



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3PSL / pdb_00003psl
Title : Fine-tuning the stimulation of MLL1 methyltransferase activity by a histone H3 based peptide mimetic
Authors : Avdic, V.; Zhang, P.; Lanouette, S.; Voronova, A.; Skerjanc, I.; Couture, J.-F.
Deposited on : 2010-12-01
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

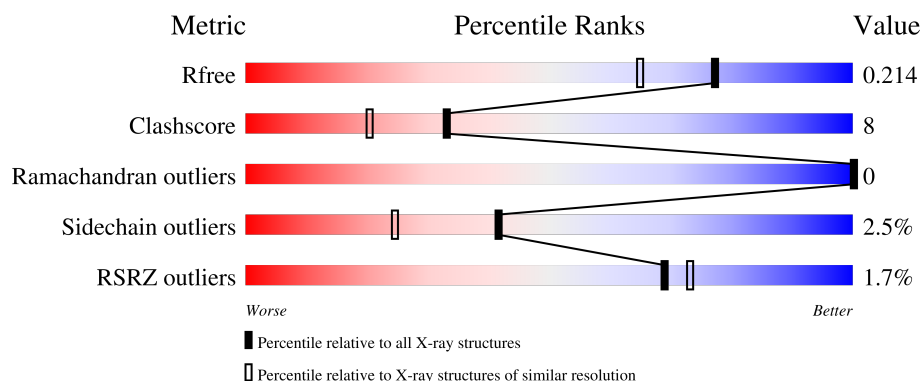
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	318	0% 78% 15% 6%
1	B	318	2% 79% 14% 6%
2	C	6	67% 17% 17%
2	D	6	67% 17% 17%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5019 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 WD repeat-containing protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	3	0
			2302	1470	382	439	11			
1	B	298	Total	C	N	O	S	0	0	0
			2299	1470	382	437	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLY	-	expression tag	UNP P61964
A	18	ALA	-	expression tag	UNP P61964
A	19	MET	-	expression tag	UNP P61964
A	20	GLY	-	expression tag	UNP P61964
B	17	GLY	-	expression tag	UNP P61964
B	18	ALA	-	expression tag	UNP P61964
B	19	MET	-	expression tag	UNP P61964
B	20	GLY	-	expression tag	UNP P61964

- Molecule 2 is a protein called N-alpha acetylated form of histone H3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			32	19	7	6			
2	D	5	Total	C	N	O	0	0	0
			35	21	8	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	197	Total	O	0	0
			197	197		
3	B	146	Total	O	0	0
			146	146		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	4	Total 4	O 4	0	0
3	D	4	Total 4	O 4	0	0

- Molecule 1: WD repeat-containing protein 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	45.95Å 48.61Å 63.31Å 98.79° 90.95° 117.48°	Depositor
Resolution (Å)	35.64 – 1.70 35.64 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.6 (35.64-1.70) 96.6 (35.64-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.51 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.155 , 0.205 0.162 , 0.214	Depositor DCC
R_{free} test set	2575 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5019	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: ACE

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	1.35	5/2372 (0.2%)	1.15	1/3216 (0.0%)
1	B	1.24	3/2354 (0.1%)	1.13	2/3192 (0.1%)
2	C	2.19	1/29 (3.4%)	1.02	0/38
2	D	2.17	1/32 (3.1%)	1.06	0/41
All	All	1.31	10/4787 (0.2%)	1.14	3/6487 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	0	ACE	C-N	10.16	1.53	1.33
2	C	0	ACE	C-N	7.73	1.48	1.33
1	A	285	ILE	CA-CB	-6.43	1.46	1.54
1	B	316	ILE	N-CA	6.00	1.53	1.46
1	A	222	PHE	N-CA	5.48	1.52	1.45
1	A	144	ILE	C-O	5.45	1.29	1.24
1	B	152	SER	C-O	5.42	1.30	1.23
1	A	163	CYS	C-O	5.17	1.30	1.24
1	A	328	LYS	N-CA	5.05	1.52	1.46
1	B	320	ALA	C-O	5.03	1.30	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	131	TYR	CB-CA-C	-5.55	101.51	109.84
1	A	227	LYS	N-CA-C	5.37	119.00	112.23
1	B	39	PHE	N-CA-C	5.13	117.05	108.99

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2302	0	2269	36	0
1	B	2299	0	2266	36	0
2	C	32	0	32	0	0
2	D	35	0	41	0	0
3	A	197	0	0	5	0
3	B	146	0	0	9	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
All	All	5019	0	4608	72	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 8.

