



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6E7O / pdb_00006e7o
Title : Crystal structure of deglycosylated human EPDR1
Authors : Wei, Y.; Prive, G.G.
Deposited on : 2018-07-27
Resolution : 3.00 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

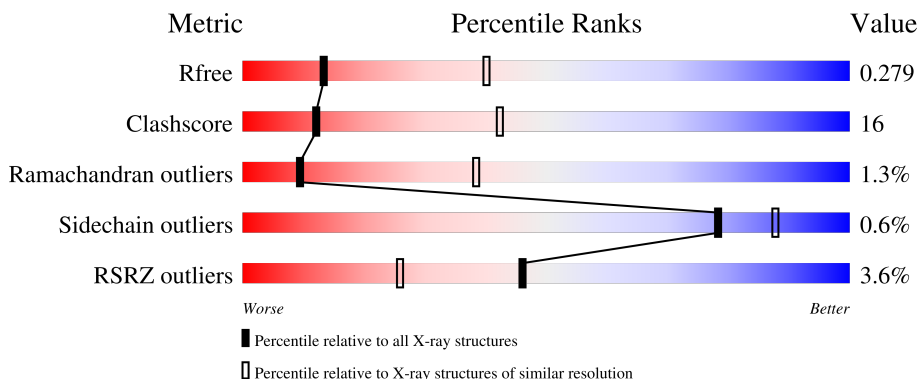
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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	194	2% 55% 29% • 14%
1	B	194	0% 53% 30% 17%
1	C	194	6% 54% 25% 21%
1	D	194	3% 58% 25% • 16%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5040 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 Mammalian ependymin-related protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	0	0	0
			1327	842	218	259	8			
1	B	161	Total	C	N	O	S	0	0	0
			1280	812	207	254	7			
1	C	154	Total	C	N	O	S	0	0	0
			1158	736	182	235	5			
1	D	163	Total	C	N	O	S	0	0	0
			1275	813	206	248	8			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	SER	-	expression tag	UNP Q9UM22
A	225	HIS	-	expression tag	UNP Q9UM22
A	226	HIS	-	expression tag	UNP Q9UM22
A	227	HIS	-	expression tag	UNP Q9UM22
A	228	HIS	-	expression tag	UNP Q9UM22
A	229	HIS	-	expression tag	UNP Q9UM22
A	230	HIS	-	expression tag	UNP Q9UM22
B	37	SER	-	expression tag	UNP Q9UM22
B	225	HIS	-	expression tag	UNP Q9UM22
B	226	HIS	-	expression tag	UNP Q9UM22
B	227	HIS	-	expression tag	UNP Q9UM22
B	228	HIS	-	expression tag	UNP Q9UM22
B	229	HIS	-	expression tag	UNP Q9UM22
B	230	HIS	-	expression tag	UNP Q9UM22
C	37	SER	-	expression tag	UNP Q9UM22
C	225	HIS	-	expression tag	UNP Q9UM22
C	226	HIS	-	expression tag	UNP Q9UM22
C	227	HIS	-	expression tag	UNP Q9UM22
C	228	HIS	-	expression tag	UNP Q9UM22
C	229	HIS	-	expression tag	UNP Q9UM22
C	230	HIS	-	expression tag	UNP Q9UM22

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Chain	Residue	Modelled	Actual	Comment	Reference
D	37	SER	-	expression tag	UNP Q9UM22
D	225	HIS	-	expression tag	UNP Q9UM22
D	226	HIS	-	expression tag	UNP Q9UM22
D	227	HIS	-	expression tag	UNP Q9UM22
D	228	HIS	-	expression tag	UNP Q9UM22
D	229	HIS	-	expression tag	UNP Q9UM22
D	230	HIS	-	expression tag	UNP Q9UM22

