



wwPDB EM Validation Summary Report ⓘ

Nov 29, 2022 – 01:25 AM EST

PDB ID : 7UFG
EMDB ID : EMD-26475
Title : Cryo-EM structure of PAPP-A in complex with IGFBP5
Authors : Judge, R.A.; Jain, R.; Hao, Q.; Ouch, C.; Sridar, J.; Smith, C.L.; Wang, J.C.K.; Eaton, D.
Deposited on : 2022-03-22
Resolution : 3.28 Å(reported)

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 ⓘ 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:

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

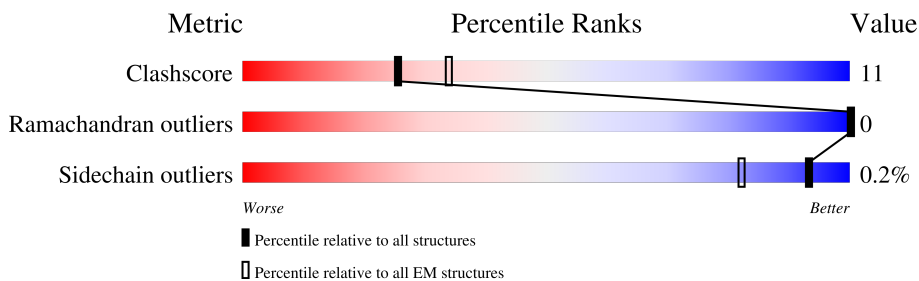
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.28 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	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1581	
1	B	1581	
2	C	272	
2	D	272	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 33028 atoms, of which 14783 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 Pappalysin-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1151	15782	5542	7002	1505	1670	63	0	0
1	B	1182	16506	5734	7411	1549	1746	66	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	483	ALA	GLU	engineered mutation	UNP Q13219
A	1144	TYR	SER	engineered mutation	UNP Q13219
A	1548	SER	-	expression tag	UNP Q13219
A	1549	GLY	-	expression tag	UNP Q13219
A	1550	PRO	-	expression tag	UNP Q13219
A	1551	THR	-	expression tag	UNP Q13219
A	1552	ARG	-	expression tag	UNP Q13219
A	1553	THR	-	expression tag	UNP Q13219
A	1554	ARG	-	expression tag	UNP Q13219
A	1555	PRO	-	expression tag	UNP Q13219
A	1556	LEU	-	expression tag	UNP Q13219
A	1557	GLU	-	expression tag	UNP Q13219
A	1558	GLN	-	expression tag	UNP Q13219
A	1559	LYS	-	expression tag	UNP Q13219
A	1560	LEU	-	expression tag	UNP Q13219
A	1561	ILE	-	expression tag	UNP Q13219
A	1562	SER	-	expression tag	UNP Q13219
A	1563	GLU	-	expression tag	UNP Q13219
A	1564	GLU	-	expression tag	UNP Q13219
A	1565	ASP	-	expression tag	UNP Q13219
A	1566	LEU	-	expression tag	UNP Q13219
A	1567	ALA	-	expression tag	UNP Q13219
A	1568	ALA	-	expression tag	UNP Q13219
A	1569	ASN	-	expression tag	UNP Q13219
A	1570	ASP	-	expression tag	UNP Q13219
A	1571	ILE	-	expression tag	UNP Q13219

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1572	LEU	-	expression tag	UNP Q13219
A	1573	ASP	-	expression tag	UNP Q13219
A	1574	TYR	-	expression tag	UNP Q13219
A	1575	LYS	-	expression tag	UNP Q13219
A	1576	ASP	-	expression tag	UNP Q13219
A	1577	ASP	-	expression tag	UNP Q13219
A	1578	ASP	-	expression tag	UNP Q13219
A	1579	ASP	-	expression tag	UNP Q13219
A	1580	LYS	-	expression tag	UNP Q13219
A	1581	VAL	-	expression tag	UNP Q13219
B	483	ALA	GLU	engineered mutation	UNP Q13219
B	1144	TYR	SER	engineered mutation	UNP Q13219
B	1548	SER	-	expression tag	UNP Q13219
B	1549	GLY	-	expression tag	UNP Q13219
B	1550	PRO	-	expression tag	UNP Q13219
B	1551	THR	-	expression tag	UNP Q13219
B	1552	ARG	-	expression tag	UNP Q13219
B	1553	THR	-	expression tag	UNP Q13219
B	1554	ARG	-	expression tag	UNP Q13219
B	1555	PRO	-	expression tag	UNP Q13219
B	1556	LEU	-	expression tag	UNP Q13219
B	1557	GLU	-	expression tag	UNP Q13219
B	1558	GLN	-	expression tag	UNP Q13219
B	1559	LYS	-	expression tag	UNP Q13219
B	1560	LEU	-	expression tag	UNP Q13219
B	1561	ILE	-	expression tag	UNP Q13219
B	1562	SER	-	expression tag	UNP Q13219
B	1563	GLU	-	expression tag	UNP Q13219
B	1564	GLU	-	expression tag	UNP Q13219
B	1565	ASP	-	expression tag	UNP Q13219
B	1566	LEU	-	expression tag	UNP Q13219
B	1567	ALA	-	expression tag	UNP Q13219
B	1568	ALA	-	expression tag	UNP Q13219
B	1569	ASN	-	expression tag	UNP Q13219
B	1570	ASP	-	expression tag	UNP Q13219
B	1571	ILE	-	expression tag	UNP Q13219
B	1572	LEU	-	expression tag	UNP Q13219
B	1573	ASP	-	expression tag	UNP Q13219
B	1574	TYR	-	expression tag	UNP Q13219
B	1575	LYS	-	expression tag	UNP Q13219
B	1576	ASP	-	expression tag	UNP Q13219
B	1577	ASP	-	expression tag	UNP Q13219

