Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 12:58 PM EST

PDB ID	:	3V4L
Title	:	Mouse MALT1(caspase-IG3 domains) in complex with a irreversible peptidic inhibitor
Authors	:	Renatus, M.; Wiesmann, C.
Deposited on	:	2011-12-15
Resolution	:	3.15 Å(reported)

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

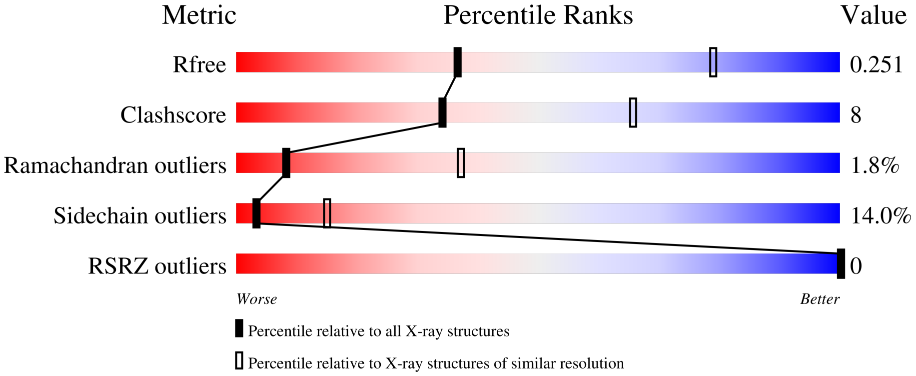
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.15 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}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	A	396	
2	B	6	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3101 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 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	386	3054	1957	502	572	23	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	GLY	-	expression tag	UNP Q2TBA3
A	335	PRO	-	expression tag	UNP Q2TBA3
A	336	GLY	-	expression tag	UNP Q2TBA3
A	337	SER	-	expression tag	UNP Q2TBA3

- Molecule 2 is a protein called MALT1 Inhibitor.

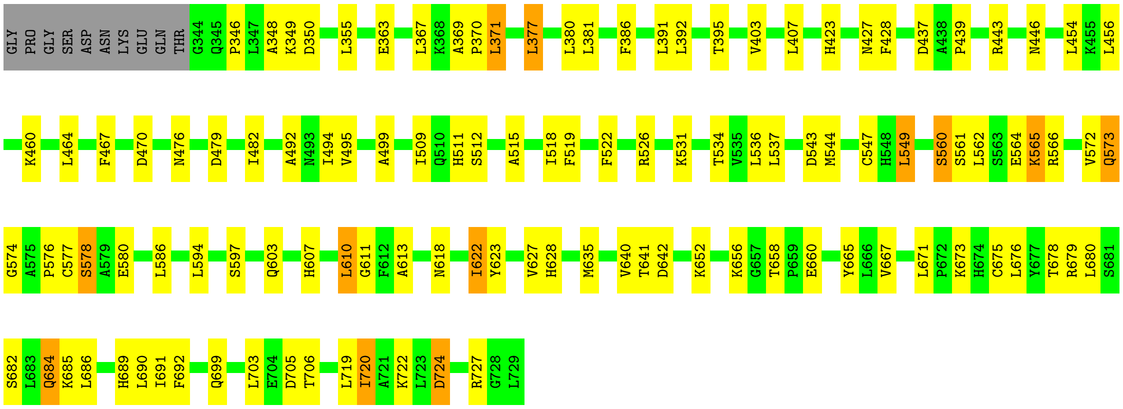
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	6	47	31	10	6	0	0	1

3 Residue-property plots ⓘ

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.

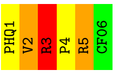
- Molecule 1: Mucosa-associated lymphoid tissue lymphoma translocation protein 1 homolog

Chain A:



- Molecule 2: MALT1 Inhibitor

Chain B:



4 Data and refinement statistics

Property	**Value**	**Source**
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α, β, γ	150.86Å 150.86Å 91.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.29 – 3.15 58.29 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.5 (58.29-3.15) 98.5 (58.29-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 3.13Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.178 , 0.231 0.188 , 0.251	Depositor DCC
R_{free} test set	548 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	69.2	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3101	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.52	0/3118	0.77	0/4220
2	B	1.27	0/36	1.80	1/47 (2.1%)
All	All	0.53	0/3154	0.79	1/4267 (0.0%)

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	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	VAL	CB-CA-C	5.37	121.60	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	3	ARG	Sidechain
2	B	5	ARG	Sidechain

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	3054	0	3078	48	0
2	B	47	0	48	8	0
All	All	3101	0	3126	52	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 8.

