Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2026 – 07:13 PM JST

PDB ID	:	9XJV / pdb_00009xjv
Title	:	Crystal structure of murine EMAP-II
Authors	:	Jiang, L.G.; Chen, L.Y.; Huang, M.D.
Deposited on	:	2025-11-05
Resolution	:	1.84 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:

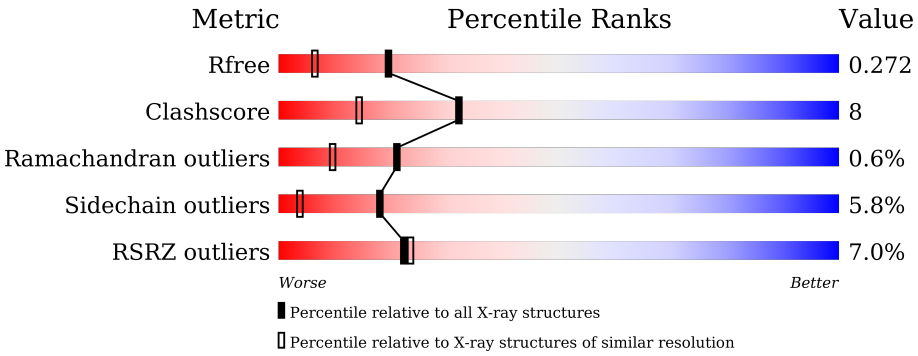
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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 <=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	166	6% 80% 16%
1	B	166	8% 78% 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2773 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 Endothelial monocyte-activating polypeptide 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1240	778	218	233	11			
1	B	164	Total	C	N	O	S	0	0	0
			1240	778	218	233	11			

- Molecule 2 is water.

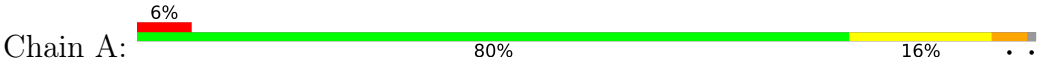
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	148	Total	O	0	0
			148	148		
2	B	145	Total	O	0	0
			145	145		

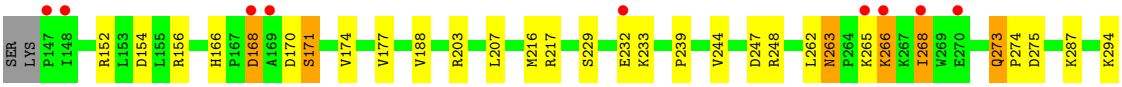
3 Residue-property plots (i)

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: Endothelial monocyte-activating polypeptide 2

Chain A:

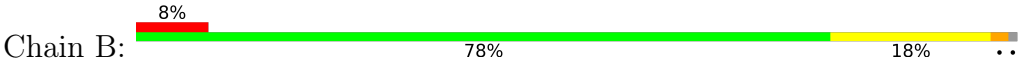


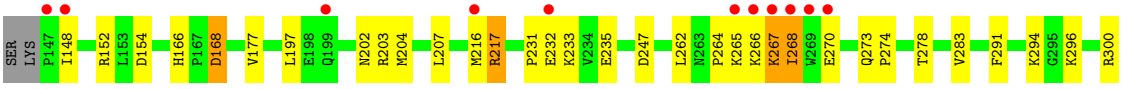




• Molecule 1: Endothelial monocyte-activating polypeptide 2

Chain B:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	37.51Å 45.18Å 55.26Å 81.18° 79.61° 66.33°	Depositor
Resolution (Å)	34.06 – 1.84 34.06 – 1.84	Depositor EDS
% Data completeness (in resolution range)	96.4 (34.06-1.84) 96.4 (34.06-1.84)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.37 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.209 , 0.267 0.216 , 0.272	Depositor DCC
R_{free} test set	1298 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	13.2	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	2773	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.71	0/1263	1.16	6/1711 (0.4%)
1	B	0.71	0/1263	1.20	4/1711 (0.2%)
All	All	0.71	0/2526	1.18	10/3422 (0.3%)

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	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	244	VAL	N-CA-CB	-6.97	101.45	111.21
1	A	154	ASP	CA-CB-CG	6.51	119.11	112.60
1	A	203	ARG	CD-NE-CZ	-6.15	115.78	124.40
1	B	247	ASP	CA-CB-CG	6.15	118.75	112.60
1	A	170	ASP	CA-CB-CG	5.85	118.45	112.60
1	B	204	MET	CG-SD-CE	5.82	113.71	100.90
1	A	239	PRO	O-C-N	-5.58	118.74	121.31
1	A	247	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	154	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	291	PHE	CA-CB-CG	5.16	118.96	113.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	ARG	Sidechain
1	B	203	ARG	Sidechain
1	B	217	ARG	Sidechain

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	1240	0	1268	19	0
1	B	1240	0	1268	21	0
2	A	148	0	0	4	1
2	B	145	0	0	6	1
All	All	2773	0	2536	40	1