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1578	ASP	-	expression tag	UNP Q13219
B	1579	ASP	-	expression tag	UNP Q13219
B	1580	LYS	-	expression tag	UNP Q13219
B	1581	VAL	-	expression tag	UNP Q13219

- Molecule 2 is a protein called Insulin-like growth factor-binding protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	25	Total	C	H	N	O	0	0
			403	127	197	43	36		
2	C	20	Total	C	H	N	O	0	0
			335	100	173	32	30		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	HIS	-	expression tag	UNP P24593
D	-7	HIS	-	expression tag	UNP P24593
D	-6	HIS	-	expression tag	UNP P24593
D	-5	HIS	-	expression tag	UNP P24593
D	-4	HIS	-	expression tag	UNP P24593
D	-3	HIS	-	expression tag	UNP P24593
D	-2	ALA	-	expression tag	UNP P24593
D	-1	ALA	-	expression tag	UNP P24593
D	0	ALA	-	expression tag	UNP P24593
D	253	ALA	-	expression tag	UNP P24593
D	254	ALA	-	expression tag	UNP P24593
D	255	ALA	-	expression tag	UNP P24593
D	256	ASP	-	expression tag	UNP P24593
D	257	TYR	-	expression tag	UNP P24593
D	258	LYS	-	expression tag	UNP P24593
D	259	ASP	-	expression tag	UNP P24593
D	260	ASP	-	expression tag	UNP P24593
D	261	ASP	-	expression tag	UNP P24593
D	262	ASP	-	expression tag	UNP P24593
D	263	LYS	-	expression tag	UNP P24593
C	-8	HIS	-	expression tag	UNP P24593
C	-7	HIS	-	expression tag	UNP P24593
C	-6	HIS	-	expression tag	UNP P24593
C	-5	HIS	-	expression tag	UNP P24593
C	-4	HIS	-	expression tag	UNP P24593
C	-3	HIS	-	expression tag	UNP P24593

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	ALA	-	expression tag	UNP P24593
C	-1	ALA	-	expression tag	UNP P24593
C	0	ALA	-	expression tag	UNP P24593
C	253	ALA	-	expression tag	UNP P24593
C	254	ALA	-	expression tag	UNP P24593
C	255	ALA	-	expression tag	UNP P24593
C	256	ASP	-	expression tag	UNP P24593
C	257	TYR	-	expression tag	UNP P24593
C	258	LYS	-	expression tag	UNP P24593
C	259	ASP	-	expression tag	UNP P24593
C	260	ASP	-	expression tag	UNP P24593
C	261	ASP	-	expression tag	UNP P24593
C	262	ASP	-	expression tag	UNP P24593
C	263	LYS	-	expression tag	UNP P24593

