



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5IBV / pdb_00005ibv
Title : Crystal Structure of Human Astrovirus capsid protein
Authors : Tao, Y.J.; Toh, Y.S.
Deposited on : 2016-02-22
Resolution : 2.15 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

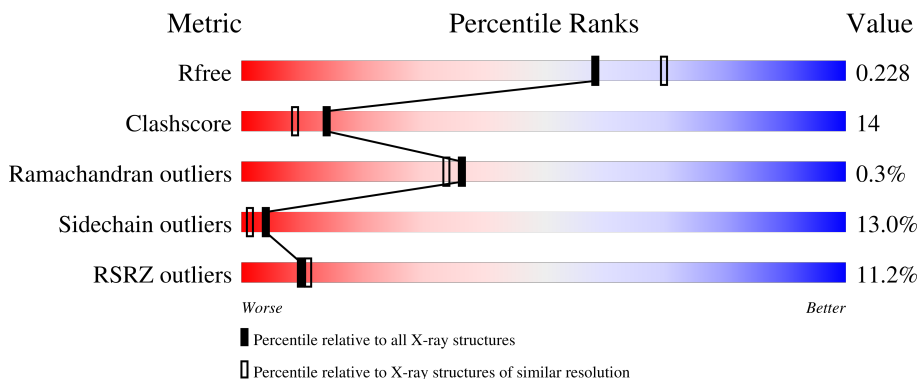
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	354	10% 64% 22% 5% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2525 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 Capsid polypeptide VP90.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	Se	0	2	0
			2452	1550	422	469	5	6			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	416	GLY	ALA	conflict	UNP Q9IFX1
A	417	GLY	-	expression tag	UNP Q9IFX1
A	418	GLY	-	expression tag	UNP Q9IFX1
A	419	HIS	-	expression tag	UNP Q9IFX1
A	420	HIS	-	expression tag	UNP Q9IFX1
A	421	HIS	-	expression tag	UNP Q9IFX1
A	422	HIS	-	expression tag	UNP Q9IFX1
A	423	HIS	-	expression tag	UNP Q9IFX1
A	424	HIS	-	expression tag	UNP Q9IFX1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	73	Total	O	0	0
			73	73		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.98Å 59.24Å 56.20Å 90.00° 91.45° 90.00°	Depositor
Resolution (Å)	30.00 – 2.15 30.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.00-2.15) 98.3 (30.00-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.80 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.209 , 0.246 0.211 , 0.228	Depositor DCC
R_{free} test set	958 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.997	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2525	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% 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

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	0.66	1/2504 (0.0%)	0.80	3/3410 (0.1%)

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	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	LEU	C-O	-5.13	1.18	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	VAL	N-CA-C	10.75	121.58	110.72
1	A	315	GLY	N-CA-C	-7.33	105.12	115.30
1	A	264	LEU	N-CA-C	5.21	118.62	111.54

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	264	LEU	Peptide
1	A	312	SER	Peptide
1	A	315	GLY	Peptide
1	A	359	ARG	Peptide
1	A	362	THR	Peptide
1	A	363	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	A	407	MSE	Peptide
1	A	410	PRO	Peptide
1	A	411	SER	Peptide

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	2452	0	2431	69	0
2	A	73	0	0	7	0
All	All	2525	0	2431	69	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 14.

