



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2017 – 04:24 PM EDT

PDB ID : 3V4O
Title : Human MALT1 (caspase domain) in complex with an irreversible peptidic inhibitor
Authors : Renatus, M.; Wiesmann, C.
Deposited on : unknown
Resolution : 2.10 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

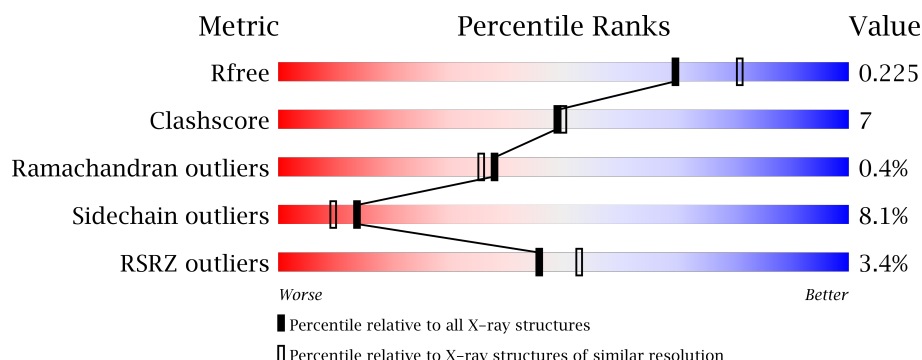
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	245	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>• •</div> </div> </div>
2	B	6	<div> <div>50%</div> <div>17%</div> <div>33%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2064 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 Mucosa-associated lymphoid tissue lymphoma translocation protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	1	0
			1867	1194	308	353	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	GLY	-	EXPRESSION TAG	UNP Q9UDY8
A	326	PRO	-	EXPRESSION TAG	UNP Q9UDY8
A	327	GLY	-	EXPRESSION TAG	UNP Q9UDY8
A	328	SER	-	EXPRESSION TAG	UNP Q9UDY8

- Molecule 2 is a protein called MALT1 Inhibitor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	0	0	1
			47	31	10	6			

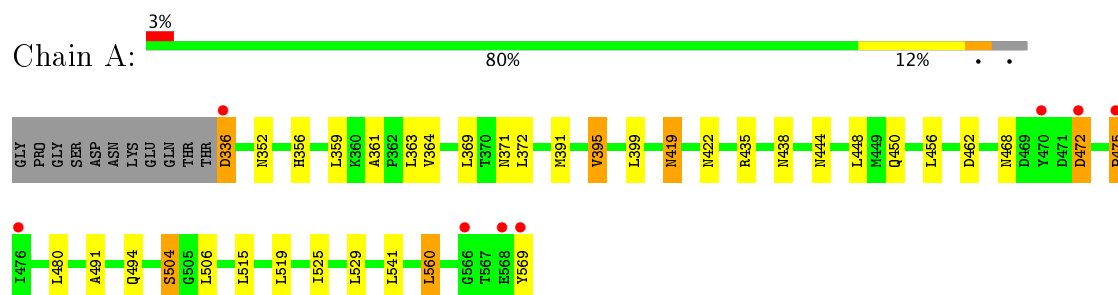
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	149	Total	O	0	0
			149	149		
3	B	1	Total	O	0	0
			1	1		

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 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: Mucosa-associated lymphoid tissue lymphoma translocation protein 1



- Molecule 2: MALT1 Inhibitor



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	77.50 Å 77.50 Å 180.49 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	53.86 – 2.10 44.80 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (53.86-2.10) 99.7 (44.80-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.176 , 0.228 0.177 , 0.225	Depositor DCC
R_{free} test set	973 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2064	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PHQ, CF0

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	0/1901	0.75	0/2567
2	B	1.14	0/36	1.92	2/47 (4.3%)
All	All	0.67	0/1937	0.79	2/2614 (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
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	3	ARG	NE-CZ-NH2	-6.89	116.86	120.30
2	B	5	ARG	NE-CZ-NH1	-5.24	117.68	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	3	ARG	Sidechain

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	1867	0	1889	26	0
2	B	47	0	48	3	0
3	A	149	0	0	8	1
3	B	1	0	0	0	0
All	All	2064	0	1937	26	1

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 7.

