



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2024 – 07:51 am BST

PDB ID : 2JAJ
Title : DDAH1 complexed with L-257
Authors : Murray-Rust, J.; O'Hara, B.P.; Rossiter, S.; Leiper, J.M.; Vallance, P.; McDonald, N.Q.
Deposited on : 2006-11-29
Resolution : 2.00 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

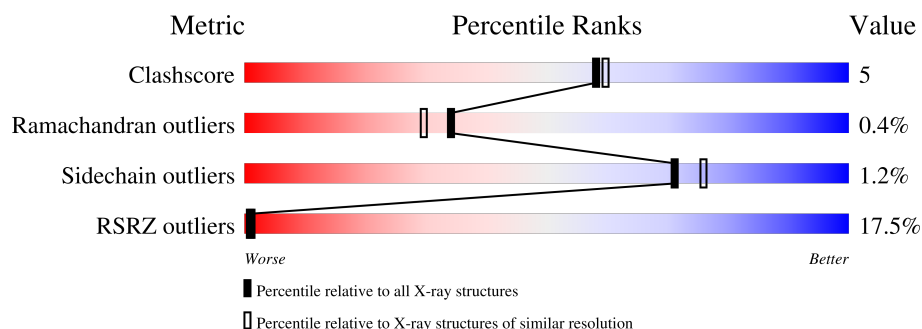
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	289	
1	B	289	

2 Entry composition [i](#)

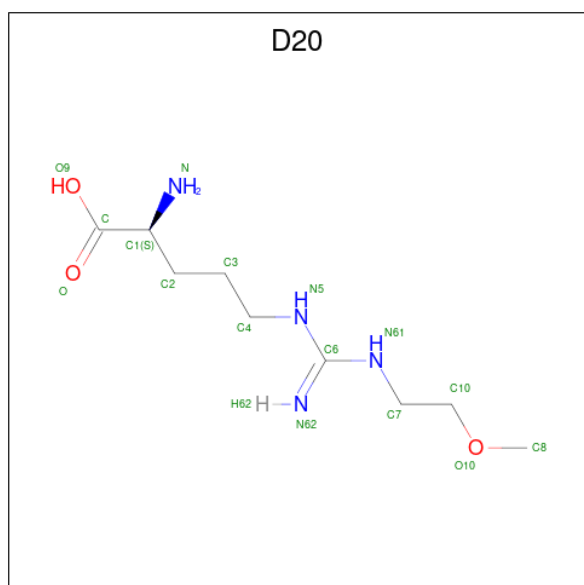
There are 3 unique types of molecules in this entry. The entry contains 4381 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NG, NG-DIMETHYLARGININE DIMETHYLAMINOHYDROLYASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	2	0
			2054	1292	347	401	14			
1	B	281	Total	C	N	O	S	0	0	0
			2014	1270	344	387	13			

- Molecule 2 is N 5 -{IMINO[(2-METHOXYETHYL)AMINO]METHYL}-L-ORNITHINE (three-letter code: D20) (formula: $C_9H_{20}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	9	4	3		
2	B	1	Total	C	N	O	0	0
			16	9	4	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	233	Total 233	O 233	0	0
3	B	48	Total 48	O 48	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.85Å 46.91Å 147.61Å 90.00° 94.56° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 32.36 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.6 (30.00-2.00) 93.6 (32.36-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.19 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.263 0.213 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4381	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% 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: D20

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	0.95	0/2091	0.86	1/2835 (0.0%)
1	B	0.59	0/2047	0.73	0/2792
All	All	0.79	0/4138	0.80	1/5627 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

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	203	MET	CG-SD-CE	6.14	110.02	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	ALA	Peptide

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	2054	0	2025	9	0
1	B	2014	0	1902	31	0
2	A	16	0	19	0	0
2	B	16	0	18	1	0
3	A	233	0	0	2	0
3	B	48	0	0	1	0
All	All	4381	0	3964	39	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.

