



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 24, 2024 – 09:17 AM EST

PDB ID : 1MKZ
Title : Crystal structure of MoaB protein at 1.6 Å resolution.
Authors : Sanishvili, R.; Skarina, T.; Joachimiak, A.; Edwards, A.; Savchenko, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2002-08-29
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

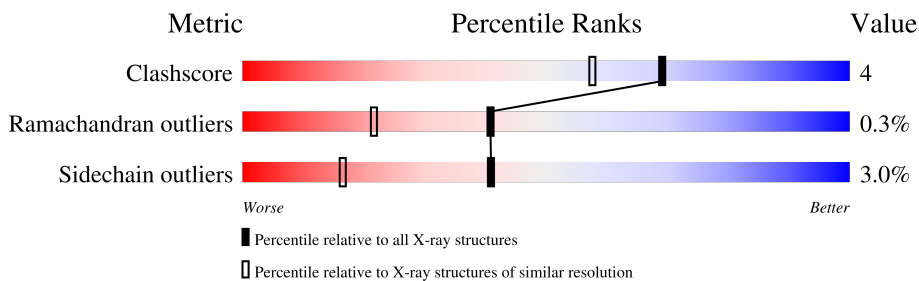
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	172	84% 13% ...
1	B	172	88% 10% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2961 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 Molybdenum cofactor biosynthesis protein B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	170	1344	841	237	262	2	2	0	11	0
1	B	171	1335	838	237	255	2	3	0	10	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P30746
A	108	MSE	MET	modified residue	UNP P30746
A	134	LEU	PHE	SEE REMARK 999	UNP P30746
A	136	MSE	MET	modified residue	UNP P30746
A	171	GLY	-	cloning artifact	UNP P30746
A	172	SER	-	cloning artifact	UNP P30746
B	1	MSE	MET	modified residue	UNP P30746
B	108	MSE	MET	modified residue	UNP P30746
B	134	LEU	PHE	SEE REMARK 999	UNP P30746
B	136	MSE	MET	modified residue	UNP P30746
B	171	GLY	-	cloning artifact	UNP P30746
B	172	SER	-	cloning artifact	UNP P30746

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



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

- Molecule 4 is water.


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	102	Total O 102 102	0	0
4	B	133	Total O 133 133	0	0

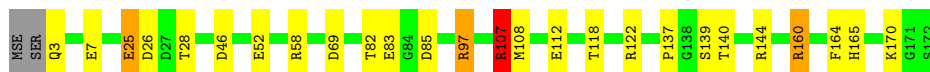
3 Residue-property plots [i](#)

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. 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. 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.


Note EDS was not executed.

- Molecule 1: Molybdenum cofactor biosynthesis protein B

Chain A:  84% 13% ...



- Molecule 1: Molybdenum cofactor biosynthesis protein B

Chain B:  88% 10% ..



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	69.17Å 69.17Å 126.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	129.10 – 1.60	Depositor
% Data completeness (in resolution range)	94.8 (129.10-1.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24, CNS	Depositor
R, R_{free}	0.183 , 0.219	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2961	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

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: ACY, SO4

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	0.71	1/1409 (0.1%)	1.04	12/1907 (0.6%)
1	B	0.84	0/1396	1.16	12/1890 (0.6%)
All	All	0.78	1/2805 (0.0%)	1.10	24/3797 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	MSE	SE-CE	-7.12	1.53	1.95

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97[A]	ARG	NE-CZ-NH1	-8.82	115.89	120.30
1	B	97[B]	ARG	NE-CZ-NH1	-8.82	115.89	120.30
1	B	122	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	B	27	ASP	CB-CG-OD2	7.31	124.88	118.30
1	B	35	ASP	CB-CG-OD2	6.76	124.38	118.30
1	B	144	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	B	160[A]	ARG	NE-CZ-NH1	-6.57	117.02	120.30
1	B	160[B]	ARG	NE-CZ-NH1	-6.57	117.02	120.30
1	A	107	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	B	107	ARG	CA-CB-CG	5.92	126.43	113.40
1	A	97[A]	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	97[B]	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	144	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	85	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	26	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	95	PHE	CB-CG-CD2	-5.67	116.83	120.80
1	B	122	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	A	122	ARG	NE-CZ-NH2	-5.25	117.67	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	160	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	95	PHE	CB-CG-CD1	5.06	124.34	120.80
1	A	97[A]	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	97[B]	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	69	ASP	CB-CG-OD2	5.01	122.81	118.30

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	1344	0	1320	14	1
1	B	1335	0	1321	6	0
2	A	20	0	0	3	0
2	B	15	0	0	1	0
3	A	4	0	3	1	0
3	B	8	0	6	0	0
4	A	102	0	0	3	0
4	B	133	0	0	0	0
All	All	2961	0	2650	20	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 4.

