



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 28, 2026 – 12:18 PM EDT

PDB ID : 9O3S / pdb_00009o3s
Title : Crystal Structure of R36A Variant of D-Dopachrome Tautomerase (D-DT)
Authors : Pilien, A.V.R.; Argueta, C.; Parkins, A.; Pantouris, G.
Deposited on : 2025-04-07
Resolution : 1.64 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
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

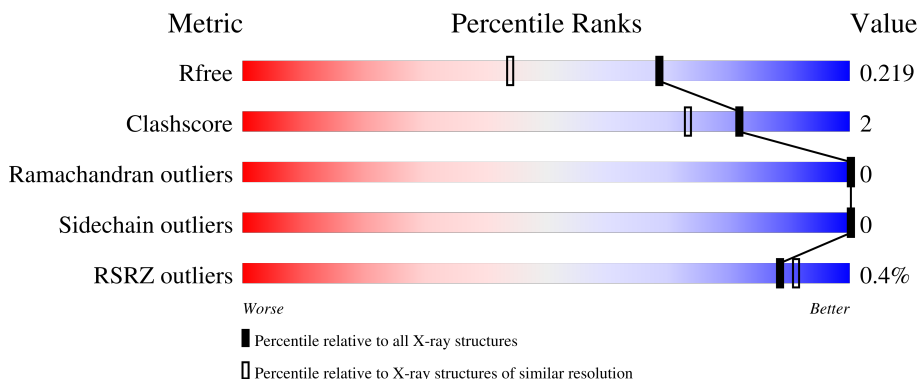
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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.



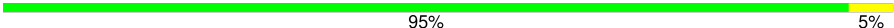





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	AAA	117	<div> <div>%</div> <div>95% 5%</div> </div>
1	BBB	117	<div> <div>%</div> <div>92% 8%</div> </div>
1	CCC	117	<div> <div>97% .</div> </div>
1	DDD	117	<div> <div>%</div> <div>94% 6%</div> </div>
1	EEE	117	<div> <div>96% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	FFF	117	 95%5%
1	GGG	117	 93%7%
1	HHH	117	 92%8%
1	III	117	 92%8%
1	JJJ	117	 90%10%
1	KKK	117	 87%13%
1	LLL	117	 2%94%6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12069 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 D-dopachrome decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	117	Total	C	N	O	S	0	2	0
			877	560	150	162	5			
1	BBB	117	Total	C	N	O	S	0	2	0
			890	569	151	165	5			
1	CCC	117	Total	C	N	O	S	0	1	0
			878	561	148	165	4			
1	DDD	117	Total	C	N	O	S	0	3	0
			889	567	150	167	5			
1	EEE	117	Total	C	N	O	S	0	0	0
			872	557	150	161	4			
1	FFF	117	Total	C	N	O	S	0	0	0
			866	554	149	159	4			
1	GGG	117	Total	C	N	O	S	0	0	0
			873	558	148	163	4			
1	HHH	117	Total	C	N	O	S	0	2	0
			885	565	151	165	4			
1	III	117	Total	C	N	O	S	0	1	0
			879	561	150	164	4			
1	JJJ	117	Total	C	N	O	S	0	1	0
			880	563	148	165	4			
1	KKK	117	Total	C	N	O	S	0	1	0
			879	561	150	163	5			
1	LLL	117	Total	C	N	O	S	0	0	0
			875	558	150	163	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	36	ALA	ARG	variant	UNP P30046
BBB	36	ALA	ARG	variant	UNP P30046
CCC	36	ALA	ARG	variant	UNP P30046
DDD	36	ALA	ARG	variant	UNP P30046
EEE	36	ALA	ARG	variant	UNP P30046

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Chain	Residue	Modelled	Actual	Comment	Reference
FFF	36	ALA	ARG	variant	UNP P30046
GGG	36	ALA	ARG	variant	UNP P30046
HHH	36	ALA	ARG	variant	UNP P30046
III	36	ALA	ARG	variant	UNP P30046
JJJ	36	ALA	ARG	variant	UNP P30046
KKK	36	ALA	ARG	variant	UNP P30046
LLL	36	ALA	ARG	variant	UNP P30046