All (26) 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:419:ASN:HD21	1:A:468:ASN:H	1.04	1.02
1:A:450:GLN:NE2	3:A:687:HOH:O	2.16	0.78
1:A:504:SER:OG	3:A:692:HOH:O	2.03	0.77
1:A:435:ARG:H	1:A:438:ASN:HD22	1.34	0.74
1:A:352:ASN:HB2	3:A:626:HOH:O	1.94	0.68
1:A:422:ASN:ND2	1:A:475:PRO:HB3	2.12	0.64
1:A:419:ASN:ND2	1:A:468:ASN:H	1.87	0.64
1:A:435:ARG:HH12	1:A:472:ASP:HB2	1.65	0.61
1:A:422:ASN:HD21	1:A:475:PRO:HB3	1.67	0.60
1:A:419:ASN:HD21	1:A:468:ASN:N	1.88	0.60
1:A:435:ARG:H	1:A:438:ASN:ND2	1.98	0.59
1:A:356:HIS:HD2	3:A:730:HOH:O	1.87	0.57
1:A:450:GLN:HE22	1:A:480:LEU:HB3	1.76	0.50
1:A:435:ARG:NH1	1:A:472:ASP:HB2	2.27	0.50
1:A:541:LEU:HD13	2:B:2:VAL:HG12	1.94	0.48
1:A:336:ASP:CG	1:A:336:ASP:O	2.54	0.46
1:A:444:ASN:HB3	3:A:719:HOH:O	2.14	0.46
1:A:361:ALA:HB3	2:B:5:ARG:HH11	1.81	0.46
1:A:494:GLN:NE2	3:A:634:HOH:O	2.49	0.46
1:A:359:LEU:HD13	2:B:5:ARG:HG2	1.99	0.44
1:A:444:ASN:CB	3:A:719:HOH:O	2.66	0.43
1:A:391:MET:O	1:A:395:VAL:HG13	2.20	0.42
1:A:525:ILE:HD13	1:A:560:LEU:HD22	2.02	0.42
1:A:462:ASP:HA	1:A:491:ALA:HB2	2.01	0.41
1:A:504:SER:HB2	3:A:649:HOH:O	2.20	0.41
1:A:515:LEU:HD11	1:A:519:LEU:HD13	2.03	0.41

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
3:A:714:HOH:O	3:A:714:HOH:O[12_565]	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	A	233/245 (95%)	225 (97%)	7 (3%)	1 (0%)	38	35
2	B	2/6 (33%)	2 (100%)	0	0	100	100
All	All	235/251 (94%)	227 (97%)	7 (3%)	1 (0%)	38	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	475	PRO

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	206/214 (96%)	188 (91%)	18 (9%)	12	8
2	B	4/4 (100%)	4 (100%)	0	100	100
All	All	210/218 (96%)	192 (91%)	18 (9%)	14	8

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	336	ASP
1	A	363	LEU
1	A	364[A]	VAL
1	A	364[B]	VAL
1	A	369	LEU
1	A	371	ASN
1	A	372	LEU
1	A	395	VAL
1	A	399	LEU
1	A	419	ASN
1	A	448	LEU
1	A	456	LEU
1	A	472	ASP
1	A	504	SER
1	A	506	LEU
1	A	529	LEU
1	A	560	LEU
1	A	569	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	HIS
1	A	419	ASN
1	A	422	ASN
1	A	438	ASN
1	A	444	ASN
1	A	450	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 [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	234/245 (95%)	-0.34	8 (3%) 46 53	13, 23, 48, 67	0
2	B	4/6 (66%)	-0.52	0 100 100	21, 22, 27, 29	0
All	All	238/251 (94%)	-0.35	8 (3%) 46 53	13, 23, 48, 67	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	569	TYR	7.8
1	A	568	GLU	5.3
1	A	336	ASP	4.0
1	A	476	ILE	3.0
1	A	566	GLY	2.8
1	A	470	TYR	2.8
1	A	475	PRO	2.0
1	A	472	ASP	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.