

Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 01:25 AM EDT

PDB ID : 5JXA

Title : Crystal structure of ligand-free VRC03 antigen-binding fragment. Authors : Zhou, T.; Moquin, S.; Joyce, M.G.; Mascola, J.R.; Kwong, P.D.

Deposited on : 2016-05-12

Resolution : 1.60 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 (i) 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.35.1

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

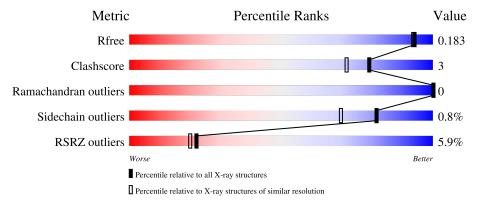
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 1.60 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 <=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	Н	235	91%	6% ••
2	L	209	96%	•

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CU	L	302	_	-	_	X



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7379 atoms, of which 3315 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.

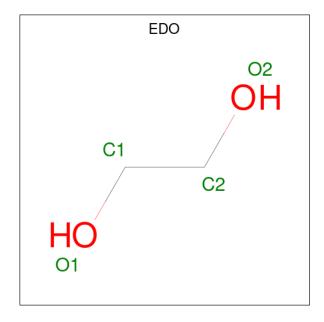
• Molecule 1 is a protein called VRC03 Heavy chain.

M	ol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
	l	Н	231	Total 3501	C 1133	H 1721	N 300	O 338	S 9	0	3	0

• Molecule 2 is a protein called VRC03 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	L	209	Total 3204	C 1023	H 1576	N 277	O 322	S 6	0	0	0

• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



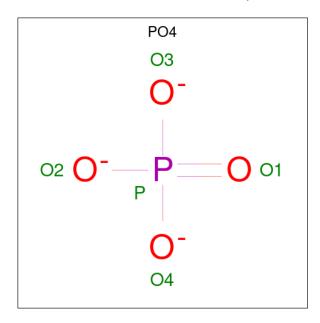
\mathbf{M}	ol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	}	Н	1	Total 10			0	0
3	}	Н	1	Total 10		H 6	0	0



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M	Iol	Chain	Residues	A	tor	ns		ZeroOcc	AltConf
	3	L	1	Total 10	C 2	H 6	O 2	0	0

• Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Н	1	Total O I	P 0	0
4	L	1	Total O I	P 1 0	0
4	L	1	Total O I	P 1 0	0

• Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Н	1	Total Cu 1 1	0	0
5	L	2	Total Cu 2 2	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Н	295	Total O 295 295	0	0



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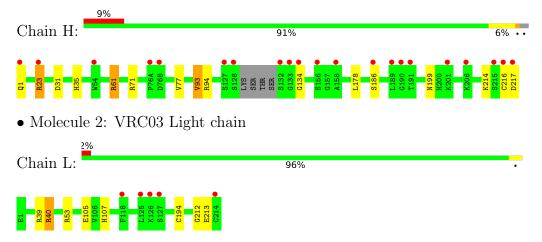
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	331	Total O 331 331	0	0



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: VRC03 Heavy chain





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	162.19Å 50.80Å 71.76Å	Donositor
a, b, c, α , β , γ	90.00° 108.15° 90.00°	Depositor
Resolution (Å)	22.95 - 1.60	Depositor
rtesolution (A)	22.95 - 1.60	EDS
% Data completeness	88.9 (22.95-1.60)	Depositor
(in resolution range)	88.9 (22.95-1.60)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.84 (at 1.60Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
D D.	0.160 , 0.180	Depositor
R, R_{free}	0.165 , 0.183	DCC
R_{free} test set	3243 reflections $(4.97%)$	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.681	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.39, 47.4	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7379	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.23% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



 $^{^1 {\}rm Intensities}$ estimated from amplitudes.

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: CU, PO4, EDO

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).

