



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:39 PM GMT

PDB ID : 3RKD
Title : Hepatitis E Virus E2s domain (Genotype I) in complex with a neutralizing antibody
Authors : Tang, X.H.; Sivaraman, J.
Deposited on : 2011-04-18
Resolution : 1.90 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

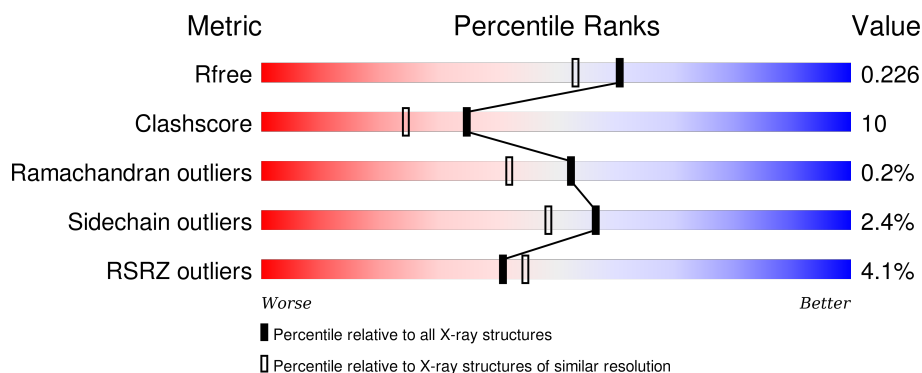
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	146	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> <div>•</div> </div>
1	B	146	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>10%</div> </div> <div>••</div> </div>
2	C	214	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>17%</div> </div> </div>
2	L	214	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>21%</div> </div> <div>•</div> </div>
3	D	230	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>20%</div> </div> <div>• 5%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	230	<div><div></div><div>4%</div><div>75%</div><div>19%</div><div>• 5%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9533 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 protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	0	0	0
			1096	697	185	214			
1	B	145	Total	C	N	O	0	0	0
			1090	694	184	212			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	532	HIS	TYR	ENGINEERED MUTATION	UNP B0VX51
A	604	PRO	-	EXPRESSION TAG	UNP B0VX51
B	532	HIS	TYR	ENGINEERED MUTATION	UNP B0VX51
B	604	PRO	-	EXPRESSION TAG	UNP B0VX51

- Molecule 2 is a protein called Monoclonal Antibody, Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1656	1034	278	338	6			
2	C	213	Total	C	N	O	S	0	0	0
			1656	1034	278	338	6			

- Molecule 3 is a protein called Monoclonal Antibody, Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	218	Total	C	N	O	S	0	0	0
			1637	1044	267	320	6			
3	D	218	Total	C	N	O	S	0	0	0
			1637	1044	267	320	6			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	118	Total 118	O 118	0	0
4	B	107	Total 107	O 107	0	0
4	L	134	Total 134	O 134	0	0
4	H	140	Total 140	O 140	0	0
4	C	133	Total 133	O 133	0	0
4	D	129	Total 129	O 129	0	0

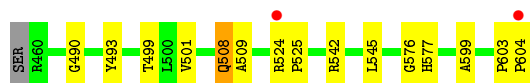
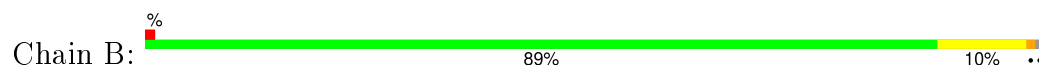
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