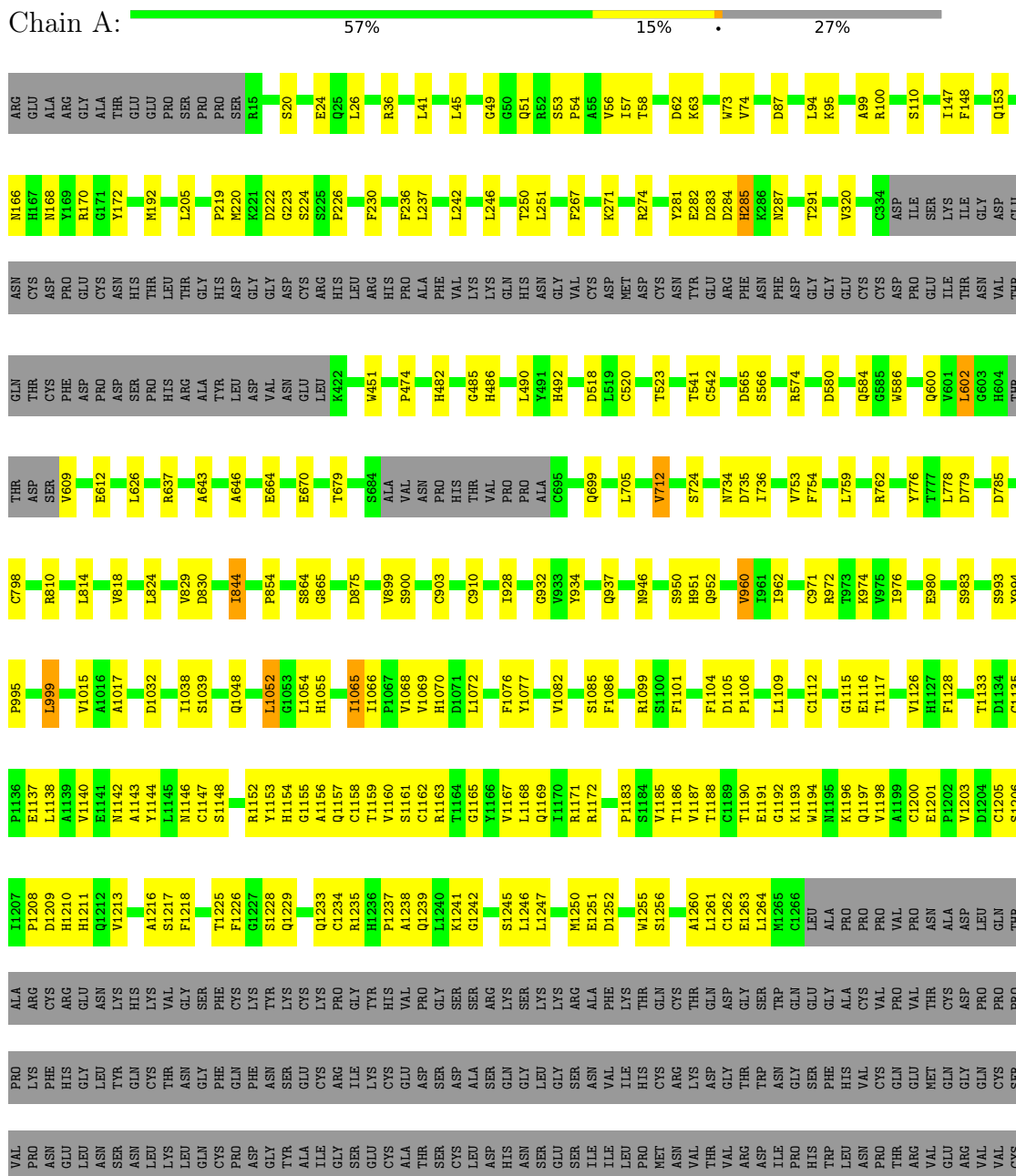
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	

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. 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: Pappalysin-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	245018	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	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:
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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/9019	0.66	41/12321 (0.3%)
1	B	0.25	0/9343	0.53	16/12757 (0.1%)
2	C	0.22	0/161	0.45	0/210
2	D	0.22	0/207	0.52	0/271
All	All	0.25	0/18730	0.59	57/25559 (0.2%)

There are no bond length outliers.

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	LYS	CD-CE-NZ	-11.24	85.85	111.70
1	A	474	PRO	C-N-CA	9.46	142.17	122.30
1	A	284	ASP	C-N-CA	9.06	144.35	121.70
1	B	542	CYS	C-N-CA	8.82	140.83	122.30
1	A	875	ASP	C-N-CA	8.25	142.33	121.70

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	A	8780	7002	8123	191	0
1	B	9095	7411	8490	224	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	162	173	183	2	0
2	D	206	197	231	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	18245	14783	17027	403	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 11.

The worst 5 of 403 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:1147:CYS:HA	1:A:1158:CYS:HA	1.39	1.03
1:A:1137:GLU:HA	1:A:1152:ARG:HD2	1.43	1.00
1:B:1144:TYR:HB2	1:B:1161:SER:HB3	1.41	0.99
1:B:1118:TYR:H	1:B:1126:VAL:HG12	1.25	0.99
1:A:1135:CYS:HA	1:A:1192:GLY:HA2	1.43	0.98

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	1143/1581 (72%)	1077 (94%)	66 (6%)	0	100	100
1	B	1176/1581 (74%)	1101 (94%)	75 (6%)	0	100	100
2	C	18/272 (7%)	18 (100%)	0	0	100	100
2	D	23/272 (8%)	21 (91%)	2 (9%)	0	100	100
All	All	2360/3706 (64%)	2217 (94%)	143 (6%)	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 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	938/1386 (68%)	938 (100%)	0	100	100
1	B	993/1386 (72%)	991 (100%)	2 (0%)	93	97
2	C	18/234 (8%)	18 (100%)	0	100	100
2	D	23/234 (10%)	22 (96%)	1 (4%)	29	59
All	All	1972/3240 (61%)	1969 (100%)	3 (0%)	93	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	734	ASN
1	B	744	LYS
2	D	143	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	529	HIS
1	A	1154	HIS
1	B	42	GLN
1	B	1050	HIS

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 2 ligands modelled in this entry, 2 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

This section contains visualisations of the EMDB entry EMD-26475. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.