Mal	Chain		nd lengths	Bond angles		
Mol Chain		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	Н	0.70	8/1840 (0.4%)	0.68	3/2510 (0.1%)	
2	L	0.67	7/1663 (0.4%)	0.67	$1/2252 \ (0.0\%)$	
All	All	0.69	15/3503~(0.4%)	0.68	4/4762 (0.1%)	

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$Ideal(\AA)$
1	Н	61	ARG	CZ-NH1	7.21	1.42	1.33
1	Н	23[A]	ARG	CZ-NH1	7.17	1.42	1.33
1	Н	23[B]	ARG	CZ-NH1	7.17	1.42	1.33
1	Н	23[A]	ARG	CZ-NH2	7.00	1.42	1.33
1	Н	23[B]	ARG	CZ-NH2	7.00	1.42	1.33
1	Н	61	ARG	CZ-NH2	6.94	1.42	1.33
2	L	40	ARG	CZ-NH2	6.88	1.42	1.33
2	L	40	ARG	CZ-NH1	6.71	1.41	1.33
2	L	53	ARG	CZ-NH1	6.68	1.41	1.33
2	L	39	ARG	CZ-NH2	6.34	1.41	1.33
2	L	39	ARG	CZ-NH1	6.34	1.41	1.33
1	Н	94	ARG	CZ-NH1	6.21	1.41	1.33
2	L	53	ARG	CZ-NH2	6.07	1.41	1.33
2	L	194	CYS	CB-SG	-6.01	1.72	1.82
1	Н	94	ARG	CZ-NH2	5.90	1.40	1.33

All (4) bond angle outliers are listed below:

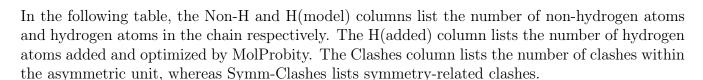
Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^o)$
1	Н	23[A]	ARG	CA-C-O	5.89	132.48	120.10
1	Н	23[B]	ARG	CA-C-O	5.89	132.48	120.10
2	L	39	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	Н	94	ARG	NE-CZ-NH1	-5.62	117.49	120.30



There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Н	1780	1721	1728	13	0
2	L	1628	1576	1576	5	0
3	Н	8	12	12	0	0
3	L	4	6	6	2	0
4	Н	5	0	0	1	0
4	L	10	0	0	0	0
5	Н	1	0	0	0	0
5	L	2	0	0	0	0
6	Н	295	0	0	6	2
6	L	331	0	0	4	0
All	All	4064	3315	3322	19	2

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 3.

All (19) 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:H:23[B]:ARG:NH1	6:H:401:HOH:O	1.95	0.97
1:H:1:GLN:N	6:H:405:HOH:O	2.14	0.78
1:H:199:ASN:OD1	6:H:402:HOH:O	2.01	0.78
1:H:134:GLY:O	1:H:186:SER:N	2.13	0.72
2:L:213:GLU:OE1	6:L:402:HOH:O	2.08	0.71
1:H:31:ASP:OD2	6:H:403:HOH:O	2.08	0.70
4:H:303:PO4:O1	6:H:404:HOH:O	2.14	0.65
1:H:216:CYS:SG	1:H:217:ASP:N	2.77	0.58
1:H:61:ARG:HH21	1:H:61:ARG:HG2	1.74	0.52
1:H:61:ARG:HD2	6:L:526:HOH:O	2.10	0.51
1:H:214:LYS:O	6:H:406:HOH:O	2.20	0.51
2:L:40:ARG:NH2	6:L:401:HOH:O	2.05	0.49
2:L:212:GLY:H	3:L:303:EDO:C1	2.26	0.47



Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	Clash overlap (Å)
2:L:212:GLY:H	3:L:303:EDO:H11	1.82	0.45
2:L:107:HIS:NE2	6:L:403:HOH:O	2.19	0.44
1:H:35:HIS:HB2	1:H:93:VAL:HG23	2.00	0.43
1:H:61:ARG:HG2	1:H:61:ARG:NH2	2.32	0.43
1:H:23[B]:ARG:HG2	1:H:77:VAL:HG22	2.01	0.41
1:H:178:LEU:C	1:H:178:LEU:HD12	2.42	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
6:H:401:HOH:O	6:H:512:HOH:O[2_555]	2.16	0.04
6:H:542:HOH:O	6:H:587:HOH:O[2_555]	2.18	0.02

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	Н	230/235~(98%)	224 (97%)	6 (3%)	0	100	100	
2	L	207/209 (99%)	203 (98%)	4 (2%)	0	100	100	
All	All	437/444 (98%)	427 (98%)	10 (2%)	0	100	100	

There are no Ramachandran outliers to report.

