



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 03:02 am BST

PDB ID : 4I1P
Title : Human MALT1 (caspase-IG3) in complex with activity based-probe
Authors : Schlauderer, F.; Lammens, K.; Hopfner, K.P.
Deposited on : 2012-11-21
Resolution : 2.40 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

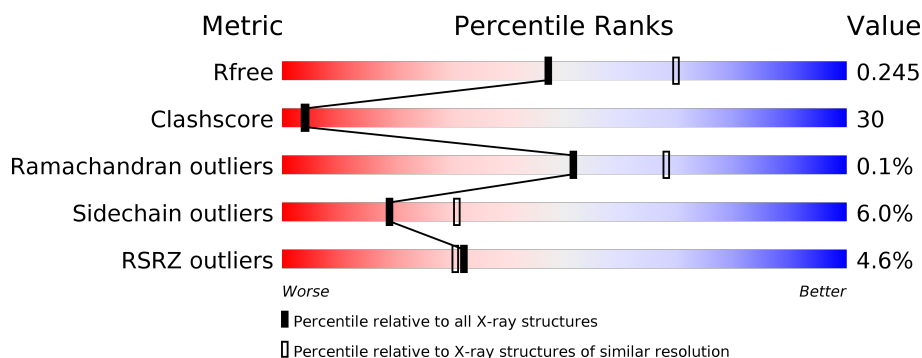
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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 $\leq 5\%$. 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	388	<div> <div>4%</div> <div> <div></div> <div>63%</div> <div>30%</div> <div>• •</div> </div> </div>
1	C	388	<div> <div>5%</div> <div> <div></div> <div>62%</div> <div>32%</div> <div>• •</div> </div> </div>
2	B	5	<div> <div></div> <div> <div>40%</div> <div>60%</div> </div> </div>
2	D	5	<div> <div></div> <div> <div>40%</div> <div>60%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	801	-	-	X	-
3	ACT	A	803	-	-	X	-
3	ACT	A	804	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6256 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	379	Total	C	N	O	S	124	0	0
			3007	1925	487	574	21			
1	C	380	Total	C	N	O	S	113	0	0
			3015	1930	488	575	22			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	338	MET	-	INITIATING METHIONINE	UNP Q9UDY8
A	720	HIS	-	EXPRESSION TAG	UNP Q9UDY8
A	721	HIS	-	EXPRESSION TAG	UNP Q9UDY8
A	722	HIS	-	EXPRESSION TAG	UNP Q9UDY8
A	723	HIS	-	EXPRESSION TAG	UNP Q9UDY8
A	724	HIS	-	EXPRESSION TAG	UNP Q9UDY8
A	725	HIS	-	EXPRESSION TAG	UNP Q9UDY8
C	338	MET	-	EXPRESSION TAG	UNP Q9UDY8
C	720	HIS	-	EXPRESSION TAG	UNP Q9UDY8
C	721	HIS	-	EXPRESSION TAG	UNP Q9UDY8
C	722	HIS	-	EXPRESSION TAG	UNP Q9UDY8
C	723	HIS	-	EXPRESSION TAG	UNP Q9UDY8
C	724	HIS	-	EXPRESSION TAG	UNP Q9UDY8
C	725	HIS	-	EXPRESSION TAG	UNP Q9UDY8

- Molecule 2 is a protein called tetrapeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	5	Total	C	N	O	0	0	1
			39	23	10	6			
2	D	5	Total	C	N	O	0	0	1
			39	23	10	6			

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	O 2	0	0
4	C	55	Total 55	O 55	0	0
4	D	1	Total 1	O 1	0	0

A0	L1	R2	S3	?4
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- Molecule 2: tetrapeptide

Chain D: 
40% 60%

A0	L1	R2	S3	?4
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	178.24Å 53.48Å 78.74Å 90.00° 103.80° 90.00°	Depositor
Resolution (Å)	43.94 – 2.40 43.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.1 (43.94-2.40) 96.3 (43.94-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.198 , 0.245 0.195 , 0.245	Depositor DCC
R_{free} test set	1370 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6256	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4AR, ACT

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	0.57	2/3062 (0.1%)	0.64	1/4141 (0.0%)
1	C	0.52	0/3070	0.61	1/4151 (0.0%)
2	B	0.18	0/26	0.25	0/32
2	D	0.25	0/26	0.48	0/32
All	All	0.54	2/6184 (0.0%)	0.63	2/8356 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	623	PRO	N-CD	5.21	1.55	1.47
1	A	622	PRO	N-CD	5.16	1.55	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	621	LYS	C-N-CD	5.74	140.46	128.40
1	C	352	ASN	C-N-CA	-5.58	107.75	121.70

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	3007	0	3029	152	0
1	C	3015	0	3037	188	0
2	B	39	0	41	8	0
2	D	39	0	41	19	0
3	A	20	0	15	12	0
3	C	20	0	15	2	0
4	A	58	0	0	8	0
4	B	2	0	0	0	0
4	C	55	0	0	3	0
4	D	1	0	0	0	0
All	All	6256	0	6178	347	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 30.

