



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 24, 2017 – 01:12 PM EDT

PDB ID : 3G0A
Title : Mth0212 with two bound manganese ions
Authors : Lakomek, K.; Dickmanns, A.; Ficner, R.
Deposited on : unknown
Resolution : 2.60 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

<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 : 1.7.2 (RC1), CSD as538be (2017)
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

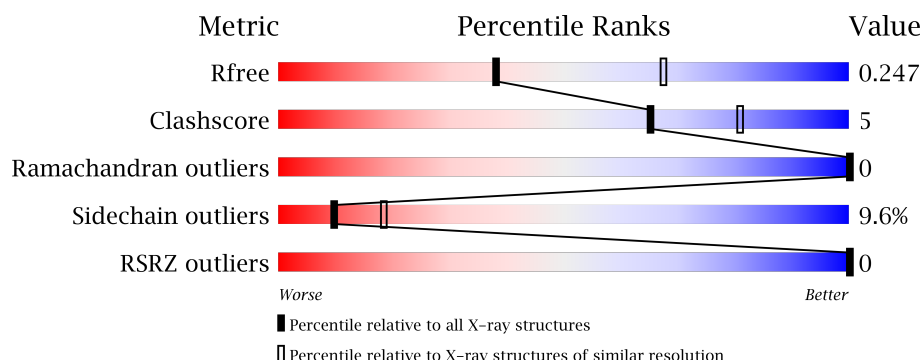
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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 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	265	

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
3	GOL	A	268	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2237 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 Exodeoxyribonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	5	0
			2153	1384	375	386	8			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	THR	ENGINEERED MUTATION	UNP O26314
A	258	LEU	-	EXPRESSION TAG	UNP O26314
A	259	GLU	-	EXPRESSION TAG	UNP O26314
A	260	HIS	-	EXPRESSION TAG	UNP O26314
A	261	HIS	-	EXPRESSION TAG	UNP O26314
A	262	HIS	-	EXPRESSION TAG	UNP O26314
A	263	HIS	-	EXPRESSION TAG	UNP O26314
A	264	HIS	-	EXPRESSION TAG	UNP O26314
A	265	HIS	-	EXPRESSION TAG	UNP O26314

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	71	Total	O	0	0
			71	71		

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- Molecule 1: Exodeoxyribonuclease

Chain A:

79% 16%

MET ALA V3 L4 N10 V11 M12 R15 Y27 K30 L34 P43 L46 P47 R48 K49 L50 R51 S58 F59 F60 K66 L82 R83 E89 D101 F102 D103 D104 F105 L106 K116 L122 L126 L133 E134 D135 V136 M137 R140 V146

