLY ALA ALA LYS GLU PHE ALA ALA ALA LEU LEU THR GLU GLU ARG ARG ILE LYS

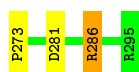
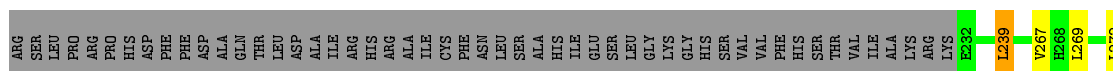
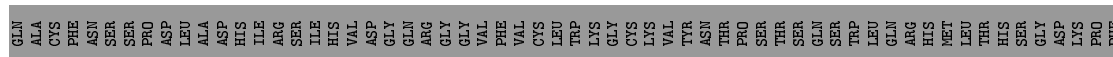




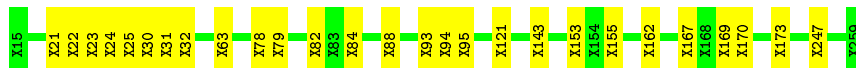
- Molecule 7: JARID2-substrate



- Molecule 8: Zinc finger protein AEBP2



- Molecule 9: SUZ12



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	249696	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: M3L

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 >2	RMSZ	# Z >2
1	A	0.53	0/890	0.78	1/1219 (0.1%)
1	M	0.48	0/983	0.70	0/1328
1	Q	1.18	3/506 (0.6%)	0.89	1/687 (0.1%)
2	B	0.48	0/40	0.38	0/53
3	E	0.46	0/185	1.04	0/250
4	C	0.42	0/1247	0.69	1/1669 (0.1%)
4	K	0.42	0/2466	0.64	1/3352 (0.0%)
5	L	0.62	0/2956	0.79	1/4012 (0.0%)
6	N	0.64	0/3146	0.77	4/4291 (0.1%)
7	O	0.52	0/51	0.71	0/66
8	P	0.46	0/492	0.79	0/666
All	All	0.59	3/12962 (0.0%)	0.75	9/17593 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	M	0	1
4	K	0	1
5	L	0	1
6	N	0	1
8	P	0	1
9	Z	0	1
All	All	0	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	146	GLY	C-O	21.12	1.57	1.23
1	Q	146	GLY	CA-C	7.68	1.64	1.51
1	Q	146	GLY	N-CA	6.97	1.56	1.46

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	146	GLY	CA-C-O	-6.82	108.32	120.60
4	C	73	SER	N-CA-C	-6.73	92.82	111.00
6	N	404	MET	CB-CG-SD	-6.49	92.94	112.40
6	N	79	LEU	CB-CG-CD2	-6.09	100.65	111.00
5	L	405	THR	N-CA-C	5.65	126.25	111.00

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	441	GLN	Peptide
1	A	478	TYR	Peptide
1	A	480	TYR	Peptide
1	A	481	HIS	Peptide
4	K	723	PHE	Peptide

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	A	867	0	736	21	0
1	M	962	0	898	16	0
1	Q	496	0	450	10	0
2	B	52	0	49	0	0
3	E	184	0	172	10	0
4	C	1227	0	1249	16	0
4	K	2406	0	2120	70	0
5	L	2881	0	2760	131	0
6	N	3062	0	2908	79	0
7	O	51	0	54	11	0
8	P	484	0	476	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	Z	674	0	166	19	0
All	All	13346	0	12038	355	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 14.

The worst 5 of 355 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)
9:Z:25:UNK:CB	9:Z:247:UNK:H	1.19	1.50
4:K:728:TYR:CE1	7:O:25:ALA:HB1	1.52	1.42
9:Z:25:UNK:CB	9:Z:247:UNK:N	1.76	1.37
4:K:440:PHE:O	4:K:444:ILE:HG12	1.23	1.36
4:K:728:TYR:CE1	7:O:25:ALA:CB	2.10	1.33

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	A	121/739 (16%)	85 (70%)	30 (25%)	6 (5%)	2	24
1	M	120/739 (16%)	105 (88%)	13 (11%)	2 (2%)	11	49
1	Q	64/739 (9%)	45 (70%)	18 (28%)	1 (2%)	11	50
2	B	4/345 (1%)	4 (100%)	0	0	100	100
3	E	25/345 (7%)	15 (60%)	6 (24%)	4 (16%)	0	3
4	C	140/746 (19%)	128 (91%)	12 (9%)	0	100	100
4	K	319/746 (43%)	275 (86%)	41 (13%)	3 (1%)	20	63
5	L	360/441 (82%)	299 (83%)	57 (16%)	4 (1%)	17	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	N	382/425 (90%)	326 (85%)	53 (14%)	3 (1%)	22	65
7	O	5/7 (71%)	4 (80%)	1 (20%)	0	100	100
8	P	62/295 (21%)	43 (69%)	18 (29%)	1 (2%)	11	50
All	All	1602/5567 (29%)	1329 (83%)	249 (16%)	24 (2%)	17	52

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	442	THR
1	A	481	HIS
3	E	160	PHE
5	L	238	GLU
1	M	581	VAL

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	A	73/646 (11%)	72 (99%)	1 (1%)	71	89
1	M	101/646 (16%)	100 (99%)	1 (1%)	80	91
1	Q	45/646 (7%)	45 (100%)	0	100	100
2	B	2/294 (1%)	2 (100%)	0	100	100
3	E	19/295 (6%)	18 (95%)	1 (5%)	26	63
4	C	138/667 (21%)	138 (100%)	0	100	100
4	K	233/667 (35%)	231 (99%)	2 (1%)	82	93
5	L	311/392 (79%)	302 (97%)	9 (3%)	48	78
6	N	341/375 (91%)	329 (96%)	12 (4%)	41	75
7	O	3/3 (100%)	3 (100%)	0	100	100
8	P	50/263 (19%)	49 (98%)	1 (2%)	60	84
All	All	1316/4894 (27%)	1289 (98%)	27 (2%)	62	84

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	L	436	ARG
6	N	55	ARG
6	N	393	VAL
1	M	563	ARG
5	L	109	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
6	N	192	HIS
4	C	117	GLN
6	N	328	HIS
6	N	88	ASN
6	N	226	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	M3L	B	116	2	11,11,12	0.54	0	11,14,16	0.91	0

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
2	M3L	B	116	2	-	0/8/10/12	0/0/0/0

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.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	Z	6

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	182:UNK	C	247:UNK	N	39.28
1	Z	45:UNK	C	55:UNK	N	34.04
1	Z	67:UNK	C	77:UNK	N	29.09
1	Z	138:UNK	C	143:UNK	N	26.06
1	Z	99:UNK	C	120:UNK	N	9.78