The worst 5 of 347 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:D:4:4AR:C2	2:D:4:4AR:C7	1.92	1.45
1:A:483:THR:HB	1:A:485:ASN:ND2	1.40	1.35
1:C:473:THR:CG2	1:C:475:PRO:HD3	1.61	1.29
1:A:464:CYS:CB	2:B:4:4AR:C7	2.17	1.22
1:C:572:GLU:O	1:C:576:ARG:HG3	1.38	1.21

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	377/388 (97%)	366 (97%)	10 (3%)	1 (0%)	41 55
1	C	378/388 (97%)	366 (97%)	12 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	2/5 (40%)	2 (100%)	0	0	100	100
2	D	2/5 (40%)	2 (100%)	0	0	100	100
All	All	759/786 (97%)	736 (97%)	22 (3%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	710	PRO

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	336/345 (97%)	316 (94%)	20 (6%)	19	31
1	C	337/345 (98%)	316 (94%)	21 (6%)	18	29
2	B	3/3 (100%)	3 (100%)	0	100	100
2	D	3/3 (100%)	3 (100%)	0	100	100
All	All	679/696 (98%)	638 (94%)	41 (6%)	19	31

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	711	LEU
1	C	401	LEU
1	C	679	LYS
1	A	716	ASP
1	C	351	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	681	HIS

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Mol	Chain	Res	Type
1	C	485	ASN
1	C	601	GLN
1	A	599	GLN
1	C	584	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	4AR	B	4	1,2	10,11,23	1.77	1 (10%)	9,13,30	6.24	1 (11%)
2	4AR	D	4	1,2	10,11,23	5.32	1 (10%)	9,13,30	5.12	1 (11%)

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
2	4AR	B	4	1,2	-	1/10/11/20	-
2	4AR	D	4	1,2	-	0/10/11/20	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	4AR	C7-C2	16.79	1.92	1.49
2	B	4	4AR	C7-C2	5.51	1.63	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	4AR	O1-C2-C7	-18.70	87.94	121.15
2	D	4	4AR	O1-C2-C7	-15.25	94.07	121.15

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4	4AR	N1-C1-C2-O1

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	4AR	3	0
2	D	4	4AR	7	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

10 ligands are modelled in this entry.

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ACT	C	802	-	1,3,3	0.11	0	0,3,3	0.00	-
3	ACT	C	801	-	1,3,3	1.46	0	0,3,3	0.00	-
3	ACT	C	803	-	1,3,3	1.36	0	0,3,3	0.00	-
3	ACT	C	804	-	1,3,3	0.51	0	0,3,3	0.00	-
3	ACT	A	804	-	1,3,3	0.50	0	0,3,3	0.00	-
3	ACT	A	803	-	1,3,3	0.73	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ACT	A	801	-	1,3,3	0.49	0	0,3,3	0.00	-
3	ACT	C	805	-	1,3,3	1.31	0	0,3,3	0.00	-
3	ACT	A	805	-	1,3,3	0.89	0	0,3,3	0.00	-
3	ACT	A	802	-	1,3,3	0.88	0	0,3,3	0.00	-

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.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	803	ACT	1	0
3	A	804	ACT	2	0
3	A	803	ACT	2	0
3	A	801	ACT	8	0
3	C	805	ACT	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, 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	379/388 (97%)	0.13	17 (4%) 33 31	42, 66, 124, 155	29 (7%)
1	C	379/388 (97%)	0.16	18 (4%) 31 30	42, 66, 122, 151	27 (7%)
2	B	4/5 (80%)	1.04	0 100 100	61, 69, 75, 84	0
2	D	4/5 (80%)	0.71	0 100 100	64, 78, 84, 87	0
All	All	766/786 (97%)	0.15	35 (4%) 32 31	42, 66, 122, 155	56 (7%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	504	SER	6.2
1	C	580	TRP	4.4
1	A	697	ASP	4.3
1	C	663	LEU	3.9
1	A	505	GLY	3.7

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	B-factors(Å ²)	Q<0.9
2	4AR	D	4	12/23	0.91	0.16	49,53,56,98	0
2	4AR	B	4	12/23	0.93	0.17	48,51,59,124	0

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. 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	B-factors(Å ²)	Q<0.9
3	ACT	C	805	4/4	0.17	0.36	122,125,126,126	0
3	ACT	A	805	4/4	0.63	0.40	109,110,111,112	0
3	ACT	C	801	4/4	0.74	0.34	88,89,90,92	0
3	ACT	A	803	4/4	0.77	0.39	82,83,84,86	0
3	ACT	C	803	4/4	0.78	0.33	98,100,100,100	0
3	ACT	A	801	4/4	0.87	0.28	77,80,80,82	0
3	ACT	A	802	4/4	0.87	0.30	106,107,108,109	0
3	ACT	A	804	4/4	0.90	0.33	81,82,83,86	0
3	ACT	C	802	4/4	0.90	0.28	94,95,95,96	0
3	ACT	C	804	4/4	0.91	0.19	97,97,98,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.