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 (40) 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:B:296:LYS:HD2	2:B:425:HOH:O	1.59	1.02
1:B:267:LYS:HB2	2:B:464:HOH:O	1.73	0.88
1:A:265:LYS:O	1:A:266:LYS:HB2	1.86	0.76
1:B:166:HIS:HD2	1:B:168:ASP:H	1.34	0.74
1:A:166:HIS:HD2	1:A:168:ASP:H	1.36	0.71
1:B:265:LYS:O	1:B:266:LYS:HB2	1.97	0.64
1:B:152:ARG:HB3	1:B:268:ILE:HD11	1.80	0.63
1:B:152:ARG:CB	1:B:268:ILE:HD11	2.30	0.62
1:A:268:ILE:HG23	2:A:426:HOH:O	2.00	0.61
1:B:202:ASN:HB3	2:B:476:HOH:O	2.01	0.60
1:B:300:ARG:HD3	2:B:475:HOH:O	2.05	0.57
1:A:233:LYS:HE2	2:A:525:HOH:O	2.06	0.56
1:A:265:LYS:O	1:A:266:LYS:CB	2.51	0.56
1:A:263:ASN:C	1:A:263:ASN:HD22	2.16	0.53
1:B:296:LYS:CE	2:B:401:HOH:O	2.55	0.52
1:A:262:LEU:HD22	1:A:268:ILE:CD1	2.40	0.52
1:A:171:SER:HB2	2:A:496:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:LYS:HE3	2:B:460:HOH:O	2.11	0.49
1:B:273:GLN:N	1:B:274:PRO:CD	2.75	0.49
1:A:166:HIS:HE1	1:A:216:MET:O	1.95	0.48
1:A:152:ARG:HB3	1:A:268:ILE:CD1	2.44	0.47
1:A:177:VAL:HG11	1:A:207:LEU:HD11	1.96	0.47
1:B:233:LYS:HE3	1:B:235:GLU:OE2	2.15	0.47
1:B:266:LYS:O	1:B:267:LYS:C	2.57	0.47
1:A:152:ARG:CB	1:A:268:ILE:CD1	2.94	0.46
1:B:267:LYS:HB3	1:B:270:GLU:HB2	1.98	0.46
1:B:152:ARG:HG3	1:B:268:ILE:HD12	1.98	0.45
1:A:152:ARG:CB	1:A:268:ILE:HD11	2.45	0.45
1:B:166:HIS:HE1	1:B:216:MET:O	2.00	0.44
1:A:229:SER:OG	1:A:310:LYS:HD3	2.17	0.43
1:B:278:THR:HA	1:B:283:VAL:O	2.18	0.43
1:A:152:ARG:HB3	1:A:268:ILE:HD11	2.00	0.43
1:B:264:PRO:O	1:B:267:LYS:HG3	2.19	0.43
1:B:177:VAL:HG11	1:B:207:LEU:HD11	2.01	0.43
1:A:174:VAL:HG22	1:A:188:VAL:HG22	2.01	0.42
1:A:248:ARG:CZ	2:A:416:HOH:O	2.67	0.41
1:A:273:GLN:N	1:A:274:PRO:CD	2.83	0.41
1:B:168:ASP:O	1:B:217:ARG:NE	2.52	0.41
1:B:262:LEU:HD22	1:B:268:ILE:HG12	2.03	0.41
1:A:275:ASP:HB3	1:A:287:LYS:HG3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:514:HOH:O	2:B:476:HOH:O[1_545]	2.01	0.19

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 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	162/166 (98%)	157 (97%)	4 (2%)	1 (1%)	21 9
1	B	162/166 (98%)	156 (96%)	5 (3%)	1 (1%)	21 9
All	All	324/332 (98%)	313 (97%)	9 (3%)	2 (1%)	21 9

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	LYS
1	B	267	LYS

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 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	138/140 (99%)	130 (94%)	8 (6%)	18 4
1	B	138/140 (99%)	130 (94%)	8 (6%)	18 4
All	All	276/280 (99%)	260 (94%)	16 (6%)	18 4

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	ASP
1	A	171	SER
1	A	217	ARG
1	A	232	GLU
1	A	263	ASN
1	A	268	ILE
1	A	273	GLN
1	A	294	LYS
1	B	148	ILE
1	B	168	ASP
1	B	197	LEU
1	B	231	PRO
1	B	232	GLU
1	B	268	ILE

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Mol	Chain	Res	Type
1	B	294	LYS
1	B	310	LYS

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	166	HIS
1	A	263	ASN
1	A	271	GLN
1	A	273	GLN
1	A	302	GLN
1	B	166	HIS
1	B	193	ASN
1	B	263	ASN
1	B	273	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 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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	164/166 (98%)	0.32	10 (6%)	27	28	7, 15, 31, 53	0
1	B	164/166 (98%)	0.33	13 (7%)	18	19	7, 15, 32, 63	0
All	All	328/332 (98%)	0.32	23 (7%)	22	23	7, 15, 32, 63	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	LYS	5.1
1	B	266	LYS	4.8
1	B	265	LYS	3.9
1	B	232	GLU	3.8
1	A	265	LYS	3.8
1	B	270	GLU	3.6
1	A	232	GLU	3.4
1	B	148	ILE	3.3
1	A	266	LYS	3.1
1	B	267	LYS	3.1
1	A	270	GLU	3.0
1	B	147	PRO	2.9
1	B	216	MET	2.9
1	A	310	LYS	2.9
1	A	148	ILE	2.7
1	B	268	ILE	2.4
1	A	268	ILE	2.4
1	A	169	ALA	2.4
1	B	269	TRP	2.2
1	B	309	ILE	2.2
1	A	168	ASP	2.1
1	A	147	PRO	2.0
1	B	199	GLN	2.0

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.