



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:14 PM GMT

PDB ID : 1EPA
Title : STRUCTURE OF THE EPIDIDYMAL RETINOIC ACID-BINDING PROTEIN AT 2.1 ANGSTROMS RESOLUTION
Authors : Newcomer, M.E.
Deposited on : 1993-06-15
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

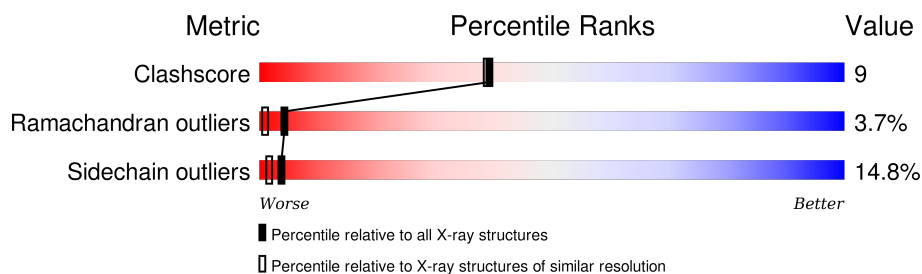
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	164	 63% 27% 5% . .
1	B	164	 65% 26% 7% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2549 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 EPIDIDYMAL RETINOIC ACID-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	0	9
			1202	774	190	233	5			
1	B	164	Total	C	N	O	S	0	0	9
			1228	789	194	240	5			

- Molecule 2 is water.

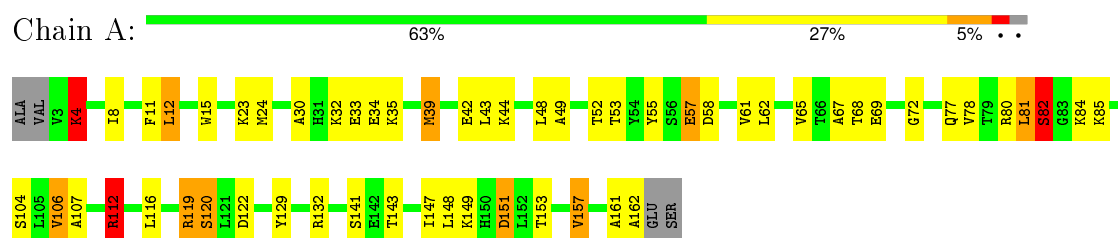
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	59	Total	O	0	0
			59	59		
2	B	60	Total	O	0	0
			60	60		

3 Residue-property plots

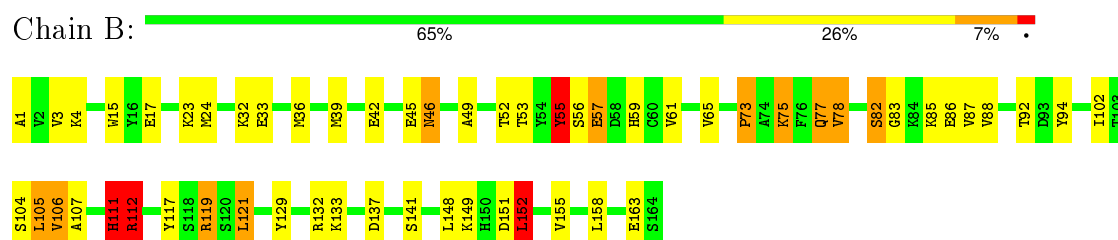
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

Note EDS was not executed.

• Molecule 1: EPIDIDYMAL RETINOIC ACID-BINDING PROTEIN



• Molecule 1: EPIDIDYMAL RETINOIC ACID-BINDING PROTEIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	39.33Å 58.67Å 66.27Å 90.00° 109.34° 90.00°	Depositor
Resolution (Å)	6.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.196 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2549	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

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	A	0.93	0/1213	1.74	17/1636 (1.0%)
1	B	0.99	0/1239	1.87	22/1673 (1.3%)
All	All	0.96	0/2452	1.81	39/3309 (1.2%)