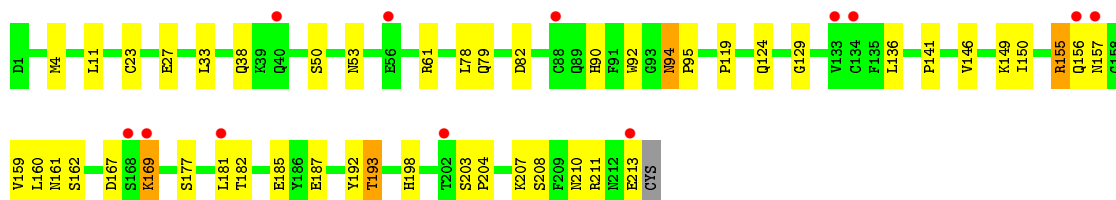
- Molecule 1: Capsid protein



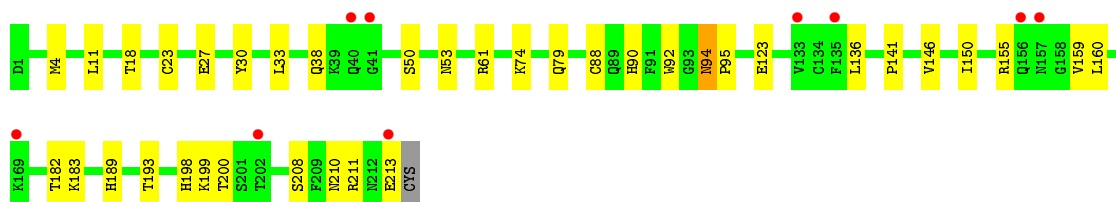
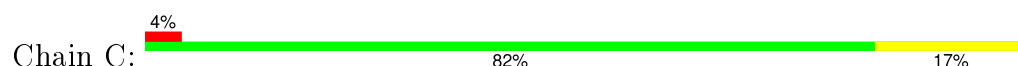
- Molecule 1: Capsid protein



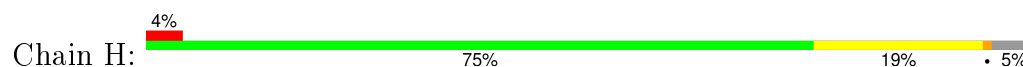
- Molecule 2: Monoclonal Antibody, Light Chain

