



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:20 PM GMT

PDB ID : 4EJR
Title : Crystal structure of major capsid protein S domain from rabbit hemorrhagic disease virus
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Deposited on : 2012-04-07
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

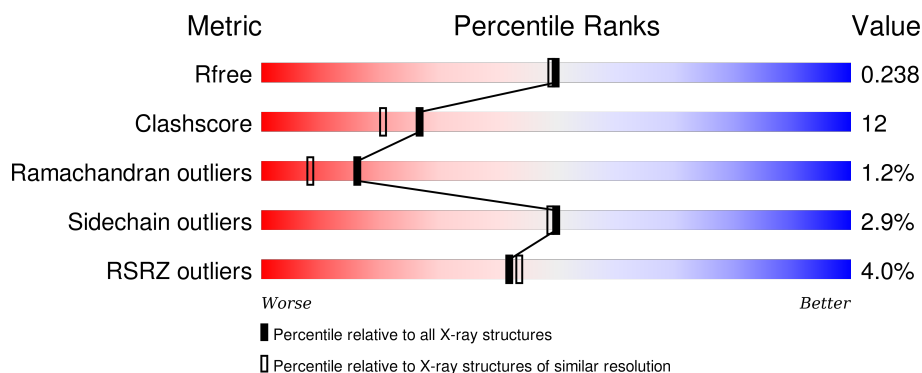
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	255	<div> <div>4%</div> <div>53%</div> <div>9%</div> <div>•</div> <div>36%</div> </div>
1	B	255	<div> <div>2%</div> <div>53%</div> <div>9%</div> <div>•</div> <div>36%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2598 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 Major capsid protein VP60.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1260	815	211	229	5			
1	B	163	Total	C	N	O	S	0	0	0
			1260	815	211	229	5			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	EXPRESSION TAG	UNP Q3HNQ1
A	-23	GLY	-	EXPRESSION TAG	UNP Q3HNQ1
A	-22	HIS	-	EXPRESSION TAG	UNP Q3HNQ1
A	-21	HIS	-	EXPRESSION TAG	UNP Q3HNQ1
A	-20	HIS	-	EXPRESSION TAG	UNP Q3HNQ1
A	-19	HIS	-	EXPRESSION TAG	UNP Q3HNQ1
A	-18	HIS	-	EXPRESSION TAG	UNP Q3HNQ1
A	-17	HIS	-	EXPRESSION TAG	UNP Q3HNQ1
A	-16	HIS	-	EXPRESSION TAG	UNP Q3HNQ1
A	-15	HIS	-	EXPRESSION TAG	UNP Q3HNQ1
A	-14	SER	-	EXPRESSION TAG	UNP Q3HNQ1
A	-13	SER	-	EXPRESSION TAG	UNP Q3HNQ1
A	-12	GLY	-	EXPRESSION TAG	UNP Q3HNQ1
A	-11	GLU	-	EXPRESSION TAG	UNP Q3HNQ1
A	-10	ASN	-	EXPRESSION TAG	UNP Q3HNQ1
A	-9	LEU	-	EXPRESSION TAG	UNP Q3HNQ1
A	-8	TYR	-	EXPRESSION TAG	UNP Q3HNQ1
A	-7	PHE	-	EXPRESSION TAG	UNP Q3HNQ1
A	-6	GLN	-	EXPRESSION TAG	UNP Q3HNQ1
A	-5	GLY	-	EXPRESSION TAG	UNP Q3HNQ1
A	-4	SER	-	EXPRESSION TAG	UNP Q3HNQ1
A	-3	LYS	-	EXPRESSION TAG	UNP Q3HNQ1
A	-2	LEU	-	EXPRESSION TAG	UNP Q3HNQ1
A	-1	GLU	-	EXPRESSION TAG	UNP Q3HNQ1
A	0	PHE	-	EXPRESSION TAG	UNP Q3HNQ1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-24	MET	-	EXPRESSION TAG	UNP Q3HNP1
B	-23	GLY	-	EXPRESSION TAG	UNP Q3HNP1
B	-22	HIS	-	EXPRESSION TAG	UNP Q3HNP1
B	-21	HIS	-	EXPRESSION TAG	UNP Q3HNP1
B	-20	HIS	-	EXPRESSION TAG	UNP Q3HNP1
B	-19	HIS	-	EXPRESSION TAG	UNP Q3HNP1
B	-18	HIS	-	EXPRESSION TAG	UNP Q3HNP1
B	-17	HIS	-	EXPRESSION TAG	UNP Q3HNP1
B	-16	HIS	-	EXPRESSION TAG	UNP Q3HNP1
B	-15	HIS	-	EXPRESSION TAG	UNP Q3HNP1
B	-14	SER	-	EXPRESSION TAG	UNP Q3HNP1
B	-13	SER	-	EXPRESSION TAG	UNP Q3HNP1
B	-12	GLY	-	EXPRESSION TAG	UNP Q3HNP1
B	-11	GLU	-	EXPRESSION TAG	UNP Q3HNP1
B	-10	ASN	-	EXPRESSION TAG	UNP Q3HNP1
B	-9	LEU	-	EXPRESSION TAG	UNP Q3HNP1
B	-8	TYR	-	EXPRESSION TAG	UNP Q3HNP1
B	-7	PHE	-	EXPRESSION TAG	UNP Q3HNP1
B	-6	GLN	-	EXPRESSION TAG	UNP Q3HNP1
B	-5	GLY	-	EXPRESSION TAG	UNP Q3HNP1
B	-4	SER	-	EXPRESSION TAG	UNP Q3HNP1
B	-3	LYS	-	EXPRESSION TAG	UNP Q3HNP1
B	-2	LEU	-	EXPRESSION TAG	UNP Q3HNP1
B	-1	GLU	-	EXPRESSION TAG	UNP Q3HNP1
B	0	PHE	-	EXPRESSION TAG	UNP Q3HNP1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	30	Total O 30 30	0	0
2	B	48	Total O 48 48	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.73 Å 48.36 Å 65.16 Å 90.00° 100.95° 90.00°	Depositor
Resolution (Å)	49.35 – 2.00 49.35 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.35-2.00) 99.8 (49.35-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.201 , 0.241 0.201 , 0.238	Depositor DCC
R_{free} test set	1330 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 26144 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2598	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.89 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.5598e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.19	3/1300 (0.2%)	1.03	5/1785 (0.3%)
1	B	1.25	3/1300 (0.2%)	1.03	3/1785 (0.2%)
All	All	1.22	6/2600 (0.2%)	1.03	8/3570 (0.2%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	156	VAL	CB-CG1	6.18	1.65	1.52
1	B	81	SER	CB-OG	-5.93	1.34	1.42
1	A	93	VAL	CB-CG2	-5.55	1.41	1.52
1	A	210	GLN	CG-CD	-5.52	1.38	1.51
1	B	78	PHE	CE1-CZ	5.40	1.47	1.37

