



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:18 PM UTC

PDB ID : 1AWQ / pdb_00001awq
Title : CYPA COMPLEXED WITH HAGPIA (PSEUDO-SYMMETRIC MONOMER)
Authors : Vajdos, F.F.
Deposited on : 1997-10-04
Resolution : 1.58 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

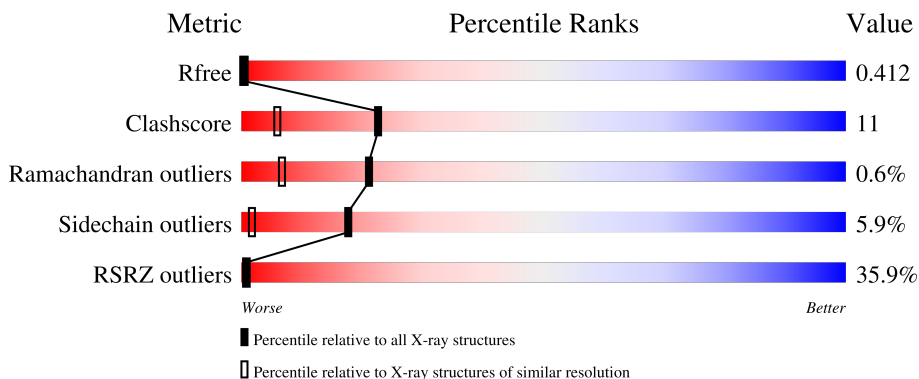
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	164	37% 72% 27% .
2	B	6	67% 33%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1350 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 CYCLOPHILIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1258	797	217	236	8			

- Molecule 2 is a protein called PEPTIDE FROM THE HIV-1 CAPSID PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	0	0	0
			40	25	8	7			

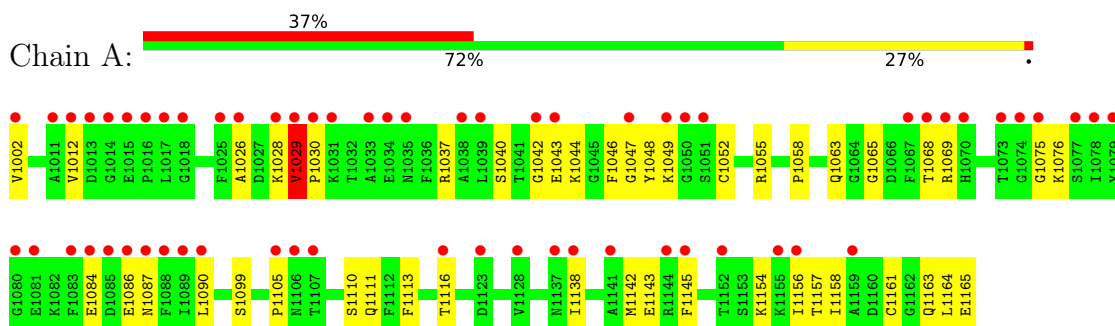
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	48	Total	O	0	0
			48	48		
3	B	4	Total	O	0	0
			4	4		

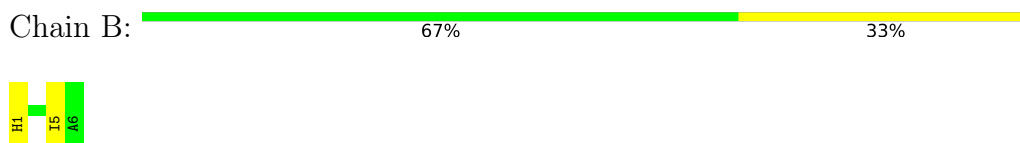
3 Residue-property plots [i](#)

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: CYCLOPHILIN A



• Molecule 2: PEPTIDE FROM THE HIV-1 CAPSID PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	51.50Å 51.50Å 62.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.58 15.00 – 1.58	Depositor EDS
% Data completeness (in resolution range)	88.3 (15.00-1.58) 88.1 (15.00-1.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 1.53Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.343 , 0.433 0.333 , 0.412	Depositor DCC
R_{free} test set	1002 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	1350	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.67% 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	A	0.53	0/1286	1.03	5/1723 (0.3%)
2	B	0.72	0/41	1.10	0/54
All	All	0.54	0/1327	1.03	5/1777 (0.3%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1029	VAL	CA-C-N	7.62	129.36	119.84
1	A	1029	VAL	C-N-CA	7.62	129.36	119.84
1	A	1047	GLY	N-CA-C	6.49	124.10	112.22
1	A	1075	GLY	N-CA-C	-6.41	102.35	112.61
1	A	1138	ILE	N-CA-C	-5.66	105.33	110.82

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	1258	0	1225	27	0
2	B	40	0	40	0	0
3	A	48	0	0	1	0
3	B	4	0	0	0	0
All	All	1350	0	1265	27	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.