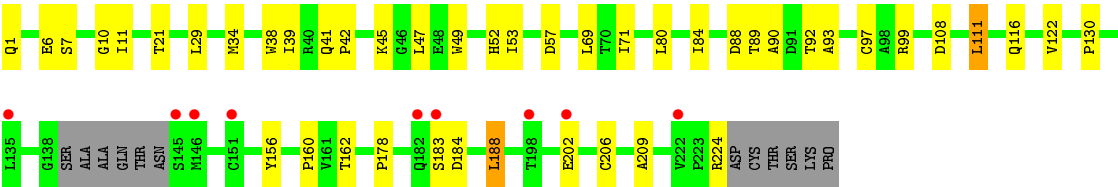


- Molecule 2: Monoclonal Antibody, Light Chain

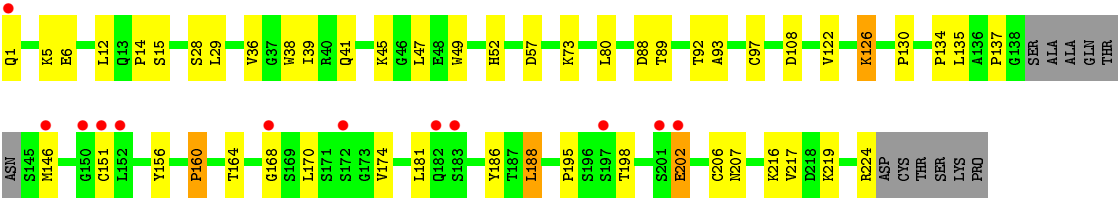


- Molecule 3: Monoclonal Antibody, Heavy Chain





● Molecule 3: Monoclonal Antibody, Heavy Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.48Å 95.20Å 108.31Å 90.00° 107.31° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 25.09 – 1.90	Depositor EDS
% Data completeness (in resolution range)	87.9 (20.00-1.90) 95.9 (25.09-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 1.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.189 , 0.217 0.199 , 0.226	Depositor DCC
R_{free} test set	10835 reflections (9.98%)	DCC
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.5	EDS
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 112736 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9533	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.57% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.34	0/1122	0.65	1/1540 (0.1%)
1	B	0.33	0/1116	0.65	1/1532 (0.1%)
2	C	0.30	0/1695	0.61	0/2302
2	L	0.31	0/1695	0.62	0/2302
3	D	0.35	1/1680 (0.1%)	0.66	0/2299
3	H	0.36	1/1680 (0.1%)	0.67	1/2299 (0.0%)
All	All	0.33	2/8988 (0.0%)	0.64	3/12274 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	202	GLU	CD-OE2	7.05	1.33	1.25
3	D	202	GLU	CD-OE2	7.05	1.33	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	493	TYR	N-CA-C	-5.51	96.13	111.00
1	A	493	TYR	N-CA-C	-5.35	96.56	111.00
3	H	111	LEU	N-CA-C	-5.18	97.02	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1096	0	1085	5	0
1	B	1090	0	1080	10	0
2	C	1656	0	1576	30	0
2	L	1656	0	1576	49	0
3	D	1637	0	1630	49	0
3	H	1637	0	1630	40	0
4	A	118	0	0	0	0
4	B	107	0	0	1	0
4	C	133	0	0	2	0
4	D	129	0	0	1	0
4	H	140	0	0	0	0
4	L	134	0	0	0	0
All	All	9533	0	8577	171	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 10.

The worst 5 of 171 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)
2:L:181:LEU:HD21	2:L:185:GLU:HB3	1.23	1.17
3:D:126:LYS:HE2	3:D:126:LYS:H	1.13	1.10
2:L:210:ASN:HB2	2:L:213:GLU:HG3	1.44	0.97
1:B:524:ARG:HE	1:B:604:PRO:HB2	1.31	0.95
2:L:181:LEU:HD21	2:L:185:GLU:CB	1.96	0.94

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	144/146 (99%)	138 (96%)	5 (4%)	1 (1%)	26 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	143/146 (98%)	137 (96%)	5 (4%)	1 (1%)	26	14
2	C	211/214 (99%)	209 (99%)	2 (1%)	0	100	100
2	L	211/214 (99%)	208 (99%)	3 (1%)	0	100	100
3	D	214/230 (93%)	205 (96%)	9 (4%)	0	100	100
3	H	214/230 (93%)	206 (96%)	8 (4%)	0	100	100
All	All	1137/1180 (96%)	1103 (97%)	32 (3%)	2 (0%)	52	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	490	GLY
1	A	490	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	119/119 (100%)	118 (99%)	1 (1%)	86	86
1	B	118/119 (99%)	117 (99%)	1 (1%)	86	86
2	C	188/189 (100%)	183 (97%)	5 (3%)	52	43
2	L	188/189 (100%)	182 (97%)	6 (3%)	46	35
3	D	189/199 (95%)	183 (97%)	6 (3%)	46	35
3	H	189/199 (95%)	184 (97%)	5 (3%)	54	45
All	All	991/1014 (98%)	967 (98%)	24 (2%)	57	49

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	160	PRO
2	C	11	LEU
3	D	206	CYS
3	H	188	LEU

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Mol	Chain	Res	Type
3	H	206	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	210	ASN
2	C	3	GLN
2	C	210	ASN
3	H	52	HIS
3	H	116	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 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	146/146 (100%)	-0.21	3 (2%) 67 70	14, 19, 27, 40	0
1	B	145/146 (99%)	-0.09	2 (1%) 78 80	14, 21, 32, 45	0
2	C	213/214 (99%)	0.13	9 (4%) 40 44	15, 26, 39, 49	0
2	L	213/214 (99%)	0.20	12 (5%) 28 31	15, 24, 39, 57	0
3	D	218/230 (94%)	0.26	12 (5%) 29 32	17, 27, 45, 54	0
3	H	218/230 (94%)	0.15	9 (4%) 41 45	15, 25, 43, 50	0
All	All	1153/1180 (97%)	0.10	47 (4%) 41 45	14, 24, 40, 57	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	202	GLU	4.0
3	D	183	SER	3.8
1	B	524	ARG	3.4
3	H	183	SER	3.3
3	D	201	SER	3.3

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.