C149 N169 V176 T204 Y208 F224 N227 E228 E229 E230 V234 E235 R236 I242 H248 E254 L257 L258 E259 H260 H261 H262 H263 H264 H265 H266 H267 H268 H269 H270 H271 H272 H273 H274 H275 H276 H277 H278 H279 H280 H281 H282 H283 H284 H285 H286 H287 H288 H289 H290 H291 H292 H293 H294 H295 H296 H297 H298 H299 H300 H301 H302 H303 H304 H305 H306 H307 H308 H309 H310 H311 H312 H313 H314 H315 H316 H317 H318 H319 H320 H321 H322 H323 H324 H325 H326 H327 H328 H329 H330 H331 H332 H333 H334 H335 H336 H337 H338 H339 H340 H341 H342 H343 H344 H345 H346 H347 H348 H349 H350 H351 H352 H353 H354 H355 H356 H357 H358 H359 H360 H361 H362 H363 H364 H365 H366 H367 H368 H369 H370 H371 H372 H373 H374 H375 H376 H377 H378 H379 H380 H381 H382 H383 H384 H385 H386 H387 H388 H389 H390 H391 H392 H393 H394 H395 H396 H397 H398 H399 H400 H401 H402 H403 H404 H405 H406 H407 H408 H409 H410 H411 H412 H413 H414 H415 H416 H417 H418 H419 H420 H421 H422 H423 H424 H425 H426 H427 H428 H429 H430 H431 H432 H433 H434 H435 H436 H437 H438 H439 H440 H441 H442 H443 H444 H445 H446 H447 H448 H449 H450 H451 H452 H453 H454 H455 H456 H457 H458 H459 H460 H461 H462 H463 H464 H465 H466 H467 H468 H469 H470 H471 H472 H473 H474 H475 H476 H477 H478 H479 H480 H481 H482 H483 H484 H485 H486 H487 H488 H489 H490 H491 H492 H493 H494 H495 H496 H497 H498 H499 H500 H501 H502 H503 H504 H505 H506 H507 H508 H509 H510 H511 H512 H513 H514 H515 H516 H517 H518 H519 H520 H521 H522 H523 H524 H525 H526 H527 H528 H529 H530 H531 H532 H533 H534 H535 H536 H537 H538 H539 H540 H541 H542 H543 H544 H545 H546 H547 H548 H549 H550 H551 H552 H553 H554 H555 H556 H557 H558 H559 H560 H561 H562 H563 H564 H565 H566 H567 H568 H569 H570 H571 H572 H573 H574 H575 H576 H577 H578 H579 H580 H581 H582 H583 H584 H585 H586 H587 H588 H589 H590 H591 H592 H593 H594 H595 H596 H597 H598 H599 H600 H601 H602 H603 H604 H605 H606 H607 H608 H609 H610 H611 H612 H613 H614 H615 H616 H617 H618 H619 H620 H621 H622 H623 H624 H625 H626 H627 H628 H629 H630 H631 H632 H633 H634 H635 H636 H637 H638 H639 H640 H641 H642 H643 H644 H645 H646 H647 H648 H649 H650 H651 H652 H653 H654 H655 H656 H657 H658 H659 H660 H661 H662 H663 H664 H665 H666 H667 H668 H669 H670 H671 H672 H673 H674 H675 H676 H677 H678 H679 H680 H681 H682 H683 H684 H685 H686 H687 H688 H689 H690 H691 H692 H693 H694 H695 H696 H697 H698 H699 H700 H701 H702 H703 H704 H705 H706 H707 H708 H709 H710 H711 H712 H713 H714 H715 H716 H717 H718 H719 H720 H721 H722 H723 H724 H725 H726 H727 H728 H729 H730 H731 H732 H733 H734 H735 H736 H737 H738 H739 H740 H741 H742 H743 H744 H745 H746 H747 H748 H749 H750 H751 H752 H753 H754 H755 H756 H757 H758 H759 H760 H761 H762 H763 H764 H765 H766 H767 H768 H769 H770 H771 H772 H773 H774 H775 H776 H777 H778 H779 H780 H781 H782 H783 H784 H785 H786 H787 H788 H789 H790 H791 H792 H793 H794 H795 H796 H797 H798 H799 H800 H801 H802 H803 H804 H805 H806 H807 H808 H809 H810 H811 H812 H813 H814 H815 H816 H817 H818 H819 H820 H821 H822 H823 H824 H825 H826 H827 H828 H829 H830 H831 H832 H833 H834 H835 H836 H837 H838 H839 H840 H841 H842 H843 H844 H845 H846 H847 H848 H849 H850 H851 H852 H853 H854 H855 H856 H857 H858 H859 H860 H861 H862 H863 H864 H865 H866 H867 H868 H869 H870 H871 H872 H873 H874 H875 H876 H877 H878 H879 H880 H881 H882 H883 H884 H885 H886 H887 H888 H889 H890 H891 H892 H893 H894 H895 H896 H897 H898 H899 H900 H901 H902 H903 H904 H905 H906 H907 H908 H909 H910 H911 H912 H913 H914 H915 H916 H917 H918 H919 H920 H921 H922 H923 H924 H925 H926 H927 H928 H929 H930 H931 H932 H933 H934 H935 H936 H937 H938 H939 H940 H941 H942 H943 H944 H945 H946 H947 H948 H949 H950 H951 H952 H953 H954 H955 H956 H957 H958 H959 H960 H961 H962 H963 H964 H965 H966 H967 H968 H969 H970 H971 H972 H973 H974 H975 H976 H977 H978 H979 H980 H981 H982 H983 H984 H985 H986 H987 H988 H989 H990 H991 H992 H993 H994 H995 H996 H997 H998 H999 H1000

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	56.38Å 56.38Å 162.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.83 – 2.60 48.83 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.83-2.60) 98.4 (48.83-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.252 0.190 , 0.247	Depositor DCC
R_{free} test set	415 reflections (4.92%)	DCC
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.093 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2237	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.57% 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: GOL, PO4, MN

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	0.54	0/2214	0.67	1/2984 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	82	LEU	CA-CB-CG	5.78	128.60	115.30

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	2153	0	2098	20	0
2	A	2	0	0	0	0
3	A	6	0	8	0	0
4	A	5	0	0	0	0
5	A	71	0	0	4	0
All	All	2237	0	2106	20	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.

The worst 5 of 20 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:43:PRO:HA	1:A:46:LEU:HD12	1.67	0.77
1:A:104:ASP:OD1	1:A:259:GLU:HA	1.99	0.62
1:A:10:ASN:HB3	1:A:248:HIS:CG	2.42	0.55
1:A:103:ASP:HB3	1:A:259:GLU:OE1	2.08	0.53
1:A:149:CYS:HB3	1:A:224:PHE:CE2	2.47	0.49

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	256/265 (97%)	245 (96%)	11 (4%)	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	Outliers	Percentiles	
1	A	229/235 (97%)	206 (90%)	23 (10%)	9	17

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116[B]	LYS
1	A	126	LEU
1	A	258	LEU
1	A	122	LEU
1	A	133	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	A	268	-	5,5,5	0.31	0	5,5,5	0.35	0
4	PO4	A	269	-	4,4,4	0.72	0	6,6,6	0.32	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	GOL	A	268	-	-	0/4/4/4	0/0/0/0
4	PO4	A	269	-	-	0/0/0/0	0/0/0/0

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 [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	257/265 (96%)	-0.38	0 100 100	18, 31, 46, 61	4 (1%)

There are no RSRZ outliers to report.

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
3	GOL	A	268	6/6	0.85	0.28	9.11	55,55,56,56	0
2	MN	A	266	1/1	0.96	0.06	-3.34	73,73,73,73	0
2	MN	A	267	1/1	0.95	0.15	-	33,33,33,33	0
4	PO4	A	269	5/5	0.92	0.24	-	74,74,74,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.