



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:17 PM GMT

PDB ID : 4EE2
Title : Crystal Structure of Anthrax Protective Antigen K446M Mutant to 1.91-A
Resolution
Authors : Kintzer, A.F.; Krantz, B.A.
Deposited on : 2012-03-28
Resolution : 1.91 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
<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

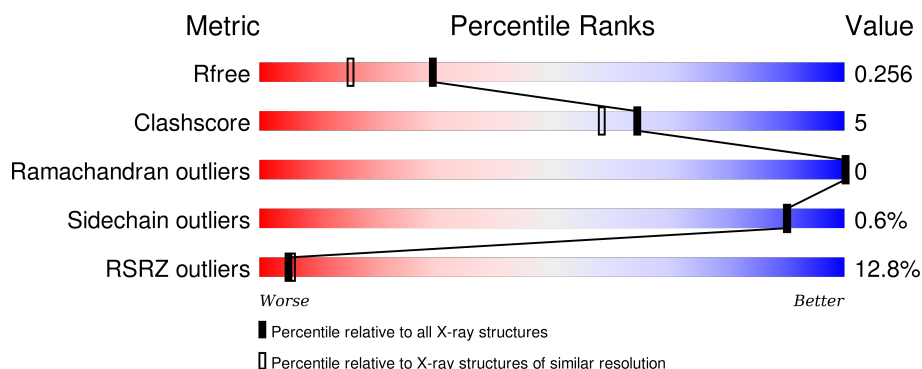
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 1.91 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	5832 (1.94-1.90)
Clashscore	102246	6540 (1.94-1.90)
Ramachandran outliers	100387	6464 (1.94-1.90)
Sidechain outliers	100360	6465 (1.94-1.90)
RSRZ outliers	91569	5846 (1.94-1.90)

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	736	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5709 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 Protective antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	701	Total	C	N	O	S	0	0	0
			5560	3474	955	1122	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	INITIATING METHIONINE	UNP P13423
A	446	MET	LYS	ENGINEERED MUTATION	UNP P13423

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

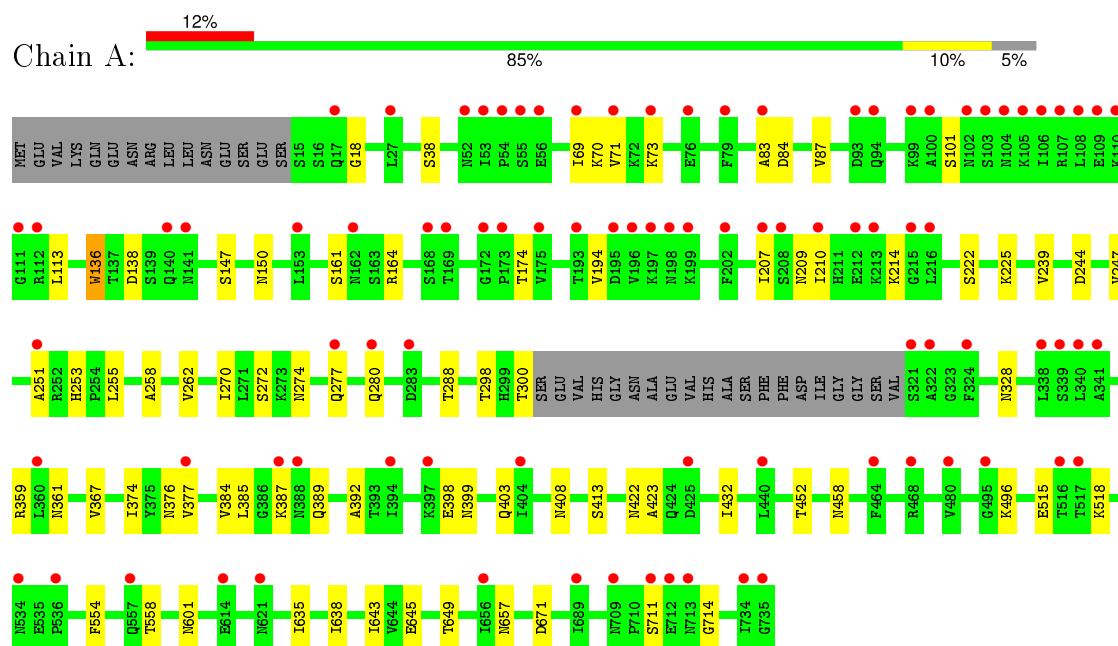
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	147	Total	O	0	0
			147	147		

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 ($\text{RSRZ} > 2$). 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: Protective antigen



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.22Å 93.51Å 116.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.69 – 1.91 40.68 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.69-1.91) 92.8 (40.68-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 1.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.229 , 0.265 0.225 , 0.256	Depositor DCC
R_{free} test set	1876 reflections (3.27%)	DCC
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 61083 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5709	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.35	0/5658	0.54	0/7668

There are no bond length outliers.

