



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 03:28 pm BST

PDB ID : 5IOI  
Title : X-RAY STRUCTURE OF THE N-TERMINAL DOMAIN OF HUMAN DOUBLECORTIN  
Authors : Ruf, A.; Benz, J.; Burger, D.; D'Arcy, B.; Debulpaep, M.; Di Lello, P.; Fry, D.; Huber, W.; Kremer, T.; Laeremans, T.; Matile, H.; Ross, A.; Rudolph, M.G.; Rufer, A.C.; Sharma, A.; Steinmetz, M.O.; Steyaert, J.; Schoch, G.; Stihle, M.; Thoma, R.  
Deposited on : 2016-03-08  
Resolution : 2.40 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

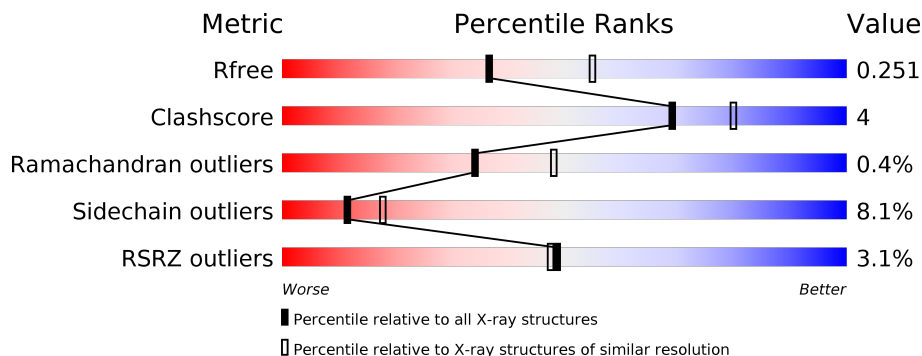
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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	107	
1	B	107	
1	C	107	
1	D	107	
1	E	107	
1	F	107	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 5085 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 Neuronal migration protein doublecortin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	107	Total 866	C 544	N 151	O 168	S 3	0	0	0
1	B	88	Total 716	C 450	N 121	O 143	S 2	0	0	0
1	C	96	Total 783	C 492	N 134	O 155	S 2	0	0	0
1	D	89	Total 724	C 455	N 122	O 144	S 3	0	0	0
1	E	107	Total 866	C 544	N 151	O 168	S 3	0	0	0
1	F	95	Total 777	C 489	N 133	O 153	S 2	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	LEU	-	expression tag	UNP O43602
A	126	VAL	-	expression tag	UNP O43602
A	127	PRO	-	expression tag	UNP O43602
A	128	ARG	-	expression tag	UNP O43602
A	129	GLY	-	expression tag	UNP O43602
A	130	SER	-	expression tag	UNP O43602
A	131	HIS	-	expression tag	UNP O43602
A	132	MET	-	expression tag	UNP O43602
A	215	ASP	LYS	engineered mutation	UNP O43602
A	216	ASP	LYS	engineered mutation	UNP O43602
B	125	LEU	-	expression tag	UNP O43602
B	126	VAL	-	expression tag	UNP O43602
B	127	PRO	-	expression tag	UNP O43602
B	128	ARG	-	expression tag	UNP O43602
B	129	GLY	-	expression tag	UNP O43602
B	130	SER	-	expression tag	UNP O43602
B	131	HIS	-	expression tag	UNP O43602

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	132	MET	-	expression tag	UNP O43602
B	215	ASP	LYS	engineered mutation	UNP O43602
B	216	ASP	LYS	engineered mutation	UNP O43602
C	125	LEU	-	expression tag	UNP O43602
C	126	VAL	-	expression tag	UNP O43602
C	127	PRO	-	expression tag	UNP O43602
C	128	ARG	-	expression tag	UNP O43602
C	129	GLY	-	expression tag	UNP O43602
C	130	SER	-	expression tag	UNP O43602
C	131	HIS	-	expression tag	UNP O43602
C	132	MET	-	expression tag	UNP O43602
C	215	ASP	LYS	engineered mutation	UNP O43602
C	216	ASP	LYS	engineered mutation	UNP O43602
D	125	LEU	-	expression tag	UNP O43602
D	126	VAL	-	expression tag	UNP O43602
D	127	PRO	-	expression tag	UNP O43602
D	128	ARG	-	expression tag	UNP O43602
D	129	GLY	-	expression tag	UNP O43602
D	130	SER	-	expression tag	UNP O43602
D	131	HIS	-	expression tag	UNP O43602
D	132	MET	-	expression tag	UNP O43602
D	215	ASP	LYS	engineered mutation	UNP O43602
D	216	ASP	LYS	engineered mutation	UNP O43602
E	125	LEU	-	expression tag	UNP O43602
E	126	VAL	-	expression tag	UNP O43602
E	127	PRO	-	expression tag	UNP O43602
E	128	ARG	-	expression tag	UNP O43602
E	129	GLY	-	expression tag	UNP O43602
E	130	SER	-	expression tag	UNP O43602
E	131	HIS	-	expression tag	UNP O43602
E	132	MET	-	expression tag	UNP O43602
E	215	ASP	LYS	engineered mutation	UNP O43602
E	216	ASP	LYS	engineered mutation	UNP O43602
F	125	LEU	-	expression tag	UNP O43602
F	126	VAL	-	expression tag	UNP O43602
F	127	PRO	-	expression tag	UNP O43602
F	128	ARG	-	expression tag	UNP O43602
F	129	GLY	-	expression tag	UNP O43602
F	130	SER	-	expression tag	UNP O43602
F	131	HIS	-	expression tag	UNP O43602
F	132	MET	-	expression tag	UNP O43602
F	215	ASP	LYS	engineered mutation	UNP O43602