All (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:28[B]:THR:HG22	4:A:1271:HOH:O	1.78	0.83
1:A:28[B]:THR:HG23	1:A:140:THR:OG1	1.80	0.81
1:A:170:LYS:HB2	2:A:304:SO4:O3	1.84	0.77
1:A:107:ARG:HG3	1:A:118[B]:THR:CG2	2.13	0.77
1:A:112:GLU:OE2	4:A:1301:HOH:O	2.10	0.68
1:B:52:GLU:OE1	2:B:402:SO4:O2	2.22	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28[B]:THR:CG2	1:A:140:THR:OG1	2.51	0.56
1:B:88:PRO:O	1:B:92[B]:LEU:HD23	2.10	0.51
1:B:92[A]:LEU:HD11	1:B:124:VAL:HG21	1.96	0.47
1:B:107:ARG:HG3	1:B:118[B]:THR:CG2	2.49	0.43
1:A:46:ASP:OD2	3:A:1201:ACY:H3	2.19	0.42
1:A:52:GLU:OE1	2:A:302:SO4:O3	2.38	0.42
1:A:107:ARG:HG3	1:A:118[B]:THR:HG23	1.99	0.41
1:A:164:PHE:O	1:A:165:HIS:C	2.58	0.41
1:B:164:PHE:O	1:B:165:HIS:C	2.57	0.41
1:A:160:ARG:NH2	4:A:1229:HOH:O	2.40	0.40
1:B:152:ALA:HB3	1:B:153:PRO:HD3	2.03	0.40
1:A:137:PRO:HA	2:A:301:SO4:O3	2.22	0.40

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)
1:A:82:THR:O	1:A:97[B]:ARG:NH1[2_655]	2.05	0.15

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	179/172 (104%)	176 (98%)	3 (2%)	0	100	100
1	B	179/172 (104%)	175 (98%)	3 (2%)	1 (1%)	25	8
All	All	358/344 (104%)	351 (98%)	6 (2%)	1 (0%)	41	21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	GLN

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	147/138 (106%)	139 (95%)	8 (5%)	22 5
1	B	144/138 (104%)	141 (98%)	3 (2%)	53 29
All	All	291/276 (105%)	280 (96%)	11 (4%)	41 10

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	7	GLU
1	A	25[A]	GLU
1	A	25[B]	GLU
1	A	83[A]	GLU
1	A	83[B]	GLU
1	A	107	ARG
1	A	139	SER
1	B	92[A]	LEU
1	B	92[B]	LEU
1	B	139	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	20	ASN
1	A	60	GLN
1	A	120	GLN
1	B	167	HIS

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](#)

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	$\# Z > 2$
2	SO4	B	402	-	4,4,4	0.17	0	6,6,6	0.39	0
3	ACY	B	1202	-	3,3,3	0.80	0	3,3,3	1.37	0
2	SO4	A	302	-	4,4,4	0.16	0	6,6,6	0.28	0
2	SO4	A	303	-	4,4,4	0.13	0	6,6,6	0.33	0
3	ACY	B	1203	-	3,3,3	0.71	0	3,3,3	1.09	0
3	ACY	A	1201	-	3,3,3	0.84	0	3,3,3	1.73	1 (33%)
2	SO4	A	304	-	4,4,4	0.22	0	6,6,6	0.62	0
2	SO4	B	403	-	4,4,4	0.13	0	6,6,6	0.32	0
2	SO4	B	401	-	4,4,4	0.31	0	6,6,6	0.63	0
2	SO4	A	301	-	4,4,4	0.34	0	6,6,6	0.78	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	1201	ACY	O-C-CH3	-2.37	113.11	122.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	SO4	1	0
2	A	302	SO4	1	0
3	A	1201	ACY	1	0
2	A	304	SO4	1	0
2	A	301	SO4	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.