All (27) 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:1099:SER:HB3	1:A:1113:PHE:CZ	2.29	0.67
1:A:1026:ALA:O	1:A:1030:PRO:HG3	1.98	0.62
1:A:1052:CYS:HB2	1:A:1156:ILE:O	1.99	0.62
1:A:1037:ARG:HH11	1:A:1163:GLN:HE22	1.50	0.58
1:A:1028:LYS:O	1:A:1030:PRO:HD3	2.07	0.55
1:A:1090:LEU:HD22	1:A:1090:LEU:N	2.22	0.54
1:A:1028:LYS:C	1:A:1030:PRO:HD3	2.35	0.51
1:A:1164:LEU:O	1:A:1165:GLU:HB3	2.11	0.51
1:A:1076:LYS:O	1:A:1110:SER:HB3	2.13	0.49
1:A:1012:VAL:HG12	1:A:1154:LYS:HD3	1.94	0.48
1:A:1037:ARG:HH11	1:A:1163:GLN:NE2	2.13	0.47
1:A:1116:THR:HB	3:A:250:HOH:O	2.13	0.47
1:A:1029:VAL:HG12	1:A:1086:GLU:HB3	1.99	0.45
1:A:1090:LEU:HD22	1:A:1090:LEU:H	1.82	0.44
1:A:1068:THR:OG1	1:A:1069:ARG:HD2	2.17	0.44
1:A:1029:VAL:HG13	1:A:1087:ASN:HD21	1.82	0.44
1:A:1040:SER:O	1:A:1161:CYS:SG	2.75	0.44
1:A:1099:SER:HB3	1:A:1113:PHE:CE1	2.52	0.44
1:A:1065:GLY:HA3	1:A:1111:GLN:HA	2.00	0.43
1:A:1157:THR:HG22	1:A:1158:ILE:N	2.33	0.43
1:A:1048:TYR:HB3	1:A:1158:ILE:HD12	2.01	0.42
1:A:1037:ARG:NH1	1:A:1163:GLN:HE22	2.17	0.42
1:A:1142:MET:HA	1:A:1145:PHE:HD2	1.84	0.42
1:A:1055:ARG:HB3	1:A:1063:GLN:HB3	2.01	0.42
1:A:1058:PRO:HG3	1:A:1143:GLU:O	2.20	0.42
1:A:1042:GLY:C	1:A:1044:LYS:H	2.29	0.40
1:A:1142:MET:HB2	1:A:1156:ILE:HG12	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	162/164 (99%)	144 (89%)	17 (10%)	1 (1%)	21	7
2	B	4/6 (67%)	4 (100%)	0	0	100	100
All	All	166/170 (98%)	148 (89%)	17 (10%)	1 (1%)	21	7

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1043	GLU

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	132/132 (100%)	126 (96%)	6 (4%)	24	3
2	B	3/3 (100%)	1 (33%)	2 (67%)	0	0
All	All	135/135 (100%)	127 (94%)	8 (6%)	18	2

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1002	VAL
1	A	1029	VAL
1	A	1046	PHE
1	A	1049	LYS
1	A	1084	GLU
1	A	1105	PRO
2	B	1	HIS
2	B	5	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1106	ASN
1	A	1163	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, 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	164/164 (100%)	1.72	61 (37%) 1 1	5, 27, 48, 55	0
2	B	6/6 (100%)	0.83	0 100 100	11, 13, 23, 27	0
All	All	170/170 (100%)	1.69	61 (35%) 1 1	5, 27, 48, 55	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1079	TYR	4.9
1	A	1016	PRO	4.8
1	A	1002	VAL	4.4
1	A	1042	GLY	4.3
1	A	1090	LEU	4.2
1	A	1141	ALA	4.2
1	A	1050	GLY	4.1
1	A	1030	PRO	4.1
1	A	1105	PRO	4.1
1	A	1074	GLY	4.1
1	A	1075	GLY	4.0
1	A	1086	GLU	4.0
1	A	1145	PHE	3.9
1	A	1029	VAL	3.7
1	A	1034	GLU	3.7
1	A	1073	THR	3.7
1	A	1087	ASN	3.6
1	A	1138	ILE	3.5
1	A	1078	ILE	3.5
1	A	1159	ALA	3.5
1	A	1012	VAL	3.5
1	A	1047	GLY	3.4
1	A	1068	THR	3.4
1	A	1014	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	1018	GLY	3.3
1	A	1017	LEU	3.2
1	A	1026	ALA	3.2
1	A	1025	PHE	3.1
1	A	1033	ALA	3.1
1	A	1077	SER	3.0
1	A	1080	GLY	2.9
1	A	1088	PHE	2.9
1	A	1015	GLU	2.9
1	A	1085	ASP	2.9
1	A	1038	ALA	2.8
1	A	1152	THR	2.8
1	A	1089	ILE	2.7
1	A	1156	ILE	2.7
1	A	1049	LYS	2.7
1	A	1043	GLU	2.7
1	A	1011	ALA	2.6
1	A	1084	GLU	2.5
1	A	1107	THR	2.5
1	A	1144	ARG	2.5
1	A	1028	LYS	2.4
1	A	1083	PHE	2.4
1	A	1081	GLU	2.4
1	A	1013	ASP	2.4
1	A	1035	ASN	2.4
1	A	1137	ASN	2.4
1	A	1106	ASN	2.4
1	A	1155	LYS	2.3
1	A	1128	VAL	2.2
1	A	1070	HIS	2.2
1	A	1051	SER	2.2
1	A	1116	THR	2.1
1	A	1123	ASP	2.1
1	A	1067	PHE	2.0
1	A	1069	ARG	2.0
1	A	1031	LYS	2.0
1	A	1039	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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.