



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 08:20 AM EDT

PDB ID : 2NQV / pdb_00002nqv
Title : MoeA D228A
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Deposited on : 2006-10-31
Resolution : 2.82 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

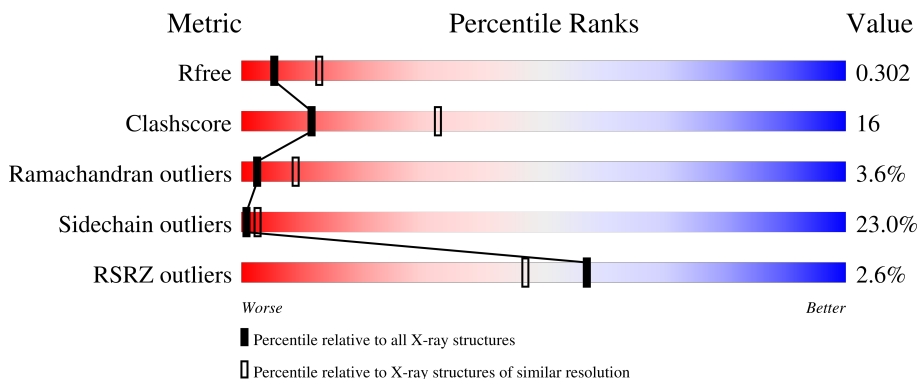
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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 $\leq 5\%$. 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	411	
1	B	411	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6148 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 Molybdopterin biosynthesis protein moeA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3050	1925	533	579	13			
1	B	403	Total	C	N	O	S	0	0	0
			3037	1917	531	576	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	ALA	ASP	engineered mutation	UNP P12281
B	228	ALA	ASP	engineered mutation	UNP P12281

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	6	Total	O	0	0
			6	6		

D358	G359	E360	L361	E362	V363	T364		H368	Q369	G370	S371	H372	I373		S378	L379	G380		L386	E387	R388	D389	R390	G391	N392	V393		V399	E400	V401	E402	F403	F404	N405	A406		G409	GLY	LEU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.67Å 98.13Å 160.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.82 50.00 – 2.82	Depositor EDS
% Data completeness (in resolution range)	73.4 (50.00-2.82) 73.4 (50.00-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.55 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.240 , 0.319 0.237 , 0.302	Depositor DCC
R_{free} test set	997 reflections (3.75%)	wwPDB-VP
Wilson B-factor (Å ²)	63.6	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6148	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: GOL

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	0.94	0/3109	1.08	5/4224 (0.1%)
1	B	1.00	2/3096 (0.1%)	1.11	6/4208 (0.1%)
All	All	0.97	2/6205 (0.0%)	1.09	11/8432 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	99	MET	SD-CE	5.67	1.93	1.79
1	B	215	GLN	CA-C	-5.29	1.45	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	GLY	N-CA-C	-6.19	106.70	115.30
1	B	27	GLN	N-CA-C	5.93	118.42	109.23
1	B	391	GLY	N-CA-C	-5.75	105.89	112.79
1	A	79	LYS	N-CA-C	5.62	117.07	108.52
1	A	373	ILE	N-CA-C	5.60	115.95	108.27

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	3050	0	3052	105	0
1	B	3037	0	3038	97	0
2	A	30	0	40	7	0
2	B	18	0	24	6	0
3	A	7	0	0	0	0
3	B	6	0	0	1	0
All	All	6148	0	6154	197	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 16.

The worst 5 of 197 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:B:189:LEU:O	2:B:907:GOL:H31	1.47	1.12
1:A:300:ASN:C	1:A:300:ASN:HD22	1.65	1.03
1:B:190:GLN:HG3	1:B:194:GLN:HE21	1.40	0.86
1:B:338:ARG:HH12	1:B:392:ASN:HD22	1.28	0.82
1:B:190:GLN:HG3	1:B:194:GLN:NE2	1.95	0.79

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	403/411 (98%)	353 (88%)	37 (9%)	13 (3%)	3	10
1	B	401/411 (98%)	351 (88%)	34 (8%)	16 (4%)	2	7
All	All	804/822 (98%)	704 (88%)	71 (9%)	29 (4%)	2	9

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ALA
1	A	89	GLU
1	A	282	LYS
1	A	404	PHE
1	B	68	ILE

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	325/330 (98%)	250 (77%)	75 (23%)	1	2
1	B	324/330 (98%)	250 (77%)	74 (23%)	1	3
All	All	649/660 (98%)	500 (77%)	149 (23%)	1	3

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	233	LEU
1	B	364	THR
1	B	264	ILE
1	B	325	SER
1	A	276	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	72	GLN
1	B	210	HIS
1	B	372	HIS
1	B	194	GLN
1	B	222	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	GOL	A	905	-	5,5,5	0.49	0	5,5,5	0.41	0
2	GOL	B	907	-	5,5,5	0.46	0	5,5,5	1.27	0
2	GOL	A	901	-	5,5,5	0.67	0	5,5,5	0.80	0
2	GOL	B	908	-	5,5,5	0.22	0	5,5,5	0.45	0
2	GOL	A	904	-	5,5,5	0.65	0	5,5,5	1.11	0
2	GOL	A	906	-	5,5,5	0.51	0	5,5,5	0.64	0
2	GOL	A	903	-	5,5,5	0.42	0	5,5,5	0.54	0
2	GOL	B	902	-	5,5,5	0.39	0	5,5,5	0.25	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
2	GOL	A	905	-	-	3/4/4/4	-
2	GOL	B	907	-	-	3/4/4/4	-
2	GOL	A	901	-	-	2/4/4/4	-
2	GOL	B	908	-	-	3/4/4/4	-
2	GOL	A	904	-	-	0/4/4/4	-
2	GOL	A	906	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	903	-	-	2/4/4/4	-
2	GOL	B	902	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	905	GOL	C1-C2-C3-O3
2	B	902	GOL	C1-C2-C3-O3
2	A	903	GOL	O1-C1-C2-O2
2	A	903	GOL	O1-C1-C2-C3
2	A	905	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	905	GOL	2	0
2	B	907	GOL	3	0
2	A	901	GOL	3	0
2	B	908	GOL	3	0
2	A	903	GOL	2	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	405/411 (98%)	0.26	14 (3%) 47 37	28, 62, 122, 159	0
1	B	403/411 (98%)	0.02	7 (1%) 69 60	30, 56, 95, 118	0
All	All	808/822 (98%)	0.14	21 (2%) 57 47	28, 59, 111, 159	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	LEU	3.2
1	A	120	MET	3.1
1	A	70	SER	3.0
1	A	69	ALA	3.0
1	A	326	GLY	2.9

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	GOL	A	906	6/6	0.69	0.22	75,75,76,76	0
2	GOL	A	903	6/6	0.76	0.17	64,66,66,67	0
2	GOL	A	904	6/6	0.80	0.14	71,73,75,75	0
2	GOL	B	908	6/6	0.85	0.22	60,62,62,63	0
2	GOL	B	902	6/6	0.86	0.14	73,77,78,78	0
2	GOL	A	905	6/6	0.86	0.10	73,74,74,74	0
2	GOL	A	901	6/6	0.88	0.15	46,50,52,54	0
2	GOL	B	907	6/6	0.92	0.09	31,34,36,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.