All (72) 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)
1:A:204:GLN:HB2	3:A:452:HOH:O	1.62	0.98
1:A:178:HIS:HD2	1:A:222:PHE:H	1.16	0.89
1:A:323:ASN:HB3	3:A:442:HOH:O	1.73	0.87
1:B:140:GLN:OE1	3:B:357:HOH:O	1.94	0.84
1:B:178:HIS:HD2	1:B:222:PHE:H	1.27	0.80
1:A:178:HIS:CD2	1:A:222:PHE:H	2.01	0.79
1:B:310:HIS:HD2	1:B:313:GLU:H	1.28	0.77
1:B:110:THR:HG22	1:B:126:LYS:HD3	1.67	0.77
1:B:170:HIS:HE1	1:B:188:SER:OG	1.67	0.77
1:B:178:HIS:CD2	1:B:222:PHE:H	2.09	0.71
1:A:292:GLU:OE1	3:A:497:HOH:O	2.09	0.70
1:A:310:HIS:HD2	1:A:313:GLU:H	1.39	0.68
1:A:35:TYR:H	1:A:295:GLN:HE22	1.40	0.68
1:B:140:GLN:HG3	3:B:357:HOH:O	1.95	0.66
1:A:196:ARG:NH2	3:A:520:HOH:O	2.32	0.63
1:A:255:HIS:CD2	1:A:255:HIS:H	2.16	0.63
1:B:110:THR:CG2	1:B:126:LYS:HD3	2.29	0.63
1:A:242:ASP:CG	1:A:245:LYS:HG3	2.25	0.62
1:A:255:HIS:HE1	3:A:363:HOH:O	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:HIS:CD2	1:B:313:GLU:H	2.15	0.61
1:A:310:HIS:CD2	1:A:313:GLU:H	2.18	0.61
1:A:195[B]:CYS:SG	1:A:217:VAL:HG11	2.41	0.61
1:B:93:VAL:HG22	1:B:102:LEU:HD22	1.83	0.60
1:B:89:GLY:HA3	3:B:3:HOH:O	2.01	0.60
1:B:255:HIS:H	1:B:255:HIS:CD2	2.20	0.59
1:A:322:GLU:H	1:A:322:GLU:CD	2.11	0.59
1:B:35:TYR:H	1:B:295:GLN:HE22	1.49	0.58
1:A:204:GLN:HG3	1:A:205:CYS:N	2.18	0.58
1:B:170:HIS:CE1	1:B:188:SER:OG	2.54	0.58
1:B:140:GLN:CG	3:B:357:HOH:O	2.50	0.57
1:A:310:HIS:CD2	1:A:312:THR:H	2.23	0.57
1:A:57:GLY:O	1:A:310:HIS:HE1	1.90	0.55
1:A:283:VAL:HB	1:A:297:LEU:HB2	1.89	0.54
1:A:310:HIS:HD2	1:A:312:THR:H	1.55	0.54
1:A:170:HIS:HE1	1:A:188:SER:OG	1.91	0.53
1:B:64:SER:HB3	1:B:66:ASP:OD1	2.08	0.53
1:B:80:GLU:OE1	3:B:421:HOH:O	2.19	0.52
1:A:255:HIS:H	1:A:255:HIS:HD2	1.55	0.52
1:A:249:LEU:O	1:A:250:LYS:HG3	2.10	0.52
1:B:55:PRO:O	1:B:311:PRO:HG3	2.10	0.52
1:B:55:PRO:HG3	3:B:387:HOH:O	2.11	0.51
1:B:56:ASN:HD22	1:B:56:ASN:C	2.18	0.50
1:B:140:GLN:CD	3:B:357:HOH:O	2.50	0.50
1:A:93:VAL:HG22	1:A:102:LEU:HD22	1.93	0.49
1:A:151:GLU:HG2	1:A:172:ASP:C	2.37	0.49
1:B:265:ASN:ND2	1:B:307:THR:OG1	2.45	0.49
1:A:56:ASN:C	1:A:56:ASN:HD22	2.19	0.49
1:A:35:TYR:N	1:A:295:GLN:HE22	2.10	0.49
1:B:191:TYR:HA	1:B:216:PRO:HB3	1.95	0.49
1:A:75:TYR:HE2	1:A:313:GLU:HG3	1.77	0.48
1:B:55:PRO:C	1:B:57:GLY:H	2.21	0.47
1:B:195:CYS:SG	1:B:217:VAL:HG11	2.54	0.47
1:B:255:HIS:H	1:B:255:HIS:HD2	1.60	0.46
1:B:55:PRO:C	1:B:57:GLY:N	2.73	0.45
1:B:303:VAL:HB	1:B:321:LEU:HD12	1.98	0.45
1:B:315:ILE:HG12	1:B:331:LYS:HD2	1.99	0.45
1:A:191:TYR:HA	1:A:216:PRO:HB3	1.98	0.44
1:B:292:GLU:CD	3:B:445:HOH:O	2.60	0.44
1:B:317:ALA:HA	1:B:328:LYS:O	2.18	0.44
1:A:288:LEU:HD23	1:A:288:LEU:C	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:VAL:CG2	1:B:102:LEU:HD22	2.48	0.44
1:A:178:HIS:CD2	1:A:222:PHE:N	2.79	0.43
1:A:242:ASP:OD2	1:A:245:LYS:HG3	2.18	0.43
1:A:218:SER:HB2	1:A:261:CYS:HA	2.00	0.43
1:A:41:LEU:HB2	1:A:327:ILE:HB	2.00	0.43
1:B:289:GLN:HG2	3:B:395:HOH:O	2.18	0.42
1:B:93:VAL:HA	1:B:103:VAL:O	2.20	0.41
1:A:282:LEU:HD12	1:A:298:GLN:HA	2.02	0.41
1:A:209:LEU:HD22	1:A:209:LEU:N	2.36	0.41
1:B:234:LEU:HD23	1:B:234:LEU:HA	1.89	0.41
1:A:233:THR:C	1:A:235:ASP:H	2.28	0.40
1:B:57:GLY:O	1:B:310:HIS:HE1	2.04	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 X-ray entries followed by that with respect to entries of similar resolution.