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ASP	CB-CG-OD2	-7.87	111.21	118.30
1	A	192	LEU	CA-CB-CG	-7.48	98.09	115.30
1	B	148	LEU	CA-CB-CG	6.08	129.29	115.30
1	B	192	LEU	CA-CB-CG	-5.84	101.88	115.30
1	A	199	ILE	CB-CA-C	-5.56	100.48	111.60

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	1260	0	1226	24	0
1	B	1260	0	1226	41	0
2	A	30	0	0	0	0
2	B	48	0	0	0	0
All	All	2598	0	2452	60	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 12.

The worst 5 of 60 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:145:GLY:HA2	1:B:148:LEU:CD2	1.49	1.39
1:B:145:GLY:CA	1:B:148:LEU:HD23	1.80	1.11
1:B:145:GLY:CA	1:B:148:LEU:CD2	2.29	1.09
1:B:145:GLY:HA2	1:B:148:LEU:HD23	1.31	1.04
1:B:145:GLY:HA2	1:B:148:LEU:HD21	1.37	1.03

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	161/255 (63%)	154 (96%)	6 (4%)	1 (1%)	30	22
1	B	161/255 (63%)	153 (95%)	5 (3%)	3 (2%)	10	4
All	All	322/510 (63%)	307 (95%)	11 (3%)	4 (1%)	16	8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	205	SER

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Mol	Chain	Res	Type
1	B	145	GLY
1	B	146	PRO
1	A	204	GLY

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	137/206 (66%)	131 (96%)	6 (4%)	35	30
1	B	137/206 (66%)	135 (98%)	2 (2%)	72	75
All	All	274/412 (66%)	266 (97%)	8 (3%)	50	49

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	B	148	LEU
1	A	202	PHE
1	A	174	ARG
1	A	198	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	94	GLN
1	B	197	ASN
1	B	152	GLN
1	A	200	ASN
1	B	118	GLN

5.3.3 RNA ⓘ

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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	163/255 (63%)	0.08	9 (5%) 29 30	13, 21, 53, 62	0
1	B	163/255 (63%)	-0.16	4 (2%) 61 61	11, 19, 40, 53	0
All	All	326/510 (63%)	-0.04	13 (3%) 42 44	11, 20, 48, 62	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	PRO	4.4
1	A	202	PHE	4.0
1	A	203	GLY	3.9
1	A	146	PRO	3.2
1	A	185	GLY	3.0

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 carbohydrates 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.