All (52) 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:427:ASN:HD21	1:A:476:ASN:H	1.19	0.87
1:A:682:SER:HB2	1:A:685:LYS:HD2	1.73	0.70
2:B:1:PHQ:H21	2:B:3:ARG:HD3	1.84	0.59
1:A:611:GLY:HA3	1:A:623:TYR:CE1	2.39	0.56
1:A:392:LEU:H	1:A:618:ASN:HD22	1.55	0.55
2:B:1:PHQ:H21	2:B:3:ARG:CD	2.36	0.55
1:A:476:ASN:HD22	1:A:479:ASP:HB2	1.71	0.55
1:A:367:LEU:HD13	2:B:5:ARG:HG2	1.90	0.53
1:A:427:ASN:HD21	1:A:476:ASN:N	1.98	0.53
1:A:443:ARG:H	1:A:446:ASN:HD22	1.57	0.53
1:A:367:LEU:HD21	1:A:423:HIS:CE1	2.43	0.53
1:A:635:MET:HB2	1:A:699:GLN:HB3	1.91	0.52
1:A:522:PHE:CZ	1:A:547:CYS:HB2	2.45	0.51
1:A:509:ILE:HG22	2:B:2:VAL:HG12	1.93	0.50
1:A:509:ILE:HG22	2:B:2:VAL:CG1	2.42	0.50
1:A:618:ASN:OD1	1:A:684:GLN:HG3	2.11	0.50
1:A:724:ASP:HB3	1:A:727:ARG:HB3	1.94	0.50
1:A:371:LEU:HD21	1:A:665:TYR:HB2	1.94	0.49
1:A:391:LEU:HD21	1:A:720:ILE:HD13	1.93	0.49
1:A:427:ASN:ND2	1:A:476:ASN:H	1.99	0.49
1:A:355:LEU:HD21	1:A:377:LEU:HB3	1.95	0.48
1:A:564:GLU:O	1:A:566:ARG:N	2.41	0.47
1:A:363:GLU:HG3	1:A:439:PRO:HA	1.96	0.47
1:A:346:PRO:HG2	1:A:565:LYS:O	2.15	0.47
1:A:470:ASP:HA	1:A:499:ALA:HB2	1.96	0.46
1:A:348:ALA:O	1:A:572:VAL:HA	2.15	0.46
1:A:428:PHE:CD2	1:A:482:ILE:HG12	2.51	0.46
1:A:381:LEU:O	1:A:386:PHE:HB2	2.15	0.46
1:A:684:GLN:HE21	1:A:685:LYS:N	2.14	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:THR:HG22	1:A:437:ASP:HB3	1.99	0.45
1:A:549:LEU:HD22	2:B:2:VAL:HG11	1.98	0.45
1:A:454:LEU:HD13	1:A:467:PHE:HE1	1.82	0.45
1:A:454:LEU:HD21	1:A:494:ILE:HD13	1.98	0.45
1:A:642:ASP:O	1:A:692:PHE:HA	2.17	0.45
1:A:594:LEU:HD13	1:A:719:LEU:HD21	1.97	0.44
1:A:576:PRO:O	1:A:578:SER:N	2.43	0.44
1:A:613:ALA:HB2	1:A:671:LEU:HD21	1.99	0.44
1:A:623:TYR:HA	1:A:676:LEU:O	2.18	0.44
2:B:1:PHQ:C2	2:B:3:ARG:HD3	2.48	0.43
2:B:3:ARG:CB	2:B:4:PRO:HD2	2.48	0.43
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.89	0.43
1:A:610:LEU:HD23	1:A:610:LEU:HA	1.88	0.43
1:A:613:ALA:CB	1:A:671:LEU:HD21	2.49	0.42
1:A:454:LEU:HD13	1:A:467:PHE:CE1	2.55	0.42
1:A:607:HIS:HB2	1:A:628:HIS:HB3	2.00	0.42
1:A:495:VAL:HG22	1:A:560:SER:HB2	2.02	0.42
1:A:369:ALA:N	1:A:370:PRO:CD	2.83	0.42
1:A:622:ILE:HD11	1:A:680:LEU:HD11	2.02	0.42
1:A:531:LYS:HB2	1:A:536:LEU:HB2	2.02	0.42
1:A:492:ALA:O	1:A:562:LEU:HA	2.21	0.41
1:A:658:THR:HB	1:A:660:GLU:OE1	2.20	0.40
1:A:519:PHE:HA	1:A:544:MET:HE2	2.02	0.40

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	385/396 (97%)	358 (93%)	20 (5%)	7 (2%)	8 37
2	B	2/6 (33%)	2 (100%)	0	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	387/402 (96%)	360 (93%)	20 (5%)	7 (2%)	8 37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	573	GLN
1	A	574	GLY
1	A	577	CYS
1	A	512	SER
1	A	565	LYS
1	A	597	SER
1	A	515	ALA

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	340/347 (98%)	293 (86%)	47 (14%)	3 16
2	B	4/4 (100%)	3 (75%)	1 (25%)	0 2
All	All	344/351 (98%)	296 (86%)	48 (14%)	3 15

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	349	LYS
1	A	350	ASP
1	A	371	LEU
1	A	377	LEU
1	A	380	LEU
1	A	403	VAL
1	A	407	LEU
1	A	456	LEU
1	A	460	LYS
1	A	464	LEU
1	A	511	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	518	ILE
1	A	526	ARG
1	A	534	THR
1	A	537	LEU
1	A	543	ASP
1	A	549	LEU
1	A	560	SER
1	A	561	SER
1	A	573	GLN
1	A	578	SER
1	A	580	GLU
1	A	586	LEU
1	A	603	GLN
1	A	610	LEU
1	A	622	ILE
1	A	627	VAL
1	A	640	VAL
1	A	641	THR
1	A	652	LYS
1	A	656	LYS
1	A	667	VAL
1	A	673	LYS
1	A	675	CYS
1	A	678	THR
1	A	679	ARG
1	A	684	GLN
1	A	686	LEU
1	A	689	HIS
1	A	690	LEU
1	A	691	ILE
1	A	703	LEU
1	A	705	ASP
1	A	706	THR
1	A	720	ILE
1	A	722	LYS
1	A	724	ASP
2	B	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	427	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	446	ASN
1	A	458	GLN
1	A	476	ASN
1	A	510	GLN
1	A	585	ASN
1	A	592	HIS
1	A	684	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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, 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	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	386/396 (97%)	-0.12	0	100	100	40, 68, 95, 115	0
2	B	4/6 (66%)	0.02	0	100	100	58, 62, 62, 77	0
All	All	390/402 (97%)	-0.12	0	100	100	40, 68, 95, 115	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.