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	ARG	NE-CZ-NH1	13.95	127.28	120.30
1	B	132	ARG	NE-CZ-NH2	-12.56	114.02	120.30
1	B	119	ARG	NE-CZ-NH2	-12.02	114.29	120.30
1	B	132	ARG	NE-CZ-NH1	11.11	125.85	120.30
1	B	94	TYR	CB-CG-CD1	-10.80	114.52	121.00
1	B	39	MET	CG-SD-CE	-9.12	85.60	100.20
1	B	56	SER	CA-C-N	-8.84	97.76	117.20
1	B	36	MET	CA-CB-CG	-8.46	98.91	113.30
1	A	119	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	B	36	MET	CG-SD-CE	-8.40	86.77	100.20
1	A	15	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	B	55	TYR	CA-CB-CG	7.63	127.90	113.40
1	B	152	LEU	CA-CB-CG	7.51	132.57	115.30
1	B	112	ARG	NE-CZ-NH1	7.48	124.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	A	55	TYR	CB-CG-CD1	-7.36	116.58	121.00
1	A	82	SER	CA-C-N	-7.31	101.58	116.20
1	A	119	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	B	15	TRP	CE2-CD2-CG	-6.75	101.90	107.30
1	A	15	TRP	CE2-CD2-CG	-6.54	102.07	107.30
1	A	162	ALA	N-CA-C	-6.49	93.49	111.00
1	B	15	TRP	CD1-CG-CD2	6.43	111.45	106.30
1	B	117	TYR	CB-CG-CD1	-6.24	117.26	121.00
1	A	129	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	B	56	SER	O-C-N	6.09	132.44	122.70
1	A	39	MET	CG-SD-CE	5.76	109.42	100.20
1	B	52	THR	N-CA-CB	-5.75	99.38	110.30
1	A	15	TRP	CG-CD1-NE1	-5.69	104.41	110.10
1	B	151	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	81	LEU	CA-C-N	-5.55	104.99	117.20
1	B	111	HIS	CA-CB-CG	-5.46	104.32	113.60
1	A	4	LYS	N-CA-C	5.45	125.73	111.00
1	A	157	VAL	CG1-CB-CG2	-5.27	102.47	110.90
1	A	120	SER	N-CA-CB	-5.25	102.63	110.50
1	B	57	GLU	CA-CB-CG	-5.16	102.05	113.40
1	A	151	ASP	CB-CG-OD1	5.11	122.89	118.30
1	A	106	VAL	N-CA-C	-5.09	97.26	111.00
1	B	4	LYS	O-C-N	-5.09	114.56	122.70
1	A	112	ARG	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	GLY	Peptide
1	B	55	TYR	Sidechain

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	1202	0	1184	22	0
1	B	1228	0	1214	20	0
2	A	59	0	0	2	0
2	B	60	0	0	0	0
All	All	2549	0	2398	42	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 9.