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	297/318 (93%)	284 (96%)	13 (4%)	0	100	100
1	B	294/318 (92%)	281 (96%)	13 (4%)	0	100	100
2	C	3/6 (50%)	3 (100%)	0	0	100	100
2	D	3/6 (50%)	3 (100%)	0	0	100	100
All	All	597/648 (92%)	571 (96%)	26 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 X-ray entries followed by that with respect to entries of similar

resolution.

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	258/276 (94%)	252 (98%)	6 (2%)	44	27
1	B	255/276 (92%)	248 (97%)	7 (3%)	39	23
2	C	2/4 (50%)	2 (100%)	0	100	100
2	D	3/4 (75%)	3 (100%)	0	100	100
All	All	518/560 (92%)	505 (98%)	13 (2%)	42	24

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	56	ASN
1	A	173	PRO
1	A	181	ARG
1	A	258	GLU
1	A	282	LEU
1	B	41	LEU
1	B	56	ASN
1	B	162	LYS
1	B	204	GLN
1	B	256	LYS
1	B	282	LEU
1	B	295	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	170	HIS
1	A	178	HIS
1	A	255	HIS
1	A	265	ASN
1	A	295	GLN
1	A	310	HIS
1	A	323	ASN
1	B	56	ASN
1	B	140	GLN

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Mol	Chain	Res	Type
1	B	170	HIS
1	B	178	HIS
1	B	255	HIS
1	B	257	ASN
1	B	295	GLN
1	B	310	HIS
1	B	314	ASN
1	B	323	ASN

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 oligosaccharides 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](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	298/318 (93%)	-0.39	4 (1%) 75 79	7, 14, 29, 39	5 (1%)
1	B	298/318 (93%)	0.05	6 (2%) 65 69	9, 22, 38, 47	3 (1%)
2	C	4/6 (66%)	-0.88	0 100 100	9, 10, 11, 18	0
2	D	4/6 (66%)	-1.05	0 100 100	10, 13, 14, 21	0
All	All	604/648 (93%)	-0.18	10 (1%) 69 73	7, 18, 34, 47	8 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	TYR	3.8
1	B	334	CYS	3.3
1	A	334	CYS	2.5
1	A	209	LEU	2.4
1	A	181	ARG	2.3
1	B	268	VAL	2.3
1	B	37	LEU	2.2
1	A	258	GLU	2.2
1	B	244	SER	2.2
1	B	333	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.