- Molecule 1: Mammalian ependymin-related protein 1



LYS
MET
SER
GLU
ASP
CYS
SER
TRP
HIS
HIS
HIS
HIS
HIS
HIS

● Molecule 1: Mammalian endymin-related protein 1



SER
A36
C42
Q46
V53
M54
Y55
Q56
G60
R61
N62
S63
R64
A65
L66
L67
S68
Y69
D70
G71
R76
V78
K83
ALA
LEU
ILE
PRO
CYS
LYS
R90
L91
Y98
F104
Q105
I106
Q112
C113
S114
L118
T119
Q120
P121
W122
I127
S138
I139
GLY

GLY
PRO
Q143
I146
T147
E150
R154
K155
SER
ALA
ARG
SER
TYR
T162
W163
I164
G165
I166
D171
G172
Y173
F174
V175
T178
I181
N182
V185
I186
L187
S188
T189
R190
F191
F192
S202
T203
F204
T205
M212
A213
S214
L215
GLU
LYS
MET
SER
GLU
ASP
CYS
SER

TRP
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	87.81Å 97.48Å 189.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.69 – 3.00 61.69 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (61.69-3.00) 92.7 (61.69-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.14_3211)	Depositor
R, R_{free}	0.255 , 0.278 0.257 , 0.279	Depositor DCC
R_{free} test set	863 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	70.6	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 72.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5040	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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](#)

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	0.20	0/1358	0.51	0/1849
1	B	0.25	0/1311	0.58	0/1788
1	C	0.16	0/1184	0.42	0/1621
1	D	0.20	0/1304	0.52	0/1780
All	All	0.21	0/5157	0.51	0/7038

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1327	0	1240	39	0
1	B	1280	0	1184	43	0
1	C	1158	0	1007	34	0
1	D	1275	0	1172	47	0
All	All	5040	0	4603	150	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 150 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:C:79:LEU:HD23	1:C:93:GLU:HB3	1.56	0.85
1:D:53:VAL:HG12	1:D:64:ARG:HB3	1.60	0.84
1:A:137:TYR:OH	1:B:64:ARG:NH2	2.18	0.76
1:C:96:LEU:HD23	1:C:103:MET:HB3	1.68	0.76
1:D:114:SER:HB2	1:D:215:LEU:HD12	1.69	0.75

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	161/194 (83%)	153 (95%)	4 (2%)	4 (2%)	4	23
1	B	155/194 (80%)	148 (96%)	5 (3%)	2 (1%)	9	38
1	C	142/194 (73%)	132 (93%)	9 (6%)	1 (1%)	18	53
1	D	155/194 (80%)	148 (96%)	6 (4%)	1 (1%)	21	56
All	All	613/776 (79%)	581 (95%)	24 (4%)	8 (1%)	9	38

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ILE
1	B	185	VAL
1	C	186	ILE
1	D	119	THR
1	A	107	ASP

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	145/179 (81%)	144 (99%)	1 (1%)	76	86
1	B	142/179 (79%)	142 (100%)	0	100	100
1	C	119/179 (66%)	118 (99%)	1 (1%)	73	86
1	D	137/179 (76%)	136 (99%)	1 (1%)	76	86
All	All	543/716 (76%)	540 (99%)	3 (1%)	78	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	CYS
1	C	72	LEU
1	D	118	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	57	GLN
1	C	176	GLN
1	D	108	GLN
1	D	62	ASN
1	C	47	GLN

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

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 [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	167/194 (86%)	0.36	4 (2%) 59 36	51, 82, 126, 149	0
1	B	161/194 (82%)	0.23	2 (1%) 76 55	42, 74, 108, 152	0
1	C	154/194 (79%)	0.59	11 (7%) 22 11	81, 114, 176, 185	0
1	D	163/194 (84%)	0.31	6 (3%) 45 25	75, 104, 144, 152	0
All	All	645/776 (83%)	0.37	23 (3%) 46 26	42, 94, 149, 185	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	194	ILE	4.5
1	C	196	LEU	4.3
1	C	62	ASN	4.0
1	C	210	CYS	3.0
1	D	181	ILE	3.0

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 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.