



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 11:40 PM GMT

PDB ID : 1EPB  
Title : STRUCTURE OF THE EPIDIDYMAL RETINOIC ACID-BINDING PROTEIN AT 2.1 ANGSTROMS RESOLUTION  
Authors : Newcomer, M.E.  
Deposited on : 1993-06-15  
Resolution : 2.20 Å(reported)

This is a full wwPDB validation 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 <http://wwpdb.org/ValidationPDFNotes.html>

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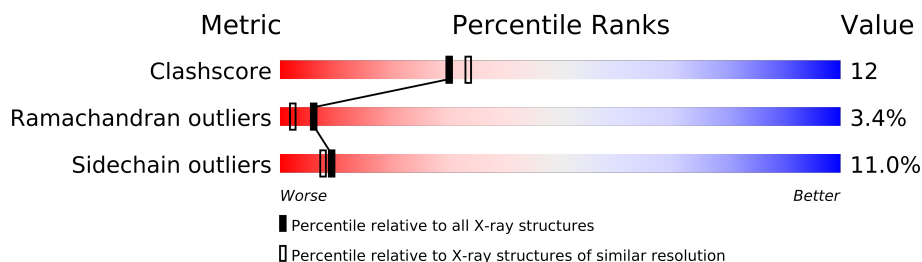
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	164	
1	B	164	

## 2 Entry composition i

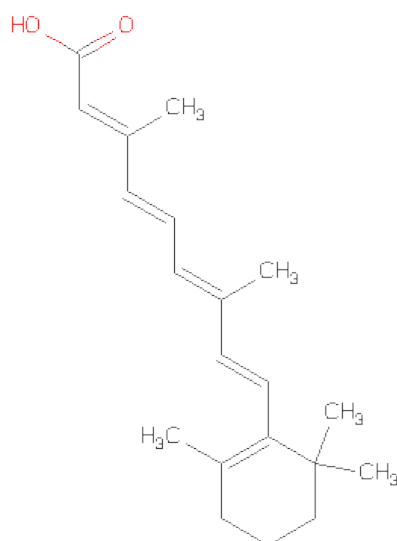
There are 3 unique types of molecules in this entry. The entry contains 2587 atoms, of which 42 are hydrogens and 0 are deuterium.

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
			1201	773	190	233	5			
1	B	164	Total	C	N	O	S	0	0	9
			1228	789	194	240	5			

- Molecule 2 is RETINOIC ACID (three-letter code: REA) (formula:  $C_{20}H_{28}O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			43	20	21	2		
2	B	1	Total	C	H	O	0	0
			43	20	21	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total 38	O 38	0	0
3	B	34	Total 34	O 34	0	0



## 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, $\alpha$ , $\beta$ , $\gamma$	39.80Å 58.89Å 66.65Å 90.00° 109.44° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2587	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: REA

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	0.87	0/1212	1.63	17/1636 (1.0%)
1	B	0.92	0/1239	1.66	14/1673 (0.8%)
All	All	0.90	0/2451	1.64	31/3309 (0.9%)

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 (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	TYR	CB-CG-CD1	-12.13	113.72	121.00
1	B	132	ARG	NE-CZ-NH2	-10.11	115.25	120.30
1	A	129	TYR	CB-CG-CD2	-9.32	115.41	121.00
1	B	15	TRP	CD1-CG-CD2	9.18	113.64	106.30
1	A	119	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	B	15	TRP	CE2-CD2-CG	-8.27	100.69	107.30
1	A	132	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	B	132	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	A	15	TRP	CD1-CG-CD2	7.21	112.07	106.30
1	A	15	TRP	CE2-CD2-CG	-6.87	101.81	107.30
1	A	112	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	117	TYR	CB-CG-CD2	-6.56	117.06	121.00
1	B	15	TRP	CG-CD1-NE1	-6.38	103.72	110.10
1	A	119	ARG	NE-CZ-NH2	-6.19	117.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	TYR	CA-CB-CG	5.98	124.76	113.40
1	B	2	VAL	CA-CB-CG2	-5.95	101.97	110.90
1	B	112	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	B	39	MET	CG-SD-CE	-5.80	90.92	100.20
1	A	69	GLU	CA-CB-CG	5.70	125.94	113.40
1	A	132	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	151	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	101	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	81	LEU	O-C-N	5.40	131.35	122.70
1	B	94	TYR	CB-CG-CD2	5.32	124.19	121.00
1	A	81	LEU	CA-C-N	-5.30	105.55	117.20
1	B	129	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	B	15	TRP	CB-CG-CD1	-5.29	120.12	127.00
1	A	15	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	B	97	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	A	80	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	33	GLU	CA-CB-CG	-5.01	102.37	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	GLY	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1201	0	1184	26	0
1	B	1228	0	1214	30	0
2	A	22	21	6	5	0
2	B	22	21	6	5	0
3	A	38	0	0	0	0
3	B	34	0	0	2	0
All	All	2545	42	2410	58	0



Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (58) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:23:LYS:C	1:A:24:MET:CA	2.45	0.84
1:A:32:LYS:CA	1:A:33:GLU:N	2.46	0.79
1:B:23:LYS:C	1:B:24:MET:CA	2.52	0.78
1:A:39:MET:HG3	1:A:52:THR:HG22	1.67	0.74
1:A:77:GLN:HB3	1:A:84:LYS:HZ1	1.56	0.71
1:B:32:LYS:CA	1:B:33:GLU:N	2.54	0.70
1:A:39:MET:SD	2:A:165:REA:H183	2.32	0.70
1:B:117:TYR:CD1	2:B:165:REA:H183	2.27	0.69
1:B:34:GLU:HB3	1:B:149:LYS:HB2	1.75	0.68
1:B:89:VAL:HG22	1:B:100:ILE:HD11	1.75	0.68
1:A:77:GLN:HB3	1:A:84:LYS:NZ	2.11	0.65
1:B:65:VAL:HG21	1:B:80:ARG:HH11	1.63	0.63
1:A:153:THR:O	1:A:157:VAL:HG23	1.98	0.63
1:A:150:HIS:HE1	3:B:179:HOH:O	1.82	0.63
1:B:82:SER:O	1:B:106:VAL:HA	1.98	0.62
1:B:53:THR:HA	1:B:61:VAL:O	1.99	0.61
1:B:1:ALA:HB1	1:B:74:ALA:HB3	1.82	0.61
1:B:117:TYR:CG	2:B:165:REA:H183	2.37	0.60
1:A:39:MET:CE	1:A:50:LEU:HD22	2.33	0.58
1:B:36:MET:HG3	1:B:155:VAL:HG21	1.84	0.58
1:A:39:MET:HE3	1:A:50:LEU:HD22	1.85	0.58
1:B:8:ILE:HG12	1:B:48:LEU:HD11	1.85	0.58
1:B:35:LYS:HE2	1:B:55:TYR:CD1	2.40	0.56
1:A:80:ARG:O	1:A:82:SER:N	2.41	0.54
1:A:117:TYR:CD2	2:A:165:REA:H182	2.43	0.53
1:A:39:MET:HE2	1:A:41:VAL:HG22	1.92	0.52
1:B:50:LEU:HD11	2:B:165:REA:H193	1.90	0.52
1:A:39:MET:CE	1:A:41:VAL:HG22	2.41	0.51
1:A:87:VAL:HA	1:A:101:ASP:O	2.10	0.51
1:A:14:PHE:HE1	1:A:16:TYR:CE1	2.33	0.46
1:B:65:VAL:HG21	1:B:80:ARG:HD3	1.98	0.46
1:A:80:ARG:HA	1:A:80:ARG:NE	2.31	0.46
1:B:79:THR:HG23	1:B:84:LYS:HG2	1.98	0.46
1:A:38:ALA:HB3	1:A:158:LEU:HD23	1.99	0.45
2:A:165:REA:H173	2:A:165:REA:H8	1.99	0.45
2:B:165:REA:H8	2:B:165:REA:H173	1.99	0.45
1:B:65:VAL:HG21	1:B:80:ARG:NH1	2.30	0.45
1:B:23:LYS:HB2	1:B:111:HIS:CE1	2.52	0.45
1:B:102:ILE:O	1:B:112:ARG:HA	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:74:ALA:HB1	1:B:89:VAL:HB	2.00	0.44
1:A:87:VAL:HG23	1:A:100:ILE:HG23	2.00	0.43
1:B:72:GLY:HA2	1:B:73:PRO:HD3	1.85	0.43
1:B:147:ILE:HG12	3:B:181:HOH:O	2.17	0.43
1:A:3:VAL:HG13	1:A:94:TYR:OH	2.18	0.43
1:A:56:SER:O	1:A:59:HIS:ND1	2.52	0.43
1:A:102:ILE:HD13	2:A:165:REA:C14	2.49	0.43
1:B:17:GLU:O	1:B:148:LEU:HD22	2.18	0.43
1:B:35:LYS:HE2	1:B:55:TYR:CE1	2.54	0.42
1:B:93:ASP:O	1:B:94:TYR:HB2	2.19	0.42
1:B:50:LEU:CD1	2:B:165:REA:H193	2.50	0.42
1:B:60:CYS:CB	1:B:154:CYS:SG	3.07	0.42
1:B:8:ILE:HD12	1:B:8:ILE:HA	1.93	0.42
1:A:90:GLU:HG3	1:A:114:MET:CE	2.50	0.41
1:A:132:ARG:NH1	1:A:145:LEU:HD12	2.35	0.41
1:A:117:TYR:CD2	2:A:165:REA:C18	3.04	0.41
1:B:148:LEU:HD12	1:B:148:LEU:N	2.35	0.41
1:B:20:PHE:HZ	1:B:29:LEU:CA	2.33	0.41
1:A:55:TYR:OH	1:A:58:ASP:HA	2.21	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	147/164 (90%)	133 (90%)	10 (7%)	4 (3%)	8	3
1	B	151/164 (92%)	135 (89%)	10 (7%)	6 (4%)	5	1
All	All	298/328 (91%)	268 (90%)	20 (7%)	10 (3%)	6	2