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	115	Total O 115 115	0	0
2	BBB	127	Total O 127 127	0	0
2	CCC	121	Total O 121 121	0	0
2	DDD	128	Total O 128 128	0	0
2	EEE	138	Total O 138 138	0	0
2	FFF	123	Total O 123 123	0	0
2	GGG	123	Total O 123 123	0	0
2	HHH	135	Total O 135 135	0	0
2	III	127	Total O 127 127	0	0
2	JJJ	128	Total O 128 128	0	0
2	KKK	141	Total O 141 141	0	0
2	LLL	120	Total O 120 120	0	0

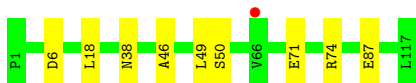
3 Residue-property plots [i](#)

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 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: D-dopachrome decarboxylase



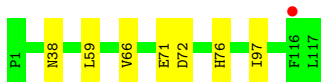
- Molecule 1: D-dopachrome decarboxylase



- Molecule 1: D-dopachrome decarboxylase



- Molecule 1: D-dopachrome decarboxylase



- Molecule 1: D-dopachrome decarboxylase



- Molecule 1: D-dopachrome decarboxylase

Chain FFF:  95% 5%



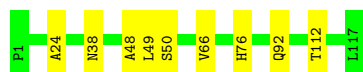
- Molecule 1: D-dopachrome decarboxylase

Chain GGG:  93% 7%



- Molecule 1: D-dopachrome decarboxylase

Chain HHH:  92% 8%



- Molecule 1: D-dopachrome decarboxylase

Chain III:  92% 8%



- Molecule 1: D-dopachrome decarboxylase

Chain JJJ:  90% 10%



- Molecule 1: D-dopachrome decarboxylase

Chain KKK:  87% 13%



- Molecule 1: D-dopachrome decarboxylase

Chain LLL:  94% 6% 2%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.97Å 49.25Å 142.75Å 84.63° 86.40° 61.06°	Depositor
Resolution (Å)	71.15 – 1.64 71.15 – 1.64	Depositor EDS
% Data completeness (in resolution range)	95.3 (71.15-1.64) 95.3 (71.15-1.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.54 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.169 , 0.210 0.180 , 0.219	Depositor DCC
R_{free} test set	6352 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.019 for h-k,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12069	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8720e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	AAA	1.16	0/900	1.28	2/1220 (0.2%)
1	BBB	1.17	0/913	1.24	1/1236 (0.1%)
1	CCC	1.10	0/898	1.25	2/1218 (0.2%)
1	DDD	1.13	0/915	1.28	1/1241 (0.1%)
1	EEE	1.14	1/889 (0.1%)	1.20	0/1206
1	FFF	1.15	1/883 (0.1%)	1.22	0/1199
1	GGG	1.18	2/890 (0.2%)	1.28	2/1207 (0.2%)
1	HHH	1.17	1/908 (0.1%)	1.24	1/1230 (0.1%)
1	III	1.15	0/899	1.24	3/1219 (0.2%)
1	JJJ	1.10	0/900	1.29	4/1220 (0.3%)
1	KKK	1.15	1/899 (0.1%)	1.21	0/1219
1	LLL	1.08	0/892	1.26	1/1210 (0.1%)
All	All	1.14	6/10786 (0.1%)	1.25	17/14625 (0.1%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	HHH	24	ALA	C-O	6.94	1.32	1.24
1	GGG	5	LEU	C-O	5.86	1.30	1.24
1	FFF	46	ALA	C-O	5.72	1.30	1.24
1	EEE	85	THR	N-CA	5.31	1.52	1.46
1	GGG	24	ALA	C-O	5.09	1.30	1.24

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	6	ASP	CA-CB-CG	5.98	118.58	112.60
1	LLL	35	ASP	CA-CB-CG	5.88	118.48	112.60
1	GGG	72	ASP	CA-CB-CG	5.63	118.23	112.60
1	HHH	92	GLN	CB-CG-CD	5.52	121.99	112.60
1	III	35	ASP	CA-CB-CG	5.47	118.08	112.60

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	AAA	877	0	891	5	0
1	BBB	890	0	913	8	0
1	CCC	878	0	888	1	0
1	DDD	889	0	902	5	0
1	EEE	872	0	885	4	0
1	FFF	866	0	874	5	0
1	GGG	873	0	887	3	0
1	HHH	885	0	908	9	0
1	III	879	0	894	6	0
1	JJJ	880	0	895	11	0
1	KKK	879	0	894	10	0
1	LLL	875	0	887	4	0
2	AAA	115	0	0	2	0
2	BBB	127	0	0	0	0
2	CCC	121	0	0	0	0
2	DDD	128	0	0	0	0
2	EEE	138	0	0	1	0
2	FFF	123	0	0	0	0
2	GGG	123	0	0	1	0
2	HHH	135	0	0	1	0
2	III	127	0	0	0	0
2	JJJ	128	0	0	0	0
2	KKK	141	0	0	0	0
2	LLL	120	0	0	0	0
All	All	12069	0	10718	53	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 2.