There are no bond angle outliers.

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	5560	0	5476	56	0
2	A	2	0	0	0	0
3	A	147	0	0	4	0
All	All	5709	0	5476	56	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 5.

All (56) 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:384:VAL:HG13	1:A:389:GLN:O	1.51	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:HIS:HD2	1:A:255:LEU:H	1.18	0.88
1:A:272:SER:HB3	1:A:288:THR:HG22	1.55	0.86
1:A:403:GLN:HE22	1:A:413:SER:H	1.34	0.76
1:A:385:LEU:O	1:A:389:GLN:HB2	1.88	0.73
1:A:384:VAL:CG1	1:A:389:GLN:O	2.39	0.61
1:A:194:VAL:HG21	1:A:239:VAL:HB	1.83	0.59
1:A:374:ILE:HG21	1:A:377:VAL:O	2.04	0.58
1:A:147:SER:OG	1:A:150:ASN:ND2	2.38	0.56
1:A:84:ASP:OD2	1:A:101:SER:HA	2.04	0.56
1:A:253:HIS:CD2	1:A:255:LEU:H	2.10	0.56
1:A:69:ILE:HD11	1:A:136:TRP:CZ3	2.42	0.55
1:A:161:SER:HB3	1:A:164:ARG:HB2	1.89	0.55
1:A:376:ASN:ND2	1:A:458:ASN:OD1	2.33	0.54
1:A:174:THR:HG23	1:A:174:THR:O	2.07	0.53
1:A:274:ASN:HD22	1:A:359:ARG:HH11	1.56	0.53
1:A:274:ASN:ND2	1:A:359:ARG:HH11	2.08	0.52
1:A:643:ILE:HA	1:A:657:ASN:HD21	1.75	0.51
1:A:253:HIS:HE1	3:A:990:HOH:O	1.91	0.51
1:A:635:ILE:O	1:A:638:ILE:HG13	2.10	0.51
1:A:422:ASN:OD1	3:A:1012:HOH:O	2.20	0.50
1:A:711:SER:O	1:A:714:GLY:N	2.44	0.50
1:A:671:ASP:N	1:A:671:ASP:OD1	2.44	0.50
1:A:398:GLU:O	1:A:399:ASN:HB2	2.11	0.49
1:A:83:ALA:O	1:A:87:VAL:HG23	2.13	0.49
1:A:277:GLN:O	1:A:280:GLN:NE2	2.46	0.49
1:A:515:GLU:OE1	1:A:518:LYS:HE2	2.12	0.48
1:A:222:SER:HB2	1:A:518:LYS:HG2	1.95	0.48
1:A:225:LYS:HD3	1:A:518:LYS:HD3	1.95	0.48
1:A:274:ASN:HD21	1:A:359:ARG:HB3	1.78	0.47
1:A:270:ILE:CG2	1:A:361:ASN:HB3	2.45	0.47
1:A:18:GLY:HA3	1:A:38:SER:O	2.15	0.46
1:A:422:ASN:HB2	3:A:1011:HOH:O	2.14	0.46
1:A:374:ILE:CG2	1:A:377:VAL:O	2.64	0.46
1:A:270:ILE:HG23	1:A:361:ASN:HB3	1.98	0.46
1:A:328:ASN:HB2	1:A:452:THR:O	2.16	0.45
1:A:210:ILE:O	1:A:214:LYS:HG2	2.18	0.44
1:A:392:ALA:HB2	1:A:432:ILE:HG23	2.00	0.44
1:A:515:GLU:OE1	1:A:518:LYS:NZ	2.50	0.43
1:A:423:ALA:O	3:A:1012:HOH:O	2.21	0.43
1:A:70:LYS:HB3	1:A:113:LEU:HD23	2.01	0.43
1:A:209:ASN:OD1	1:A:210:ILE:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ASN:HD21	1:A:496:LYS:NZ	2.16	0.42
1:A:71:VAL:HG22	1:A:73:LYS:H	1.84	0.42
1:A:138:ASP:OD1	1:A:138:ASP:C	2.57	0.42
1:A:403:GLN:NE2	1:A:413:SER:H	2.10	0.42
1:A:174:THR:CG2	1:A:174:THR:O	2.68	0.42
1:A:207:ILE:HG22	1:A:209:ASN:OD1	2.20	0.41
1:A:244:ASP:HB3	1:A:247:VAL:HG23	2.03	0.41
1:A:251:ALA:HB1	1:A:258:ALA:HB2	2.01	0.41
1:A:225:LYS:CD	1:A:518:LYS:HD3	2.50	0.41
1:A:387:LYS:HB2	1:A:387:LYS:HE2	1.74	0.41
