



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:14 AM GMT

PDB ID : 2NQM
Title : MoeA T100A mutant
Authors : Nicoas, J.; Xiang, S.; Schindelin, H.; Rajagopalan, K.V.
Deposited on : 2006-10-31
Resolution : 3.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

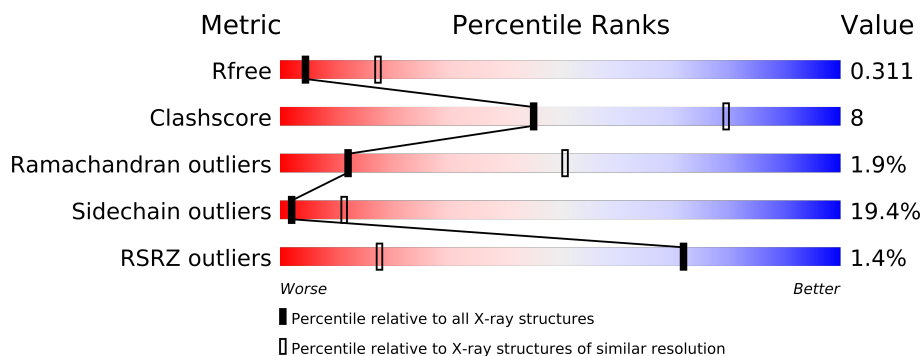
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	411	
1	B	411	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5482 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Molybdopterin biosynthesis protein moeA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2444	1550	426	461	7			
1	B	403	Total	C	N	O	S	0	0	0
			3038	1917	531	577	13			

There are 2 discrepancies between the modelled and reference sequences:

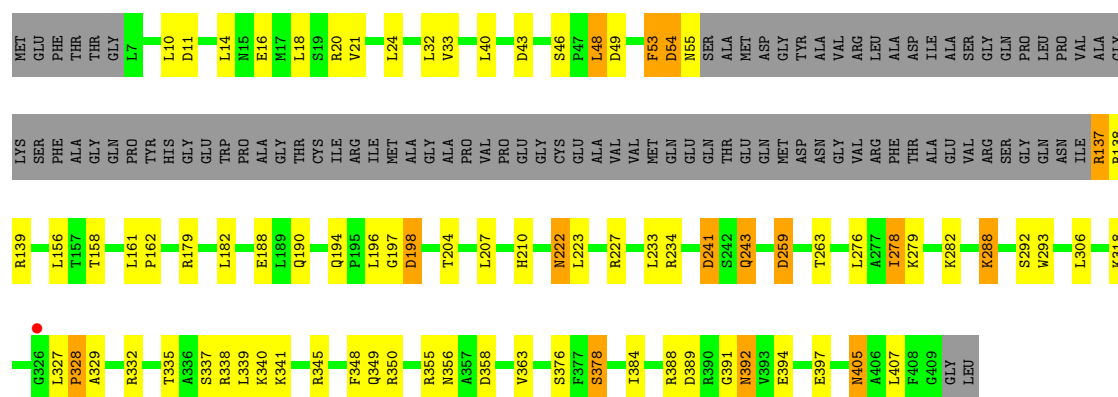
Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ALA	THR	ENGINEERED	UNP P12281
B	100	ALA	THR	ENGINEERED	UNP P12281

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

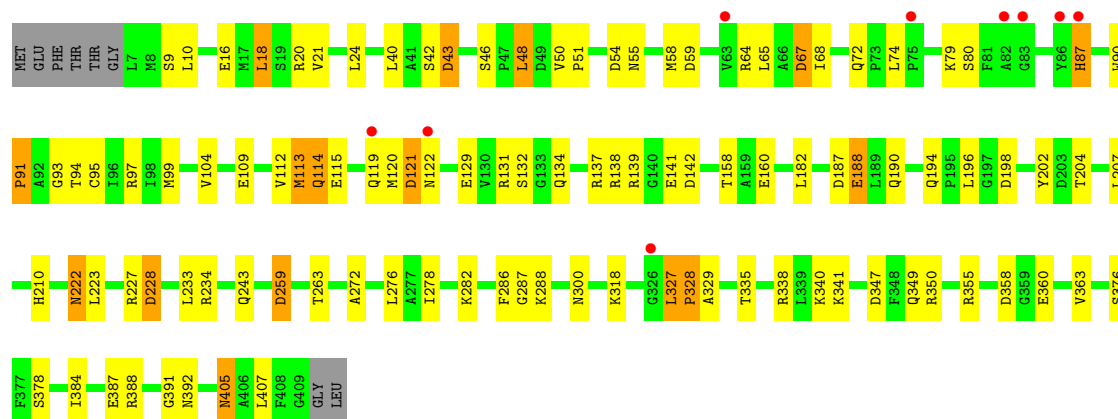
- Molecule 1: Molybdopterin biosynthesis protein moeA