All (42) 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:32:LYS:CA	1:B:33:GLU:N	2.43	0.81
1:B:23:LYS:C	1:B:24:MET:CA	2.52	0.78
1:A:23:LYS:C	1:A:24:MET:CA	2.54	0.76
1:A:77:GLN:HB3	1:A:84:LYS:HD2	1.68	0.76
1:A:32:LYS:CA	1:A:33:GLU:N	2.49	0.75
1:B:121:LEU:H	1:B:121:LEU:HD12	1.52	0.72
1:B:78:VAL:HG13	1:B:85:LYS:HB2	1.74	0.69
1:B:75:LYS:HD2	1:B:88:VAL:HG22	1.84	0.59
1:A:112:ARG:HB3	2:A:221:HOH:O	2.01	0.59
1:A:8:ILE:HD12	1:A:11:PHE:HB2	1.87	0.56
1:A:39:MET:HG3	1:A:52:THR:HG22	1.87	0.56
1:A:33:GLU:HB3	1:A:149:LYS:NZ	2.22	0.55
1:B:75:LYS:NZ	1:B:86:GLU:HG2	2.21	0.55
1:B:102:ILE:O	1:B:112:ARG:HA	2.07	0.55
1:B:83:GLY:HA3	1:B:105:LEU:O	2.07	0.53
1:A:78:VAL:HB	1:A:85:LYS:HB3	1.91	0.53
1:B:53:THR:HA	1:B:61:VAL:O	2.08	0.53
1:A:35:LYS:HA	1:A:151:ASP:HB3	1.91	0.51
1:A:80:ARG:O	1:A:82:SER:N	2.45	0.49
1:A:84:LYS:HG3	1:A:85:LYS:N	2.28	0.49
1:A:53:THR:HA	1:A:61:VAL:O	2.11	0.49
1:A:80:ARG:HA	1:A:80:ARG:NE	2.28	0.48
1:B:75:LYS:HZ1	1:B:86:GLU:HG2	1.79	0.48
1:B:3:VAL:HG11	1:B:92:THR:HG22	1.95	0.48
1:A:132:ARG:NH2	1:A:147:ILE:HD11	2.29	0.48
1:B:23:LYS:HB2	1:B:111:HIS:CE1	2.50	0.46
1:A:48:LEU:HB3	1:A:67:ALA:HB3	1.98	0.46
1:A:30:ALA:CB	1:A:34:GLU:HG2	2.47	0.45
1:B:1:ALA:HB2	1:B:73:PRO:N	2.32	0.45
1:B:75:LYS:HZ1	1:B:86:GLU:CG	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ILE:O	1:A:12:LEU:HD13	2.18	0.44
1:B:85:LYS:NZ	1:B:104:SER:HB3	2.33	0.44
1:B:129:TYR:O	1:B:133:LYS:HG3	2.20	0.42
1:A:141:SER:OG	1:A:143:THR:HB	2.20	0.42
1:A:42:GLU:HB2	1:A:49:ALA:HB3	2.02	0.41
1:B:77:GLN:HE21	1:B:86:GLU:HG3	1.86	0.41
1:B:17:GLU:O	1:B:148:LEU:HD22	2.20	0.41
1:B:42:GLU:HB3	1:B:49:ALA:HB3	2.02	0.41
1:A:106:VAL:HG11	2:A:216:HOH:O	2.21	0.41
1:A:4:LYS:HB3	1:A:4:LYS:NZ	2.36	0.41
1:B:152:LEU:HB3	1:B:155:VAL:HB	2.03	0.40
1:A:153:THR:O	1:A:157:VAL:HG23	2.21	0.40

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	147/164 (90%)	132 (90%)	10 (7%)	5 (3%)	5	1
1	B	151/164 (92%)	136 (90%)	9 (6%)	6 (4%)	4	1
All	All	298/328 (91%)	268 (90%)	19 (6%)	11 (4%)	4	1

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	GLU
1	B	45	GLU
1	B	57	GLU
1	B	106	VAL
1	B	107	ALA
1	A	82	SER

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Mol	Chain	Res	Type
1	A	161	ALA
1	B	82	SER
1	A	81	LEU
1	A	107	ALA
1	B	46	ASN

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	130/139 (94%)	113 (87%)	17 (13%)	5	2
1	B	133/139 (96%)	111 (84%)	22 (16%)	3	1
All	All	263/278 (95%)	224 (85%)	39 (15%)	4	2

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	12	LEU
1	A	43	LEU
1	A	44	LYS
1	A	57	GLU
1	A	58	ASP
1	A	62	LEU
1	A	65	VAL
1	A	68	THR
1	A	69	GLU
1	A	104	SER
1	A	112	ARG
1	A	116	LEU
1	A	119	ARG
1	A	120	SER
1	A	122	ASP
1	A	148	LEU
1	B	46	ASN

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Mol	Chain	Res	Type
1	B	55	TYR
1	B	59	HIS
1	B	65	VAL
1	B	73	PRO
1	B	75	LYS
1	B	77	GLN
1	B	78	VAL
1	B	82	SER
1	B	87	VAL
1	B	105	LEU
1	B	106	VAL
1	B	111	HIS
1	B	112	ARG
1	B	119	ARG
1	B	121	LEU
1	B	137	ASP
1	B	141	SER
1	B	149	LYS
1	B	152	LEU
1	B	158	LEU
1	B	163	GLU

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

Mol	Chain	Res	Type
1	A	77	GLN
1	B	77	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

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.