The worst 5 of 53 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:KKK:103:GLU:H	1:KKK:106:GLN:HE21	1.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JJJ:18:LEU:HD13	1:JJJ:87:GLU:CG	2.18	0.73
1:AAA:114:MET:SD	2:AAA:306:HOH:O	2.50	0.69
1:DDD:38:ASN:HD22	1:EEE:49:LEU:HA	1.61	0.65
1:JJJ:18:LEU:HD13	1:JJJ:87:GLU:HG2	1.79	0.64

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	AAA	117/117 (100%)	112 (96%)	5 (4%)	0	100	100
1	BBB	117/117 (100%)	112 (96%)	5 (4%)	0	100	100
1	CCC	116/117 (99%)	112 (97%)	4 (3%)	0	100	100
1	DDD	118/117 (101%)	114 (97%)	4 (3%)	0	100	100
1	EEE	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	FFF	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
1	GGG	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	HHH	117/117 (100%)	115 (98%)	2 (2%)	0	100	100
1	III	116/117 (99%)	112 (97%)	4 (3%)	0	100	100
1	JJJ	116/117 (99%)	112 (97%)	4 (3%)	0	100	100
1	KKK	116/117 (99%)	112 (97%)	4 (3%)	0	100	100
1	LLL	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
All	All	1393/1404 (99%)	1348 (97%)	45 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	93/94 (99%)	93 (100%)	0	100	100
1	BBB	96/94 (102%)	96 (100%)	0	100	100
1	CCC	93/94 (99%)	93 (100%)	0	100	100
1	DDD	96/94 (102%)	96 (100%)	0	100	100
1	EEE	92/94 (98%)	92 (100%)	0	100	100
1	FFF	90/94 (96%)	90 (100%)	0	100	100
1	GGG	93/94 (99%)	93 (100%)	0	100	100
1	HHH	96/94 (102%)	96 (100%)	0	100	100
1	III	94/94 (100%)	94 (100%)	0	100	100
1	JJJ	94/94 (100%)	94 (100%)	0	100	100
1	KKK	94/94 (100%)	94 (100%)	0	100	100
1	LLL	93/94 (99%)	93 (100%)	0	100	100
All	All	1124/1128 (100%)	1124 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes 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 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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	AAA	117/117 (100%)	-0.19	1 (0%) 81 85	8, 13, 22, 28	2 (1%)
1	BBB	117/117 (100%)	-0.14	1 (0%) 81 85	7, 13, 21, 28	2 (1%)
1	CCC	117/117 (100%)	-0.14	0 100 100	9, 14, 24, 34	1 (0%)
1	DDD	117/117 (100%)	-0.27	1 (0%) 81 85	6, 11, 22, 25	3 (2%)
1	EEE	117/117 (100%)	-0.40	0 100 100	8, 11, 17, 22	0
1	FFF	117/117 (100%)	-0.19	0 100 100	9, 14, 20, 30	0
1	GGG	117/117 (100%)	-0.10	0 100 100	8, 13, 25, 31	0
1	HHH	117/117 (100%)	-0.18	0 100 100	7, 13, 20, 39	2 (1%)
1	III	117/117 (100%)	-0.16	0 100 100	8, 14, 20, 28	1 (0%)
1	JJJ	117/117 (100%)	-0.09	0 100 100	7, 14, 23, 32	1 (0%)
1	KKK	117/117 (100%)	-0.20	0 100 100	9, 13, 20, 26	1 (0%)
1	LLL	117/117 (100%)	0.05	2 (1%) 69 74	10, 15, 28, 46	0
All	All	1404/1404 (100%)	-0.17	5 (0%) 88 91	6, 13, 23, 46	13 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	66	VAL	2.4
1	DDD	116	PHE	2.3
1	LLL	13	ARG	2.1
1	AAA	65	GLY	2.0
1	LLL	16	ALA	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.