Chain A:



- Molecule 1: Molybdopterin biosynthesis protein moeA

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.91Å 99.36Å 104.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 3.00 40.95 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.2 (49.39-3.00) 90.3 (40.95-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.268 , 0.345 0.240 , 0.311	Depositor DCC
R_{free} test set	808 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	79.4	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.7	EDS
Estimated twinning fraction	0.033 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 15898 reflections (0.013%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5482	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.67	0/2489	0.85	7/3381 (0.2%)
1	B	0.66	0/3097	0.82	9/4209 (0.2%)
All	All	0.66	0/5586	0.83	16/7590 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	ASP	CB-CG-OD2	6.64	124.27	118.30
1	B	59	ASP	CB-CG-OD2	6.54	124.19	118.30
1	B	142	ASP	CB-CG-OD2	6.52	124.17	118.30
1	A	241	ASP	CB-CG-OD2	5.99	123.69	118.30
1	B	358	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	358	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	43	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	389	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	43	ASP	CB-CG-OD2	5.73	123.46	118.30
1	B	259	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	228	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	121	ASP	CB-CG-OD2	5.55	123.29	118.30
1	A	49	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	67	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	11	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	347	ASP	CB-CG-OD2	5.12	122.91	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2444	0	0	22	0
1	B	3038	0	0	25	0
All	All	5482	0	0	46	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (46) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:241:ASP:OD2	1:A:292:SER:OG	2.02	0.76
1:B:21:VAL:O	1:B:318:LYS:NZ	2.27	0.68
1:A:405:ASN:C	1:A:405:ASN:ND2	2.49	0.66
1:B:405:ASN:ND2	1:B:405:ASN:C	2.49	0.65
1:A:55:ASN:O	1:A:137:ARG:N	2.31	0.64
1:B:405:ASN:ND2	1:B:407:LEU:N	2.46	0.64
1:A:210:HIS:CD2	1:A:222:ASN:OD1	2.55	0.60
1:A:278:ILE:O	1:A:345:ARG:NH1	2.37	0.56
1:A:405:ASN:ND2	1:A:407:LEU:N	2.53	0.55
1:A:327:LEU:O	1:A:328:PRO:C	2.45	0.55
1:A:21:VAL:O	1:A:318:LYS:NZ	2.41	0.54
1:B:46:SER:OG	1:B:48:LEU:O	2.26	0.53
1:A:259:ASP:OD1	1:A:259:ASP:C	2.48	0.52
1:B:272:ALA:N	1:B:286:PHE:O	2.42	0.52
1:B:187:ASP:OD2	1:B:188:GLU:N	2.43	0.52
1:B:87:HIS:N	1:B:87:HIS:ND1	2.58	0.51
1:B:387:GLU:OE1	1:B:387:GLU:N	2.43	0.51
1:A:349:GLN:O	1:A:384:ILE:N	2.44	0.51
1:A:53:PHE:O	1:A:54:ASP:CB	2.59	0.50
1:A:394:GLU:N	1:A:397:GLU:OE2	2.46	0.49
1:B:327:LEU:O	1:B:328:PRO:C	2.51	0.49
1:B:327:LEU:O	1:B:328:PRO:O	2.31	0.49
1:A:378:SER:OG	1:B:160:GLU:OE1	2.31	0.49
1:B:341:LYS:NZ	1:B:388:ARG:O	2.47	0.48
1:A:46:SER:OG	1:A:48:LEU:O	2.32	0.48
1:B:194:GLN:O	1:B:202:TYR:OH	2.32	0.48
1:B:349:GLN:O	1:B:384:ILE:N	2.48	0.47
1:A:161:LEU:N	1:A:162:PRO:CD	2.78	0.46
1:B:18:LEU:O	1:B:318:LYS:NZ	2.49	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:279:LYS:O	1:A:348:PHE:N	2.49	0.46
1:B:259:ASP:C	1:B:259:ASP:OD1	2.53	0.46
1:B:42:SER:O	1:B:43:ASP:C	2.54	0.45
1:B:210:HIS:CD2	1:B:222:ASN:OD1	2.70	0.45
1:A:18:LEU:O	1:A:318:LYS:NZ	2.50	0.45
1:B:90:TRP:CD1	1:B:91:PRO:O	2.71	0.44
1:B:391:GLY:O	1:B:392:ASN:C	2.56	0.44
1:A:197:GLY:O	1:A:198:ASP:O	2.36	0.43
1:B:50:VAL:CA	1:B:51:PRO:C	2.86	0.43
1:A:391:GLY:O	1:A:392:ASN:C	2.57	0.43
1:B:113:MET:O	1:B:115:GLU:N	2.52	0.43
1:A:288:LYS:CG	1:A:293:TRP:CZ3	3.02	0.42
1:B:95:CYS:O	1:B:95:CYS:SG	2.78	0.42
1:B:286:PHE:CG	1:B:287:GLY:N	2.88	0.41
1:A:179:ARG:NH1	1:A:243:GLN:O	2.53	0.41
1:B:328:PRO:O	1:B:329:ALA:C	2.58	0.41
1:A:341:LYS:NZ	1:A:388:ARG:O	2.53	0.41