All (69) 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:412:LEU:HD21	2:A:507:HOH:O	1.44	1.12
1:A:412:LEU:CD2	2:A:507:HOH:O	2.00	0.99
1:A:291:VAL:O	1:A:364:ALA:HB1	1.77	0.84
1:A:360:ALA:HB1	1:A:361:ARG:O	1.76	0.84
1:A:360:ALA:HA	1:A:361:ARG:HB2	1.60	0.83
1:A:360:ALA:HA	1:A:361:ARG:CB	2.11	0.80
1:A:211:THR:HA	1:A:218:THR:HG21	1.65	0.76
1:A:132:TYR:O	1:A:209:THR:HG21	1.87	0.73
1:A:195:LYS:HG3	1:A:197:SER:H	1.54	0.73
1:A:412:LEU:C	1:A:412:LEU:HD13	2.15	0.72
1:A:262:PRO:O	1:A:263:ASN:HB2	1.91	0.70
1:A:361:ARG:N	1:A:363:GLY:O	2.25	0.68
1:A:290:ASN:HD22	1:A:366:ARG:HG2	1.59	0.66
1:A:203:ARG:NH1	1:A:217:ASP:OD2	2.26	0.66
1:A:79:PRO:O	2:A:501:HOH:O	2.13	0.65
1:A:158:VAL:HG22	1:A:227:THR:HG22	1.80	0.63
1:A:210:ASN:HD21	1:A:412:LEU:HD22	1.64	0.62
1:A:359:ARG:N	1:A:360:ALA:HB2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ASN:HB2	1:A:412:LEU:HD23	1.81	0.61
1:A:310:SER:OG	2:A:502:HOH:O	2.14	0.60
1:A:312:SER:OG	1:A:313:ARG:HB2	2.02	0.60
1:A:290:ASN:ND2	1:A:366:ARG:HG2	2.16	0.60
1:A:147[A]:MSE:HA	1:A:147[A]:MSE:HE2	1.85	0.58
1:A:336:LEU:HB2	1:A:346:VAL:HG21	1.86	0.58
1:A:330:ALA:HB3	1:A:400:THR:HA	1.86	0.57
1:A:224:GLU:HG2	2:A:566:HOH:O	2.06	0.55
1:A:306:SER:CB	1:A:410:PRO:HG2	2.36	0.55
1:A:232[B]:MSE:CE	1:A:239:GLN:HA	2.37	0.54
1:A:412:LEU:HD23	2:A:507:HOH:O	1.85	0.53
1:A:138:LYS:O	1:A:196:PRO:HG3	2.09	0.53
1:A:265:VAL:HG22	1:A:409:GLN:OE1	2.10	0.52
1:A:342:PHE:CZ	1:A:382:ALA:HB1	2.45	0.52
1:A:360:ALA:CA	1:A:361:ARG:CB	2.85	0.52
1:A:147[B]:MSE:HE2	1:A:245:PHE:N	2.23	0.52
1:A:231:THR:O	1:A:232[B]:MSE:HE2	2.10	0.51
1:A:268:VAL:HG11	1:A:300:THR:HG21	1.92	0.51
1:A:230:GLN:CD	1:A:232[B]:MSE:HE3	2.35	0.51
1:A:97:THR:HG23	1:A:101:GLU:OE2	2.10	0.50
1:A:114:LYS:O	1:A:114:LYS:HG2	2.10	0.50
1:A:195:LYS:HG3	1:A:197:SER:N	2.25	0.50
1:A:195:LYS:HG3	1:A:196:PRO:N	2.24	0.50
1:A:147[B]:MSE:HE3	1:A:243:GLY:C	2.38	0.49
1:A:131:GLN:NE2	2:A:504:HOH:O	2.31	0.48
1:A:312:SER:O	1:A:313:ARG:C	2.54	0.47
1:A:109:ASN:OD1	1:A:111:VAL:HG22	2.14	0.47
1:A:166:SER:HB2	1:A:219:LEU:HD23	1.96	0.47
1:A:306:SER:HB2	1:A:410:PRO:HG2	1.97	0.47
1:A:330:ALA:CB	1:A:400:THR:HA	2.45	0.47
1:A:107:LEU:HD23	1:A:222:SER:OG	2.16	0.46
1:A:265:VAL:CG2	1:A:409:GLN:OE1	2.64	0.46
1:A:300:THR:HA	1:A:303:GLU:HG3	1.99	0.45
1:A:360:ALA:HA	1:A:361:ARG:HB3	1.98	0.44
1:A:270:SER:HB3	1:A:404:PHE:CE1	2.52	0.44
1:A:140:LEU:HD11	1:A:249:LEU:HD11	1.99	0.44
1:A:138:LYS:HG3	1:A:254:CYS:SG	2.59	0.43
1:A:210:ASN:HD21	1:A:412:LEU:CD2	2.31	0.43
1:A:232[B]:MSE:HE1	1:A:239:GLN:HA	2.00	0.43
1:A:109:ASN:HB3	1:A:112:LEU:HD12	2.01	0.42
1:A:195:LYS:CG	1:A:197:SER:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ALA:O	1:A:262:PRO:HA	2.20	0.42
1:A:147[B]:MSE:HE2	1:A:245:PHE:C	2.44	0.42
1:A:219:LEU:HD11	1:A:407:MSE:CE	2.49	0.42
1:A:399:ARG:HG2	1:A:400:THR:HG23	2.02	0.41
1:A:270:SER:HB3	1:A:404:PHE:CZ	2.55	0.41
1:A:359:ARG:H	1:A:360:ALA:HB2	1.85	0.41
1:A:267:LEU:HD23	1:A:406:GLN:OE1	2.21	0.40
1:A:232[B]:MSE:HE2	1:A:239:GLN:HA	2.02	0.40
1:A:336:LEU:HD23	1:A:399:ARG:HH11	1.86	0.40
1:A:170:SER:HB3	1:A:344:TRP:CE3	2.56	0.40