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	Rotameric Outliers		Percentiles		
1	Н	200/201 (100%)	198 (99%)	2 (1%)	76	61		
2	L	182/182 (100%)	181 (100%)	1 (0%)	88	80		
All	All	382/383 (100%)	379 (99%)	3 (1%)	81	70		

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Н	71	ARG
1	Н	93	VAL
2	L	105	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Trino	Chain	ain Res Link		В	ond leng	gths	В	ond ang	gles
MIOI	Type	$ m pe \mid Chain \mid Res$			Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	EDO	L	303	-	3,3,3	0.45	0	2,2,2	0.34	0
4	PO4	L	305	-	4,4,4	0.87	0	6,6,6	0.52	0
3	EDO	Н	302	-	3,3,3	0.55	0	2,2,2	0.23	0
3	EDO	Н	301	-	3,3,3	0.44	0	2,2,2	0.30	0
4	PO4	L	304	-	4,4,4	0.78	0	6,6,6	0.46	0
4	PO4	Н	303	-	4,4,4	1.00	0	6,6,6	0.88	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	Н	302	-	-	0/1/1/1	-
3	EDO	L	303	-	-	0/1/1/1	-
3	EDO	Н	301	-	-	0/1/1/1	-

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.

2 monomers are involved in 3 short contacts:

Mo	l Ch	ain	Res	Type	Clashes	Symm-Clashes
3		_	303	EDO	2	0
4	I	I	303	PO4	1	0

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, 95^{th} 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	$\langle { m RSRZ} \rangle$	$\# \mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	Н	$231/235\ (98\%)$	0.14	21 (9%) 9 8	15, 25, 56, 105	0
2	L	209/209~(100%)	-0.21	5 (2%) 59 56	12, 20, 41, 70	0
All	All	440/444~(99%)	-0.03	26 (5%) 22 20	12, 23, 51, 105	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Н	216	CYS	8.6
1	Н	133	GLY	7.6
1	Н	215	SER	6.8
1	Н	132	SER	6.4
1	Н	191	THR	6.2
1	Н	217	ASP	6.1
1	Н	134	GLY	5.6
2	L	214	CYS	5.6
1	Н	54	TRP	3.6
2	L	126	LYS	3.4
	Н	190	GLY	3.3
1	Н	128	SER	3.2
1	Н	76(A)	PRO	3.0
1	Н	127	SER	2.6
2	L	127	SER	2.4
2	L	125	LEU	2.3
1	Н	186	SER	2.3
1	Н	1	GLN	2.3
1	Н	156	SER	2.3
1	Н	158	ALA	2.2
1	Н	189	LEU	2.2
1	Н	206	LYS	2.1
2	L	118	PHE	2.1
1	Н	23[A]	ARG	2.1



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Mol	Chain	Res	Type	RSRZ
1	Н	76(B)	ASP	2.1
1	Н	201	LYS	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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
5	CU	L	302	1/1	0.64	0.54	161,161,161,161	0
3	EDO	L	303	4/4	0.81	0.20	36,43,52,56	0
4	PO4	Н	303	5/5	0.94	0.19	25,41,45,54	0
4	PO4	L	305	5/5	0.94	0.22	62,68,70,71	0
3	EDO	Н	302	4/4	0.94	0.08	23,28,34,34	0
3	EDO	Н	301	4/4	0.95	0.07	18,23,33,33	0
4	PO4	L	304	5/5	0.95	0.18	52,55,57,58	0
5	CU	Н	304	1/1	0.97	0.10	74,74,74,74	0
5	CU	L	301	1/1	1.00	0.03	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.

