



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 05:51 AM EDT

PDB ID : 7OIQ / pdb_00007oiq
Title : Crystal structure of AP2 Mu2 in complex with FCHO2 WxxPhi motif (C2 crystal form)
Authors : Zaccai, N.R.; Kelly, B.T.; Evans, P.R.; Owen, D.J.
Deposited on : 2021-05-12
Resolution : 1.85 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
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

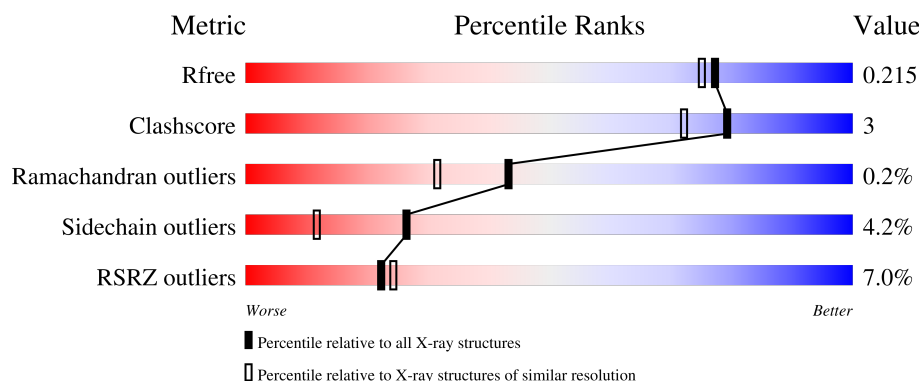
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	AAA	285	4% 81% 8% 10%
1	BBB	285	7% 78% 9% 12%
2	CCC	11	18% 100%
2	DDD	11	18% 73% 18% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4604 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 AP-2 complex subunit mu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	257	Total	C	N	O	S	0	0	0
			2075	1334	364	363	14			
1	BBB	250	Total	C	N	O	S	0	0	0
			2011	1293	353	351	14			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	151	MET	-	initiating methionine	UNP P84092
AAA	152	HIS	-	expression tag	UNP P84092
AAA	153	HIS	-	expression tag	UNP P84092
AAA	154	HIS	-	expression tag	UNP P84092
AAA	155	HIS	-	expression tag	UNP P84092
AAA	156	HIS	-	expression tag	UNP P84092
AAA	157	HIS	-	expression tag	UNP P84092
BBB	151	MET	-	initiating methionine	UNP P84092
BBB	152	HIS	-	expression tag	UNP P84092
BBB	153	HIS	-	expression tag	UNP P84092
BBB	154	HIS	-	expression tag	UNP P84092
BBB	155	HIS	-	expression tag	UNP P84092
BBB	156	HIS	-	expression tag	UNP P84092
BBB	157	HIS	-	expression tag	UNP P84092

- Molecule 2 is a protein called F-BAR domain only protein 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	CCC	11	Total	C	N	O	0	0	0
			87	59	12	16			
2	DDD	10	Total	C	N	O	0	0	0
			81	56	11	14			

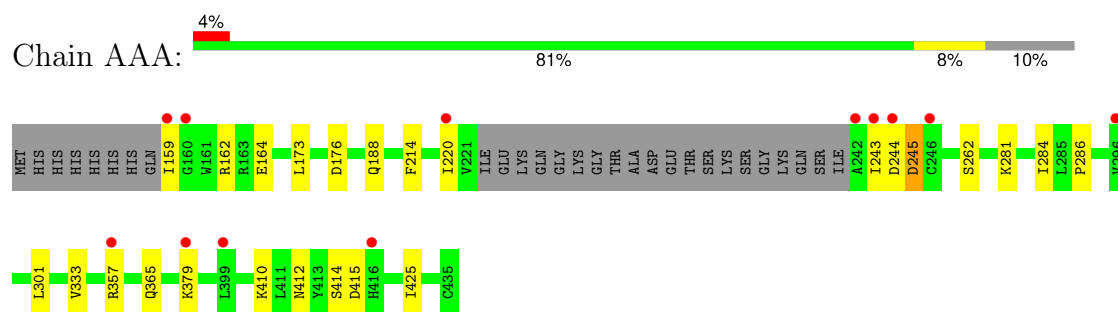
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	180	Total 180	O 180	0	0
3	BBB	148	Total 148	O 148	0	0
3	CCC	13	Total 13	O 13	0	0
3	DDD	9	Total 9	O 9	0	0