All (39) 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:116:VAL:HG11	1:B:156:THR:OG1	1.90	0.71
1:A:197:LEU:O	1:A:201:GLN:HG3	1.91	0.70
1:B:251:LEU:HB2	1:B:256:LEU:HD21	1.77	0.66
1:B:44:ARG:NH2	1:B:47:GLN:OE1	2.32	0.62
1:B:-4:GLY:N	3:B:2001:HOH:O	2.32	0.62
1:B:142:SER:OG	1:B:145:THR:N	2.30	0.60
1:A:224:LEU:HD23	3:A:2002:HOH:O	2.05	0.55
1:B:41:ARG:HB3	1:B:263:GLU:HG3	1.89	0.54
1:A:198:LYS:NZ	3:A:2173:HOH:O	2.43	0.52
1:B:46:HIS:O	1:B:49:TYR:HB3	2.09	0.52
1:B:251:LEU:HB3	1:B:254:HIS:HB2	1.91	0.51
1:B:75:PHE:CE2	1:B:269:GLY:HA3	2.45	0.51
1:B:215:ASP:CB	1:B:241:TYR:CD2	2.94	0.51
1:B:5:HIS:HB2	1:B:6:PRO:HD2	1.93	0.51
1:B:237:THR:HB	1:B:238:PRO:HD2	1.93	0.50
1:B:214:PRO:HG2	1:B:243:GLU:HB3	1.94	0.49
1:B:231:HIS:HB3	1:B:254:HIS:CD2	2.48	0.49
1:A:64:LEU:HD13	1:A:103:MET:HG2	1.94	0.48
1:B:215:ASP:CB	1:B:241:TYR:HD2	2.27	0.47
1:B:91:ARG:HB2	1:B:118:MET:HG2	1.97	0.47
1:B:176:PHE:HA	1:B:216:ASP:O	2.15	0.46
1:B:5:HIS:HB2	1:B:6:PRO:CD	2.46	0.46
1:A:187:ILE:HG12	1:A:197:LEU:HD22	1.99	0.45
1:B:18:ARG:HD3	1:B:73:CYS:HB2	1.97	0.45
1:B:153:LEU:O	1:B:156:THR:HB	2.16	0.45
1:B:215:ASP:HB3	1:B:241:TYR:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:LEU:C	1:B:278:ILE:HG13	2.37	0.44
1:B:185:ILE:O	1:B:211:LEU:N	2.47	0.44
1:A:141:LEU:HG	1:A:164:THR:HB	2.00	0.43
1:B:76:VAL:O	1:B:79:VAL:HG22	2.19	0.43
1:A:147:GLN:HE22	1:B:-2:LEU:HD21	1.84	0.43
1:A:154:ALA:HA	1:A:162:VAL:HG21	2.02	0.42
1:B:178:SER:O	1:B:185:ILE:HG23	2.19	0.42
1:B:187:ILE:HG23	1:B:212:THR:HG23	2.01	0.42
1:B:125:LEU:HD12	1:B:145:THR:HG23	2.03	0.41
1:B:237:THR:HB	1:B:238:PRO:CD	2.50	0.41
1:B:133:THR:HA	1:B:179:MET:SD	2.60	0.41
1:B:72:ASP:OD1	2:B:500:D20:N	2.49	0.41
1:A:77:GLU:HB3	1:A:273:CYS:HA	2.02	0.40

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	270/289 (93%)	261 (97%)	8 (3%)	1 (0%)	34	30
1	B	275/289 (95%)	256 (93%)	18 (6%)	1 (0%)	34	30
All	All	545/578 (94%)	517 (95%)	26 (5%)	2 (0%)	34	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	B	121	GLU

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	220/241 (91%)	219 (100%)	1 (0%)	88	92
1	B	197/241 (82%)	193 (98%)	4 (2%)	55	58
All	All	417/482 (86%)	412 (99%)	5 (1%)	71	76

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	B	44	ARG
1	B	158	LYS
1	B	213	VAL
1	B	256	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	GLN
1	B	206	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry

2 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	D20	A	500	-	12,15,15	1.12	1 (8%)	16,17,17	0.93	0
2	D20	B	500	-	12,15,15	1.19	1 (8%)	16,17,17	0.76	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	D20	A	500	-	-	0/16/16/16	-
2	D20	B	500	-	-	1/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	D20	C6-N62	2.29	1.36	1.29
2	B	500	D20	C2-C1	2.11	1.57	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	D20	C2-C3-C4-N5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	D20	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

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	272/289 (94%)	0.36	17 (6%) 20 19	25, 31, 40, 52	0
1	B	281/289 (97%)	1.43	80 (28%) 0 0	29, 47, 70, 73	0
All	All	553/578 (95%)	0.91	97 (17%) 1 1	25, 37, 68, 73	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	213	VAL	7.8
1	B	189	SER	7.5
1	B	192	SER	6.4
1	B	200	MET	5.2
1	B	204	SER	5.0
1	B	242	PRO	4.8
1	B	165	VAL	4.5
1	B	238	PRO	4.4
1	A	34	GLY	4.3
1	B	209	ASP	4.3
1	B	250	LYS	4.3
1	B	163	SER	4.3
1	B	241	TYR	4.2
1	B	156	THR	4.1
1	B	114	ASN	3.9
1	B	205	ASP	3.9
1	B	246	LYS	3.9
1	B	115	ILE	3.8
1	B	188	GLY	3.8
1	B	76	VAL	3.7
1	B	252	LYS	3.6
1	A	272	THR	3.6
1	B	202	GLN	3.6
1	B	214	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	-1	GLY	3.5
1	B	211	LEU	3.5
1	B	249	GLU	3.5
1	B	131	LEU	3.5
1	B	248	TYR	3.5
1	B	130	VAL	3.4
1	B	187	ILE	3.3
1	B	166	PRO	3.3
1	A	274	CYS	3.3
1	A	277	LEU	3.2
1	A	222	ILE	3.2
1	B	247	VAL	3.2
1	B	234	LEU	3.1
1	B	128	GLY	3.1
1	A	276	VAL	3.1
1	B	197	LEU	3.0
1	B	141	LEU	3.0
1	B	245	ALA	3.0
1	A	270	LEU	3.0
1	B	185	ILE	2.9
1	B	203	MET	2.9
1	B	32	ALA	2.9
1	B	53	LEU	2.9
1	A	271	LEU	2.8
1	A	76	VAL	2.7
1	A	81	VAL	2.7
1	B	138	PHE	2.7
1	A	130	VAL	2.7
1	B	0	MET	2.7
1	B	259	VAL	2.6
1	B	235	HIS	2.6
1	B	154	ALA	2.6
1	B	258	PRO	2.6
1	B	271	LEU	2.6
1	B	149	GLY	2.5
1	B	1	ALA	2.5
1	B	123	ALA	2.5
1	B	127	GLY	2.5
1	B	215	ASP	2.5
1	A	128	GLY	2.5
1	B	174	LYS	2.5
1	A	275	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	276	VAL	2.4
1	B	198	LYS	2.4
1	B	151	GLU	2.4
1	B	222	ILE	2.4
1	B	251	LEU	2.3
1	B	228	ASN	2.3
1	B	40	ALA	2.3
1	B	272	THR	2.3
1	B	273	CYS	2.3
1	B	161	ALA	2.2
1	A	273	CYS	2.2
1	A	79	VAL	2.2
1	B	118	MET	2.2
1	B	159	ASP	2.2
1	A	131	LEU	2.2
1	B	93	GLY	2.1
1	A	221	CYS	2.1
1	B	275	SER	2.1
1	B	206	HIS	2.1
1	B	230	GLY	2.1
1	B	132	PHE	2.1
1	B	178	SER	2.1
1	B	17	VAL	2.1
1	B	196	ALA	2.1
1	B	244	SER	2.1
1	B	120	ASP	2.1
1	B	139	VAL	2.0
1	B	145	THR	2.0
1	B	180	ALA	2.0
1	B	243	GLU	2.0
1	B	190	SER	2.0

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 monosaccharides 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
2	D20	B	500	16/16	0.86	0.14	39,41,47,47	0
2	D20	A	500	16/16	0.92	0.17	28,32,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.