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	318/411 (77%)	291 (92%)	20 (6%)	7 (2%)	10	45
1	B	401/411 (98%)	349 (87%)	45 (11%)	7 (2%)	14	54
All	All	719/822 (88%)	640 (89%)	65 (9%)	14 (2%)	12	51

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	198	ASP
1	A	282	LYS

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Mol	Chain	Res	Type
1	A	392	ASN
1	B	91	PRO
1	B	114	GLN
1	B	198	ASP
1	B	282	LYS
1	A	328	PRO
1	B	328	PRO
1	B	93	GLY
1	A	329	ALA
1	B	68	ILE
1	A	32	LEU

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	264/330 (80%)	219 (83%)	45 (17%)	3	15
1	B	324/330 (98%)	255 (79%)	69 (21%)	1	8
All	All	588/660 (89%)	474 (81%)	114 (19%)	2	11

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	14	LEU
1	A	16	GLU
1	A	20	ARG
1	A	24	LEU
1	A	33	VAL
1	A	40	LEU
1	A	48	LEU
1	A	53	PHE
1	A	137	ARG
1	A	138	ARG
1	A	139	ARG
1	A	156	LEU
1	A	158	THR

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Mol	Chain	Res	Type
1	A	182	LEU
1	A	188	GLU
1	A	190	GLN
1	A	194	GLN
1	A	196	LEU
1	A	204	THR
1	A	207	LEU
1	A	222	ASN
1	A	223	LEU
1	A	227	ARG
1	A	233	LEU
1	A	234	ARG
1	A	243	GLN
1	A	263	THR
1	A	276	LEU
1	A	278	ILE
1	A	288	LYS
1	A	306	LEU
1	A	332	ARG
1	A	335	THR
1	A	337	SER
1	A	338	ARG
1	A	339	LEU
1	A	340	LYS
1	A	350	ARG
1	A	355	ARG
1	A	356	ASN
1	A	363	VAL
1	A	376	SER
1	A	378	SER
1	A	405	ASN
1	B	9	SER
1	B	10	LEU
1	B	16	GLU
1	B	18	LEU
1	B	20	ARG
1	B	24	LEU
1	B	40	LEU
1	B	48	LEU
1	B	54	ASP
1	B	55	ASN
1	B	58	MET

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Mol	Chain	Res	Type
1	B	64	ARG
1	B	65	LEU
1	B	67	ASP
1	B	72	GLN
1	B	74	LEU
1	B	79	LYS
1	B	80	SER
1	B	87	HIS
1	B	94	THR
1	B	97	ARG
1	B	99	MET
1	B	104	VAL
1	B	109	GLU
1	B	112	VAL
1	B	113	MET
1	B	114	GLN
1	B	119	GLN
1	B	120	MET
1	B	121	ASP
1	B	122	ASN
1	B	129	GLU
1	B	131	ARG
1	B	132	SER
1	B	134	GLN
1	B	137	ARG
1	B	138	ARG
1	B	139	ARG
1	B	141	GLU
1	B	158	THR
1	B	182	LEU
1	B	188	GLU
1	B	190	GLN
1	B	196	LEU
1	B	204	THR
1	B	207	LEU
1	B	222	ASN
1	B	223	LEU
1	B	227	ARG
1	B	228	ASP
1	B	233	LEU
1	B	234	ARG
1	B	243	GLN

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Mol	Chain	Res	Type
1	B	263	THR
1	B	276	LEU
1	B	278	ILE
1	B	288	LYS
1	B	300	ASN
1	B	327	LEU
1	B	335	THR
1	B	338	ARG
1	B	340	LYS
1	B	350	ARG
1	B	355	ARG
1	B	360	GLU
1	B	363	VAL
1	B	376	SER
1	B	378	SER
1	B	405	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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, 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	322/411 (78%)	-0.14	1 (0%) 91 48	30, 55, 76, 86	0
1	B	403/411 (98%)	0.07	9 (2%) 59 12	31, 59, 113, 141	0
All	All	725/822 (88%)	-0.03	10 (1%) 72 18	30, 57, 103, 141	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	75	PRO	3.0
1	B	326	GLY	2.9
1	A	326	GLY	2.9
1	B	82	ALA	2.8
1	B	122	ASN	2.6
1	B	87	HIS	2.5
1	B	83	GLY	2.2
1	B	86	TYR	2.1
1	B	63	VAL	2.1
1	B	119	GLN	2.1

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 carbohydrates 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.