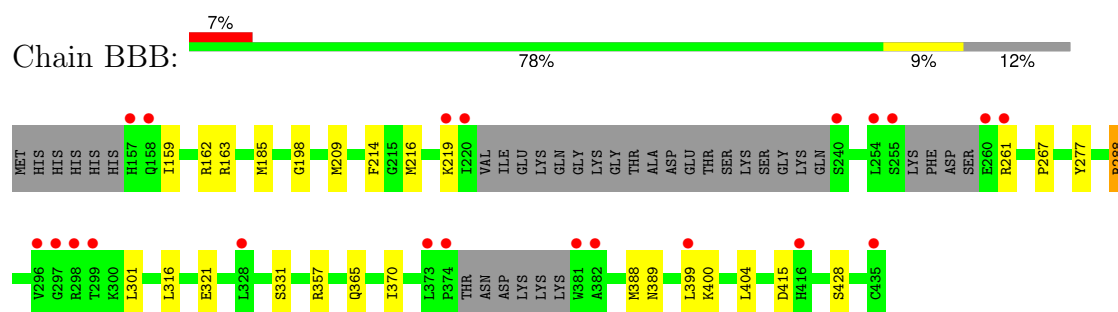
3 Residue-property plots [i](#)

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 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.

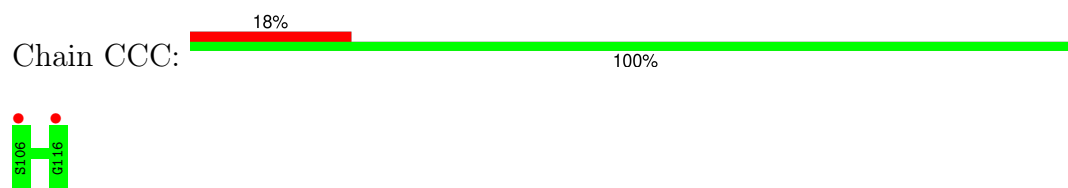
- Molecule 1: AP-2 complex subunit mu



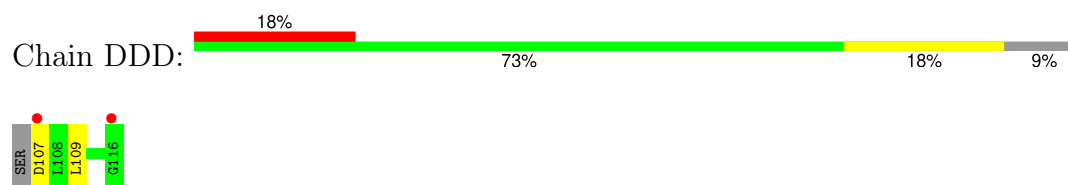
- Molecule 1: AP-2 complex subunit mu



- Molecule 2: F-BAR domain only protein 2



- Molecule 2: F-BAR domain only protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.89Å 64.54Å 108.44Å 90.00° 111.95° 90.00°	Depositor
Resolution (Å)	55.70 – 1.85 55.70 – 1.85	Depositor EDS
% Data completeness (in resolution range)	89.4 (55.70-1.85) 89.4 (55.70-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0267, PHENIX 1.19rc1_4016	Depositor
R, R_{free}	0.186 , 0.209 0.195 , 0.215	Depositor DCC
R_{free} test set	2932 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4604	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% 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](#)

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	AAA	1.09	2/2118 (0.1%)	1.25	4/2848 (0.1%)
1	BBB	1.05	0/2051	1.22	0/2757
2	CCC	0.84	0/90	0.98	0/123
2	DDD	0.90	0/84	1.09	0/115
All	All	1.06	2/4343 (0.0%)	1.23	4/5843 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	245	ASP	C-O	5.11	1.30	1.24
1	AAA	333	VAL	C-O	-5.09	1.18	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	415	ASP	CA-CB-CG	-8.39	104.20	112.60
1	AAA	425	ILE	CA-C-N	5.56	127.48	122.20
1	AAA	425	ILE	C-N-CA	5.56	127.48	122.20
1	AAA	415	ASP	CA-C-O	-5.20	115.04	120.55

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	AAA	2075	0	2163	6	0
1	BBB	2011	0	2090	16	0
2	CCC	87	0	79	0	0
2	DDD	81	0	74	1	0
3	AAA	180	0	0	0	0
3	BBB	148	0	0	1	0
3	CCC	13	0	0	0	0
3	DDD	9	0	0	0	0
All	All	4604	0	4406	23	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 3.