1:A:298:THR:HB	1:A:601:ASN:HB3	2.02	0.41
1:A:515:GLU:OE1	1:A:518:LYS:CE	2.69	0.41
1:A:262:VAL:HA	1:A:367:VAL:O	2.21	0.41
1:A:554:PHE:HB3	1:A:558:THR:HB	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	697/736 (95%)	685 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	630/662 (95%)	626 (99%)	4 (1%)	90	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	TRP
1	A	300	THR
1	A	645	GLU
1	A	649	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	158	GLN
1	A	180	ASN
1	A	246	ASN
1	A	253	HIS
1	A	274	ASN
1	A	280	GLN
1	A	400	GLN
1	A	403	GLN
1	A	408	ASN
1	A	437	ASN
1	A	541	GLN
1	A	560	GLN
1	A	601	ASN
1	A	670	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	701/736 (95%)	0.87	90 (12%) 5 5	26, 41, 70, 90	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	SER	7.0
1	A	198	ASN	6.8
1	A	199	LYS	6.3
1	A	324	PHE	5.7
1	A	93	ASP	5.2
1	A	210	ILE	5.1
1	A	53	ILE	4.8
1	A	713	ASN	4.7
1	A	71	VAL	4.6
1	A	339	SER	4.6
1	A	341	ALA	4.5
1	A	79	PHE	4.4
1	A	172	GLY	4.3
1	A	56	GLU	4.3
1	A	712	GLU	4.3
1	A	102	ASN	4.1
1	A	213	LYS	4.1
1	A	735	GLY	3.8
1	A	207	ILE	3.5
1	A	27	LEU	3.5
1	A	212	GLU	3.5
1	A	338	LEU	3.5
1	A	107	ARG	3.5
1	A	215	GLY	3.4
1	A	197	LYS	3.4
1	A	321	SER	3.4
1	A	340	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	99	LYS	3.3
1	A	104	ASN	3.3
1	A	173	PRO	3.2
1	A	112	ARG	3.2
1	A	162	ASN	3.1
1	A	711	SER	3.1
1	A	54	PRO	3.0
1	A	536	PRO	3.0
1	A	377	VAL	3.0
1	A	196	VAL	2.9
1	A	397	LYS	2.9
1	A	175	VAL	2.9
1	A	69	ILE	2.9
1	A	169	THR	2.8
1	A	404	ILE	2.7
1	A	517	THR	2.7
1	A	106	ILE	2.7
1	A	468	ARG	2.7
1	A	464	PHE	2.7
1	A	195	ASP	2.6
1	A	83	ALA	2.6
1	A	322	ALA	2.6
1	A	52	ASN	2.6
1	A	734	ILE	2.6
1	A	656	ILE	2.6
1	A	557	GLN	2.5
1	A	76	GLU	2.5
1	A	109	GLU	2.5
1	A	140	GLN	2.5
1	A	100	ALA	2.5
1	A	425	ASP	2.4
1	A	108	LEU	2.4
1	A	277	GLN	2.4
1	A	388	ASN	2.3
1	A	94	GLN	2.3
1	A	689	ILE	2.3
1	A	141	ASN	2.3
1	A	111	GLY	2.3
1	A	105	LYS	2.3
1	A	73	LYS	2.2
1	A	283	ASP	2.2
1	A	103	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	709	ASN	2.2
1	A	440	LEU	2.2
1	A	614	GLU	2.1
1	A	495	GLY	2.1
1	A	55	SER	2.1
1	A	168	SER	2.1
1	A	534	ASN	2.1
1	A	216	LEU	2.1
1	A	110	LYS	2.1
1	A	387	LYS	2.1
1	A	621	ASN	2.1
1	A	280	GLN	2.1
1	A	394	ILE	2.1
1	A	153	LEU	2.1
1	A	193	THR	2.1
1	A	516	THR	2.1
1	A	202	PHE	2.1
1	A	251	ALA	2.1
1	A	360	LEU	2.1
1	A	480	VAL	2.1
1	A	17	GLN	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CA	A	801	1/1	0.98	0.14	-0.60	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	A	800	1/1	0.98	0.14	-0.65	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.