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	216	ASP	LYS	engineered mutation	UNP O43602


- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	95	Total O 95 95	0	0
2	B	50	Total O 50 50	0	0
2	C	58	Total O 58 58	0	0
2	D	26	Total O 26 26	0	0
2	E	69	Total O 69 69	0	0
2	F	55	Total O 55 55	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Neuronal migration protein doublecortin

Chain A: 




- Molecule 1: Neuronal migration protein doublecortin

Chain B: 




- Molecule 1: Neuronal migration protein doublecortin

Chain C: 




- Molecule 1: Neuronal migration protein doublecortin

Chain D: 

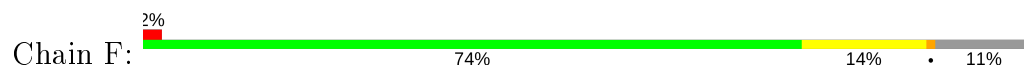


- Molecule 1: Neuronal migration protein doublecortin

Chain E: 



- Molecule 1: Neuronal migration protein doublecortin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.72Å 97.72Å 377.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.14 – 2.40 35.10 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.14-2.40) 100.0 (35.10-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 2.39Å)	Xtrriage
Refinement program	BUSTER 2.9.2	Depositor
R, $R_{free}$	0.196 , 0.234 0.211 , 0.251	Depositor DCC
$R_{free}$ test set	2200 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.0	Xtrriage
Anisotropy	0.060	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5085	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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	0.55	0/884	0.79	0/1193
1	B	0.49	0/729	0.72	0/980
1	C	0.48	0/799	0.72	0/1077
1	D	0.97	1/737 (0.1%)	1.63	3/990 (0.3%)
1	E	0.53	0/884	0.78	0/1193
1	F	0.52	0/793	0.77	0/1069
All	All	0.61	1/4826 (0.0%)	0.95	3/6502 (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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	132	MET	C-N	-22.87	0.81	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	132	MET	O-C-N	-35.17	66.43	122.70
1	D	132	MET	CA-C-N	24.65	171.43	117.20
1	D	132	MET	C-N-CA	17.91	166.47	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	132	MET	Mainchain

## 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	866	0	829	14	0
1	B	716	0	679	7	0
1	C	783	0	741	4	0
1	D	724	0	687	4	0
1	E	866	0	829	8	0
1	F	777	0	736	10	0
2	A	95	0	0	0	0
2	B	50	0	0	1	0
2	C	58	0	0	2	0
2	D	26	0	0	0	0
2	E	69	0	0	0	0
2	F	55	0	0	1	0
All	All	5085	0	4501	34	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 4.

The worst 5 of 34 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:230:ASN:HD22	1:E:150:VAL:H	1.19	0.90
1:A:224:ASN:HD22	1:A:224:ASN:H	1.27	0.81
1:B:147:LYS:HE3	1:B:147:LYS:H	1.49	0.77
1:A:128:ARG:NH2	1:B:171:SER:OG	2.26	0.68
1:A:150:VAL:H	1:E:230:ASN:HD22	1.46	0.60

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	105/107 (98%)	104 (99%)	1 (1%)	0	100	100
1	B	86/107 (80%)	84 (98%)	2 (2%)	0	100	100
1	C	94/107 (88%)	90 (96%)	3 (3%)	1 (1%)	14	20
1	D	87/107 (81%)	85 (98%)	2 (2%)	0	100	100
1	E	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
1	F	93/107 (87%)	91 (98%)	1 (1%)	1 (1%)	14	20
All	All	570/642 (89%)	552 (97%)	16 (3%)	2 (0%)	34	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	227	TRP
1	F	173	SER

### 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	96/96 (100%)	89 (93%)	7 (7%)	14	22
1	B	78/96 (81%)	72 (92%)	6 (8%)	13	20
1	C	86/96 (90%)	77 (90%)	9 (10%)	7	9
1	D	79/96 (82%)	72 (91%)	7 (9%)	9	14
1	E	96/96 (100%)	90 (94%)	6 (6%)	18	28

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	85/96 (88%)	78 (92%)	7 (8%)	11	17
All	All	520/576 (90%)	478 (92%)	42 (8%)	11	18

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	180	GLN
1	D	135	LYS
1	F	211	ASP
1	C	211	ASP
1	C	228	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	180	GLN
1	F	226	ASN
1	E	230	ASN
1	A	230	ASN
1	F	180	GLN

### 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 carbohydrates 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	132:MET	C	133:ALA	N	0.81

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	107/107 (100%)	-0.46	0 <b>100</b> <b>100</b>	24, 34, 53, 72	0
1	B	88/107 (82%)	0.12	5 (5%) <b>23</b> <b>22</b>	30, 49, 86, 89	0
1	C	96/107 (89%)	-0.19	2 (2%) <b>63</b> <b>61</b>	30, 47, 78, 82	0
1	D	89/107 (83%)	0.37	8 (8%) <b>9</b> <b>8</b>	33, 63, 94, 105	0
1	E	107/107 (100%)	-0.26	1 (0%) <b>84</b> <b>82</b>	27, 41, 67, 79	0
1	F	95/107 (88%)	-0.26	2 (2%) <b>63</b> <b>61</b>	31, 45, 74, 83	0
All	All	582/642 (90%)	-0.13	18 (3%) <b>49</b> <b>47</b>	24, 45, 81, 105	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	213	PHE	4.7
1	B	213	PHE	4.3
1	E	213	PHE	3.9
1	B	176	ILE	3.8
1	F	212	ASN	3.5

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.