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 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	320/354 (90%)	309 (97%)	10 (3%)	1 (0%)	36 34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	ARG

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	271/284 (95%)	236 (87%)	35 (13%)	4 1

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	LYS
1	A	136	LYS
1	A	148	VAL
1	A	169	SER
1	A	172	SER
1	A	180	LYS
1	A	185	THR
1	A	195	LYS
1	A	209	THR
1	A	219	LEU
1	A	222	SER
1	A	233	SER
1	A	237	ASN
1	A	248	GLU
1	A	250	SER
1	A	261	ASN
1	A	262	PRO
1	A	265	VAL
1	A	266	ASN
1	A	274	SER
1	A	280	GLU
1	A	291	VAL
1	A	303	GLU
1	A	307	LEU
1	A	313	ARG
1	A	317	GLU
1	A	318	SER
1	A	335	GLU
1	A	343	ASN
1	A	347	LYS
1	A	359	ARG
1	A	388	VAL
1	A	399	ARG
1	A	411	SER
1	A	412	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	210	ASN
1	A	304	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 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	320/354 (90%)	0.60	36 (11%) 10 11	18, 35, 76, 90	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312	SER	4.4
1	A	264	LEU	4.1
1	A	262	PRO	3.9
1	A	412	LEU	3.9
1	A	314	ALA	3.8
1	A	313	ARG	3.8
1	A	260	ALA	3.5
1	A	363	GLY	3.4
1	A	358	GLY	3.3
1	A	360	ALA	3.3
1	A	316	GLY	3.2
1	A	265	VAL	3.0
1	A	311	LEU	2.9
1	A	361	ARG	2.9
1	A	336	LEU	2.8
1	A	214	ASN	2.8
1	A	315	GLY	2.8
1	A	261	ASN	2.7
1	A	331	VAL	2.7
1	A	238	THR	2.5
1	A	359	ARG	2.5
1	A	411	SER	2.5
1	A	308	SER	2.5
1	A	408	ASN	2.4
1	A	259	ALA	2.4
1	A	303	GLU	2.4
1	A	389	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	263	ASN	2.2
1	A	291	VAL	2.2
1	A	235	TYR	2.2
1	A	307	LEU	2.2
1	A	266	ASN	2.2
1	A	387	GLY	2.1
1	A	213	ASP	2.1
1	A	151	SER	2.1
1	A	277	VAL	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.