All (23) 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:BBB:216:MET:HE2	1:BBB:399:LEU:HD21	1.68	0.74
1:BBB:288:ARG:HH11	1:BBB:288:ARG:HG3	1.53	0.73
1:BBB:216:MET:CE	1:BBB:399:LEU:HD21	2.20	0.71
1:BBB:185:MET:HE2	3:BBB:603:HOH:O	2.00	0.59
1:BBB:288:ARG:HH11	1:BBB:288:ARG:CG	2.16	0.58
1:BBB:301:LEU:HB3	1:BBB:370:ILE:HB	1.98	0.46
1:BBB:162:ARG:HD2	1:BBB:267:PRO:O	2.16	0.45
1:BBB:216:MET:HE1	1:BBB:399:LEU:HD21	1.97	0.45
1:BBB:159:ILE:HD11	1:BBB:209:MET:HE1	2.00	0.43
1:BBB:288:ARG:CG	1:BBB:288:ARG:NH1	2.77	0.43
1:AAA:159:ILE:HD11	1:AAA:162:ARG:HB3	2.00	0.43
1:BBB:316:LEU:HD13	1:BBB:357:ARG:HD2	2.00	0.43
1:AAA:173:LEU:C	1:AAA:173:LEU:HD12	2.44	0.42
1:AAA:220:ILE:HG22	1:AAA:243:ILE:CD1	2.49	0.42
1:AAA:284:ILE:O	1:AAA:286:PRO:HD3	2.20	0.42
1:BBB:389:ASN:HA	1:BBB:428:SER:OG	2.19	0.42
1:BBB:216:MET:SD	1:BBB:399:LEU:HD11	2.60	0.42
2:DDD:107:ASP:OD2	2:DDD:109:LEU:HB2	2.20	0.41
1:AAA:214:PHE:O	1:AAA:262:SER:HA	2.20	0.41
1:AAA:357:ARG:NH1	1:AAA:357:ARG:HB3	2.36	0.41
1:BBB:214:PHE:CE2	1:BBB:216:MET:HE3	2.56	0.41
1:BBB:321:GLU:O	1:BBB:388:MET:HA	2.21	0.41
1:BBB:198:GLY:HA3	1:BBB:277:TYR:CZ	2.56	0.41

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	AAA	253/285 (89%)	244 (96%)	8 (3%)	1 (0%)	30	17
1	BBB	242/285 (85%)	236 (98%)	6 (2%)	0	100	100
2	CCC	9/11 (82%)	9 (100%)	0	0	100	100
2	DDD	8/11 (73%)	8 (100%)	0	0	100	100
All	All	512/592 (86%)	497 (97%)	14 (3%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	245	ASP

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	AAA	233/257 (91%)	222 (95%)	11 (5%)	23	9
1	BBB	225/257 (88%)	216 (96%)	9 (4%)	28	13
2	CCC	9/9 (100%)	9 (100%)	0	100	100
2	DDD	8/9 (89%)	8 (100%)	0	100	100
All	All	475/532 (89%)	455 (96%)	20 (4%)	26	12

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	164	GLU
1	AAA	176	ASP
1	AAA	188	GLN
1	AAA	244	ASP
1	AAA	281	LYS
1	AAA	301	LEU
1	AAA	365	GLN
1	AAA	379	LYS
1	AAA	410	LYS
1	AAA	412	ASN
1	AAA	414	SER
1	BBB	163	ARG
1	BBB	219	LYS
1	BBB	261	ARG
1	BBB	288	ARG
1	BBB	331	SER
1	BBB	365	GLN
1	BBB	400	LYS
1	BBB	404	LEU
1	BBB	415	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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, 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	AAA	257/285 (90%)	0.20	12 (4%) 36 39	23, 33, 64, 84	0
1	BBB	250/285 (87%)	0.38	21 (8%) 17 17	24, 36, 76, 108	0
2	CCC	11/11 (100%)	0.73	2 (18%) 3 3	26, 32, 66, 80	0
2	DDD	10/11 (90%)	0.77	2 (20%) 3 2	29, 34, 53, 69	0
All	All	528/592 (89%)	0.31	37 (7%) 22 24	23, 35, 67, 108	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	220	ILE	8.2
1	AAA	242	ALA	5.5
1	BBB	381	TRP	5.0
1	BBB	374	PRO	4.5
2	DDD	116	GLY	4.3
1	BBB	260	GLU	4.1
1	BBB	373	LEU	4.1
1	BBB	296	VAL	4.0
1	BBB	254	LEU	3.6
1	BBB	255	SER	3.5
1	BBB	382	ALA	3.4
1	AAA	220	ILE	3.3
1	BBB	157	HIS	3.2
2	CCC	106	SER	3.0
1	BBB	399	LEU	2.9
1	AAA	159	ILE	2.7
2	CCC	116	GLY	2.6
1	AAA	296	VAL	2.6
1	BBB	299	THR	2.5
2	DDD	107	ASP	2.5
1	BBB	435	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	BBB	158	GLN	2.4
1	AAA	246	CYS	2.4
1	BBB	328	LEU	2.4
1	AAA	379	LYS	2.4
1	AAA	243	ILE	2.3
1	BBB	219	LYS	2.3
1	AAA	416	HIS	2.2
1	AAA	160	GLY	2.2
1	BBB	240	SER	2.2
1	AAA	399	LEU	2.2
1	BBB	261	ARG	2.2
1	AAA	244	ASP	2.1
1	BBB	298	ARG	2.1
1	BBB	416	HIS	2.1
1	BBB	297	GLY	2.0
1	AAA	357	ARG	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.