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	57	GLU

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Mol	Chain	Res	Type
1	B	71	ASP
1	B	106	VAL
1	B	107	ALA
1	A	57	GLU
1	A	73	PRO
1	A	81	LEU
1	B	74	ALA
1	A	161	ALA
1	B	73	PRO

### 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%)	117 (90%)	13 (10%)	11	10
1	B	133/139 (96%)	117 (88%)	16 (12%)	7	6
All	All	263/278 (95%)	234 (89%)	29 (11%)	9	8

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	22	SER
1	A	64	LYS
1	A	77	GLN
1	A	84	LYS
1	A	86	GLU
1	A	87	VAL
1	A	104	SER
1	A	105	LEU
1	A	112	ARG
1	A	116	LEU
1	A	122	ASP
1	A	152	LEU
1	B	46	ASN
1	B	50	LEU
1	B	52	THR

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Mol	Chain	Res	Type
1	B	59	HIS
1	B	65	VAL
1	B	71	ASP
1	B	77	GLN
1	B	78	VAL
1	B	119	ARG
1	B	121	LEU
1	B	122	ASP
1	B	141	SER
1	B	143	THR
1	B	153	THR
1	B	158	LEU
1	B	163	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	150	HIS
1	B	59	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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	REA	A	165	-	22,22,22	1.01	2 (9%)	30,30,30	1.22	2 (6%)
2	REA	B	165	-	22,22,22	1.01	2 (9%)	30,30,30	1.22	2 (6%)

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	REA	A	165	-	-	0/15/32/32	0/1/1/1
2	REA	B	165	-	-	0/15/32/32	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	165	REA	O1-C15	3.45	1.32	1.23
2	A	165	REA	O1-C15	3.43	1.32	1.23
2	A	165	REA	O2-C15	-2.62	1.22	1.30
2	B	165	REA	O2-C15	-2.60	1.22	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	165	REA	O2-C15-C14	4.02	126.00	113.59
2	A	165	REA	O2-C15-C14	4.01	125.98	113.59
2	A	165	REA	O1-C15-C14	-3.77	112.07	124.10
2	B	165	REA	O1-C15-C14	-3.76	112.08	124.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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.